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Air quality impacts of fuel cell electric hydrogen vehicles with high levels of renewable power generation

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ABSTRACT

The introduction of fuel cell electric vehicles (FCEV) operating on hydrogen is a key strategy to mitigate pollutant emissions from the light duty vehicle (LDV) transportation sector in pursuit of air quality (AQ) improvements. Further, concomitant increases in renewable power generation could assist in achieving benefits via electrolysis-provided hydrogen as a vehicle fuel. However, it is unclear (1) reductions in emissions translate to changes in primary and secondary pollutant concentrations and (2) how effects compare to those from emissions in other transport sectors including heavy duty vehicles (HDV). This work assesses how the adoption of FCEVs in counties expected to support alternative LDV technologies affect atmospheric concentrations of ozone and fine particulate matter (PM_{2.5}) throughout California (CA) in the year 2055 relative to a gasoline vehicle baseline. Further, impacts of reducing HDV emissions are explored to facilitate comparison among technology classes. A base year emissions inventory is grown to 2055 representing a business-as-usual progression of economic sectors, including primarily petroleum fuel consumption by LDV and HDVs. Emissions are spatially and temporally resolved and used in simulations of atmospheric chemistry and transport to evaluate distributions of primary and secondary pollutants relative to baseline. Results indicate that light-duty FCEV Cases achieve significant reductions in ozone and PM_{2.5} when LDV market shares reach 50–100% in early adoption counties, including areas distant from deployment sites. Reflecting a cleaner LDV baseline fleet in 2055, emissions from HDVs impact ozone and PM_{2.5} at comparable or greater levels than light duty FCEVs. Additionally, the importance of emissions from petroleum fuel infrastructure (PFI) activity is demonstrated in impacts on ozone and PM_{2.5} burdens, with large refinery complexes representing a key source of air pollution in 2055. Results presented provide insight into light duty FCEV deployment strategies that can achieve maximum reductions in ozone and PM_{2.5} and will assist decision makers in developing effective transportation sector AQ mitigation strategies.

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Introduction

Transportation sources account for an important fraction of total emissions driving AQ concerns in many U.S. regions, including ambient concentrations of ozone and particulate matter (PM) associated with detrimental human health outcomes [1]. In California (CA), emissions from the combustion of fossil fuels by transportation sources including light duty (LDV) and heavy duty vehicles (HDV) have been shown to be major contributors to total regional pollutant burdens [2]. A shift to cleaner alternative propulsion systems is being pursued in CA to reduce the environmental impacts of the LDV transportation sector, including reducing the emissions of greenhouse gases (GHG) and pollutant emissions and improving regional AQ [3,4]. A key strategy to attain emission reductions from LDVs includes the use of hydrogen in tandem with fuel cell electric power trains (FCEVs) as FCEVs have no direct emissions during operation [5]. In addition to LDV, FCEV technologies can be applied to reduce emissions in other transportation sub-sectors including HDV such as tractor-trailers, refuse trucks, transit buses, drayage trucks and others [6]. FCEV technologies also offer the benefits of high efficiencies [7], similar ranges and refueling times compared to combustion engines [8,9], and the promotion of domestic energy independence via displacement of petroleum fuels.

Impacts of transitioning to FCEVs include the full life cycle of deployed vehicle and hydrogen pathways [10]. Currently, widely-used hydrogen supply chain strategies are fossil-based including steam methane reformation which itself results in emissions [11]. However, hydrogen production methods with enhanced sustainability are desirable and can be pursued as GHG, AQ and additional environmental goals drive technological development and deployment [12]. Clean options include centralized and distributed electrolysis of water using electricity from renewable sources, representing a pathway for FCEVs to notably reduce GHG and pollutant emissions from transportation [13]. Additional renewable hydrogen systems include processes associated with biomass or biogas feedstock (e.g., gasification, pyrolysis, fermentation, anaerobic digestion) and routes using solar energy directly including thermochemical splitting of water [14,15]. Further, the integration of hydrogen production with the future electric grid could have benefits in terms of system operation by providing complementary services as a form of energy storage and could allow for enhanced integration of renewables, particularly those characterized by intermittencies including wind and solar power [16]. Therefore, hydrogen has been proposed as a complement to renewable electricity as a means of coupling GHG mitigation strategies in the utilities and transportation sectors [17–19].

The deployment of FCEVs can reduce total LDV and HDV emissions across a range of hydrogen infrastructure options from the potential for very low lifecycle GHG and criteria pollutant emissions compared to current and future conventional LDVs, including oxides of nitrogen (NO_x), volatile organic compounds (VOC), PM, and carbon monoxide (CO) [20–24]. Replacing the current on-road LDV fleet with FCEVs would reduce net GHG emissions in the U.S [25,26] and CA [27] with similar findings reported for pollutant emissions at

various scales [28–30]. In particular, FCEVs supplied with hydrogen produced via renewably powered electrolysis can achieve large-scale reductions in total emissions from transportation [31]. As many places around the world (including CA) are pursuing greater procurement of renewable energy in coming decades, including significant amounts expected from intermittent wind and solar technologies, the incorporation of hydrogen energy systems to provide fueling for vehicles and stationary sources could represent an important opportunity to maximize criteria pollutant and GHG reductions and maintain grid reliability [32]. However, it is unknown how emission reductions from using renewable hydrogen as a vehicle fuel translates to reductions in primary and secondary pollutant distributions.

In addition to direct emissions from vehicles, the existing petroleum fuel infrastructure (PFI) encompassing the production, storage, transport, and distribution of petroleum fuels (including gasoline and distillate fuels predominantly used by LDV and HDV) emits pollutants and GHG [33,34]. Deploying FCEVs in CA could reduce the consumption of petroleum fuels – potentially offsetting emissions from PFI sources. The specific response of, for example, large in-state refinery complexes are unknown and how PFI emission perturbations impact AQ is subject to the same uncertainty as those from direct vehicles. Thus, further information is needed regarding the importance of PFI emissions to regional AQ in 2055, notably in regards to interactions with State goals for transportation strategies targeting GHG reductions and AQ improvements.

Assessing regional AQ impacts resulting from FCEV displacement of conventional LDV and HDV is multifaceted and exceeds simply quantifying emission perturbations. The complexity associated with the formation and fate of atmospheric pollutant species complicates an understanding of how FCEVs deployed in select counties will impact regional AQ generally in CA air basins. In particular, the dynamics associated with the production of ground-level ozone from pre-cursor emissions lessens the value of solely quantifying emission reductions in pursuit of AQ outcomes [35]. Similarly, atmospheric levels and compositions of PM in CA are governed by a large range of factors including sources of particulate and atmospheric processes that control particle formation that could lead to spatial and temporal variation in source-related impacts and potential mitigation strategies [36]. Therefore, detailed atmospheric models must be used to account accurately for the spatial and temporal distribution of pollutant concentrations in order to conduct a detailed assessment of how FCEVs may affect ground-level ozone and $\text{PM}_{2.5}$.

The goal of this work is to assess impacts on AQ of emission sources in the transportation, electric, and industrial sector under high renewable and advanced vehicle technology penetrations. For the first time this work uses advanced atmospheric modeling to examine how county-level FCEV adoption in the LDV and HDV sector impacts the spatial and temporal distribution of primary and secondary pollutants in CA. Although previous studies have evaluated the emissions [25,28] or AQ [37,38] impacts of FCEVs, few have utilized detailed three dimensional eulerian AQ models to account for spatial and temporal emissions perturbations and

atmospheric chemistry and transport processes. While studies have shown that FCEV driven reductions in direct emissions result in improvements in secondary air pollutants, including ground-level ozone and $\text{PM}_{2.5}$ [37,38], the body of available literature quantifying impacts on secondary air pollutants is limited. Use of a novel methodology for future hydrogen infrastructure development in the South Coast Air Basin (SoCAB) of CA reported substantial reductions emissions including NO_x for the majority of Cases [30] translating to significant AQ improvements (e.g., reductions in peak 8-h-averaged ozone and 24-h-averaged $\text{PM}_{2.5}$ concentrations) [27]. However, existing studies were spatially restricted to select regions of CA (e.g., the SoCAB, Sacramento) or the entire U.S., and assume FCEV penetration is universal throughout the study domain. This work assesses the AQ impacts at the State-level of FCEV deployment in only certain areas of CA – those counties expected to have rates of early adoption of FCEVs based on vehicle registration data for alternative LDV technologies. Furthermore, this work for the first time compares the AQ impact of HDV emission changes to those from LDV. Baseline AQ in the horizon year (2055) is established accounting for changes in various emission drivers, including demand growth in economic sectors, efficiency improvements, and utilized technologies and fuels according to a business-as-usual progression. Cases are developed for FCEV deployment accounting for spatial and temporal distribution of fundamental sources to evaluate impacts on ambient pollutant concentrations from emission perturbations, including ozone and $\text{PM}_{2.5}$.

Methodology

Regional energy system projection

The sources, magnitudes, and spatial/temporal distributions of future anthropogenic emissions are determined by many drivers including socio-economic factors, energy resources, and regulatory statutes. The year 2055 is selected for the study year to provide a feasible temporal period for FCEV deployment at high levels. Assessing AQ impacts in 2055 requires projection of all pertinent emission sources by consistent methods. First, the comprehensive accounting of regional emissions evolution under business-as-usual (BAU) conditions to provide a Reference Case for comparison with FCEV and HDV Cases. The approach for the developed 2055 Reference Case follows the methodology described by Loughlin et al., 2011 [39]. Energy system progression and the evolution of emissions in major economic sectors is estimated using output from the Market Allocation (MARKAL) model. MARKAL is a data-intensive energy systems economic optimization model utilizing EPA developed and maintained regional databases characterizing regional energy systems evolution from 2005 to 2055. For this work, MARKAL is applied using the U.S. EPA 9-region MARKAL database [40], version EPAUS9R_2010_1.3. The database is calibrated to the U.S. Energy Information Agency's Annual Energy Outlook 2010 [41]. Model outputs include demands, technologies, fuel use and emissions of pollutants to 2055. MARKAL's regional-, technology-, and pollutant-specific emission projections are then

used to develop growth and control factors to grow the base year emission inventory to 2055 [39]. Following expected BAU trends, in the Reference Case used for this work the LDV sector is predominantly comprised of gasoline combustion engine technologies (a moderate to minor amount of LDV demand is assumed to be met with alternative technologies and fuels including electricity). The HDV sector is similarly assumed to be reliant on fossil-based fuels including distillate fuels, compressed natural gas, etc.

Development of emissions fields and atmospheric modeling

Construction of spatially and temporally resolved emission fields by the Sparse Matrix Operator Kernel Emissions (SMOKE) Modeling System is necessary to generate air quality model inputs representative of assessed Cases [42]. SMOKE accomplishes the core functions of emissions processing including spatial and temporal allocation, chemical speciation, biogenic emission estimates and control of area-, mobile-, and point-source anthropogenic emissions [43]. MARKAL-developed growth and control factors are applied to the 2005 US Environmental Protection Agency (EPA) National Emissions Inventory [44] via SMOKE, including disaggregation of emissions into constituent chemical species via SCC-specific chemical speciation profiles. Spatial and temporal allocation of both point and area-source emissions into a three-dimensional modeling grid is performed via source coordinates and spatial surrogates at the county level and SCC-specific temporal allocation profiles. Source-specific information used in allocation methodologies includes land use, census data, employment information, and others.

Simulations of atmospheric chemistry and transport are accomplished via the Community Multi-scale Air Quality model (CMAQ) version 4.7, with the Carbon Bond 05 (CB05) chemical mechanism [45]. CMAQ is a comprehensive AQ modeling system developed by the EPA and widely used for a various AQ needs, e.g., regulatory simulation applications [46,47]. CMAQ is designed from the “one atmosphere” perspective and is used for studies on tropospheric ozone, PM, acid deposition and visibility. Model inputs include meteorological conditions, initial and boundary conditions, land use and land cover information, and anthropogenic and biogenic source emissions. The CB05 chemical mechanism includes the photochemical formation of ozone, oxidation of volatile organic compounds and formation of organic aerosol precursors. For the simulations presented, the model grid resolution of CA is $4 \text{ km} \times 4 \text{ km}$, with a vertical height of 10,000 m above ground divided into 30 layers of variable height. Meteorological input data for CMAQ was generated by the Advanced Research Weather Research and Forecasting Model (WRF-ARW) [48].

Simulations are conducted for the week of July 7–13 as this period encompasses conditions typically associated with high ground-level ozone formation, including high temperatures, an abundance of sunlight, lack of natural scavengers, and the presence of inversion layers [49]. The first six days of simulations are used to dissipate the effects of the initial conditions as this has been shown to be sufficient [49]. Results are obtained from the seventh day of simulation (July 13) and reported as maximum 8-hr average ozone and 24-hr average

PM_{2.5}. Model performance evaluation is conducted for the episode prior to projection (July 13, 2005) using observations from the California Air Resources Board's AQ monitoring network. Hourly measurements for ozone and daily average for PM_{2.5} were used to calculate Mean Normalized Bias (MNB) and Mean Normalized Gross Error (MNGE), recommended for model evaluation [50]. Model performance is within acceptable parameters (Table 1).

Following application of projection factors, in the 2055 Reference Case simulated ground-level concentrations of ozone and PM_{2.5} show some regions of CA experience greater ambient concentrations which heighten the importance of achieving reductions, including the SoCAB, the San Francisco (S.F.) Bay Area, the Central Valley, and the Greater Sacramento area (Fig. 1). These areas currently experience high levels of ground-level ozone that often exceed Federal health-based standards and contain large urban populations [51] and improvements are desirable to CA in terms of mitigating deleterious human health outcomes from air pollution [52]. The Reference Case serves as a basis for comparison for FCEV and HDV Case with results presented as difference plots for pollutant distributions.

Case development

Cases assessed in this work are designed to span a range of potential emission outcomes from light- and heavy-duty vehicles, PFI, and the electricity sector to provide insights into impacts on primary and secondary atmospheric pollutants. A set of cases representing FCEV deployment in the LDV sector are developed and analyzed at various penetration levels in select CA counties in 2055. The counties are chosen based on plug-in hybrid and battery electric vehicle (BEV) new vehicle registration data [53] as it is likely to correspond to early adoption of LDV FCEVs. Table 1 lists the seven counties with the highest populations of plug-in hybrid and battery electric vehicles in CA. Further, the bulk of the counties are located in CA air basins requiring regional AQ improvement including the SoCAB and S.F. Bay. Case assessment comprises the development of spatially and temporally resolved emission fields appropriately accounting for all mobile and stationary source perturbations followed by simulations of atmospheric chemistry and transport. Resulting output is assessed for changes in ground-level maximum 8 h (8-hr) average ozone and 24 h (24-h) average PM_{2.5} relative to the baseline gasoline dominated vehicle Reference Case.

LDV FCEV Cases encompass penetrations of 1%, 10%, 30%, 50% and 100% of the total LDV fleet in counties in Table 2 in 2055 and are labeled accordingly, i.e., FCEV 1, FCEV 50, etc. Correspondingly, direct emissions are reduced fleet-wide in the counties of deployment across all road types. Declines in

gasoline consumption are assumed to translate to reductions in baseline PFI emissions including those from refineries, gasoline storage, fueling stations, etc. The largest source of PFI emissions include large refinery complexes that produce a range of products in addition to motor gasoline. Hence, reductions in emissions are assumed to correspond only to the fraction of refinery output attributable to motor gasoline (assumed to be 52% for CA refineries in 2055). It should be noted that one FCEV Case is included without PFI reductions (FCEV 50 No PFI) to provide comparison of the impact of PFI emissions relative to vehicle emissions. Emissions from the infrastructure needed to produce and distribute hydrogen for vehicle fueling is an essential component of overall FCEV AQ impacts. For this work it is assumed that hydrogen is generated from water electrolysis using renewable electricity and distributed to fueling site via pipeline as modeled in Tarroja et al., [54]. Therefore, emissions from hydrogen infrastructure are not assumed to increase over background levels in 2055.

Large increases in renewable resources will reduce emissions from electricity generators which are estimated from modeling of the CA electric grid through use of the Holistic Grid Resource Integration and Deployment (HiGRID) model [55]. The systems modeled in HiGRID are composed of generation resources, both renewable and conventional, and additional complementary resources such as energy storage and demand side-management strategies that all act to balance the system by not only providing sufficient energy to meet the demand, but also providing sufficient generation reserves to maintain reliability. The methodology of the energy storage model developed in HiGRID, which uses settings for power and energy capacity to smooth the net load profile of the grid, is available from Eichman et al. [56] and Tarroja et al., [54]. While the absolute energy values from HiGRID are not directly applicable here; they provide a reasonable estimate of potential emission reductions from the electricity sector under high renewable penetrations supporting the fueling needs of FCEV via renewable electrolysis in CA. The 35% reduction level is representative of several of the cases in Ref. [54] for 205 GW installed renewables in CA, and the 75% reduction level is representative of several of the cases in Ref. [54] for 475 GW installed renewables in CA. One Case, the FCEV 50 No Electric, is assessed with power plant emissions held constant to the baseline to provide insight into the comparative impacts relative to other sources.

In addition, Cases are analyzed for the removal of direct emissions from the HDV fleet in the same counties at 1%, 50%, and 100% to facilitate comparison of the impacts relative to LDV and labeled HDV 1, HDV 50, and HDV 100 Cases. While the HDV Cases do not specifically represent fuel cell propulsion systems, reductions in vehicle emissions are representative of advanced technologies including FCEV and all-electric drive. HDV Cases do not include reductions in emissions from power generation or PFI and account for tail pipe reductions as HiGRID does not account for advanced HDV technologies. However, to facilitate comparison with LDV FCEV a Case (HDV 50 PFI) with the corresponding PFI and power sector emissions reductions from the LDV FCEV 50 Case is included. Table 3 displays emission perturbations associated with assessed Cases.

Table 1 – Summary of model performance for ozone and PM_{2.5} for Jul 13, 2005.

	MNB	MNGE
O ₃ (hourly)	–7.6%	29.3%
PM _{2.5} (24-hour)	–2.8%	31.9%

Fig. 1 – Predicted ground-level concentrations of (a) max 8-hr average ozone and (b) 24-hr average $PM_{2.5}$ for the Reference Case during a typical summer day in 2055. Projected peak levels exceed 90 ppb and $78 \mu\text{g}/\text{m}^3$ for the final day of simulation.

Results

LDV FCEV AQ results

For all Cases evaluated, the use of LDV FCEVs in the selected counties contributes to improvements in ground-level ozone and $PM_{2.5}$, as displayed in Fig. 2 for the FCEV 1, FCEV 50, and FCEV 100 Cases relative to the Reference Case. Concentrations of pollutants for a typical episode in 2055 are modeled using the Reference Case assumptions for all economic sectors and expected changes in stationary and mobile sources between now and 2055 are accounted for. The use of LDV FCEVs as assumed in this work will further reduce pollutant emissions from various sources and consequently when pollutant formation in LDV FCEV Cases is compared to that of the Reference Case improvements in ozone and $PM_{2.5}$ are observed.

Peak impacts on ozone and $PM_{2.5}$ for all Cases are listed in Table 4. With respect to ozone, improvements occur in the S.F. Bay Area and the SoCAB – including locations of peak baseline concentrations in San Bernardino and Riverside Counties (quantitatively reductions in range from -0.27 ppb in the FCEV 1 Case to -3.17 in the FCEV 100 Case). Reductions are also predicted in the Central Valley for Cases with higher LDV FCEV

penetrations including the FCEV 50 and FCEV 100 Cases. These areas currently experience high levels of ground-level ozone that often exceed Federal health-based standards and contain large urban populations [51]. Thus, improvements in these areas are desirable to CA in terms of mitigating deleterious human health outcomes from air pollution.

The locations of the most pronounced impacts occur as a result of the displacement of emissions from conventional LDVs, petroleum refineries, and additional PFI sources. Urban airsheds such as the SoCAB and S.F. Bay Area contain great numbers of these sources and experience reductions in emissions in areas of importance to secondary pollutant formation. However, the most prominent reductions occur distant from the sites of deepest emission reduction from the temporal period required for the formation dynamics associated with ozone which results in the transport of precursor emissions [57]. For example, peak ozone benefits occur in the

Table 2 – 2013 vehicle populations of plug-in hybrid (PHEV) and battery electric vehicles (BEV) in 2013 by county in CA.

County	PHEVs [vehicles]	BEVs [vehicles]	Combined [vehicles]	CA air basin
Los Angeles	6385	4737	11,121	SoCAB
Santa Clara	2477	3828	6305	S.F. Bay
Orange	3109	1898	5007	SoCAB
San Diego	1329	2343	3672	San Diego
Alameda	1267	1619	2887	S.F. Bay
San Mateo	678	1438	2116	S.F. Bay
Contra Costa	783	741	1523	S.F. Bay

Table 3 – Emission reductions from the Reference Case for notable sources in analyzed Cases in 2055. NC=No Change in emissions. PFI=Petroleum Fuel Infrastructure emissions.

Case	Power emissions	LDV emissions	HDV emissions	PFI emissions
FCEV 1	–0%	–1%	NC	–1%
FCEV 10	–0%	–10%	NC	–5%
FCEV 30	–0%	–30%	NC	–15%
FCEV 50	–35%	–50%	NC	–26%
FCEV 50 No PFI	–35%	–50%	NC	–0%
FCEV 50 No Electric	–0%	–50%	NC	–26%
FCEV 100	–75%	–100%	NC	–52%
HDV 1	NC	NC	–1%	NC
HDV 50	NC	NC	–50%	NC
HDV 50 PFI	–35%	NC	–50%	–26%
HDV 100	NC	NC	–100%	NC

Fig. 2 – Predicted differences in ground-level maximum 8-hr average ozone and 24-h average $\text{PM}_{2.5}$ between the FCEV 1, FCEV 50 and FCEV 100 Cases and the Reference Case.

Table 4 – Peak reduction in ground-level ozone and PM_{2.5} from the Reference Case for LDV FCEV Cases.

Case	Δ 8-hr ozone [ppb]	Δ 24-hr PM _{2.5} [$\mu\text{g}/\text{m}^3$]
FCEV 1	–0.27	–0.05
FCEV 30	–0.92	–3.22
FCEV 50	–1.62	–2.82
FCEV 50 No PFI	–1.48	–0.30
FCEV 50 No Electric	–1.52	–2.80
FCEV 100	–3.17	–5.82

northeastern section of the SoCAB including portions of San Bernardino and Riverside County despite emission reductions in Los Angeles County from LDV and PFI. In addition, impacts of displaced emissions from power generators can be seen as plumes of reduction extending from sources northeast of the S.F. Bay Area in the FCEV 50 Case.

Reductions in emissions also improve ambient PM_{2.5} concentrations in CA in regions associated with both high LDV populations and/or the presence of large refineries in the SoCAB, S.F. Bay Area, and Central Valley. LDVs emit PM_{2.5} directly from tailpipes [58] as well as NO_x emissions that contribute to the formation of secondary PM_{2.5}. Thus, reducing emissions from both sources results in improvements of ground-level PM_{2.5} concentrations. Quantitatively, peak impacts range from –0.05 to –5.82 $\mu\text{g}/\text{m}^3$ for the FCEV 1 and FCEV 100 Cases, respectively. Relative to ozone, PM_{2.5} reductions occur with increased localization to source emissions as evident in reductions corresponding with locations of major petroleum refinery complexes in Long Beach, Los Angeles, and Santa Maria. Improvements in ground-level PM_{2.5} are attributable to both the reduction of primary PM and secondary PM, which has been shown to form largely from NO_x conversion to nitrate aerosol in Southern CA [2].

LDV FCEV no electricity reduction case

Fig. 3 displays difference plots for ozone and PM_{2.5} for the FCEV 50 No Electric Case relative to the FCEV 50 Case to show only the impact of emission perturbations from generators. Increases in concentrations result from maintaining baseline power sector emission profiles in place of the reduction assumed in the FCEV 50 Case (–35%) as no other emission source is altered. Generally, impacts are moderate with peak increases for maximum 8-h ozone exceeding 1 ppb, although most impacts are less than 0.25 ppb. Similarly, small differences in 24-h PM_{2.5} are observed that peak at –0.09 $\mu\text{g}/\text{m}^3$. Given the significant reduction in total sector emissions and the moderate observed AQ perturbations; electricity generators can be considered a minor driver of the total impacts of Cases. This is expected due to the mix of resources providing power to the CA grid, which includes low PM-emitting natural gas, renewables, and nuclear generation [59].

LDV FCEV no PFI case

Fig. 4 presents the data in terms of a difference plot between the FCEV 50 vs. the FCEV 50 No PFI Cases to show impacts only from PFI emission reductions. As emissions from all other sources remain constant (i.e., direct vehicle and generators), variance in ground-level concentrations are attributed solely to gasoline production, distribution and storage. PFI emissions contribute a notable fraction of the total PM_{2.5} benefits observed in the FCEV 50 Case. Localized reductions in concentrations between the cases exceed 2 $\mu\text{g}/\text{m}^3$, including areas directly adjacent with the Long Beach-area refinery complexes. Smaller reductions also occur in the S.F. Bay Area and Central Valley. Ozone impacts from PFI emissions are lesser with peak differences equivalent to –0.2 ppb in the S.F. Bay, the SoCAB, San Diego and Bakersfield and associated with the presence of large refinery complexes in those regions. Additional reductions of lesser magnitude occur across large areas

Fig. 3 – Predicted differences in ground-level (a) maximum 8-hr average ozone and (b) 24-h average PM_{2.5} between the FCEV 50 Case with no electricity sector emission reduction assumed (FCEV 50 No Electric) and FCEV 50 Case.

Fig. 4 – Maximum difference in (a) 8-hr ozone and (b) 24-h $PM_{2.5}$ between the FCEV 50 and FCEV 50 PFI Cases.

of CA and likely result from the distributed impacts of fueling stations.

HDV FCEV AQ impacts

The reduction of emissions from the HDV sector in counties under study attains improvements in both ground-level ozone and $PM_{2.5}$, with peak impacts reported in Table 5. It should again be noted that the only emission source altered in HDV Cases is direct vehicle emissions and comparison with LDV FCEV Cases should consider this caveat. Deployment in 1% of all HDV achieves minor AQ improvements similar in spatial dimension to those from FCEVs, i.e., less than -0.02 ppb and -0.01 $\mu\text{g}/\text{m}^3$. As would be expected impacts are more pronounced as the assumed HDV penetration level reaches 50 and 100% (Fig. 5). Reductions in ozone peak at approximately 2 and 4 ppb while reductions in $PM_{2.5}$ reach -0.31 and -0.62 $\mu\text{g}/\text{m}^3$ in the HDV 50 and HDV 100 Cases, respectively. To add context relative to LDV FCEV deployment, despite a lack of emission reduction from PFI and power generators the HDV 50 and HDV 100 Cases achieves comparable or enhanced ozone benefits relative to corresponding LDV FCEV Cases (i.e., -4.23 ppb in the HDV 100 and -3.17 in the FCEV 100). The results highlight the importance of HDV emissions to regional ozone burdens in 2055. Relative to the LDV FCEV Cases, lesser impacts on PM are incurred, attributable to the lack of refinery turn down in the bulk of HDV Cases.

Table 5 – Maximum reduction in ground-level ozone and $PM_{2.5}$ from the Reference Case for HDV Cases.

Case	Δ 8-hr ozone [ppb]	Δ 24-hr $PM_{2.5}$ [$\mu\text{g}/\text{m}^3$]
HDV 1	-0.02	-0.01
HDV 50	-1.98	-0.31
HDV 50 PFI	-2.32	-2.85
HDV 100	-4.23	-0.62

To better facilitate comparison with the LDV FCEV Cases, a Case (i.e., HDV 50 PFI Case) is evaluated reducing HDV tail pipe emissions in concert with emissions from PFI and power sector. All PFI and power sector emissions are reduced equivalently to the LDV FCEV 50 Case to facilitate direct comparison, although it should be noted that PFI reductions do not correspond directly with HDV fuel production and consumption. The resulting impacts on ozone and $PM_{2.5}$ for the HDV 50 PFI Case include impacts exceeding -2 ppb and -2.8 $\mu\text{g}/\text{m}^3$. As can be seen in Table 5, reductions in $PM_{2.5}$ are enhanced by the inclusion of PFI emission reductions in HDV Cases with peak impacts of -2.85 relative to -0.31 $\mu\text{g}/\text{m}^3$ in the HDV 50 Case. Additional ozone reductions also occur from the removal of power plant emissions in the northern central area of CA with similarity to the FCEV 50 Case.

Discussion

Meeting a large fraction of the LDV fleet with FCEVs (e.g., 50–100%) in counties likely to support early adoption of advanced vehicle technologies in tandem with high renewable penetration of the power grid achieves AQ benefits in CA, including improvements in ground-level ozone and $PM_{2.5}$, e.g., reductions in maximum 8-hr average ozone and 24-h $PM_{2.5}$ exceed 3 ppb and 5 $\mu\text{g}/\text{m}^3$ for complete LDV fleet penetration by FCEVs. LDV FCEV impacts on ozone are driven by direct vehicle tail pipe reductions while $PM_{2.5}$ levels are affected most by reductions in emissions across the gasoline life cycle. Emissions from the power sector exhibit a lower impact and reflect the relatively clean nature of CA's power grid. However, it should be considered that the summer modeling period was selected for high ambient ozone conditions and impacts on $PM_{2.5}$ may be more pronounced during winter months. Results here are similar in both magnitude and spatial scope to those reported in Ref. [32] for ozone and $PM_{2.5}$ in the SoCAB. However, improvements are less in this work (i.e., 3 ppb vs. 10 ppb)

Fig. 5 – Peak impacts on 8-hr ozone and 24-h $PM_{2.5}$ for the HDV 50 ((a) and (b)) and HDV 100 ((c) and (d)) Cases.

due to the use of updated emission inventories accounting for a cleaner, more efficient baseline gasoline LDV fleet.

Assumptions regarding hydrogen fuel infrastructure needed to support FCEVs are highly optimistic in that hydrogen production occurs from excess renewable electricity and does not incur emissions introduction from hydrogen fueling infrastructure. However, the goal of this work is to quantify the magnitude of ozone and $PM_{2.5}$ impacts attributable to major sources of emissions including vehicles, power plants, and PFI and the horizon of 2055 provides a feasible period for the development of infrastructure to support renewable hydrogen production and distribution. Similar assumptions were made in Ref. [34] for the assessment of AQ impacts of FCEV utilizing wind energy at the national scale. Therefore, the results are a “best-case” for FCEV, but it should also be considered that such a system may be needed to meet long-term transportation sustainability goals including deep reductions in GHG emissions. Further, these results also provide insight into potential impacts that

can be expected from high penetrations of all-electric vehicles in both the LDV and HDV sector as vehicle emissions and PFI changes would be largely equivalent to those assumed here for FCEV. Potential differences could occur in emissions from the electricity sector due to vehicle charging impacts, however emissions from generators were shown to have a lesser impact to emissions from both vehicle and PFI sources.

While LDV FCEV deployment achieves AQ benefits, the magnitude of observed pollutant reductions are moderate when viewed in the full context of Cases – those experiencing notable AQ improvements represent a considerably successful outcome for FCEVs, i.e., a penetration of 50–100% of the sector in counties of interest. Increases in efficiency and improved pollutant control technologies in LDVs result in a significantly lower-emitting fleet in 2055 relative to current in the Reference Case, despite an increase in vehicle-miles-traveled. In contrast, some non-LDV transportation technologies could have a proportionately larger impact on AQ in

2055, including HDVs. Demonstrating this, reducing HDV emissions in the same counties achieves similar or enhanced AQ benefits relative to the LDV FCEV Cases despite the lack of reductions from PFI and power generation. Further, when similar reductions are assumed (i.e., the HDV 50 PFI) the corresponding reductions in ozone and $PM_{2.5}$ are greater, both quantitatively and spatially. Thus, incorporating fuel cell technologies in all transportation sub-sectors, including HDVs, can assist in improving AQ and should be considered moving forward in the development of AQ improvement strategies. Indeed, pursuit of policies designed to encourage FCEV deployment should consider that HDV targets may have more value in terms of AQ benefits than LDV FCEV.

Emissions from PFI supporting motor gasoline production and distribution have important influences on ozone and $PM_{2.5}$ concentrations in CA in 2055. Contributions to regional $PM_{2.5}$ levels drive peak impacts for both LDV and HDV Cases. Moreover, reductions from PFI occur in regions of CA currently experiencing poor AQ which heightens the importance of the results, including ozone reductions in the Southern Central Valley, S.F. Bay Area, and the SoCAB and $PM_{2.5}$ in the SoCAB. However, while programs and policies are in place to promote the deployment of alternative, low or zero-emitting LDV technologies that will concurrently reduce gasoline consumption, e.g., CA's Zero Emission Vehicle Program [3], it is unknown if emissions will also decrease from PFI. A potential outcome is that gasoline production at CA refineries may remain constant with excess product exported. Thus, designing and implementing LDV adoption strategies that maximize AQ and GHG benefits should consider also reductions from sources associated with gasoline production and storage including petroleum refinery complexes.

The results show the complex relationship between the formation and fate of atmospheric pollutants and the spatial distribution of direct emissions, most notably in regards to ground-level ozone. Due to the temporal period required for ozone production from precursor emissions the spatial distributions of reductions are not necessarily correlated directly with sites of emission subtraction from vehicle operation and others, e.g., in the SoCAB maximum ozone reductions occur in Riverside and San Bernardino Counties from emission reductions in Los Angeles and Orange Counties. However, as the highest background levels of ozone occur in the affected areas which support large urban populations the observed ozone impacts are beneficial. Similarly, $PM_{2.5}$ benefits are most prominent in areas adjacent to large refinery complexes which may not necessarily be located in counties of FCEV deployment. This has importance to CA in understanding how “disadvantaged communities” will experience quantifiable AQ benefits with FCEV deployment in areas expected to see high rates or early adoption.

Understanding the regional AQ impacts of FCEV adoption only in select areas is important from both an environmental justice and regulatory perspective. Specifically, reducing exposure to air pollution from transportation sources in CA has been targeted as being an important environmental justice concern [60]. Furthermore, there is legislation (Senate Bill 535) in CA that requires a certain amount of funds from the Greenhouse Gas Reduction Fund (GGRF) to be spent in

“disadvantaged communities”, i.e., degraded AQ, low income, etc [61]. The money collected during Cap-and-Trade auctions is deposited into the GGRF, and this fund is expected to be substantial in future years and the determination of appropriate funding opportunities will be of importance. Results suggest that projects comprising the deployment of cleaner transportation technologies can result in reductions in air pollutant exposure for residents of disadvantaged communities – even if technologies are deployed or utilized in non-disadvantaged areas.

Conclusions

Atmospheric modeling is used to assess the impacts on ground-level ozone and $PM_{2.5}$ from the deployment of FCEVs comprehensively relying on renewable energy electrolysis-produced hydrogen in CA counties expected to support early adoption of advanced LDV technologies. Projecting the AQ implications of the early adoption of FCEVs requires spatial and temporal emission field development followed by detailed modeling of atmospheric chemistry and transport. Results obtained in this work for CA establish that (1) a significant penetration of LDVs with FCEVs in 2055 will improve AQ in many regions of CA including areas not encompassing FCEVs, and (2) reductions in emissions from the production and distribution of petroleum fuels play a key role in AQ benefits. Ground-level ozone concentration reductions are wide-spread through the State and occur in areas distant from the counties of emission displacement as a result of the dynamics of ozone formation and fate in relation to precursor emissions. In addition, deploying strategies to mitigate HDV emissions in the same counties may achieve greater reductions in ozone and $PM_{2.5}$ than those for LDV and highlights the importance in coming decades of non-LDV transportation technologies in regional AQ planning. As would be expected, improvements rise in parallel with penetrations of FCEVs in counties under study with the FCEV 1 Case exhibit a minor effect on concentrations and FCEV 50 and 100 Cases achieving significant AQ benefits. AQ impacts from PFI emissions are important with regards to both magnitude and spatial distribution and the results highlight the importance of considering emissions from PFI in maximizing AQ benefits from the deployment of advanced alternative transportation technologies. Specifically, the most important impacts on $PM_{2.5}$ occurred from emission reductions from major refinery complexes in the State.

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