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Journal

International Journal of Hydrogen Energy, 34(2)

ISSN

0360-3199

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Publication Date

2009

DOI

10.1016/j.ijhydene.2008.10.045

INTERNATIONAL JOURNAL OF HYDROGEN ENERGY 34 (2009) 628–641

Available at www.sciencedirect.com

ScienceDirect

journal homepage: www.elsevier.com/locate/he

Demonstration of a novel assessment methodology for hydrogen infrastructure deployment

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ARTICLE INFO

Article history:
Received 11 June 2008
Received in revised form
2 October 2008
Accepted 2 October 2008
Available online 11 December 2008

Keywords:
Hydrogen economy
Hydrogen infrastructure
Hydrogen generation
Hydrogen distribution
Hydrogen vehicles
Hydrogen life cycle
Hydrogen greenhouse gas
Fuel cell vehicle

ABSTRACT

To reduce criteria pollutant emissions and greenhouse gases from mobile sources, the use of hydrogen as a transportation fuel is proposed as a new paradigm in combination with fuel cells for vehicle power. The extent to which reductions can and will occur depends on the mix of technologies that constitute the hydrogen supply chain. This paper introduces an analysis and planning methodology for estimating emissions, greenhouse gases, and the energy efficiency of the hydrogen supply chain as a function of the technology mix on a life cycle, well to wheels (WTW) basis. The methodology, referred to as the *preferred combination assessment* (PCA) model, is demonstrated by assessing an illustrative set of hydrogen infrastructure (generation and distribution) deployment scenarios in California's South Coast Air Basin. Each scenario reflects a select mix of technologies for the years 2015, 2030, and 2060 including (1) the proportion of fossil fuels and renewable energy sources of the hydrogen and (2) the rate of hydrogen fuel cell vehicle adoption. The hydrogen deployment scenarios are compared to the existing paradigm of conventional vehicles and fuels with a goal to reveal and evaluate the efficacy and utility of the PCA methodology. In addition to a demonstration of the methodology, the salient conclusions reached from this first application include the following.

- Emissions of criteria pollutants increase or decrease, depending on the hydrogen deployment scenario, when compared to an evolution of the existing paradigm of conventional vehicles and fuels.
- For all scenarios, pipeline distribution from a centrally located generation source reduces criteria pollutant emissions when compared to distribution by truck.
- With one qualification, greenhouse gas emissions are reduced for the scenarios considered with the extent of reduction increasing in proportion to the renewable sources of hydrogen. When natural gas is utilized as a source for hydrogen, leakage of methane from the U.S. natural gas infrastructure is a significant contributor to the greenhouse gases associated with a hydrogen economy.
- For all scenarios considered, the WTW energy efficiency improves whereas the consumption of water (and the associated energy) increases.

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doi:10.1016/j.ijhydene.2008.10.045

Nomenclature

CARB	California Air Resources Board
CO	carbon monoxide
CO_2	carbon dioxide
H_2 ICE	hydrogen internal combustion engine
H_2I	hydrogen infrastructure scenario
HFCV	hydrogen fuel cell vehicle
HTFC	high temperature fuel cell
MCFC	molten carbonate fuel cell
NFCRC	National Fuel Cell Research Center, UC Irvine
NMHC	non-methane hydrocarbons
NO_x	oxides of nitrogen
NREL	National Renewable Energy Laboratory
PEM	polymer electrolyte membrane
PM	particulate matter
PSA	pressure swing absorption
SoCAB	South Coast Air Basin of California
SOFC	solid oxide fuel cell
SO_x	oxides of sulfur
U.S.DOE	United States Department of Energy
VMT	vehicle miles traveled
WTW	well to wheels
ZEV	zero emission vehicle

1. Introduction

Hydrogen is an alternative under consideration to replace conventional transportation fuels. Interest in transitioning to hydrogen is being driven by the contribution of today's vehicles to the carbon burden in the troposphere, and the concentrations of photochemical oxidant, carbon monoxide, hydrocarbon, and particulate in urban air sheds [1]. Concerns about the availability of petroleum reserves and geopolitics are also creating a push for alternative fuels that can be sourced from plentiful reserves within the country borders [2]. In addition, hydrogen enables a cleaner and more efficient alternative to the internal combustion engine. The prime example is the fuel cell, which operates on pure hydrogen and today powers prototype automobiles and buses at high efficiencies with water as the principal byproduct. The supply chain for hydrogen, however, can produce emissions of both primary (''criteria'') pollutants and greenhouse gases (GHGs), require a significant input of energy, and place a substantial demand on water resources. To mitigate this and assure an energy efficient, environmentally sensitive, and economically viable generation and delivery of hydrogen, the specification of the hydrogen supply chain requires care and, ideally, a systematic evaluation of options.

Many technology options exist to support the supply chain including the generation of hydrogen from a feedstock, the distribution of hydrogen to fueling stations (as needed), and the dispensing of the hydrogen into a vehicle. The impact signature of a hydrogen infrastructure will vary widely depending on which technologies are used along the supply chain. Because transitioning to hydrogen will require massive investments, it is important to understand, through advanced planning and modeling, the effects of different infrastructure scenarios. Though previous studies have assessed either hydrogen production pathways [3–7] or vehicle and fueling station deployments [8–11], few have considered the (1) integration of a variety of technology options in a hydrogen supply chain, and (2) mix of technology options in the context of deployment. This study introduces a novel tool, the *preferred combination assessment* (PCA) model, designed to analyze the impacts of an integrated hydrogen supply chain with respect to criteria pollutant emissions, greenhouse gas (GHG) emissions, water consumption, and energy utilization. The PCA model is introduced and described herein, and the efficacy and utility of the model is illustrated by a set of hydrogen infrastructure deployment scenarios for the South Coast Air Basin (SoCAB) in California.

2. Methodology for hydrogen infrastructure scenario assessment

A systematic evaluation of a hydrogen infrastructure scenario must encompass the full scope of hydrogen deployment from a life cycle perspective. The PCA model operates on a life cycle, or well to wheels (WTW) basis such that the generation, distribution, and utilization of hydrogen are integral to the analysis (Fig. 1).

The PCA model integrates the variety of technologies and pathways for hydrogen into a comprehensive supply chain. The total demand for hydrogen in a region and the distances over which it must be delivered are two of the required inputs. Outputs include criteria pollutant emissions, GHG emissions, energy consumption, and water consumption. The model is

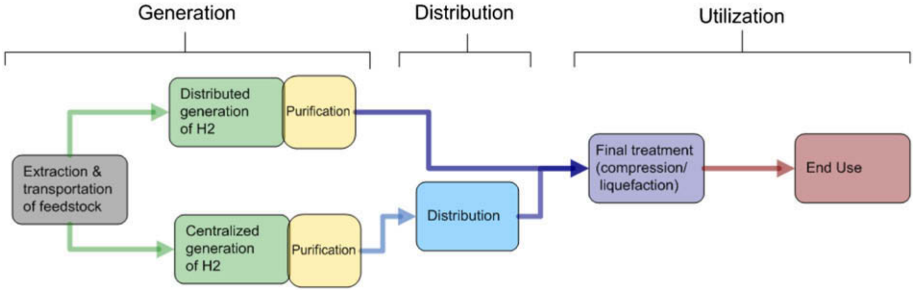

Fig. 1 – WTW hydrogen infrastructure processes considered for impact assessment.

also compatible with existing cost analysis tools [12] providing as needed the opportunity to incorporate an economic examination. Fig. 2 represents a simplified description of the model. The contribution by each technology option can be adjusted to explore how various permutations affect the outputs.

The technologies that have been incorporated into the PCA model to date are cataloged in Table 1. Included are various technologies for hydrogen *generation* (on both a central and distributed scale), hydrogen *distribution*, and *utilization* (compression and dispensing). They are selected based on the likelihood of implementation, level of maturity, preparedness for the marketplace, and ability to meet infrastructure and regulation requirements [13–15]. Hydrogen supply technologies that have not been fully demonstrated are excluded. The model is friendly to including next generation technologies once maturation establishes the (1) viability for deployment, and (2) impacts associated with deployment.

For each technology included in the model, emission factors are established for criteria pollutants and GHGs (Table 2). Energy and water consumption factors are also established for each technology. These factors serve as parameters in the model such that emissions and energy consumption outputs can be produced. The model provides the ability to adjust the contribution by each technology to the comprehensive supply chain allowing for the design of various infrastructure scenarios. It also takes into consideration the evolution of technologies over time, and changes in performance.

Of the impact categories included in a full LCA [16,17], four are addressed in the PCA model: (1) emission of criteria pollutants, (2) emission of greenhouse gases, (3) energy consumption, and (4) water consumption. Furthermore, the model incorporates the impacts associated with the operation of equipment on a WTW basis so that the entire supply chain of the fuel, from the extraction of a hydrogen feedstock to the end use, is included. The model does not include the impacts associated with the construction and decommissioning of the equipment.

3. Illustrative example

To evaluate the utility and efficacy of the PCA model, HFCV deployment scenarios and hydrogen infrastructure deployment scenarios were established for the South Coast Air Basin (SoCAB) of California. The SoCAB is of particular interest due to the (1) complex and severe air quality challenges associated with the basin, (2) history of the Basin as a leader in clean technologies, and (3) fact that many stakeholders, including the U.S. Department of Energy [18] view the Basin as a test-bed for the early deployment of hydrogen fuel cell vehicles (HFCVs). That California was the first U.S. state to pass legislation mandating reductions in GHG emissions is also noteworthy [19]. The PCA model was employed to assess the impact of selected combinations of the vehicle and infrastructure scenarios for the years 2015, 2030, and 2060. To provide a basis for comparison to the hydrogen scenarios, a reference case for conventional vehicles and fuels was established for each of the years analyzed.

3.1. *Cases for vehicle deployment in SoCAB*

The PCA model was applied to several cases for vehicle deployment to explore the utility and potential effectiveness of the model. Vehicle deployment cases were established by defining the following set of variables.

1. Geographic region. The SoCAB was selected as the geographic region.

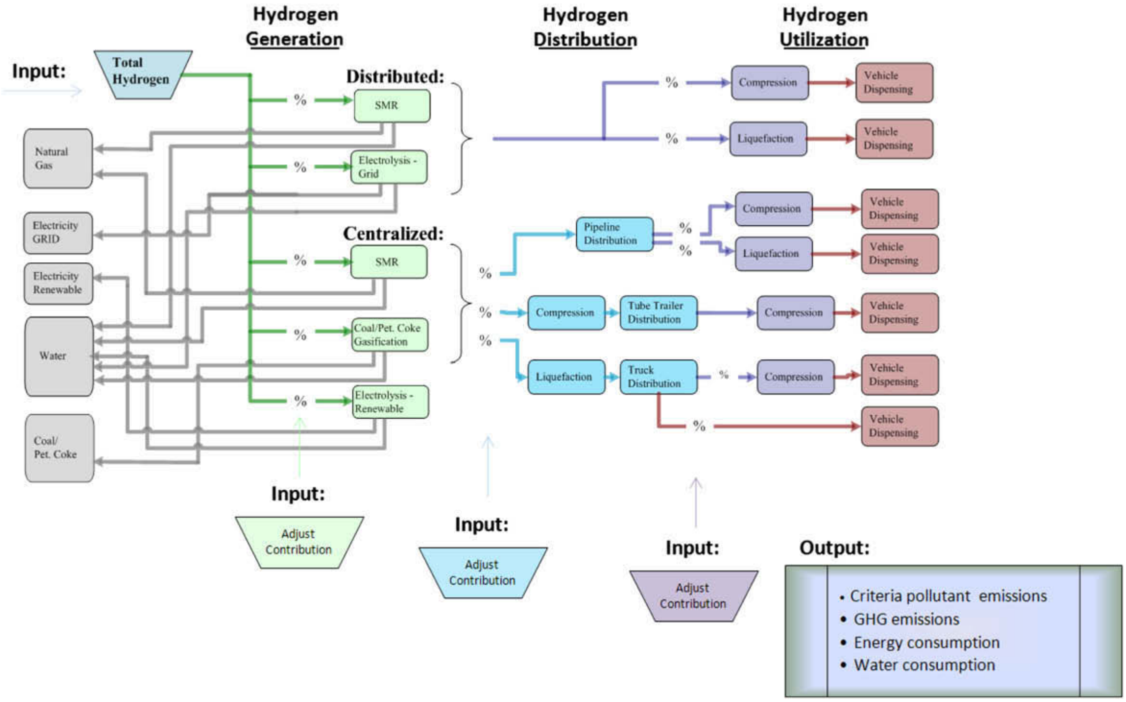

Fig. 2 – Simplified schematic of the PCA model.

Table 1 – Technologies under consideration for hydrogen infrastructure assessment.

Hydrogen generation	
Feedstock extraction and transportation	
Natural gas	
Water	
Electricity	
Petroleum coke	
Coal	
Strategy for conversion to hydrogen	
Centralized	Distributed
SMR[a]	SMR[a]
Electrolysis (renewable)	HTFC cogeneration with natural gas[b]
Petroleum coke (cogeneration)	Electrolysis (grid)
Coal gasification (cogeneration; CO2 sequestration)	Electrolysis (renewable)
Hydrogen distribution	
Truck – tube trailer (pressurized gas)	
Truck – liquid tanker	
Pipeline (gaseous hydrogen)	
Hydrogen utilization (dispensing)	
350 bar (pressurized gas)	
700 bar (pressurized gas)	
Liquid hydrogen	
140 bar (pressurized gas)	

[a] SMR refers to steam methane reformation using natural gas as the feed.

[b] HTFC cogeneration with natural gas refers to use of a high temperature fuel cell operating on natural gas feed to produce three useful products: electricity, heat, and hydrogen for use in vehicles.

2. Temporal setting. Cases for vehicle deployment were developed for the years 2015, 2030, and 2060. Year 2015 provides a starting point from which a 2030 case can be produced to show the effects of significant HFCV market penetration, followed by a 2060 case in which HFCVs account for a majority of the vehicle population. By modeling vehicle deployment in these years, it is possible to explore the manner by which a hydrogen infrastructure might evolve to achieve a preferred outcome.
3. HFCV adoption. A realistic percentage of adoption was extrapolated for each timeframe under consideration [18]. In 2015 the assumed HFCV adoption was 0.25%. Government and private fleet adoption, along with consumer test programs will account for the majority of the vehicles in 2015. For the year 2030 a 12.5% HFCV penetration was assumed, and 75% penetration was assumed for 2060.

Table 2 – List of emissions species included in this study.

Emissions category	Pollutant	Abbreviation
Criteria pollutants	Non-methane hydrocarbons	NMHC
	Carbon monoxide	CO
	Oxides of nitrogen (refers to both NO and NO2)	NO_x
	Oxides of sulfur (refers to SO2)	SO_x
	Total particulate matter	PM
Greenhouse gases	Carbon dioxide	CO_2
	Methane	CH_4

The California Air Resources Board (CARB) Emission Factors (EMFAC) [20] model provides a method for determining the current and predicted vehicle miles traveled (VMT) by passenger vehicles in SoCAB. Because the EMFAC model only forecasts VMT up to and including the year 2040, it was necessary to extrapolate data into the year 2060. Penetration of HFCVs was calculated on a VMT basis. HFCV gains in fuel economy compared to a conventional passenger vehicle were taken into account when calculating the demand for hydrogen fuel. HFCV fuel economy was assumed as 45 miles/kg in 2015, 55 miles/kg in 2030, and 60 miles/kg in 2060. Fig. 3 shows the increase in vehicle miles traveled in SoCAB from 2005 to 2060, and the penetration of HFCVs that is predicted in this study.

The cases for vehicle deployment were confined to HFCVs for the sake of illustration of the PCA model. Other types of hydrogen-powered vehicles are being proposed and tested (e.g., hydrogen internal combustion engine vehicles, hydrogen buses) and plug-in hybrid electric vehicles (PHEVs) are currently under evaluation and hydrogen PHEVs are a possibility. The PCA model is designed to accommodate these vehicle options.

3.2. *Establishing hydrogen infrastructure scenarios*

The PCA model requires the input of a hydrogen infrastructure scenario, which encompasses the following set of parameters.

1. Total demand of hydrogen in the region.
2. The contribution by each technology that constitutes the hydrogen supply chain.
3. The emissions, energy consumption, and water consumption associated with each hydrogen supply chain technology.

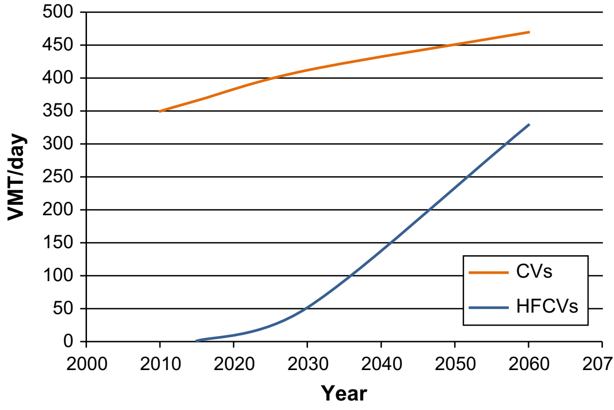

Fig. 3 – HFCV penetration rates as a portion of total VMT in SoCAB.

4. The number of fueling stations and hydrogen generation facilities located in the region of interest.
5. The characterization of emissions from hydrogen-powered vehicles.

For the present case, each hydrogen infrastructure scenario considered was defined by assuming that all of the infrastructure was placed in the SoCAB with three exceptions: processes involving the extraction and transportation of feedstocks for hydrogen (e.g., natural gas, coal), coal IGCC plants providing hydrogen and electricity to the basin but located outside the basin, and power plants providing electricity for the basin but located outside the basin. Since all hydrogen-powered vehicles were characterized as fuel cell vehicles in this study, tailpipe emissions were limited to water.

For the 2015 timeframe, an early adoption scenario for hydrogen infrastructure was designed by assigning appropriate values to each parameter. When designing subsequent scenarios for the timeframes 2030 and 2060, two different strategies were considered for the adoption of hydrogen infrastructure: one in which fossil fuels account for most of the hydrogen feedstock, and a second in which renewable energy sources account for most of the feedstock. Table 3 provides a complete list of the scenarios included in this study. Table 4 provides detailed characterization of the hydrogen supply chain technologies assigned to each scenario. It is important to affirm that these scenarios are for illustrative purposes in order to demonstrate the utility and potential efficacy of the PCA.

3.3. *Establishing scenarios with conventional vehicles for comparison*

Reference base case scenarios were established for the years 2015, 2030, and 2060, in which all passenger vehicles in SoCAB were assumed to be conventional vehicles fueled by conventional fuels. The ARB EMFAC model was used to establish the criteria pollutant emissions, GHG emissions, and gasoline consumption from passenger vehicles [20]. Emissions from petroleum refineries were established in correlation to the amount of gasoline provided to passenger vehicles in those years [21,22]. By combining the results from the passenger vehicles and petroleum refining, the WTW emissions, and energy consumption values associated with conventional vehicles in SoCAB were estimated.

3.4. *Energy and water consumptions, and emission factors*

Energy consumption, water consumption, and emission factors for the hydrogen supply chain technologies were established from both literature sources and experimental data collected at the National Fuel Cell Research Center (NFCRC) [23]. Literature sources include reports from the California Air Resources Board that catalogue emissions from both the California electrical grid [24] and mobile sources in the state [20], reports on advanced coal technologies [25] and hydrogen production from high temperature fuel cells [26] prepared by the Advanced Power and Energy Program at UC Irvine, various LCA reports from the U.S. National Renewable Energy Laboratories [27–30], and reports from the California Energy Commission on the relationship between energy and water [31].

The water consumption model includes processes that are used across the entire supply chain for hydrogen. For example, the mining and drilling for hydrogen feedstocks, the Rankine Cycle generation of power, and the technologies for hydrogen conversion all require water [32,33]. Generally, well to tank (WTT) processes for hydrogen production will take place in the southwestern United States whether they are inside the SoCAB or outside. Because this entire region faces water resource issues, water use across the life cycle of hydrogen production was considered in this study rather than placing focus on the SoCAB. In the case of Rankine Cycle power production, the amount of water withdrawn from the environment can greatly exceed the net water consumed by the plant because much of the cooling water is returned back to the environment [32]. This study utilizes data based on Rankine Cycle water consumption. However, the difference between Rankine Cycle water withdrawal and consumption is relatively small when compared to the overall water use of the hydrogen infrastructure scenarios that are described below.

4. Results

4.1. *Well to wheels criteria pollutant emissions from urban sources*

The PCA model was used to establish the criteria pollutant emissions from the urban sources for each hydrogen infrastructure scenario evaluated in this study. Urban emissions were defined as those coming from sources located within the

Table 3 – Characterization of hydrogen infrastructure scenarios analyzed in this study.

Scenario[a]	EA-H2I/FCHV	FF-H2I/FCHV	R-H2I/FCHV	FF-H2I/FCHV	R-H2I/FCHV
Year	2015	2030	2030	2060	2060
Technology mix	Early adoption mix	Mostly fossil fuel sources	Mostly renewable sources	Mostly fossil fuel sources	Mostly renewable sources
HFCV penetration (%)	0.25	12.5	12.5	75	75
Population of HFCVs	26,294	1,508,487	1,508,487	10,162,500	10,162,500
Demand for H_2 (kg/day)	20,264	935,895	935,895	5,868,750	5,868,750

a Abbreviations for various scenarios. H2I: hydrogen infrastructure scenario. EA: early adoption infrastructure scenario. FF: fossil fuel weighted infrastructure scenario. R: renewable weighted infrastructure scenario.

Table 4 – Detailed characterization of supply chain technology mix for hydrogen infrastructure scenarios.

Scenario[a]	EA-H2I/FCHV	FF-H2I/FCHV	R-H2I/FCHV	FF-H2I/FCHV	R-H2I/FCHV
Year	2015	2030		2060	
Hydrogen conversion technology					
Central scale technologies					
SMR	65%	45%	40%	30%	20%
Electrolysis (renewable)	–	–	5%	5%	30%
Petroleum coke (cogeneration)	–	20%	10%	10%	5%
Coal gasification (cogeneration)	–	–	–	30%	10%
Distributed scale technologies					
SMR	20%	10%	10%	5%	5%
HTFC cogeneration with natural gas	5%	15%	15%	15%	15%
Electrolysis (grid)	7%	5%	5%	–	–
Electrolysis (renewable)	3%	5%	10%	5%	15%
Hydrogen distribution					
Truck – tube trailer (pressurized gas)	15%	–	–	–	–
Truck – liquid tanker	83%	85%	85%	40%	40%
Pipeline (gaseous hydrogen)	2%	15%	15%	60%	60%
Hydrogen utilization (dispensing)					
350 bar (pressurized gas)	60%	60%	60%	30%	30%
700 bar (pressurized gas)	25%	15%	15%	–	–
Liquid hydrogen	5%	5%	5%	–	–
140 bar (pressurized gas)	–	20%	20%	70%	70%

a Abbreviations for various scenarios. H2I: hydrogen infrastructure scenario. EA: early adoption infrastructure scenario. FF: fossil fuel weighted infrastructure scenario. R: renewable weighted infrastructure scenario.

SoCAB. As a result, sources of criteria pollutant emissions excluded from this category are processes for the generation of hydrogen feedstocks located outside of the basin (e.g., power plants providing electricity to the basin in support of the hydrogen infrastructure, coal IGCC plants with hydrogen cogeneration). This section presents the results for the impact on urban air shed air quality. The impact of hydrogen infrastructure on the regional emission of criteria pollutants is presented in the Appendix.

Fig. 4 compares the hydrogen infrastructure (EA-H2I/HFCV) and vehicle urban emissions for a 0.25% HFCV adoption in SoCAB in a 2015 timeframe to those from an equal quantity of conventional vehicles (CVs). At such a small rate of adoption, the effects of HFCV deployment on total passenger vehicle emissions are negligible. However, the adoption levels that were assumed in the years 2030 and 2060 (12.5% and 75%, respectively) produce a visible effect on the total emissions associated with passenger vehicles. Fig. 5(a)–(e) exhibits the change in urban criteria pollutant emissions as a portion of total passenger vehicle emissions for the 2030 and 2060 timeframes. The different scenarios represent the fossil fuel dominated H2 infrastructure (FF-H2/HFCV), the renewable dominated H2 infrastructure (R-H2/HFCV), and conventional vehicles for each of the two years.

The emissions of NMHC, CO, and PM are substantially reduced in each hydrogen infrastructure scenario considered. The emission of NO_x is also reduced, but not to the same extent. The emission of SO_x is increased in every hydrogen infrastructure scenario in comparison with conventional vehicles, with the exception of the R-H2I/HFCV scenario in 2060, which is only slightly decreased. The PCA model allows a detailed evaluation of this result. For example, Fig. 6 shows the contribution by source to the total urban SO_x emissions in the 2030 and 2060 hydrogen infrastructure scenarios. The use of petroleum coke to generate hydrogen is clearly the largest contributor to the emission of SO_x. A significant portion of SO_x also comes from the use of trucks for the distribution of hydrogen. The case is similar for NO_x emissions (Fig. 7). One difference is that the distribution of hydrogen by truck accounts for most of the NO_x emissions in 2030, whereas the generation of hydrogen from Pet Coke gasification is the most prominent single source of NO_x in the 2060 timeframe.

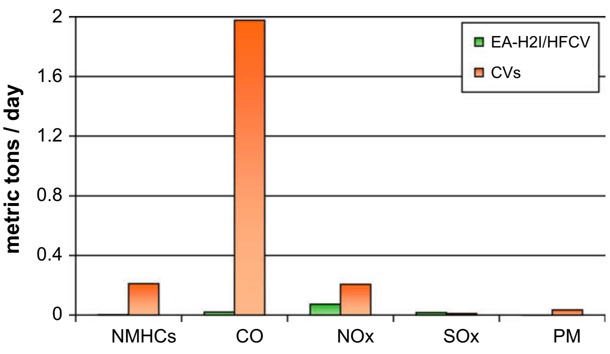

Fig. 4 – Comparison of urban emissions from a 0.25% HFCV adoption rate to an equal quantity of conventional vehicles in the year 2015.

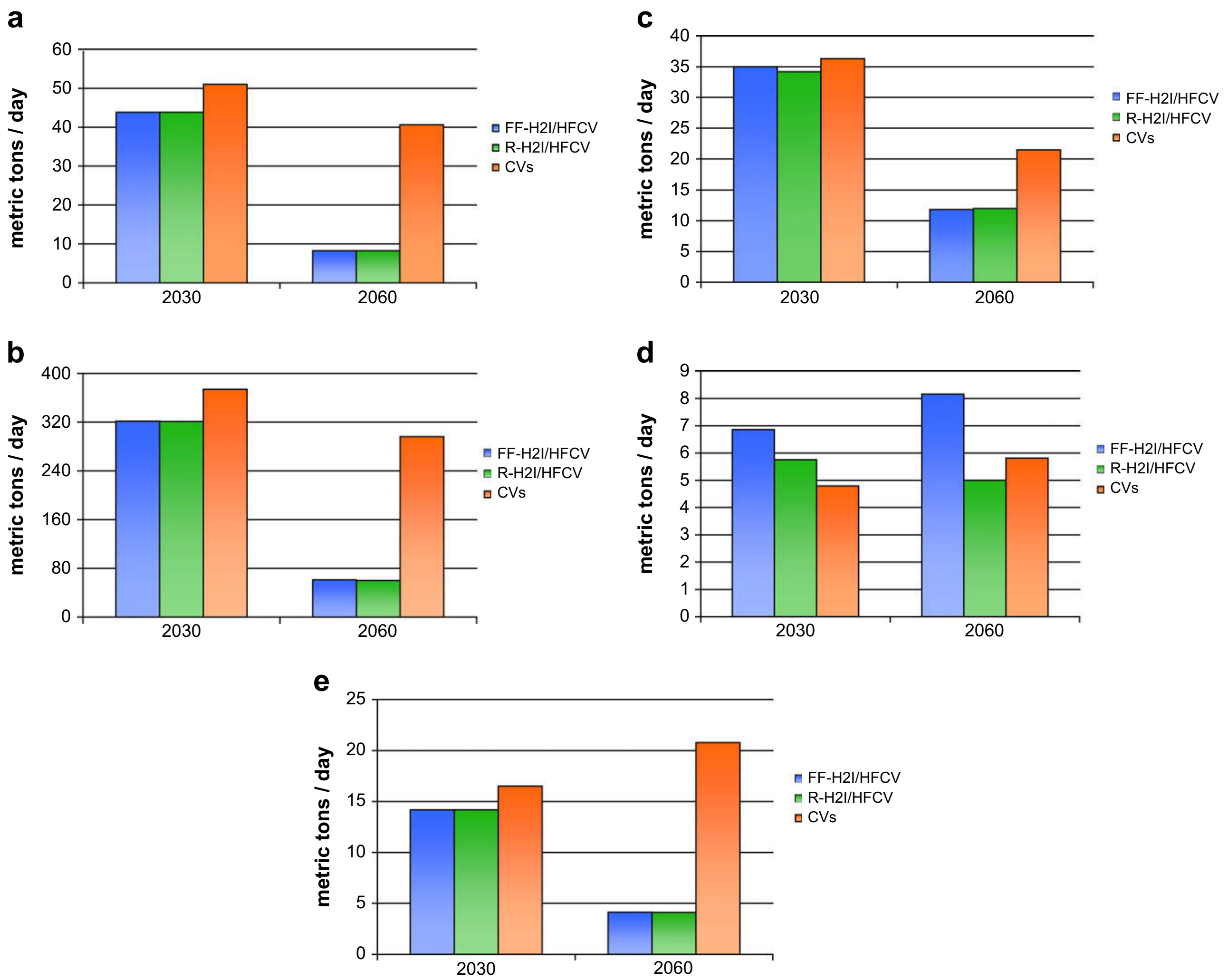

Fig. 5 – Emissions displaced by adoption of hydrogen infrastructure scenarios in 2030 and 2060. (a) NMHC emissions; (b) CO emissions; (c) NO_x emissions; (d) SO_x emissions; and (e) PM emissions.

4.2. *Well to wheels GHG emissions*

Well to wheels GHG emissions for each hydrogen infrastructure scenario were also established with the PCA model. Fig. 8 presents the GHG emissions for 2030 and 2060. (The reduction in GHG emissions is negligible for the 2015 scenario.) The FF-H2I scenario yields a 7.8% reduction in GHG emissions by 2030 and a 64.2% reduction by 2060. The R-H2I/HFCV scenario yields a 9.3% reduction in GHG emissions by 2030, and a 70.2% reduction by 2060.

4.3. *Well to wheels energy consumption*

The PCA model establishes the energy consumed in each hydrogen infrastructure scenario from which the efficiency of the integrated hydrogen supply chain can be calculated. To produce the well to wheels energy consumed per VMT, the supply chain efficiency was combined with the fuel economy of HFCVs assumed to be an average of 45 miles/kg in 2015, 55 miles/kg in 2030, and 60 miles/kg in 2060.

Fig. 9 compares the WTW energy consumption per VMT of each hydrogen infrastructure scenario to that of the baseline scenarios (CVs) that were developed using the EMFAC model. The WTT efficiency of conventional fuels (i.e., petroleum refining) was assumed as 84% [34–36].

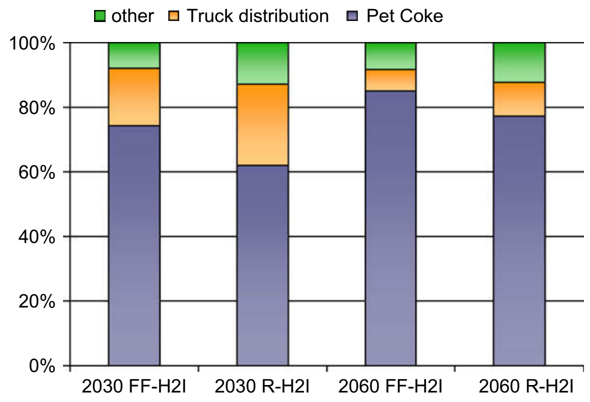

Fig. 6 – SO_x emission shown by source as a portion of the total emissions associated with hydrogen infrastructure scenarios.

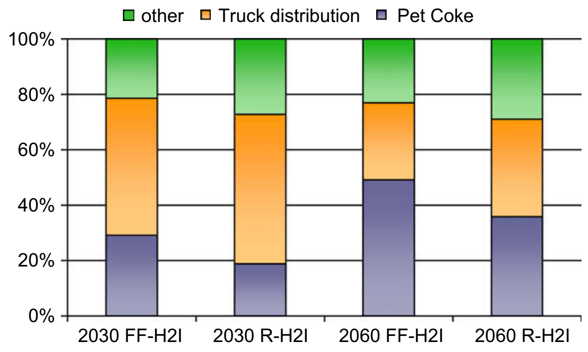

Fig. 7 – NO_x emissions shown by source as a portion of the total emissions associated with hydrogen infrastructure scenarios.

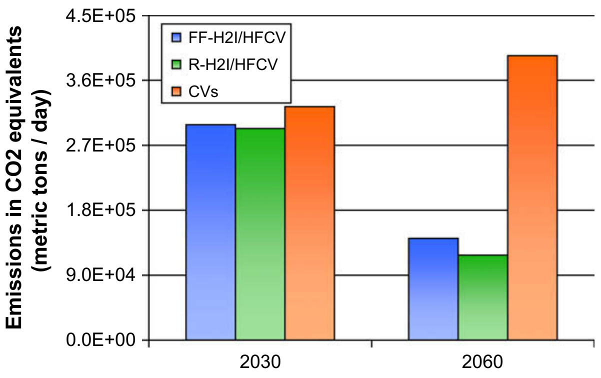

Fig. 8 – Well to wheels GHG emissions displaced by adoption of hydrogen infrastructure scenarios in 2030 and 2060.

Because the electrical infrastructure plays a role in many of the supply chain processes (i.e., electrolysis, liquefaction, pipeline distribution, compression), the efficiency of the electrical power grid has a large impact on the efficiency of the hydrogen infrastructure scenario. In this study the electrical power grid servicing the SoCAB was assumed for illustration to have an efficiency of 35% in 2015, 38% in 2030, and 45% in 2060.

4.4. *Well to wheels water consumption*

The PCA model revealed several notable observations regarding the demand for water associated with hydrogen infrastructure deployment. For direct processes, the amount of water required for electrolysis is about half of that required for hydrogen generation from SMR, and 12% of that for hydrogen generated via coal gasification. However, if the Rankine Cycle water demand for electrolysis is taken into account, then the water use for hydrogen produced from electrolysis can have a wide range depending on whether it is produced from wind and photovoltaic (PV), solar thermal, or grid power sources. Table 5 summarizes the different water requirement for generation of hydrogen.

Water demand is important to take into consideration for hydrogen generation, particularly in basins such as the SoCAB where water resource constraints have been an issue throughout the history of the region's development. In particular, using the PCA and the data of Table 5, the relative increase in water demand for a hydrogen infrastructure can be compared to conventional vehicles in a region. Fig. 10 compares the water use associated with the hydrogen infrastructure scenarios in this study to petroleum refining for continued use of conventional passenger vehicles in the SoCAB. To place this into perspective, Fig. 11 compares projections for total water use in SoCAB (based on current trends [37,38]), with and without the adoption of a hydrogen infrastructure. The adoption of hydrogen as a transportation fuel will likely increase the demand for water in the SoCAB. Water demands in scenario FF-H2I/HFCV in 2060 are 2.3% greater than those of scenario R-H2I/HFCV in 2060. This is attributed to the relatively high water demands of coal-fired and petroleum coke-fired IGCC plants as a strategy for co-generating hydrogen and electricity. A push towards air-cooled Rankine Cycle power plants can reduce water consumed by coal and petroleum coke based hydrogen generation. However, this strategy faces two challenges: a reduction in system efficiencies and an increase in the footprint of the plants [39].

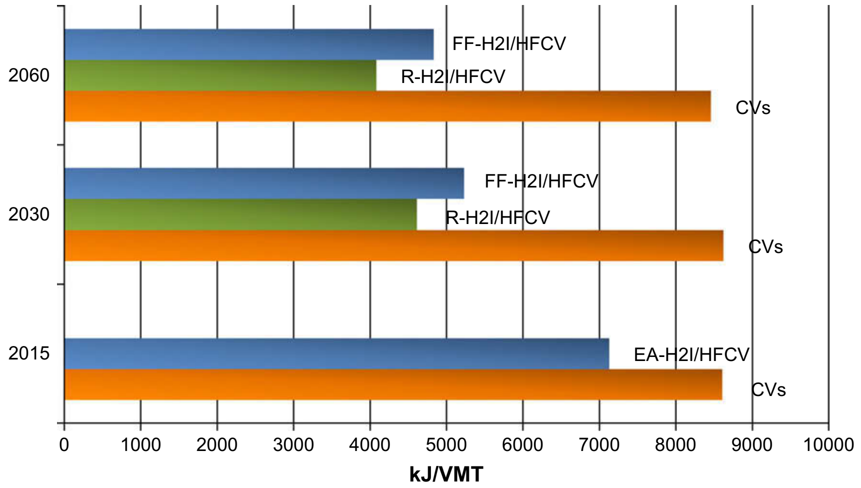

Fig. 9 – WTW energy consumption per VMT comparing hydrogen infrastructure scenarios with baseline scenarios (CVs).

Table 5 – Life cycle water consumption associated with hydrogen generation strategies.

Fuel	Generation strategy	Gallons of water Per Gallon	Gallons of water Per kg
Gasoline		3.0	
Hydrogen	Steam methane reformation		6.3
	Electrolysis (wind and PV)		2.8
	Electrolysis (solar thermal)		3.6
	Electrolysis (grid)		3.4
	Petroleum coke gasification		17.9
	Coal gasification		24.2

4.5. *Sensitivity analysis with respect to hydrogen distribution*

A key attribute of the PCA model is the amenability to the conduct of sensitivity analyses. To demonstrate and evaluate this attribute, a sensitivity analysis was performed to determine the effect of the distribution strategies on the criteria pollutant emissions and GHG emissions of a hydrogen infrastructure in the SoCAB. For example, in the 2030 and 2060 timeframes, the hydrogen distribution strategy was shifted to either all pipeline, or all truck with liquid tanker. Fig. 12(a), (d) shows the effect of distribution strategy on criteria pollutant emissions for each of the scenarios in 2030 and 2060. In 2030, the use of pipeline distribution can result in significant reductions of emissions, particularly those of NO_x and SO_x. In 2060, the use of pipeline distribution results in a less significant improvement of the total urban emissions. This is due to (1) an anticipated modernization of the truck fleet, and (2) an increase of petroleum coke gasification as a strategy for generating hydrogen. Distribution strategy had little or no effect on GHG emissions for any of the scenarios under consideration.

4.6. *Emissions from the natural gas infrastructure*

While the current results are presented to demonstrate and illustrate the utility of the PCA model, the application of the model to the SoCAB revealed a number of general insights. For example, in cases where natural gas is an input feedstock, the emissions of criteria pollutants and GHGs associated with the extraction and transport of the natural gas have a significant impact on the LCA of a hydrogen infrastructure. In Fig. 13, the incremental change in criteria pollutant emissions in the SoCAB (''urban emissions'') are compared to the incremental change in criteria pollutant emissions associated with the extraction and transport of the natural gas (''NG emissions'') for the 2015 H2I scenario. (The natural gas criteria pollutant emissions are not presented in the previous graphs because their source is remote from the urban air shed.) In the case of NMHCs, SO_x, and PM, NG emissions are in orders of magnitude greater than urban emissions related to hydrogen production using natural gas. In the case of CO and NO_x, NG emissions are two and four times greater than urban emissions related to hydrogen production using natural gas. Fig. 14 presents the contribution of the methane leakage from the natural gas infrastructure to the GHG impact relative to emissions of CO_2. Though not as dramatic as the increase in criteria pollutant emissions, methane leakage from the U.S. natural gas infrastructure is a significant contributor to the GHG footprint associated with natural gas use in a hydrogen infrastructure. In the scenarios R-H2I/HFCV and FF-H2I/HFCV, 7.6 million and 9.4 million kg of natural gas are, respectively, consumed to provide hydrogen in the SoCAB by the year 2060. To put this into perspective, the average daily demand for natural gas in the SoCAB from the regional utility was 50.1 million kg in 2005 [40].

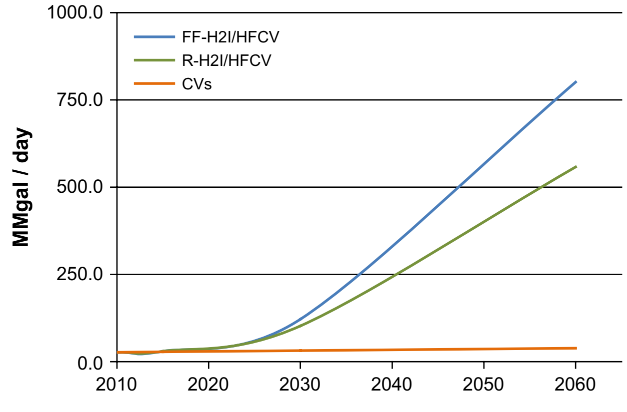

Fig. 10 – Water consumption associated with fuel preparation for passenger vehicles in SoCAB: hydrogen infrastructure plotted with conventional vehicles.

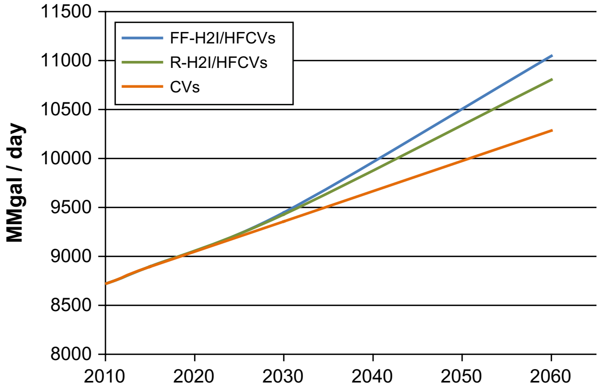

Fig. 11 – Projections for total water consumption in SoCAB with hydrogen infrastructure deployment based on current.

5. Conclusions

As governments around the world, automobile manufacturers, energy companies, and other major stakeholders begin to seriously explore a transition towards hydrogen as a transportation fuel, it is prudent to evaluate the impacts associated with the deployment of a hydrogen infrastructure and identify paths that combine and optimize energy efficiency and enable environmental stewardship. Impacts can vary widely depending on the hydrogen technologies that are employed. California will likely serve as a test-bed for early hydrogen infrastructure deployment and therefore set an example that will be closely observed.

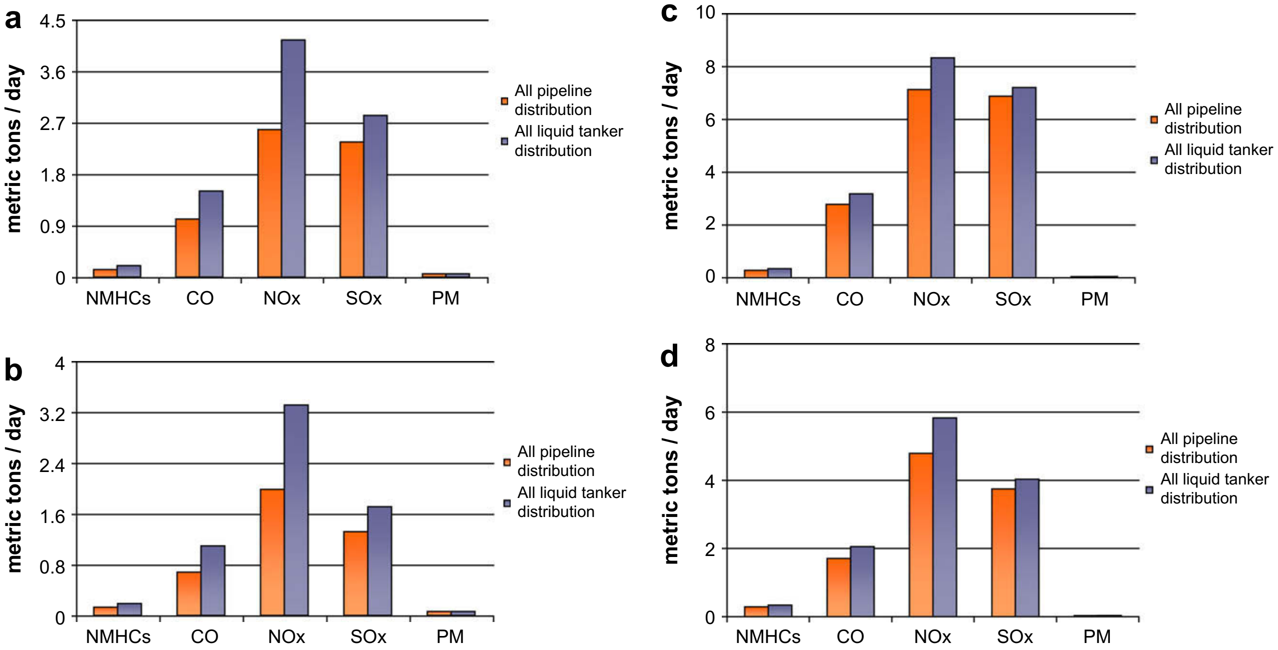

Fig. 12 – Effect of distribution strategy on urban emissions in 2030 for (a) FF-H2I; and (b) R-H2I scenarios. Effect of distribution strategy on urban emissions in 2060 for (c) FF-H2I; and (d) R-H2I scenarios.

Currently, no study has considered (1) integrating several technologies to simulate a realistic hydrogen supply chain and (2) modeled the deployment of that supply chain in a specific region of California to estimate the associated impacts with regards to emissions and water and energy consumption. To address this need, the present study illustrates the efficacy and utility of the PCA model, a methodology that integrates hydrogen technologies while allowing for adjustment of the contribution by each technology to the hydrogen supply chain on a WTW basis.

5.1. *PCA model utility*

The PCA model is designed for versatility in utility and applicability. The model integrates hydrogen technologies while allowing for adjustment of the contribution by each technology to the hydrogen supply chain on a WTW basis. The capabilities of the PCA model also include the ability to trace emissions to an exact source. This allows the inclusion of sensitivity analyses as part of the assessment process.

The versatility of the PCA allows for potentially wide set of applications. While at this point the model is well adapted for southern California, it can be applied to any geographic region in the world with appropriate adjustments. Certain characteristics about a region must be understood, such as projections for vehicle use, available resources, and the performance of the electrical grid. Similarly, these characteristics can be adjusted so as to apply the model in a variety of temporal settings.

5.2. *PCA model applicability*

As an illustration of applicability, various scenarios for hydrogen infrastructure deployment in the SoCAB were evaluated with the PCA model for the years 2015, 2030 and 2060 to test both the efficacy and potential utility of the methodology for the assessment of

- criteria pollutants,
- greenhouse gases (GHGs),
- water consumption, and
- energy efficiency

5.2.1. *Criteria pollutants*

For criteria pollutants, the PCA methodology reveals the following.

- In 2015 (0.25% penetration of HFCVs) the emission of all criteria pollutants are reduced compared to a population of conventional vehicles with the exception of SO_x, which increases.

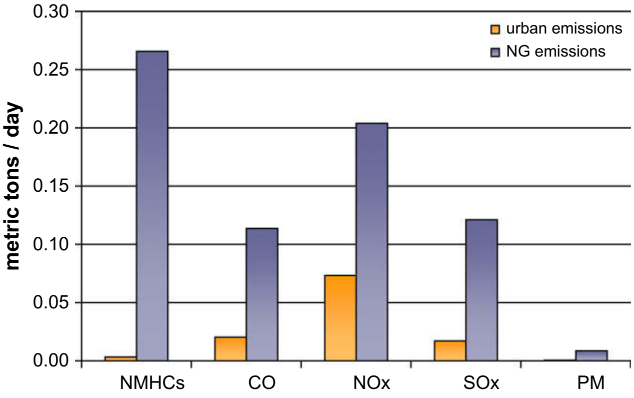

Fig. 13 – Urban emissions plotted against emissions from the extraction and transportation of natural gas for the EA-H2I/HFCVs scenario in 2015.

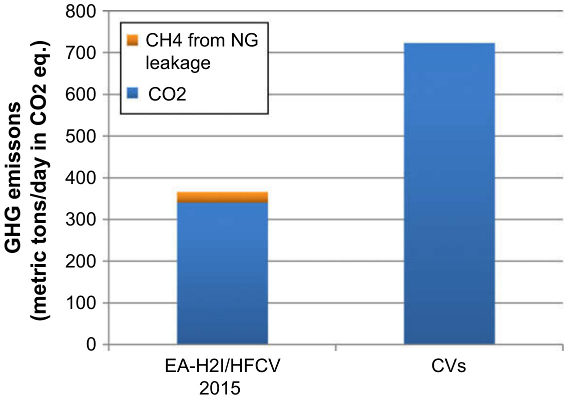

Fig. 14 – WTW CO2 emissions plotted against CH4 emissions from natural gas leakage for the EA-H2I/HFCVs scenario in 2015.

- For the years 2030 (12.5% penetration) and 2060 (75% penetration), the emission of NMHCs, CO, and PM are reduced significantly as a portion of total emissions from conventional vehicles.
- For scenarios in which fossil fuels constitute a larger portion of the technology mix in the hydrogen supply chain, SO_x emissions increase in comparison to cases with all conventional vehicles, and reductions in NO_x emissions are not as significant as for other pollutant species.
- As renewable energy sources constitute a larger portion of the technology mix, NO_x and SO_x are reduced.
- Most of the NO_x and SO_x emissions in each scenario are associated with the use of petroleum coke to generate hydrogen via gasification processes. Hydrogen distribution processes also contributed to a significant portion of these emissions.

5.2.2. *GHG emissions*

The PCA results reveal a significant reduction in GHGs by introducing a hydrogen infrastructure. With a 12.5% assumed penetration of HFCVs as a portion of total passenger vehicles in 2030, a reduction of approximately 8% is projected. With an assumed HFCV penetration of 75% in 2060, GHG emissions are reduced by 60–70%. The PCA methodology facilitates parametric variation to readily assess, for example, variations in the makeup of the supply chain on the emissions of GHGs.

5.2.3. *Fuel Consumption*

On a WTW basis, fuel consumption per VMT is less for HFCVs than for conventional vehicles. Compared with the baseline vehicle scenario the HFCVs in the EA-H2I scenario consume 17% less fuel per VMT with respect to energy content. In 2030 and 2060, HFCVs consume 50% less fuel per VMT when compared to the baseline. HFCVs in the R-H2I scenario consume about 15% less fuel than the FF-H2I scenario in 2030 and in 2060.

5.2.4. *Water consumption*

In comparison with gasoline, preparation of hydrogen for commercial fuel use consumes significantly more water. Based on current trends in the absence of a hydrogen economy, the SoCAB is projected to consume water in 2060 at a rate of 10,300 million gallons per day [31]. The cases analyzed in this study predict that, by 2060, water consumption could increase by 5.1% by the deployment of a hydrogen infrastructure with more renewable hydrogen sources (R-2030 and R-2060), or a 7.4% increase with more fossil fuel hydrogen sources (FF-2030 and FF-2060).

5.3. *Sensitivity evaluation*

Further demonstrating the capabilities of the PCA model, a sensitivity analysis was performed on the distribution of hydrogen from a location of central generation to the fueling station. The analysis explored an all pipeline distribution versus all truck distribution strategy in each scenario. In every case an all pipeline distribution strategy significantly reduced the criteria pollutant emissions (particularly emissions of NO_x) compared to all truck distribution. Scenarios in which fossil fuels were used more prominently as a source for hydrogen showed fewer reductions in criteria pollutant emissions in an all pipeline strategy because emissions from distribution were eclipsed by the relatively high emissions from petroleum coke sources.

5.4. *Generic observations*

In addition to conclusions associated with the SoCAB application, the following general conclusions are drawn.

- The potential gains associated with a hydrogen infrastructure that relies heavily on renewable energy sources rather than fossil fuel sources are significant regarding criteria pollutant emissions, GHG emissions, efficiency, and water consumption. An aggressive push towards using renewable energy sources to generate hydrogen merits serious consideration.
- Pipeline distribution of hydrogen has the potential to significantly reduce both criteria pollutant emissions and GHG emissions.
- Where natural gas serves as a feedstock for the generation of hydrogen: emissions from the natural gas infrastructure in the U.S. as well as leakage, affects the environmental signature of the hydrogen infrastructure. Results show that though producing little or no emissions in the urban environment, the natural gas infrastructure external to the air shed contributes significant criteria pollutant emissions upstream of the urban-based processes. Furthermore, methane emissions from pipeline leakage account for a significant greenhouse gas emission footprint. It is important that this issue be closely monitored considering that hydrogen infrastructure deployment in the SoCAB could increase natural gas demand by as much as 9.4 million kg per day.
- The use of petroleum coke to generate hydrogen could potentially be a large contributor to urban criteria pollutant emissions and greenhouse gas emissions in a hydrogen infrastructure. However, the utilization of waste (in this case petroleum coke) to produce a useful fuel yields many benefits: the cost of the feedstock is low, the impacts associated

with extraction or mining are avoided, and an otherwise toxic waste product is broken down. Furthermore, the plant design that was used in this study for hydrogen generation from petroleum coke did not include carbon capture. By designing carbon capture into the plant, the associated GHG emissions can be mitigated.

- The use of hydrogen as a transportation fuel can improve efficiencies, and reduce emissions and greenhouse gases on a well to wheels basis. However, hydrogen infrastructure adoption does not guarantee these improvements. It is important to understand how technology adoption strategies influence the WTW impacts of hydrogen as a transportation fuel. Engineering tools such as the PCA model will be needed in order to establish rollout strategies for hydrogen infrastructure that achieve and optimize the potential benefits.

Acknowledgements

This study was performed under a contract from the U.S. Department of Energy (Number DE-FC36-05GO85026), awarded to Air Products and Chemicals, Inc. (APCI) for the development and deployment of hydrogen infrastructure. The National Fuel Cell Research Center was a collaborating partner on the contract with the responsibility for the development and application of a generic methodology for assessing hydrogen deployment scenarios for the State of California. The authors thank Ed Heydorn and Brian Bonner from APCI for their collaboration and valuable input throughout the research effort.

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Appendix A
WTW criteria pollutant emissions within and outside of the urban air shed

Figs. A-1–A-3 show the complete WTW criteria pollutant emissions for each of the scenarios considered in this study. Both urban and non-urban criteria pollutant emissions associated with a hydrogen infrastructure are included in these figures. Fig. A-1 shows the emissions associated only with a hydrogen infrastructure in the year 2015 H2I scenario. Figs. A-2 and A-3 show the emissions associated with total passenger vehicles in the SoCAB in the year 2030 and 2060

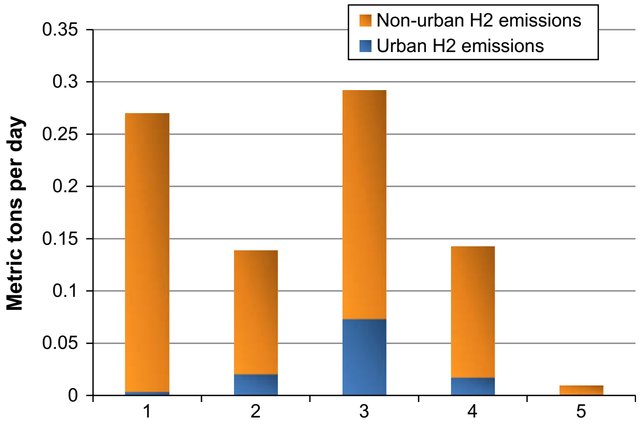

Fig. A-1 – WTW (urban and non-urban) criteria pollutant emissions associated with hydrogen infrastructure EA-H2I/HFCV scenario in 2015.

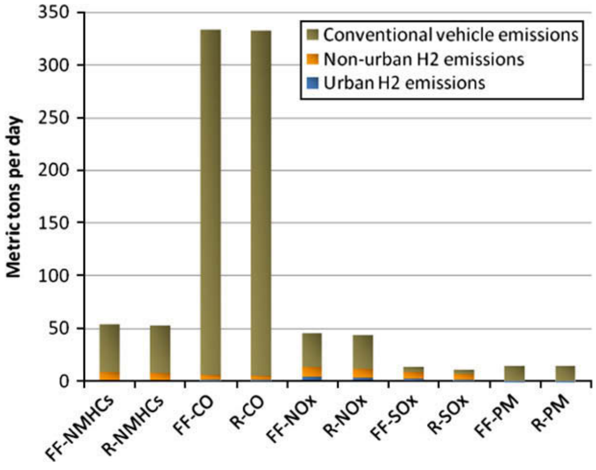

Fig. A-2 – Total (urban and non-urban) criteria pollutant emissions associated with passenger vehicles for the FF-H2I/HFCV and R-H2I/HFCV scenarios in 2030.

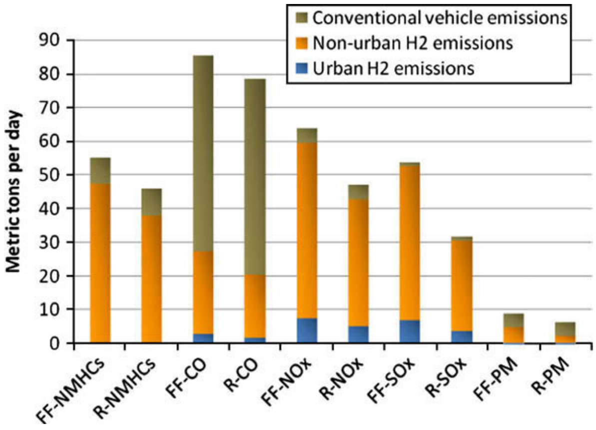

Fig. A-3 – Total (urban and non-urban) criteria pollutant emissions associated with passenger vehicles for the FF-H2I/HFCV and R-H2I/HFCV scenarios in 2060.

scenarios meaning that hydrogen infrastructure contributes only a portion of the total emissions while conventional vehicles contribute the rest.

In the scenarios modeled for the years 2015 and 2030, most of the non-urban criteria pollutant emissions can be attributed to the extraction of natural gas, and its transportation to the SoCAB region, while a small portion can be attributed to electric power production outside the basin. In the year 2060, the gasification of coal to generate hydrogen contributes significantly to the non-urban emissions associated with a hydrogen infrastructure as well.

Moving criteria pollutant emissions outside of the SoCAB will help mitigate many air quality issues and health risks in that region. However, it is clear that hydrogen infrastructure deployment could be a significant source of non-urban criteria pollutant emissions and this issue should be carefully monitored as we consider and adopt strategies to facilitate such a future.

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