

Air quality impacts of liquefied natural gas in the South Coast Air Basin of California



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ABSTRACT

The effects of liquefied natural gas (LNG) on pollutant emission inventories and air quality in the South Coast Air Basin (SoCAB) of California are evaluated using recent appliance emissions measurements by Lawrence Berkeley National Laboratory and the Southern California Gas Company (SoCalGas), and use of a state-of-the-art air quality model. Pollutant emissions can be impacted by LNG operation because of differences in composition and physical properties including the Wobbe index, a measure of energy delivery rate. Various LNG distribution scenarios are evaluated to determine the potential impacts of LNG. Projected penetration of LNG in the SoCalGas pipeline network in SoCAB is expected to be limited, which could cause increases in overall (area-wide) emissions of nitrogen oxides that are smaller than 0.05%. Based on the photochemical state of the South Coast Air Basin of California, any increase in NO_x is expected to cause an increase in the highest local ozone concentrations, which is observed in model results. However, the magnitude of NO_x emissions increases due to LNG use is determined to be within the uncertainty range of natural gas combustion sources and would not be discernible with the existing monitoring network.

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1. Introduction

Most of California's natural gas (NG) supply is from out of state. In 2008, California customers received 46% of their natural gas supply from basins located in the Southwest, 19% from Canada, 22% from the Rocky Mountains, and 13% from basins located within California (CPUC, 2010). With a growing demand for natural gas in California, the state has been investigating additional sources of natural gas. An alternative for current natural gas supply by pipeline from other regions in the North American sub-continent is the use of liquefied natural gas (LNG) obtained from areas such as Indonesia, South America and Australia. LNG is used in other parts of the US, with terminals in Massachusetts, Maryland, Georgia, Puerto Rico, Louisiana, Texas and Alaska (FERC, 2013). While there are currently no LNG terminals located in California, Sempra Energy commissioned and started operations at the Energia Costa Azul (ECA) LNG terminal, in Ensenada, Baja California (Mexico) which

can supply part of the terminal's natural gas capacity to Southern California (ECA, 2012). In addition, the increased extraction of shale gas in the United States occurring in the last five years and expected to keep increasing in the future provides an alternative source to conventional NG sources (EIA, 2013).

One of the most important issues the state of California faces with the possible increased use of LNG or shale gas is the potential impact of the changes in natural gas composition on pollutant emissions and associated exposure and health effects. The new NG supplies will likely differ in composition, e.g. lower fraction of methane, higher fraction of ethane and other non-methane hydrocarbons, and properties, e.g. higher heating value and Wobbe index (Suellentrop, 2005; Bulba and Krouskop, 2009). The Wobbe index (WI) is particularly relevant as it is a measure of energy delivery to devices that control gas flow with a fixed orifice and it is an indicator of interchangeability of fuel gases. It is defined by: where HHV and G_s are the higher heating value and the specific gravity of the gas, respectively. Maintaining a constant WI ensures that appliances will operate within the specifications they were designed for. Conversely, operating appliances with fuels that have WI far from standard specifications could cause incomplete combustion, higher nitrogen oxides (NO_x) and carbon monoxide (CO) emissions,

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reduced efficiency and problems with flame lift or flashback, which could lead to hazardous conditions of operation. In Southern California, the California Public Utilities Commission (CPUC) issued a revised Rule 30 tariff that directed the Southern California Gas Company (SoCalGas) to limit the maximum WI of pipeline NG to 1385 British Thermal Units per standard cubic feet (BTU/scf), which is equivalent to 51.60 MJ/Nm³. Moreover, the South Coast Air Quality Management District (SCAQMD) proposed a reduction of the WI limit to 1360 BTU/scf in the 2007 Air Quality Management Plan (SCAQMD, 2007), to reduce potential NO_x emissions from NG combustion.

$$WI = \frac{HHV}{\sqrt{G_s}} \quad (1)$$

This study evaluates possible changes in air pollutant emissions in the South Coast Air Basin of California (SoCAB) due to the use of LNG, and investigates the possible impacts on air quality. The SoCAB is the region of the United States with the worst air pollution by ozone, according to the American Lung Association (ALA, 2013). The SoCAB exceeds the ozone National Ambient Air Quality Standards (NAAQS) over 100 days a year (ARB, 2014), and future increases in nitrogen oxide (NO_x) emissions associated with LNG use would exacerbate ozone pollution and hinder efforts to attain ozone standards. Approximately 9% of NO_x emissions in the SoCAB are produced by NG combustion in the residential, commercial, industrial, and utilities sectors (SCAQMD, 2007). As controls on NO_x emissions from other sources are tightened, the relative contribution of NG sources is projected to increase. The work presented here integrates emission factors determined experimentally by the Lawrence Berkeley National Laboratory (LBNL) (Singer et al., 2010)

and Southern California Gas Company (SoCalGas, 2006), with current emissions inventories generated by the South Coast Air Quality Management District (SCAQMD). The goal of this effort is to determine for the first time emission changes due to the use of LNG in natural gas combustion processes. The resulting spatially and hourly resolved emissions scenarios are used as inputs to a state-of-the-art air quality model to determine the potential impacts of LNG on ozone and secondary particulate matter concentrations. As a result, the contribution of this work is the update of emissions from natural gas combustion in the South Coast Air Basin of California, the quantification of the potential air pollutant emission increases due to changes in natural gas composition, and the air quality modeling of those emission scenarios.

2. Materials and methods

2.1. Modeling LNG distribution

SoCalGas supplies natural gas throughout the SoCAB and other parts of California, including San Diego. A system map of the transmission system is shown in Fig. 1. Gasified LNG is expected to enter the SoCalGas system through the Otay Mesa receipt point, on the border between Tijuana and San Diego, and in lesser amount through the Blythe receipt point, near the California–Arizona border. To understand the transmission of LNG throughout the system, it is important to understand the direction of the natural gas flow. From Otay Mesa, natural gas flows northwards towards the RAINBOW-MORENO pipeline, merging with the CACTUS CITY-MORENO segment, whose supply originates in the Blythe receipt point. Therefore, the natural gas provided from Otay Mesa is first consumed in the San Diego area and the remnant is transmitted to

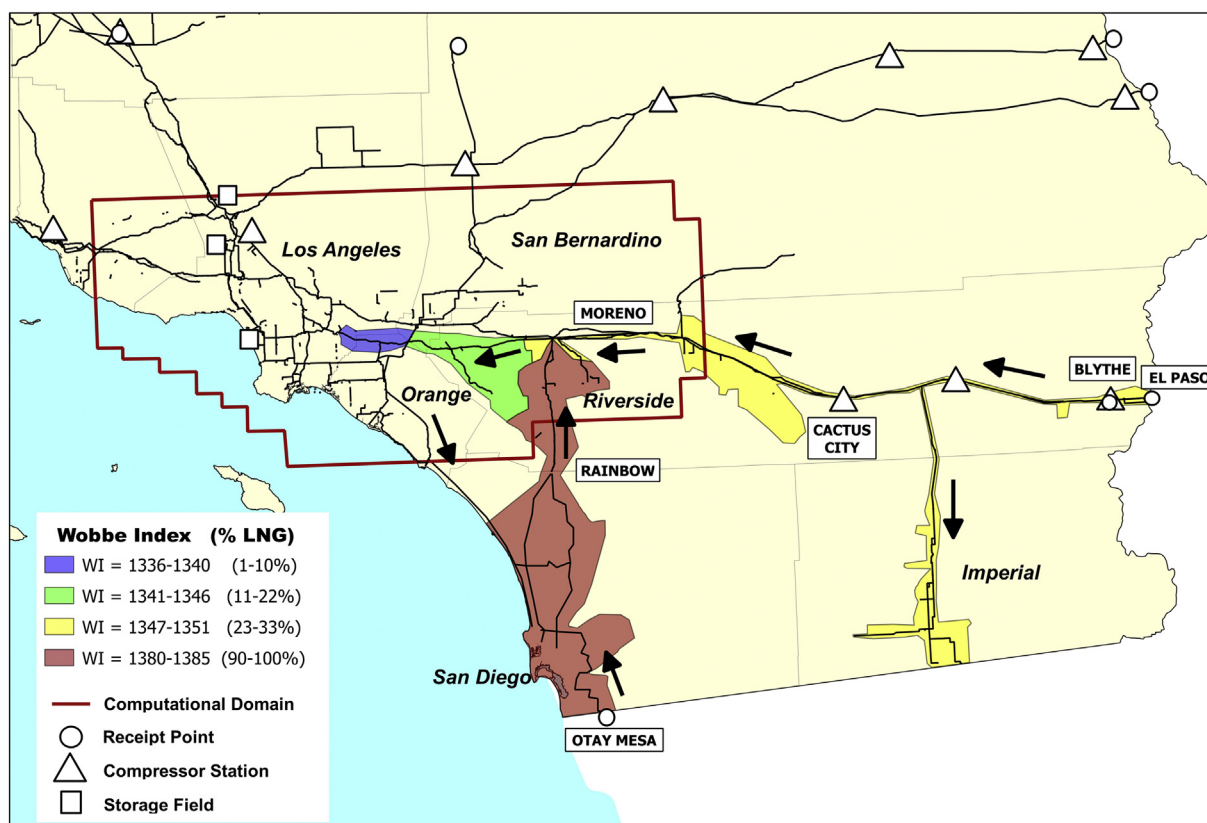


Fig. 1. Southern California Gas Company and San Diego Gas and Electric Company (SDG&E) natural gas distribution system map and Wobbe Index distribution for the maximum penetration of gasified LNG in the SoCalGas/SDG&E system.

Riverside, and then towards Los Angeles. From Los Angeles, the natural gas flows southwards towards Orange County, along the coastal pipeline through San Clemente. Based on this configuration, San Diego County will receive the highest concentration of gasified LNG, followed by Riverside County. Due to the limited capacity of the ECA terminal, the supply of LNG to San Bernardino, Los Angeles and Orange County should be marginal. Only those locations within the SoCAB that receive some fraction of LNG should have modified emissions in the air-quality model; the other locations will receive the same baseline NG as has been delivered historically, a hence, no impacts in emissions should be expected.

Natural gas flow through the SoCalGas system is modeled by Sempra with a proprietary model that is based on changes in hydrostatic pressure that depend upon pipeline diameters, location of compression stations and spatially resolved gas delivery, among other factors. The distribution of potential LNG receipts is assessed by including in the model a simulated inert tracer that is mixed and transmitted along with the existing natural gas. The tracer concentration is then assumed as the fraction of LNG present in the natural gas stream.

The current analysis focuses on summer demand because this is when ozone concentration is typically the highest, and thus will result in air quality impacts that will be most sensitive to changes in emissions. The highest expected LNG fraction during summer 2023 with a typical NG demand of 76 million Nm³/day results from: (1) maximizing the output from ECA, 27 million Nm³/day, which ends up supplying 11 and 2 million Nm³/day into the Ota and Blythe receipt points, respectively, and (2) minimizing the receipts of natural gas from El Paso, 3 million Nm³/day. The pipeline network model produces a spatial distribution of the Wobbe index based upon the fraction of gasified LNG in that area of the SoCalGas distribution network. In this model, the lower limit for Wobbe index is 1335 BTU/scf, equivalent to 49.74 MJ/Nm³; this occurs when there is no LNG introduced into the system. The upper limit for an area receiving only LNG is 1385 BTU/scf, equivalent to 51.60 MJ/Nm³, which is the maximum allowable Wobbe index according to current gas tariffs. The resulting spatially-resolved Wobbe Index distribution for the highest expected penetration of gasified LNG is presented in Fig. 1. Additional information on modeling and analysis of LNG penetration is presented in the Supplemental Material.

2.2. Air quality impact assessment modeling scenarios

The simulation of LNG distribution by Sempra's model represents a realistic scenario used as the basis to investigate the potential impacts of expected LNG use on ambient air quality in the SoCAB. In addition, several hypothetical bounding scenarios are used to investigate whether LNG use at any plausible scale would have substantial impacts on overall emissions and ambient air quality. Both realistic and hypothetical scenarios are compared to a baseline case scenario, which is adapted from a projected emission inventory developed by SCAQMD.

The scenarios investigated are the following:

- **Sempra Scenario:** This scenario considers the highest expected LNG penetration modeled by Sempra, based upon modeling of expected LNG receipts, gas demand and other supplies, as discussed above and presented in Fig. 1. The baseline Wobbe index for natural gas with no LNG is 1335 Btu/scf (typical Wobbe index for NG delivered to Southern California), and the maximum Wobbe index assumed for 100% LNG is 1385 Btu/scf (which is the maximum Wobbe index currently allowed in California).
- **100% LNG penetration:** Although the scenario of 100% LNG penetration into the SoCAB is not possible with current infrastructure, this case is considered as a bounding case that could

inform consideration of any future proposals to expand significantly distribution of higher Wobbe Index natural gas in the SoCAB. This bounding scenario assumes that 100% of distributed NG in the SoCAB has a Wobbe index of 1385 (50 Btu/scf higher than the baseline fuel and the maximum allowed by current tariff limits).

- **100% LNG penetration with increased Wobbe index limit:** this scenario assumes that 100% of all natural gas used in the basin comes from LNG, and that Wobbe index of the re-gasified LNG is 1400 Btu/scf (52.16 MJ/Nm³). Even though this WI exceeds California's tariff limits, laboratory experiments have shown that equipment was able to operate with NG with such high WI without incidents. This scenario represents a hypothetical worst-case for LNG impacts in the SoCAB.
- **100% LNG penetration with commercial and industrial equipment tuning:** This scenario assumes that due to the high penetration of LNG, the basin experiences a prolonged supply of LNG. With a steady inflow of LNG as the primary source for natural gas, businesses would be able to plan adjustments of commercial and industrial equipment, retuning them for a high Wobbe index gas, and hence, minimizing the impacts of LNG on emissions from these installations. Namely, this scenario assumes no impacts on NO_x emissions in commercial and industrial equipment due to retuning of appliances. Only residential sources and fugitive emissions are affected by LNG penetration.

2.3. Modeling emissions from natural gas-related sources

In order to evaluate the potential impacts of the emissions from LNG use on air quality in the SoCAB, first it is necessary to establish the baseline inventory of emissions from all sources in the basin. From this inventory, the emissions specifically due to natural gas sources need to be identified and modified for changes in gas quality due to LNG use. Modifications of the emissions inventory requires an understanding of the factors used to produce the inventory, including items like the emission factors for specific technologies and any information regarding the distribution of these technologies within the different sectors of the inventory.

2.3.1. Baseline emissions inventories

The baseline emissions inventory for the South Coast Air Basin is obtained from the South Coast Air Quality Management District. The inventory is gridded, with emissions assigned to specific 5 by 5 km locations within the SoCAB modeling domain. This inventory was presented in the 2007 Air Quality Management Plan (AQMP) developed by the SCAQMD (SCAQMD, 2007), and contains emissions from 6410 different sources, including on-road and off-road mobile sources, stationary and area sources, and biogenic sources.

The overall contribution to total NG-related NO_x emissions in the year 2023 by all of the different area and point sources categorized by 'General Activity Sector' and 'Technology' is presented in Fig. 2. The NG-related emissions of NO_x add up to 26 tons/day out of basin-wide total NO_x emissions of 114 tons/day. One thing to note in Fig. 2 is the significant fraction of emissions by Technology that are assigned to the 'other' category, particularly for area emissions. These emissions are not assigned to a specific technology either due to a large mix of miscellaneous sources or sources that are difficult to characterize.

2.3.2. Adjustments to the baseline inventory

LBNL performed experiments to measure emissions with NG and LNG on a number of residential appliances (Singer et al., 2010). These measurements provide an opportunity to compare emission

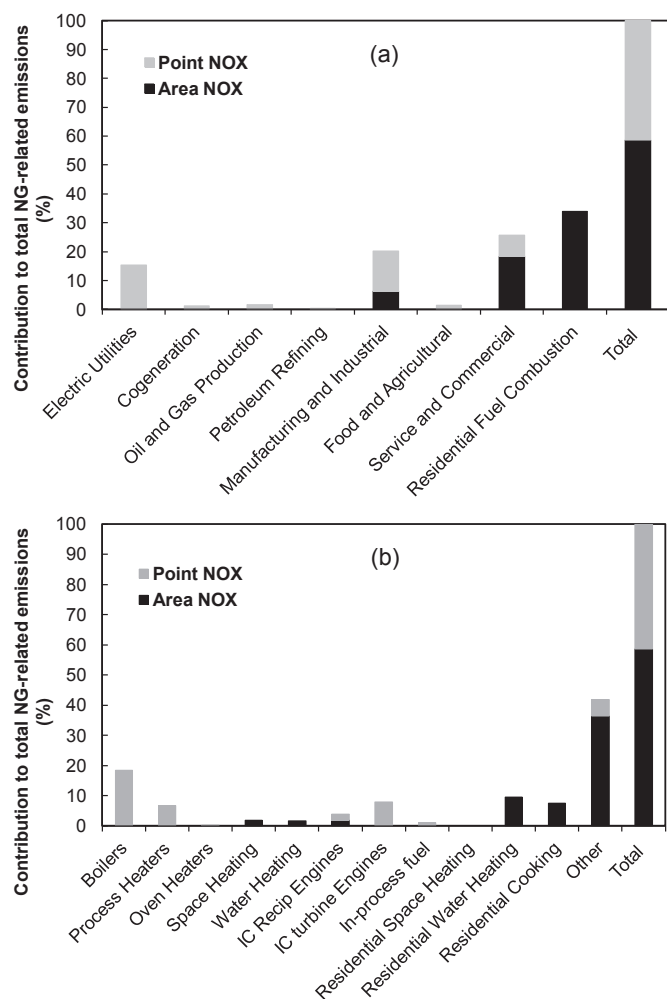


Fig. 2. Contribution to total NG-related sources – both area and point sources – to NO_x emissions estimated for the year 2023 by: (a) general activity sector and (b) technology.

factors resulting from recent field and lab measurements of devices covering a suite of technologies with emission factor provided for all residential sources in AP-42, which is a compendium of emission factors for a variety of sources developed by the United States Environmental Protection Agency (USEPA, 1995). The average experimental emission factors for NO_x and CO obtained by LBNL are shown in Fig. 3. Thorough statistical analyses of the measurements were performed by Singer et al., 2010 and Martinez et al., 2014. For NO_x , emission factors for all technologies fall below the AP-42 value of 0.64 g/Nm^3 . The measured technology specific CO emission factors are much higher than the AP-42 values for cooking burners and tankless water heaters, and much lower for storage water heaters and residential furnaces.

Results presented in Fig. 3 suggest that emission factors in AP-42 do not represent emissions from the residential technologies currently in place in the state of California. Even newly measured furnace emission factor for NO_x is lower than the AP-42 value, which was based on measurements performed several decades ago on the residential furnaces available at that time. The current population of California furnaces includes many designed for lower NO_x emissions. In addition, the changes in residential emissions as a function of Wobbe index were computed in relation to these experimental emission factors. Therefore, the SCAQMD 2023 Baseline inventory for residential appliances was modified to use

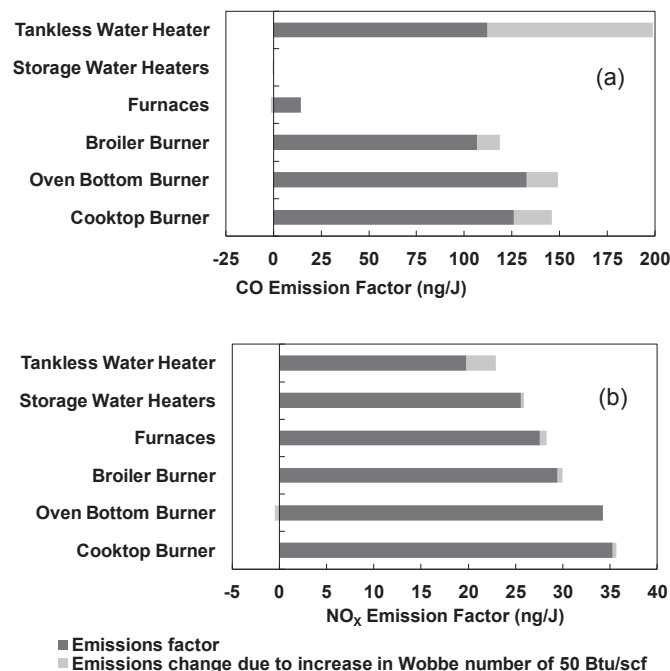


Fig. 3. Emission testing results for residential appliances obtained by Lawrence Berkeley National Lab (Singer et al., 2010).

newer emission factors. This updated inventory is called the 2023 LBNL Baseline inventory.

The emission factors $EF_{i,j,m}$ for general activity sector i , technology j and pollutant m are calculated with Eq. (2), as follows: using the information from emissions testing ($et_{l,m}$) shown in Fig. 3. The emission factors obtained by the experimental measurements are technology specific, which are not directly comparable with the generic technology specified in the inventory. Consequently, technology mix factors ($f_{i,j,l}$) are required to link a specific technology l , with general activity sector i and technology j . The $f_{i,j,l}$ factors, presented in Table 1, were established after discussions with stakeholders, including SCAQMD, ARB, SoCalGas and San Diego Air Pollution Control District (APCD), and the insights from technology survey by LBNL.

$$EF_{i,j,m} = \sum_l f_{i,j,l} \cdot et_{l,m} \quad (2)$$

SoCalGas conducted a series of experiments to analyze the effect of changing gas quality on emissions for several low and ultra-low NO_x technologies. The experiments examined a limited number of installations that were expected to be sensitive to changes in natural gas composition. Consequently, SoCalGas test results provide an upper bound for equipment sensitivity, although there is not enough information to attest that the technologies studied by SoCalGas are representative of the overall technology mix in commercial and industrial applications. As a result, the emission testing results by SoCalGas are not used to update the baseline emissions, but they are used later to incorporate the effects of LNG on commercial and industrial emissions. In summary, only the LBNL measurements on residential appliances are used to update the baseline emissions inventory. In addition, the baseline assumed that emissions from commercial space and water heating, which had been based on uncontrolled boilers, would be better represented by the emission factors measured for the same technologies in the residential sector. The resulting emission factors used in the 2023 LBNL Baseline inventory are presented in Table 2.

Table 1Technology distribution factors ($f_{i,j,l}$) among area sources to relate emission testing with natural gas combustion emissions source categories in the inventory.

Description	Furnace	Storage water heater	Tank-less water heater	Cook-top	Oven burner	Broiler burner	Low- NO _x burner
Industrial							1.00
Commercial Water Heating		0.70	0.30				
Commercial Space Heating	1.00						
Commercial Other							1.00
Residential Cooking				0.80	0.15	0.05	
Residential Water Heating		0.70	0.30				
Residential Space Heating	1.00						
Residential Other	0.34	0.23	0.10	0.26	0.05	0.02	

2.3.3. Modeling emissions changes due to LNG

The updated emissions from the 2023 LBNL Baseline emissions inventory are considered as the baseline reference to evaluate the impacts of LNG use. Changes in emissions related to LNG use, which depend on changes in Wobbe index, need to be assessed by the available experimental data. The available emissions data can be divided into two groups: (1) residential appliances and commercial space and water heating, and (2) 'other' commercial and industrial natural gas combustion area sources and industrial and commercial boilers and process heaters, included in point sources. Changes in NO_x and CO emissions in the first group are calculated using the factors presented in Table 2. Changes in NO_x emissions in the second group are calculated assuming the increases reported by SoCalGas (shown in Fig. 4). Commercial and industrial area sources are expected to be smaller units that employ low- NO_x burner technology, and commercial and industrial point sources are expected to be large installations that employ ultra-low NO_x technologies. These assumptions are based on an internal equipment survey conducted by SCAQMD (Baez et al., 2010).

The use of LNG not only impacts emissions from natural gas combustion, it can also impact emissions from fugitive sources released during the transmission and distribution of natural gas. In California, natural gas generally has a lower fraction of non-methane hydrocarbons (NMHC) than most of the potential supply of LNG available for the ECA terminal. Emissions of NMHC are important because they are precursors of ozone formation and significant increases in NMHC can lead to increases in ozone concentrations. As a result, switching to LNG would increase the emissions of these volatile organic compounds (VOC) from fugitive sources in the NG transmission and distribution lines. Table 3 presents the composition of natural gas from different origins. The ECA terminal has been receiving natural gas from Peru and potentially could receive from the Tangguh project in Indonesia. While gas composition from each source will vary over time, the differences between supply sources are generally much larger. All

gas delivered into SoCalGas and SDG&E transmission system has to meet specification limits for heat content, Wobbe Index, and inert components. The limits for compressed natural gas set by the California Air Resources Board (ARB) are used as a reference for comparison, and provide the upper limit for the fraction of non-methane hydrocarbons allowed in the natural gas. Compared to the median natural gas distributed throughout Southern California, the ARB specifications allow an increase the fraction of NMHC of 200%.

For air quality modeling purposes, the emissions of ethane through hexane are lumped in a group that represents short-chain alkanes (ALKL). The basin-wide emissions of ALKL from fugitive NG transmission and distribution are 1.2 tons/day, out of 99.8 tons/day of total emissions of ALKL.

2.4. Air quality modeling of the South Coast Air Basin of California

The California Institute of Technology (CIT) Airshed Model has been updated and modified over the course of more than a decade of work at UC Irvine (UCI). This model, now dubbed the UCI-CIT Airshed Model, is used as the host model for the chemical and aerosol mechanisms (Harley et al., 1993; Griffin et al., 2002b; Meng et al., 1998). The grid used by the UCI-CIT model encompasses Orange County and part of Los Angeles, Ventura, San Bernardino and Riverside counties (Fig. 5). The grid consists of cells with an area of 25 km². Additionally the vertical resolution is described through 5 vertical layers with the following dimensions from ground level upward: (1) 0 m–39 m, (2) 39 m–154 m, (3) 154 m–308 m, (4) 308 m–671 m, and (5) 671 m–1100 m.

The gas-phase chemical mechanism used in the present simulations is the Caltech Atmospheric Chemical Mechanism (CACM, see Griffin et al., 2002a). CACM is based upon the work of Stockwell et al., 1997, Jenkin et al., 1997, and Carter 2000a,b, and includes O₃ chemistry and a state-of-the-art mechanism of the gas phase precursors of secondary organic aerosol (SOA). The full mechanism

Table 2Updated emission factors for area sources based on emission testing by LBNL, and increments in emissions due to an increase of 50 Btu/scf (1.86 MJ/Nm³) in the Wobbe number tested by LBNL and SoCalGas.

Description	Updated emission factor ($EF_{i,j,m}$)		Increase in emission factor $\Delta EF_{i,j,m}$ ($\Delta WNI = 50$)	
	NO _x	CO	NO _x	CO
	g/Nm ³		g/Nm ³	
Industrial	0.99 ^a	0.56 ^a	0.40 ^b	–
Commercial Water Heating ^c	0.95	1.33	0.05	1.03
Commercial Space Heating ^c	1.09	0.56	0.03	–0.06
Commercial Other	0.72 ^a	0.56 ^a	0.29 ^b	–
Residential Cooking ^d	1.27	4.84	0.00	0.59
Residential Water Heating ^d	0.95	1.33	0.05	1.03
Residential Space Heating ^d	1.09	0.56	0.03	–0.06
Residential Other ^d	1.11	2.28	0.02	0.51

^a No new data. Emission factor is the same as in SCAQMD inventory.

^b Emission increase of 40% in the WI range of 1335–1385 btu/scf based on low- NO_x technologies tested by SoCalGas (Fig. 4).

^c Assume same emission factor as in 'Residential'.

^d Measurements by LBNL.

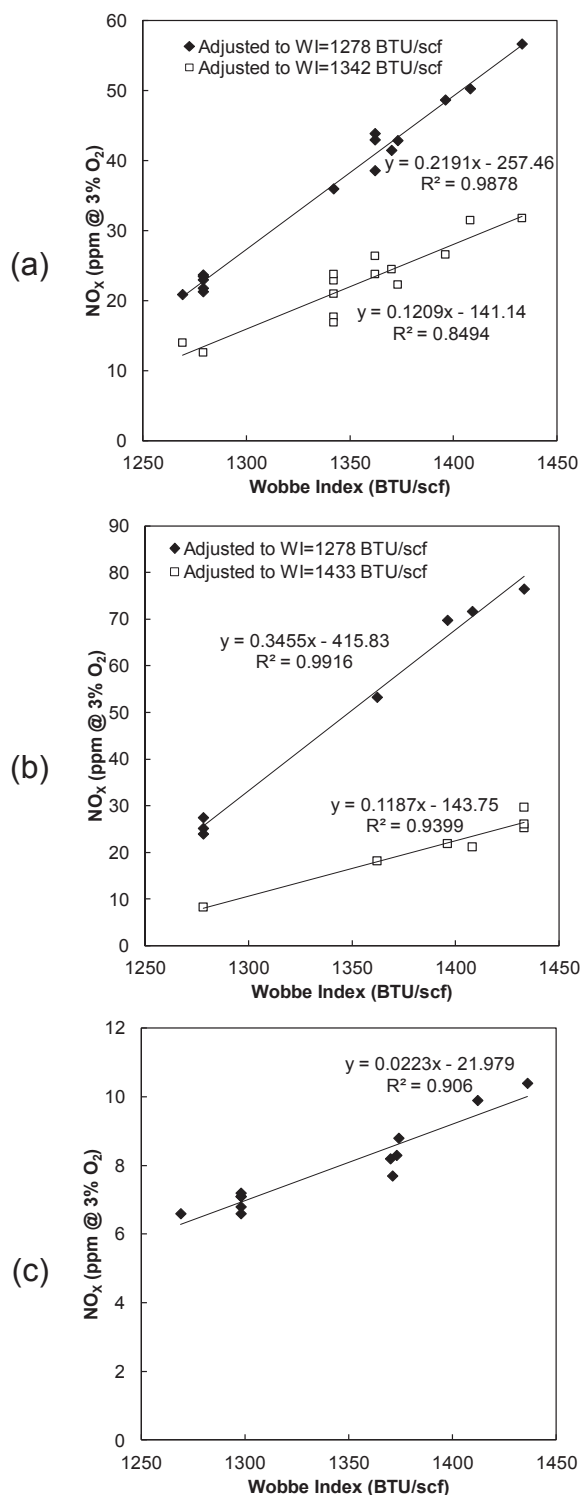


Fig. 4. Emission testing results for commercial and industrial burners obtained by SoCalGas: (a) steam boiler with premixed gun-type power burner, (b) low- NO_x steam boiler, and (c) ultra low NO_x steam boiler (SoCalGas, 2006).

consists of 361 chemical reactions and 191 gas-phase species, which describe a comprehensive treatment of VOCs oxidation. Inorganic aerosol formation is calculated using the Simulating Inorganic Composition of Atmospheric Particles at Equilibrium 2 model (SCAPE2, Meng et al., 1995), whereas organic aerosol formation is calculated using the Model to Predict the Multiphase Partitioning of

Table 3

Mass composition of natural gas from different origins (Suellentrop, 2005).

	SoCalGas median	ARB ^a	Peru	Tanggub
Methane	89.74%	75.32%	81.29%	92.62%
Ethane	4.43%	9.82%	18.07%	4.69%
Propane	1.30%	7.20%	0.05%	1.32%
Butanes	0.00%	0.00%	0.00%	0.70%
Hexane and higher	0.21%	0.79%	0.00%	0.00%
CO_2	3.25%	0.00%	0.00%	0.00%
N_2	1.07%	6.87%	0.59%	0.67%

^a ARB corresponds to the specification limits for ethane, higher hydrocarbons and inert compounds allowed by ARB for compressed natural gas (CNG) (California Code of Regulations, Title 13 – Motor Vehicles, Division 3 – Air Resources Board, Chapter 5 – Standards for Motor Vehicle Fuels, Article 3 – Specifications for Alternative Motor Vehicle Fuels, Section 2292.5).

Organics (MPMPO, Griffin et al., 2002b). MPMPO allows the simultaneous formation of SOA in a hydrophobic organic phase and a hydrophilic aqueous phase. In addition, MPMPO modifies SCAPE2 to account for the interaction between organic ions present in the aqueous phase and the inorganic aerosol components. The module consists of 37 size-resolved aerosol-phase species, in 8 different size bins ranging from 0.04 to 10 μm . The integrated module, allows particulate matter to undergo advection, turbulent diffusion, condensation/evaporation, nucleation, emissions and dry deposition processes.

The UCI-CIT Airshed Model is an Eulerian air quality model that solves the atmospheric diffusion and advection equation (Eq. (3)).

$$\frac{\partial C_m^k}{\partial t} = -\nabla \cdot (u C_m^k) + \nabla \cdot (K \nabla C_m^k) + \left(\frac{\partial C_m^k}{\partial t} \right)_{\text{sources/sinks}} + \left(\frac{\partial C_m^k}{\partial t} \right)_{\text{aerosol}} + \left(\frac{\partial C_m^k}{\partial t} \right)_{\text{chemistry}} \quad (3)$$

The above equation is integrated numerically in time t for concentration C of each species m , and phase k (gas or aerosol) over a series of discrete time steps in each of the spatially distributed discrete cells of the model. The method to solve Eq. (3) is by operator splitting, which is a numerical technique that splits each term in Eq. (2), making the solution computationally efficient (Yanenko, 1971). Each term in the right hand side of Eq. (3) represents a major process in the atmosphere. From left to right: (1) advective transport due to wind transport, (2) turbulent diffusion due to atmospheric stability/instability, (3) emissions (sources) and deposition (sinks) of pollutants (4) mass transfer between gas and aerosol phases, and (5) chemical reactions.

The outputs from the UCI-CIT Airshed model are spatially and temporally resolved concentration profiles of major and trace species of interest over a geographic region. In order to minimize the effects of initial conditions and conduct various analyses, air quality modeling involves simulation of episodes involving multiple days. This modeling approach greatly facilitates the study of various scenarios involving changes in emissions and associated impacts on the air quality in a particular region.

The Southern California Air Quality Study (SCAQS) was a comprehensive campaign of atmospheric measurements that took place in the SoCAB, during August 27–29, 1987. The study collected an extensive set of meteorological and air quality data that has been used widely to validate air quality models (Meng et al., 1998; Griffin et al., 2002a, 2002b; Moya et al., 2002). Zeldin et al. (1990) found that August 28, 1987 is representative of the meteorological conditions in the SoCAB, which makes it suitable for modeling. In addition, the August 27–28, 1987 episode is statistically within the top 10% of severe ozone-forming meteorological conditions. Hence, meteorological conditions for August 27–29 are considered

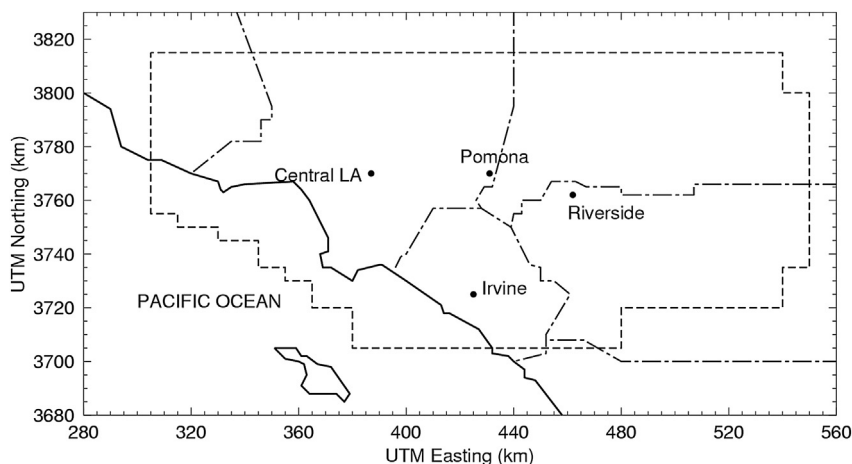


Fig. 5. UCI-CIT Airshed modeling domain of the South Coast Air Basin of California.

representative for the evaluation of air quality impacts of LNG emissions under high-ozone forming conditions.

The SCAQS episode in August 27–29, 1987 was characterized by a weak onshore pressure gradient and warming temperatures aloft. The wind flow was characterized by a sea breeze during the day and a weak land-mountain breeze at night. The presence of a well-defined diurnal inversion layer at the top of neutral and unstable layers near the surface, along with a slightly stable nocturnal boundary layer, facilitated the accumulation of pollutants over the SoCAB, which lead to a high ozone concentration occurrence.

Griffin et al. (2002a) and Ensberg et al. (2010) evaluated model performance of the UCI-CIT model and the CACM chemical mechanism using the August 27–29th 1987 meteorology and emissions inventory by comparison to measurements at dozens of monitoring locations in SoCAB. Model performance was evaluated following USEPA recommended metrics for Mean Normalized Gross Error (MNGE) and Mean Normalized Bias (MNB) for ozone (USEPA, 2007), showing 41–46% MNGE and –5 to 21% MNB.

3. Results and discussion

3.1. Summary of estimated emissions for the LNG modeling scenarios

The impacts on emissions from the LNG scenarios described in Section 2.2 are summarized in Table 4. The overall impact of the Sempra Scenario on emissions is less than 0.1% of total emissions for all pollutants, even assuming the largest realistic LNG penetration in the SoCAB. The hypothetical scenario '100% LNG' assumes 100% penetration (use) of LNG throughout the SoCAB. While this is not feasible with current or planned LNG receiving infrastructure, it does provide a bound on the maximum air quality impact that can be expected from LNG use. In this scenario the NO_x emissions

Table 4
Impacts on emissions of CO , NO_x and short-chain alkanes (ALKL) estimated for all LNG scenarios. Increases in emissions are expressed with respect to the LBNL Baseline case, in tons per day (tpd) and percentage (%).

Case	CO increase		NO_x increase		ALKL increase	
	tpd	%	tpd	%	tpd	%
Realistic LNG Distribution Scenario						
Sempra Scenario	0.111	0.01%	0.092	0.08%	0.008	0.01%
Hypothetical Bounding Scenarios						
100% LNG	2.651	0.12%	2.763	2.46%	1.001	1.02%
100% LNG ($\text{WI}_{\max} = 1400$)	3.493	0.15%	3.581	3.19%	1.001	1.02%
100% LNG with tuning	2.651	0.12%	0.166	0.15%	1.001	1.02%

increase by 2.76 tons/day, corresponding to a 2.5% increase in total basin-wide emissions of NO_x from natural gas combustion. This scenario also adds 2.6 and 1.0 tons/day of CO and short-chain alkanes to basin-wide emissions, respectively, which represent increases of 0.1% and 1%. The recommendation by the SCAQMD to reduce the WI limit from 1385 BTU/scf to 1360 BTU/scf would reduce the WI range in Southern California by half – from 50 BTU/scf to 25 BTU/scf – assuming a baseline WI of 1335 BTU/scf. The reduced WI limit would result in potential NO_x emission increases that are half the emissions increases caused by scenario '100% LNG', potentially avoiding 1.4 tons/day of NO_x .

A second hypothetical scenario explores the effects of increasing the limit of Wobbe index in the SoCAB to 1400 BTU/scf: 100% LNG ($\text{WI}_{\max} = 1400$). Although this is currently not feasible under current gas quality tariff limits, experimental results suggest that increasing the Wobbe index to 1400 BTU/scf will not impact significantly safe operation of most equipment. Assuming linear changes in emissions within the expected range of the Wobbe index, incremental changes in emissions ($\Delta E_{i,j,m}$) for NO_x and CO due to a Wobbe index of 1400 BTU/scf are 30% larger than for 1385 BTU/scf. The resulting increases in emissions for Scenario 100% LNG ($\text{WI} = 1400$) add up to 3.6 tons/day (3.2%) of total basin-wide NO_x emissions. In addition, emissions of CO and ALKL increase by 3.5 and 1.0 tons/day, respectively.

Finally, the hypothetical scenario '100% LNG with tuning' investigates the possible mitigating effects of basin-wide adjustments of burners to optimize operation with LNG. This scenario assumes that due to the high penetration of LNG, the basin experiences a prolonged supply of LNG. With a steady inflow of LNG as the primary source for natural gas, businesses would be able to plan adjustments of commercial and industrial equipment, retuning them for a high Wobbe index gas, and hence, lowering the impacts of LNG on emissions from these installations. This tuning reduces the overall impacts of LNG on NO_x emissions to 0.17 tons/day (0.15% of total basin-wide emissions of NO_x). The impacts on CO remain the same as in scenario 100% LNG because increases of CO emissions from industrial and commercial installations were not accounted for due to lack of data. The impacts on ALKL emissions also remain the same as in scenario 100% LNG because burner tuning does not affect fugitive emissions.

3.2. Baseline air quality in 2023

The 2023 SCAQMD Baseline corresponds to a controlled future emissions inventory that includes long-term emissions controls

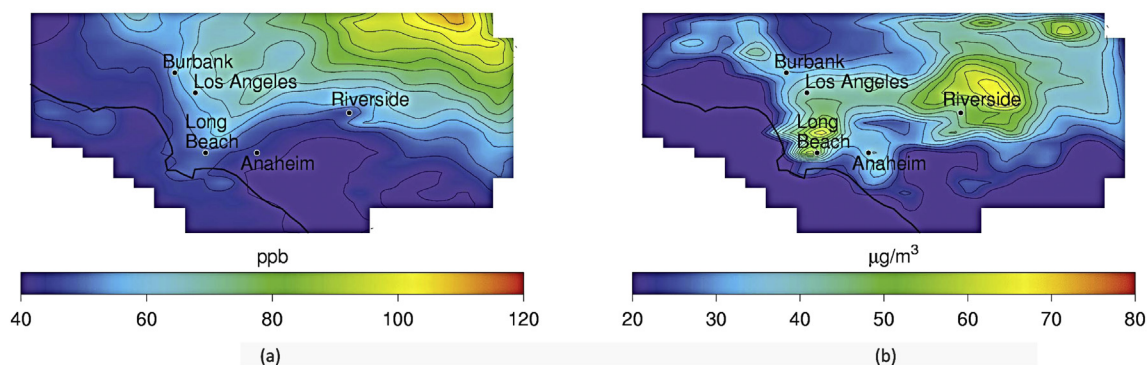


Fig. 6. Baseline air quality for the year 2023: a) 8-h ozone concentration, and b) 24-h $PM_{2.5}$ concentrations.

that limit total NO_x emissions in the South Coast Air Basin of California to 114 tons per day (SCAQMD, 2007). NG-related emissions from area sources are based upon emission factors from the USEPA's AP-42. NG-related emissions from point sources are directly obtained by SCAQMD through its emission reporting system for permitted sources. The 2023 SCAQMD Baseline emission inventory as received from the SCAQMD for the year 2023 and the meteorological conditions of the August 27–29, 1987 episode are used to simulate the baseline air quality conditions for 2023. Results show that ozone and $PM_{2.5}$ concentrations peak at locations downwind from Los Angeles. CO concentrations, however, peak in Central Los Angeles. Ozone, NO_2 and $PM_{2.5}$ peaks occur downwind from main emissions because they are secondary pollutants, whereas CO is a primary pollutant and its concentrations depend mainly on direct emissions.

Although baseline simulations for the year 2023 use emission inventories that have been developed for the 2007 AQMP to demonstrate attainment of ozone and $PM_{2.5}$ air quality standards, ozone and $PM_{2.5}$ concentrations exceed the established air quality standards (75 parts per billion (ppb) for ozone; 35 μg per cubic meter ($\mu g/m^3$) for $PM_{2.5}$) as shown in Fig. 6. The CACM chemical mechanism used in the CIT-UCI model predicts higher oxidative capacity that leads to higher concentrations of O_3 than those predicted by other chemical mechanisms, such as SAPRC-99, which was used to produce the results in the AQMP (Jimenez et al., 2003).

3.3. Air quality resulting from updating area sources emissions inventory

The updated inventory, using emission testing results from LBNL for residential sources, reduces the basin-wide emissions of NO_x by 2.1 tons/day. This reduction translates into a reduction of 1.8% in

NO_x emissions with respect to the SCAQMD Baseline emissions inventory. Because the decreases in emissions are due to changes in the emission factors for the residential natural gas sector, the largest decreases occur near Los Angeles, where the highest population density exists.

The differences in the concentration of air pollutants calculated using the 2023 SCAQMD baseline inventory compared to the updated LBNL baseline inventory are shown in Fig. 7. The decrease in NO_x emissions leads to a slight increase in O_3 concentration around Los Angeles, due to the high overall amount of NO_x emissions and the VOC-limited regime in that area. In contrast, ozone concentration decreases in the eastern portion of the domain, where the highest ozone concentrations typically occur. Overall, the peak 8-h ozone concentration in the LBNL Baseline case is 1 ppb lower than in the SCAQMD Baseline case. Due to the reduction of NO_x emissions and ozone concentrations around Riverside, $PM_{2.5}$ concentrations also decrease, by a maximum of 1 μg per cubic meter.

These results show that updating emission factors that are currently used by air regulatory agencies (SCAQMD) for natural gas combustion in residential appliances reduces its overall emissions contribution to current inventories used to demonstrate the efficiency of air pollution control measures. This could affect the assessment of additional policies to control emissions from natural gas combustion.

3.4. Air quality impacts of LNG

The increase of 92 kg of NO_x per day in the Sempra Scenario (0.08% with respect to total emissions) results in small impacts on ozone and secondary particulate matter concentrations. The maximum increase in peak ozone concentrations and 24-h $PM_{2.5}$

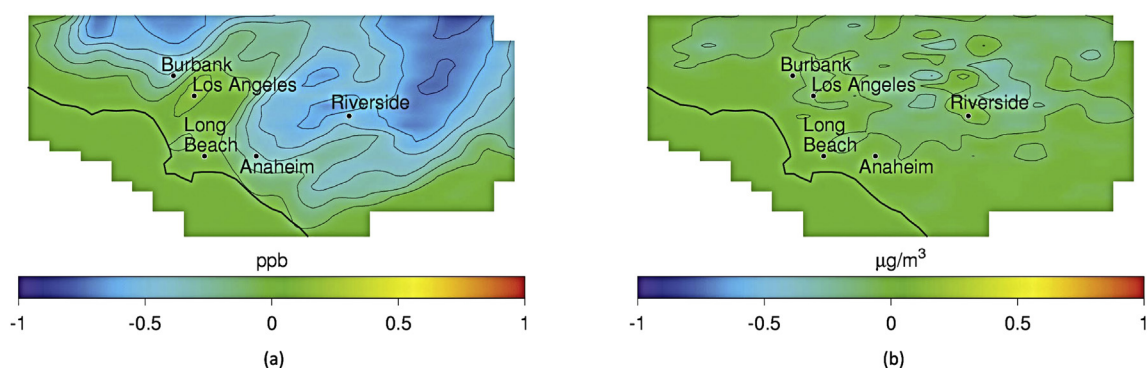


Fig. 7. Differences in air pollutant concentrations of the Baseline LBNL minus Baseline SCAQMD cases: (a) peak 8-h average ozone, (b) 24-h average $PM_{2.5}$.

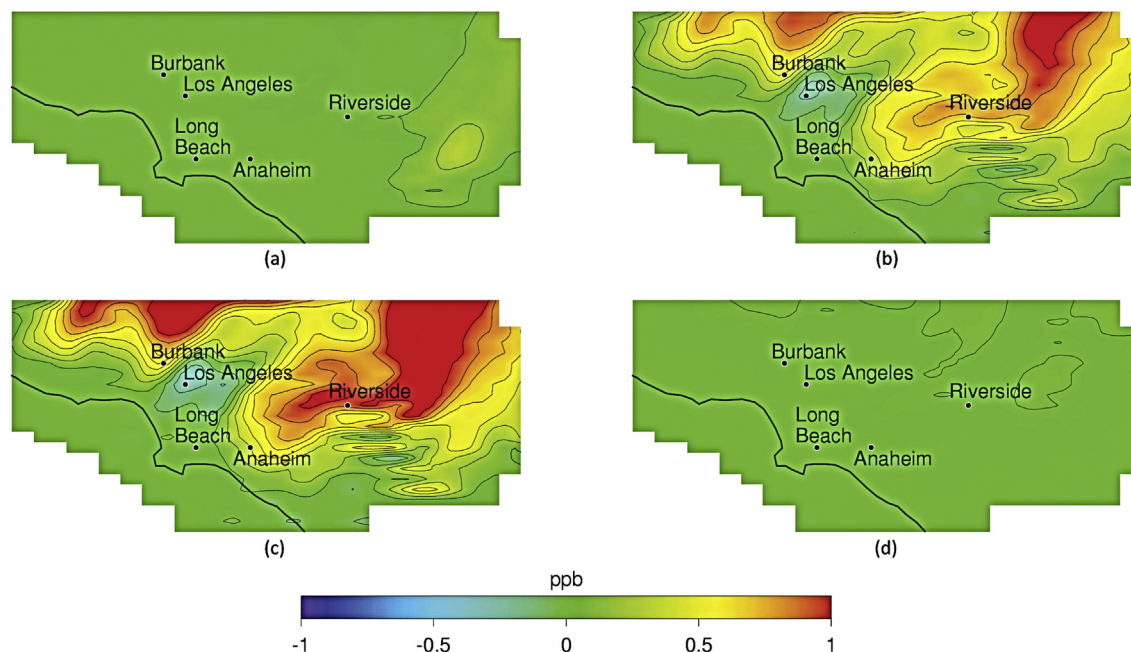


Fig. 8. Impacts on peak ozone concentrations due LNG implementation scenarios projected the year 2023: (a) Sempra scenario, (b) 100% LNG penetration scenario, (c) 100% LNG penetration with increased Wobbe index limit, (d) 100% LNG penetration with commercial and industrial equipment tuning.

concentrations are 0.5 ppb and $0.6 \mu\text{g}/\text{m}^3$, respectively (Fig. 8a and Fig. 9a, and Table 5).

As presented in Table 4, hypothetical bounding scenarios introduce significantly higher emissions due to LNG implementation that is greater than the realistic delivery scenario. Scenario 100% LNG increases NO_x emissions by 2.5%, which leads to an increase in the average model-predicted peak ozone concentrations of 0.4 ppb, and maximum increases in some locations in the model domain are 1.9 ppb (shown in Fig. 8b). As discussed above, a

reduction in the WI limit from 1385 BTU/scf to 1360 BTU/scf proposed by the SCAQMD would reduce the emission impacts from LNG by half, potentially reducing the air quality impacts by half.

Scenario 100% LNG with $\text{WI}_{\text{max}} = 1400$ increases emissions of NO_x by 3.2%, resulting in an increase in predicted peak ozone concentrations of 2.3 ppb (shown in Fig. 8c). The impact on ozone concentration due to these two scenarios is an expected outcome of moderate increases in NO_x emissions in the SoCAB. Increasing NO_x emissions leads to a reduction of ozone concentrations around

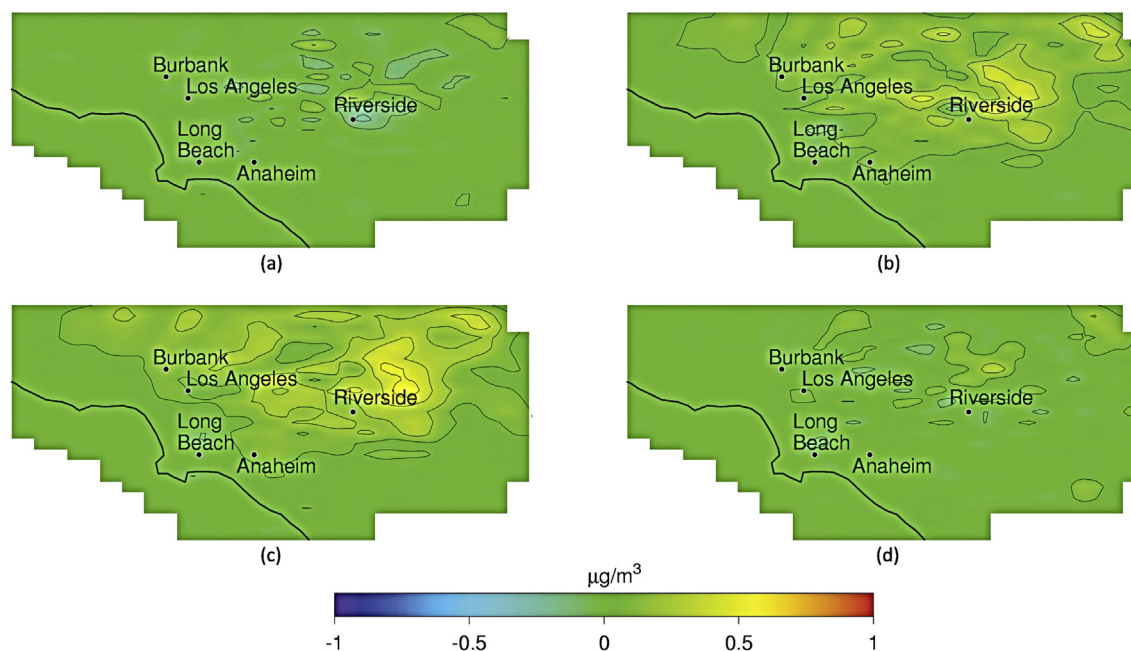


Fig. 9. Impacts on 24-h average $\text{PM}_{2.5}$ concentrations due LNG implementation scenarios projected the year 2023: (a) Sempra scenario, (b) 100% LNG penetration scenario, (c) 100% LNG penetration with increased Wobbe index limit, (d) 100% LNG penetration with commercial and industrial equipment tuning.

Table 5
Summary of impacts on peak ozone and 24-h PM_{2.5} due to LNG scenarios.

Case	$\Delta[\text{O}_3]_{\text{max}}$ (ppb)		$\Delta[\text{PM}_{2.5}]_{24\text{-h}}$ ($\mu\text{g}/\text{m}^3$)	
	Maximum	Minimum	Maximum	Minimum
Sempre Scenario	0.42	−0.22	0.55	−0.36
100% LNG	1.90	−0.99	0.66	−0.39
100% LNG ($\text{WI}_{\text{max}} = 1400$)	2.27	−1.23	0.66	−0.21
100% LNG with tuning	0.30	−0.13	0.49	−0.33

central Los Angeles and an increase in ozone concentrations farther downwind in the eastern segment of the domain where typically the highest ozone concentrations occur. In addition, increases in ozone concentrations occur in the northwestern part of the domain (Ventura County) due to high ozone productivity caused by incoming clean air from the coast coupled with local NO_x emissions. Finally, Scenario 100% LNG with tuning presents the potential benefits of tuning NG commercial and industrial installations to minimize NO_x emissions. As shown in Table 4, increases in NO_x emissions due to LNG use in conjunction with equipment tuning are less than 0.2%, even with 100% penetration of LNG. The resulting impacts on ozone concentrations are marginal, less than ± 0.3 ppb (Fig. 8d). Even though the increase in reactive organic gases in the tuning case is the same as in the 100% LNG case, short-chain alkanes have low ozone production potential, as reported by Carter (2000a,b) based on VOC reactivity scales. As a result, the impact of fugitive emissions of VOC on ozone formation is determined to be marginal, even for a high penetration of LNG. It should be noted that it is uncertain how many facilities could implement the maintenance and equipment tuning necessary to use high Wobbe number LNG.

Fig. 9 presents the impact of all LNG scenarios on 24-h PM_{2.5} concentrations. As in the case of ozone, scenarios 100% LNG and 100% LNG with $\text{WI}_{\text{max}} = 1400$ lead to the highest model-predicted impacts. Scenario 100% LNG with $\text{WI}_{\text{max}} = 1400$ increases the average model-predicted PM_{2.5} by $0.1 \mu\text{g}/\text{m}^3$, and maximum increase in PM_{2.5} of less than $1 \mu\text{g}/\text{m}^3$. As for ozone, tuning of equipment minimizes the impacts on secondary particulate matter, producing impacts that are comparable to the impacts caused by the Sempre scenario.

4. Conclusions

The work presented here integrates laboratory measurements obtained by LBNL and SoCalGas with current emissions inventories generated by the SCAQMD to determine spatially and temporally resolved emission changes due to the potential use of LNG in natural gas combustion processes. The resulting emissions are used as inputs to a state-of-the-art air quality model to determine the potential impacts of LNG on ozone and secondary particulate matter formation in SoCAB. Results provide valuable information for decision makers to determine the effect of policies aimed at controlling the Wobbe Index of natural gas from alternative sources.

The residential appliance experiments performed by LBNL provided technology specific emission factors that are used to update the baseline SCAQMD emission inventory. For most technologies, the more relevant NO_x emission factors are lower than the emission factors currently used that are based on AP-42 values. Updating the emission factors for residential natural gas appliances used in the original inventory with emission factors obtained in experimental measurements decreased projected nitrogen oxide emissions by a total of 2.4 tons/day in the SoCAB. This reduction translates to a reduction of 2.1% in projected NO_x emissions from all sources in the basin.

Projections based upon the ECA LNG plant capacity show that the penetration of liquefied natural gas to the SoCAB is limited and the resulting impacts on emissions are marginal. In addition, three hypothetical bounding scenarios are included to investigate whether LNG use at any plausible scale would have substantial impacts on overall emissions and ambient air quality. The hypothetical scenario that considers 100 percent LNG penetration into the basin increases NO_x emissions by 2.8 tons/day and corresponds to a 2.5% in total basin-wide NO_x emissions. It is important to note that additional LNG facilities would be required to reach this level and that this increase in emissions is of the same order as the difference between the SCAQMD baseline inventory and the emissions inventory updated with the measurements of LBNL. In addition, 100% penetration of LNG increases emissions of CO and short-chain alkanes by 2.6 and 1.0 tons/day, respectively. An increase in the Wobbe index limit results in linear increases in emissions from LNG use. Conversely, a reduction in the WI limit from 1385 BTU/scf to 1360 BTU/scf as proposed by the SCAQMD would reduce the potential emissions and air quality impacts of LNG by half.

In the United States, NO_x emissions from NG combustion in residential and commercial area sources and industrial boiler add up to an average of 2900 tons/day in 2011 (USEPA, 2011). A shift of 50 BTU/scf in the NG Wobbe Index could increase emissions of NO_x by nearly 72 tons per day. Changes in gas composition – an as a result, changes in Wobbe Index – can be expected in the future as the extraction of shale gas as a source of domestic NG continues in the US (Bulba and Krouskop, 2009). As a result, the findings in this study on potential emission changes are not only relevant to LNG use in Southern California, but also relevant to other regions in the United States. However, this study focuses only on emissions from combustion. Domestic natural gas production can also contribute to pollutant emissions from the extraction process, which this study did not address.

The implementation of tuning strategies to adjust equipment to changes in Wobbe index in commercial and industrial installations would reduce the impacts of LNG even in high penetration cases. Even though tuning of equipment would not avoid fugitive emissions from LNG distribution, adjustment of NO_x emissions could practically offset the potential increases in NO_x emissions due to widespread LNG use. It should be noted that it is uncertain how many facilities could implement the maintenance and equipment tuning necessary to use high Wobbe index LNG. Nonetheless, tuning strategies could be an alternative for the reduction of the current WI limit proposed by SCAQMD.

These results indicate that the impact of LNG on overall basin-wide nitrogen oxides emissions should be very small, and may be below the level at which the models can discern. Indeed, even when the SoCAB is assumed to receive a hypothetical 100 percent LNG, the impact on the ozone concentrations are small, and may be within the predictive error limits of the model. The difference in emissions between the 2023 SCAQMD baseline and the LBNL baseline is of the same order of magnitude as that predicted by the hypothetical 100 percent LNG penetration. Thus, the available emissions data and air quality model results suggest that the impact of LNG use on air quality in the South Coast Air Basin of California is within the uncertainty limits of the emission estimates from residential appliances alone, even with the current WI limits established by Rule 30 for Southern California.

This work focused on stationary sources in the SoCAB. Future work is underway to include additional sources of emissions that could be affected by a change in natural gas composition, such as mobile sources, and to analyze other geographical areas in the state of California where those sources of emissions may affect air quality.

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Appendix A. Supplementary material

Supplementary material associated with this article can be found, in the online version, at <http://dx.doi.org/10.1016/j.jngse.2014.09.025>.

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