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Ozone Source Apportionment Technique Development and Its Applications in Southern
California

By

YUSHENG ZHAO
DISSERTATION

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Approved:

Michael Kleeman, Chair

Christopher D. Cappa

Ian C. Faloona

Committee in Charge

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List of Abbreviations

AB32	Assembly Bill 32
ACS	American Community Survey
AQG	Air quality guidelines
BAU	Business-as-usual scenario
BCIC	Boundary conditions and initial conditions
BenMAP-CE	Environmental Benefits Mapping and Analysis Program – Community Edition
CAM-chem	Community Atmosphere Model with Chemistry
CAMx-OSAT	Comprehensive Air Quality Model with extensions with O3 Source Apportionment Technology
CA-REMARQUE	California Regional Multisector Air Quality Emissions model
CARB	California Air Resource Board
CMAQ-ISAM	Community Multiscale Air Quality Integrated Source Apportionment Method
CCSM	Community Climate System Model
CESM	Community Earth System Model
CTM	Chemical transport model
EJ	Environmental justice
ENSO	El Nino Southern Oscillation
EPA	Environmental Protection Agency
FDDA	Four-dimensional data assimilation
FNR	Formaldehyde to NO2 ratio
GHG	Greenhouse Gases
GHGAi	Greenhouse Gases reduction scenario
IPCC	Intergovernmental Panel on Climate Change
LA	Los Angeles
LAX	Los Angeles International Airport
MARPOL	International Convention for the Prevention of Pollution from Ships
MD8H	Maximum Daily 8-hour Average
MEGAN	Model of Emissions of Gases and Aerosols from Nature
MFB	Mean fractional bias

MOZART	Model for Ozone and Related chemical Tracers
NAAQS	National Ambient Air Quality Standards
NARR	North American Regional Reanalysis
NEI	National Emission Inventory
NMB	Normalized Mean Bias
NME	Normalized Mean Error
NMVOC	None-Methane VOC
NO _x	Nitrogen oxides, NO + NO ₂
NO _x SA	NO _x source apportionment
NO _y	Sum of NO _x and all oxidized atmospheric odd-nitrogen species
PM	Particulate Matter
RCP	Representative concentration pathway
RMSE	Root mean square errors
SAN	San Diego International Airport
SD	San Diego
SFO	San Francisco International Airport
SMOKE	Sparse Matrix Operator Kernel Emissions
SoCAB	South Coast Air Basin
UCD/CIT	University of California Davis/California Institute of Technology airshed model
UNFCCC	United Nations Framework Convention on Climate Change
VCPs	Volatile chemical products
VOCs	Volatile organic compounds
VOC SA	VOC source apportionment
WHO	World Health Organization
WRF	Weather Research and Forecasting model
WRF-Chem	Weather Research and Forecasting with Chemistry model

Abstract

Ground-level ozone (O_3) is widely recognized as a significant air pollutant that affects public health across the globe. O_3 is formed from precursor emissions of oxides of nitrogen (NO_x) and volatile organic compounds (VOCs) that react in the atmosphere in the presence of sunlight. Understanding the source contributions to O_3 formation is a critical step in the design of efficient O_3 control strategies. However, due to the nonlinear nature of O_3 chemistry, it is challenging to identify the major source contributions to O_3 concentrations. The research in this thesis addresses such issue by using O_3 source apportionment calculations within a chemical transport model (CTM), which is a specialized approach to resolve the source contributions to O_3 .

In Chapter 2, a novel O_3 source apportionment technique is developed to explicitly resolve the contributions from both NO_x and VOC sources to O_3 formation. The new technique is flexible and can be configured to identify the original source of precursors that contribute to O_3 formation or the most recent source depending on the choice of the tagging method. The detailed features of the new technique are demonstrated during a peak O_3 event in September 2010 in Los Angeles, California, while trends in O_3 source contributions over time are evaluated during two additional simulations in July 2005 and August 2015. Quality control checks show that the new source apportionment methodology does not alter predicted total O_3 concentrations, and the detailed source apportionment information can be averaged to yield results that are consistent with traditional O_3 source apportionment calculations. The detailed O_3 source apportionment results during Sept 2010 show that the major NO_x sources that contribute to O_3 are gasoline and diesel engines from on-road vehicles, diesel combustion in off-road engines, and soil-derived NO_x , while the majority of VOCs are VOCs emitted from upwind boundary conditions that are outside the domain and biogenic VOCs within the domain. The formaldehyde to NO_2 ratio (FNR) suggest that the chemical regime was VOC-limited, but given the uncontrollable nature of the identified

major VOC emissions, the source apportionment results suggest that NO_x emission controls would have been the preferred emission control strategy to reduce O₃ concentration in Los Angeles at that time, with the understanding that some period of O₃ disbenefits would need to be tolerated until the emissions control program shifts the atmospheric chemistry back into the NO_x-limited regime.

In Chapter 3, the newly developed O₃ source apportionment is applied to resolve a puzzle found in Zapata et al. (2018a) that O₃ concentrations within major California cities in the year 2050 are predicted to increase and continue to violate the 8-h O₃ standard despite the adoption of low-carbon energy. This O₃ penalty is largely due to the persistent NO_x-rich chemistry within urban cores that causes O₃ concentrations to increase when traditional combustion sources are replaced by renewable energy sources and reductions in NO_x emissions are not enough. By simulating Zapata's case again but employing a CTM equipped with the novel O₃ source apportionment technique, the major sources that contribute to the O₃ violations are identified and three cumulative Supplemental Control Steps are developed based on Zapata's low-carbon energy scenario. All three Control Steps successfully lower O₃ concentrations significantly in the South Coast Air Basin (SoCAB), with residual O₃ violations mainly predicted in non-populated wilderness areas. The significant reductions in O₃ produced by the Supplemental Control Steps decrease the predicted incidence of hay fever/ rhinitis, asthma, and all-cause mortality by an order of magnitude compared to the previous scenario where low-carbon energy is adopted. The predicted public health savings associated with the Supplemental Control Steps are valued at \$19.70-30.36B/yr.

Chapter 4 extends the scope of Chapter 3 by analyzing the environmental justice aspect within the Supplemental Control Steps designed in Chapter 3. The exposure disparities, defined as departures from the population average exposure, are calculated for O₃ and NO₂ in Southern California. Future air quality fields are simulated using a CTM under five emission scenarios

including the business-as-usual (BAU) scenario, Greenhouse Gasses reduction (GHGAi) scenario, and the three Control Steps. We find that traditional O₃ control strategies reduce O₃ exposure disparities by <1.6 % and reduce NO₂ exposure disparities by <9 % in Southern California. For the Black and African residents living in the urban core of Los Angeles, the relative NO₂ exposure disparities increase from +23.1 % to +66.2 % and O₃ exposure disparities increase from -3.3 % to +0.1 % due to NO_x emissions reductions mainly in outlying regions and the NO_x-rich environment in the urban core. To reduce the exposure disparities, additional analysis is performed with complete elimination of NO_x emissions from Los Angeles International Airport (LAX), which is not practical but able to reduce the NO₂ exposure disparities by up to 50 %.

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Chapter 1 Introduction

Ambient air pollution is one of the greatest environmental threats to global human health, causing an estimated 4.2 million premature deaths in 2019 alone (World Health Organization, 2022). As one of the six criteria air pollutants regulated by the United States Environmental Protection Agency (US EPA), ground-level ozone (O_3) has adverse impact on public health mainly through human's respiratory systems and exacerbates problems such as coughing, chest tightness, and other asthmatic symptoms (Burnett et al., 1997; Gent et al., 2003; Lippmann, 1989).

With several decades of control efforts, O_3 concentrations have significantly decreased in California, while residual O_3 pollution still persists (Faloona et al., 2020). In 2023, the national average of Fourth Daily Max 8-hour O_3 was 69 ppb among 484 national sites, with a maximum value of 107 ppb in a site in California (U.S. EPA, 2024a). There were 189 sites exceeding the 70-ppb National Ambient Air Quality Standards (NAAQS), with 37 sites in California. Another study that simulated the future conditions in the year 2050 with reduced Greenhouse Gases (GHG) emissions predicted that O_3 concentrations would continue to violate the NAAQS in major California cities (Zapata et al., 2018a). It becomes crucial to understand source contributions to O_3 formation and to design efficient O_3 controls for both present and future conditions.

O_3 is formed through a complex sequence of photochemical reactions between volatile organic compounds (VOCs) and nitrogen oxides (NO_x) in the presence of sunlight (Atkinson, 2000). However, due to the complexity of O_3 chemistry, it is difficult to quantify the final source contributions to O_3 formation. Therefore, Chapter 2 of this thesis develops a specialized approach to resolve such difficulty, which is a novel O_3 source apportionment technique within a chemical transport model (CTM) that can comprehensively resolve the source contributions. The O_3 source apportionment technique uses the species tagging method that can probe relationships between initial emissions and final concentrations produced by photochemical reaction mechanisms. It can quantify the contributions from emissions in

different geographical regions to concentrations in other geographical regions (Ying and Kleeman, 2006), or emissions in different source categories to the concentrations at receptor locations (Cohan and Napelenok, 2011; Ying et al., 2004; Ying and Kleeman, 2006). Previous studies that performed O₃ source apportionment only attribute the production of O₃ to either VOC or NO_x sources depending on the O₃ formation regime (Dunker et al., 2002; Kwok et al., 2015; Sillman, 1995; Tonnesen and Dennis, 2000). While in this thesis, the O₃ source apportionment addresses the separate roles of NO_x and VOC sources in O₃ formation, which is more comprehensive. The O₃ source apportionment results are mainly calculated for Los Angeles during a peak O₃ event in September 2010 (Venecek et al., 2019), while two additional simulations in July 2005 and August 2015 are used to evaluate the source apportionment trends over time.

As a top 10 world economy and having a long-standing commitment to a clean environment, California has both the resources and the motivation to lead a role on fighting climate change. Assembly Bill 32 (AB32) commits California to reducing GHG emissions by 80% of 1990 levels by the year 2050 (California Air Resources Board, 2006), which will be achieved mainly by transforming the energy system to low-carbon energy. Such transition of energy system may result in the immediate public health savings from reduced air pollution over \$20B/yr, much of which is associated with reduced concentrations of airborne particulate matter (PM_{2.5}) (Li et al., 2022b; Zapata et al., 2018a). O₃, however, does not respond as beneficially due to the predicted increases of O₃ concentrations in urban areas.

In Chapter 3, the new O₃ source apportionment technique is applied to identify the major sources that contribute to future O₃ violations and to assist in the development of future O₃ mitigation plans that can reach California's GHG emissions reduction goals. By using a CTM configured with the O₃ source apportionment technique, we quantify the NO_x and VOC source contributions in the GHG emissions reduction scenario and design supplemental control programs that focus on the major O₃ sources from NO_x and VOCs. The supplemental control programs are aimed to comply with the O₃ NAAQS. The public health benefits associated with the supplemental control program are also estimated using established epidemiological relationships.

While designing future O₃ control programs, we also need to consider another important factor, which is environmental justice (EJ) (Anderson et al., 2018; Boyce and Pastor, 2013; Gallagher and Holloway, 2022; Mitchell et al., 2015; Morelli et al., 2019; Picciano et al., 2023; Yuzhou Wang et al., 2023). EJ is important especially for California because California has the second highest racial diversity index among all states in the U.S. (U.S. Census Bureau, 2021). EJ can protect people from disproportionate and adverse human health and environment risks and hazards, and provide people with equitable access to a healthy, sustainable, and resilient environment. Based on the work in Chapter 3, Chapter 4 further analyzes the environmental disparities related to O₃ and NO₂ exposures for the year 2050 after the adoption of low carbon energy and supplemental programs. The environmental disparities for historical periods between 2000-2019 are also analyzed for comparison. Exposure disparities under different future scenarios are analyzed for different race/ethnicity groups defined by the American Community Survey (ACS). With residual exposure disparities found, additional control strategies are explored to reach exposure equity for all race/ethnicity groups as much as possible.

Chapter 2 Separately resolving NO_x and VOC contributions to ozone formation

2.1. Introduction

Ground-level ozone (O₃) is one of the six criteria pollutants regulated by the United States Environmental Protection Agency (US EPA). O₃ is formed through a complex sequence of photochemical reactions between volatile organic compounds (VOCs) and nitrogen oxides (NO_x) in the presence of sunlight (Atkinson, 2000). O₃ harms public health by exacerbating respiratory problems such as coughing, chest tightness, and other asthmatic symptoms (Burnett et al., 1997; Gent et al., 2003; Lippmann, 1989). O₃ also damages plants leading to reduced crop yields (Rich, 1964) and harms the built environment by damaging rubber compounds and fading paint (Lee et al., 1996).

O₃ concentrations have decreased significantly over the past 40 years in California due to the adoption of stringent emissions controls, but residual O₃ continues to threaten public health (Faloona et al., 2020). The EPA 2019 design value reports show that there are 74 nonattainment areas violating the 2015 8-Hour O₃ National Ambient Air Quality Standard (NAAQS) across the United States, with 25 of these areas in California.

Understanding source contributions to O₃ formation is a critical first step in the design of efficient O₃ controls in NAAQS nonattainment areas. Both natural and anthropogenic sources can emit O₃ precursors to the atmosphere. Once in the atmosphere, these precursors undergo complex chemical reactions, making it difficult to quantify final source contributions to O₃ formation. One of the specialized approaches developed to handle these complicating factors is species tagging within reactive chemical transport models (CTMs).

Species tagging within CTMs can probe relationships between initial emissions and final concentrations produced by photochemical reaction mechanisms. Species tagging can quantify the contributions from

emissions in different geographical regions to concentrations in other geographical regions (Ying and Kleeman, 2006), or emissions in different source categories to the concentrations at receptor locations (Cohan and Napelenok, 2011; Ying et al., 2004; Ying and Kleeman, 2006). Previous studies have performed O₃ source apportionment using the Comprehensive Air Quality Model with extensions (CAMx) with O₃ Source Apportionment Technology (OSAT) (Collet et al., 2014; Li et al., 2012), the EPA's Community Multiscale Air Quality (CMAQ) Integrated Source Apportionment Method (ISAM) (Collet et al., 2018; Kwok et al., 2015), and the Weather Research and Forecasting with Chemistry model (WRF-Chem) (Gao et al., 2017, 2016). The source apportionment methods in these models are very similar. NO_x and VOCs are grouped into multiple families and tracked during all the model processes while mass balance is maintained. The production of O₃ is attributed to either VOC or NO_x sources depending on the O₃ formation regime. The CAMx-OSAT model and the CMAQ-ISAM model use the ratio of hydrogen peroxide (H₂O₂) production rates to nitric acid (HNO₃) production rates ($P_{H_2O_2}/P_{HNO_3}$) to determine whether O₃ formation is limited by NO_x or VOCs (Dunker et al., 2002; Kwok et al., 2015; Tonnesen and Dennis, 2000), while the WRF-Chem model uses the ratio of HCHO/NO_y (Sillman, 1995). Once the O₃ formation regime is determined, the contributions of O₃ are attributed to different source groups based on the ratio of the limited precursor in the source group to the total limited precursors in all source groups.

Attributing O₃ formation to the sources of the limiting precursor makes the source apportionment results easier to interpret, but ignoring the separate roles that NO_x and VOC sources play in O₃ formation can miss important features. The dominant sources of NO_x in the VOC-limited regime or the dominant sources of VOC in the NO_x-limited regime are relevant and important to understand when designing an efficient emissions control program to reduce O₃ concentrations. For example, conventional wisdom states that reducing VOC emissions is the most effective way to control O₃ formation when NO_x is abundant. Reducing NO_x in this regime may cause O₃ concentrations to increase in the short term. However, this simplified view ignores cases under which VOC cannot be reduced because further

controls are too expensive or impractical. Understanding the contributions from both NO_x and VOC sources in the context of the O₃ formation regime is therefore necessary for the design of effective emission control programs.

Here we propose a new O₃ source apportionment technique within the framework of a regional CTM to address shortcomings in the traditional O₃ source apportionment approaches by fully apportioning NO_x and VOC contributions to O₃ concentrations.

2.2. Methodology

2.2.1. Model configuration

The University of California Davis/California Institute of Technology (UCD/CIT) air quality model was used to predict the O₃ source apportionment results. The UCD/CIT air quality model is a reactive CTM that predicts the evolution of gas- and particle-phase pollutants with emissions, transport, deposition, chemical reaction, and phase change (Kleeman and Cass, 2001; Yu et al., 2019). The model solves the core equation

$$\frac{\partial C_i}{\partial t} + \nabla \cdot u C_i = \nabla K \nabla C_i + E_i - S_i + R_i^{gas}(C) + R_i^{particle}(C) + R_i^{phase}(C)$$

where C_i is the concentration of gas- or particle-phase species i at a particular location as a function of time t , u is the wind vector, K is the turbulent eddy diffusivity tensor (assumed to be diagonal), E_i is the emissions rate, S_i is the loss rate, R_i^{gas} is the change in concentration due to gas-phase reactions, $R_i^{particle}$ is the change in concentration due to particle-phase reactions, and R_i^{phase} is the change in concentration due to phase change.

The UCD/CIT model can be configured to use any gas-phase chemical mechanism. Gas-phase chemistry in the current study is described using two versions of the SAPRC11 chemical mechanism (Carter and Heo, 2013). The first version of SAPRC11 was configured to track NO_x source contributions to O₃ formation, while the second version was configured to track VOC source contributions to O₃ formation. Both versions of the mechanism enforce mass balance.

O₃ source apportionment results were calculated for Los Angeles from Sep 21 to Sep 27, 2010, corresponding to the highest regional O₃ concentrations in Southern California in this year (Venecek et al., 2019). Two domains were used in the simulation: one parent domain with 24-km resolution covers all of California, and one subdomain with 4-km resolution covers southern California (Figure S2.1).

Meteorology inputs were generated by the Weather Research and Forecasting (WRF) model (WRFv3.4).

Anthropogenic emissions were generated based on the California Air Resource Board (CARB) 2010 Emission Inventory processed using the Sparse Matrix Operator Kernel Emissions (SMOKEv3.7). Biogenic emissions were generated using the Model of Emissions of Gases and Aerosols from Nature (MEGANv2.1). Initial and boundary conditions were generated from the global concentration field predicted by the Model for Ozone and Related chemical Tracers (MOZART).

2.2.2. NO_x source apportionment

The NO_x source apportionment (NO_x SA) method follows the tagging approach previously used to track source contributions to particulate nitrate formation (Kleeman et al., 2005). Nitrogen atoms contained in NO_y species NO, NO₂, NO₃, N₂O₅, HNO₃, HNO₄, PAN, etc., are automatically tagged with the source suffix _N using a modified version of the “prep” mechanism compiler distributed as part of the SAPRC software suite. The current formulation expands the method to include O³P, O¹D, and O₃ using nitrogen source tags that are passed from NO_x species. The automated process enforces tag balance so that the total number of tags is identical for reactants and products. For example, the SAPRC11 reaction



is automatically expanded to



Two special cases do not follow the tag balance rules and must be handled separately. The first special case passes the nitrogen source tag information from the reactant NO₂ or NO₃ species with a single tag to the product NO or NO₂ species and to the product O³P species. Reactions following this pattern are listed in Table 2.1.

Table 2.1: Reactions of the first special case to track NO_x-source contributions to O₃ formation. Only the first typed reaction in each sequence is shown to be concise. The total number of reactions matching each format is shown in the far-right column when tracking contributions from nine sources plus initial/boundary conditions.

Reaction Label	SAPRC11 Rate Constant	Modified Reaction	Total Prep Reactions
1-N	PF=NO2-06	NO2_N1 + HV = NO_N1 + O3P_N1	9

17-N	PF=NO3NO2-6	NO3_N1 + HV = NO2_N1 + O3P_N1	9
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The second special case passes the source tag information from the reactant NO_x species and discards the source tag information from the reactant O₃ or O³P species. The reaction templates for this case are listed in Table 2.2.

Table 2.2: Reaction templates for the second special case to track NO_x-source contributions to O₃ formation. The source tags _N[1-9] in the reactants are matched to the source tags in the product list. The total number of additional reactions matching each format is shown in the far-right column when tracking contributions from nine sources plus initial/boundary conditions.

Reaction Label	SAPRC11 Rate Constant	Modified Reaction	Total Prep Reactions
4O3+N	FALLOFF 9.00e-32 0.000 -1.50 3.00e-11 0.000 0.00 0.60 1.00	O3P[_N1] + NO[_N2] = NO2[_N2]	99
5O3+N	5.50e-12 -0.374 0.00	O3P[_N1] + NO2[_N2] = NO[_N2] + O2	99
6O3+N	FALLOFF 2.50e-31 0.000 -1.80 2.20e-11 0.000 -0.70 0.60 1.00	O3P[_N1] + NO2[_N2] = NO3[_N2]	99
7O3+N	3.00e-12 2.981 0.00	O3[_N1] + NO[_N2] = NO2[_N2] + O2	99
8O3+N	1.40e-13 4.908 0.00	O3[_N1] + NO2[_N2] = O2 + NO3[_N2]	99

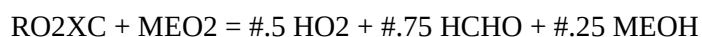
Although the two special cases purposefully do not enforce source tag balance, they still follow the mass balance, and all reactions conserve the total concentrations of reactive nitrogen species and odd oxygen species. A total of nine source tags representing different emission source groups are used in the current NO_x source apportionment exercise, leading to the expanded reaction count listed in the final columns of Table 2.1 and Table 2.2. The combined automatic tagging procedures and the special case tagging procedures summarized in Table 2.1 and Table 2.2 produce 2439 tagged chemical reactions with nine source tags in addition to the base SAPRC11 mechanism.

2.2.3. VOC source apportionment

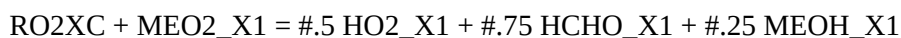
The VOC source apportionment (VOC SA) tagging approach is similar to the NO_x source apportionment approach, but tags are used to track sources of odd oxygen instead of nitrogen. VOCs emitted from

different source groups are tagged with the suffix _X. Each tag is then passed to the peroxy radicals and other compounds containing odd oxygen produced in the chemical reactions. The complexity of the VOC reactions produces multiple special cases that cannot balance the oxygen tag between reactants and products. Reaction templates are used to specify the tagging pattern in these cases, as described below.

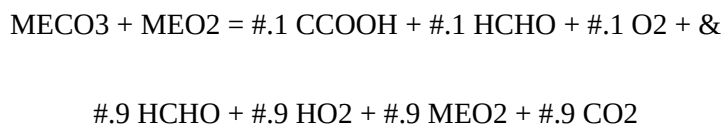
The first special case involves reactions that have one single-tag reactant but multiple tagged products. The single reactant tag is passed to all the specified tagged products in this case. For example, the following reaction in SAPRC11



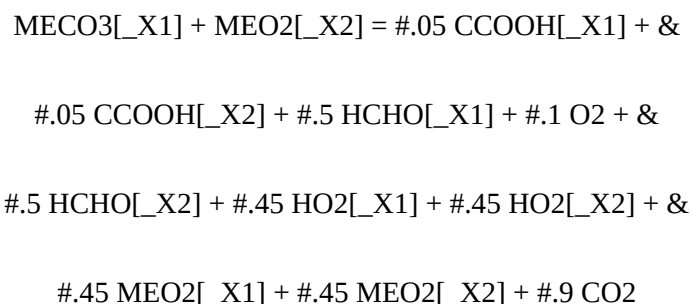
is tagged with the template



For reactants involving two VOCs, source tags are evenly distributed to the products. For example, the following reaction in SAPRC11



is tagged with the template

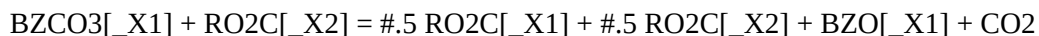


where _X1 represents source tag1 and X2 represents source tag2.

In cases where specific products can be traced to the specific reactants, the source tag of that products is the same as the specific reactants. For example, the following reaction in SAPRC11

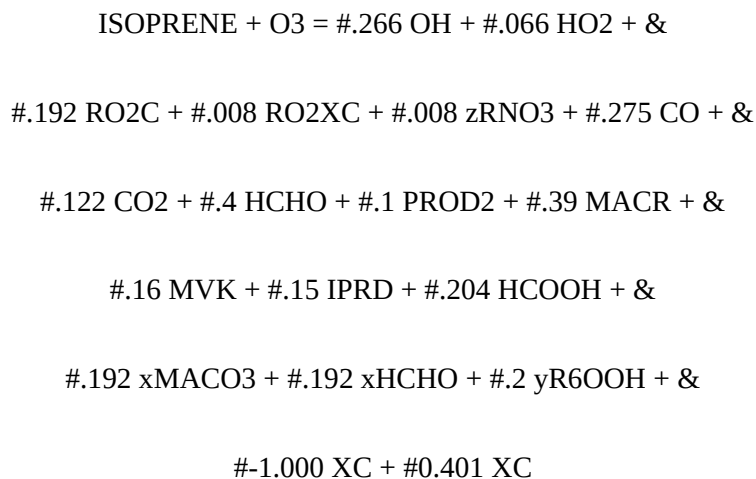


is tagged with the template

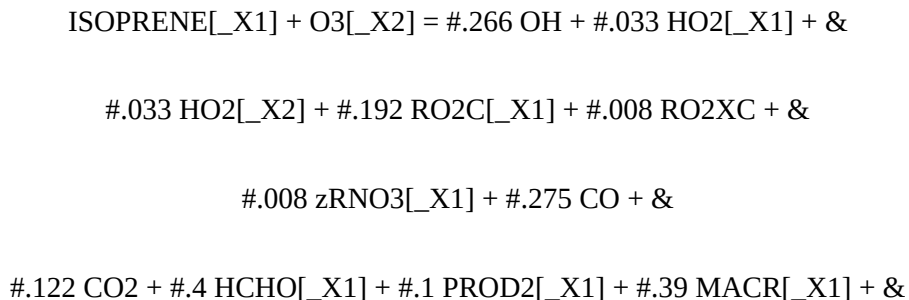


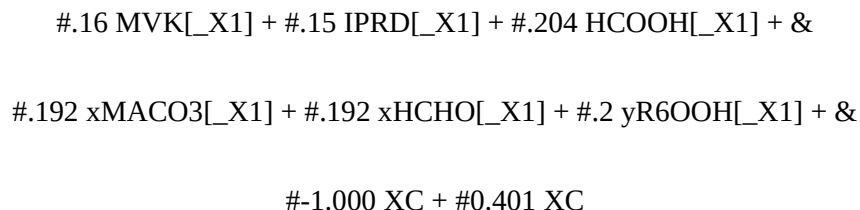
where RO₂C can be traced to both reactants, and BZO can be traced to BZCO₃ based on the BZCO₃ chemistry in SAPRC11 mechanism.

For parent VOCs and peroxy radicals reacting with tagged O₃ or O³P, the source tag in O₃ and O³P is only passed to half of HO₂ and xHO₂ products. The rest of the products are tagged with the identity of the parent VOC or peroxy radical. For example, the following reaction in SAPRC11



is tagged with the template

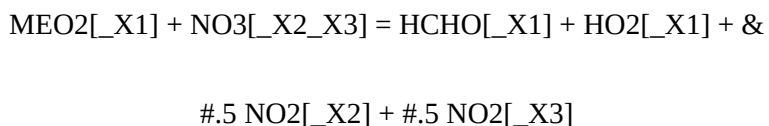




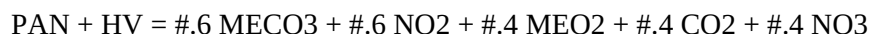
When odd oxygen is passed to reactive nitrogen compounds, the original VOC source tags are also preserved since they will eventually be passed from reactive nitrogen compounds back to O₃. The reactive nitrogen species that contain odd oxygen are NO₂, NO₃, N₂O₅, PAN-species, HNO₄, RNO₃, and xRNO₃. For reactions that have both tagged parent VOC and tagged reactive nitrogen compounds as reactants, the source tags in the nitrogen compounds are only passed to reactive nitrogen compound in the products. The rest of the products are tagged with the source identity of the VOC reactants. For example, the following reaction in SAPRC11



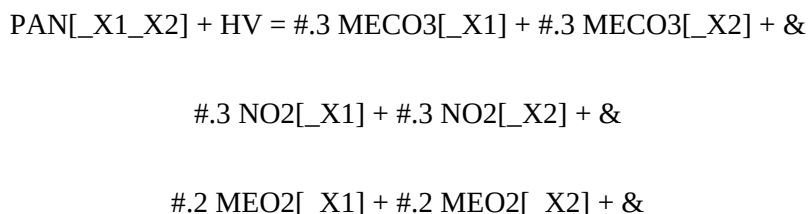
is tagged with the template

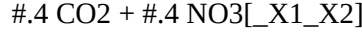


For photolysis reactions involving PAN species with two source tags, the two source tags are evenly distributed to the products. For example, the following reaction in SAPRC11



is tagged with the template





The number of variables and reactions within the SAPRC11 mechanism grows non-linearly with the number of tracked VOC sources. A total of six VOC source tags were tracked in the current study with the upper bound constrained by the limits of the FORTRAN compiler on the host computer system. The combined SAPRC11 mechanism generated using automatic tag balancing along with the reaction templates described above contained 18132 tagged reactions in addition to the base SAPRC11 mechanism.

2.2.4. Model refinements to support source apportionment calculations

2.2.4.1. Advection equation solver

Source apportionment calculations embedded into CTMs should not change the predicted total concentrations of the tagged species (Dunker et al., 2002). Achieving this consistent behavior can be challenging for some model processes such as advection. Many CTMs decompose the 3D advection problem into a series of 1D advection problems described by the equation

$$\frac{\partial C}{\partial t} + \frac{v \partial C}{\partial x} = 0$$

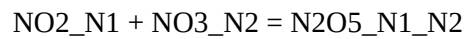
where C is the concentration, t is time, and v is the velocity in the direction of interest. Numerical solutions to the advection equation produce numerical noise that degrades the accuracy of the predicted pollutant concentration fields around sharp concentration gradients. Chock (Chock, 1991, 1985; Chock and Dunker, 1983) investigated multiple algorithms for solving the advection equation and found that the Forester (Forester, 1977) smoothing scheme can be used to dampen computational noise around sharp wave fronts. The method approximates a diffusive process selectively applied in regions of oscillating concentrations using the equation

$$C_i^{k+1} = C_i^k + (\mu/2) \left(\Delta C_{i+1/2}(\phi_i + \phi_{i+1}) - \Delta C_{i-1/2}(\phi_i + \phi_{i-1}) \right)^k$$

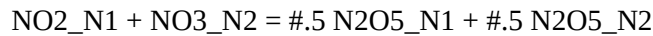
where i is the grid cell location and k is the smoothing application count, $k = 1$ for atmospheric modeling; μ is diffusion coefficient (typically < 0.5); $\Delta C_{i-1/2} \equiv C_i - C_{i-1}$; ϕ is the grid function variable, $\phi = 1$ for grid locations around oscillating concentrations where smoothing is required and $\phi = 0$ for the other grid locations. Separating parent NO_x or VOC species into source-oriented groups naturally creates sub-group fields with sharp spatial gradients. The spatial pattern of numerical noise that develops around these fields can change according to the source-apportionment configuration. This leads to slightly different results from advection calculations carried out using different source apportionment configurations. This undesirable behavior was corrected by modifying the Forester smoothing algorithm so that the spatial smoothing pattern (ϕ_i values) for all source-oriented concentrations within the same parent species were based on the spatial patterns of the total parent species concentrations (summed across all source-oriented groups). The consistent smoothing pattern (ϕ_i values) applied to all source-oriented species within the same parent family regardless of the source-apportionment configuration largely produces consistent results across the advection calculations.

2.2.4.2. Simplified tagging mechanism

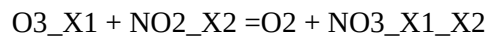
To enable our source apportionment technique to track nine emission source sectors simultaneously, we simplified both NO_x SA and VOC SA by modifying multi-tagged species to single-tagged species. The reaction templates are also modified to be compatible with the simplified method. For example, the tagged template in NO_x SA



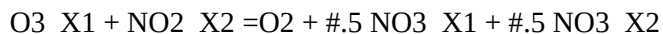
is modified to



The tagged template in VOC SA



is modified to



The simplified tagging mechanism has reduced the number of tagged chemical reactions from 2836 to 2566 in NO_x SA and 18132 to 11782 in VOC SA in addition to the base SAPRC11 mechanism, respectively.

2.2.5. Model comparison with CMAQ-ISAM

O₃ source apportionment results from the UCD/CIT model were also compared to the results generated by the CMAQ-ISAM model developed by the United States EPA. The model configuration during this comparison test was similar to the configuration described in section 2.1 with the exception that a single domain with 12 km spatial resolution covering Southern California was used to expedite the calculations. The anthropogenic emissions were generated from the SMOKEv3.7 using the 2011 National Emission Inventory (NEI). CMAQ-ISAM used the saprc07tic_ae7i_aq chemical mechanism while UCD/CIT used SAPRC11 (Carter and Heo, 2013). For aerosol-phase chemical mechanism, CMAQ-ISAM used AERO7 while UCD/CIT used ISSOROPIA for inorganics and n-product model with adjusted coefficients for SOA. A summary comparing the model details is provided in Table S2.1.

2.3. Results

2.3.1. Model improvements

2.3.1.1. Advection equation solver

Simulations over California were performed using different VOC source apportionment configurations to test the effects of the updated Forester smoothing algorithm during an 8-day period in Aug 2009 (Aug 21 - 28). Figure 2.1 shows four concentration difference plots for NO₂ at hour 12 on the final simulation day. Each panel of Figure 2.1 shows the difference in NO₂ concentrations between a simulation with source apportionment (SA) and a simulation without source apportionment (NonSA). The top row of Figure 2.1 is configured with chemical reactions disabled while the bottom row is configured with chemical reactions enabled. The left column of Figure 2.1 is configured using the original Forester smoothing algorithm while the right column is configured using the updated algorithm. The results displayed in the top row of Figure 2.1 indicate that adoption of the updated Forester smoothing algorithm reduces the maximum value of the computational noise in the NO₂ concentrations from 1.64 ppb to 0.12 ppb in the absence of chemical reactions. NonSA NO_x concentrations range from 0.09 ppb to 5.51 ppb with a mean value of 0.95 ppb in these simulations. The bottom row of Figure 2.1 shows that the adoption of the new Forester smoothing algorithm reduces the maximum value of the computational noise in the NO₂ concentrations from 1.17 ppb to 0.55 ppb when chemical reactions are enabled. NonSA NO_x concentrations range between 0.08 ppb and 29.96 ppb with a mean value of 1.60 ppb in these simulations.

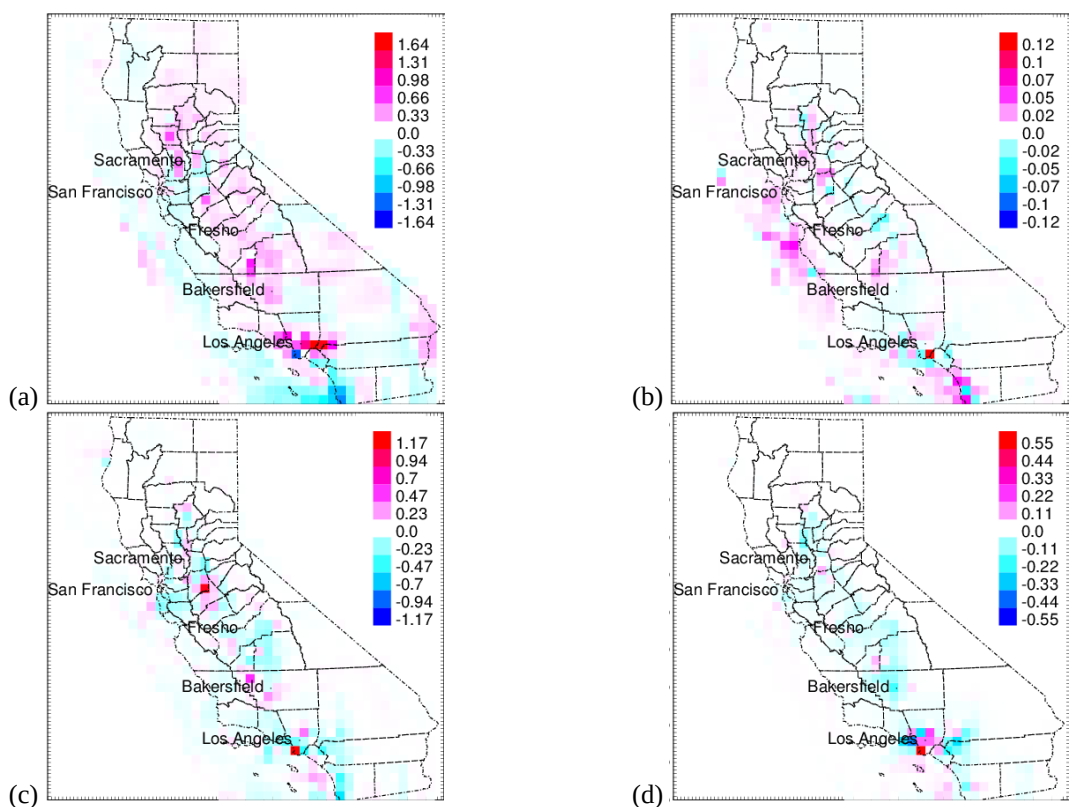


Figure 2.1: NO_2 difference plots at hour 12 on August 28, 2009 for test cases with (a) chemical reactions off and no uniform smoothing pattern; (b) chemical reaction off and uniform smoothing pattern applied; (c) chemical reactions on and no uniform smoothing pattern; (d) chemical reaction on and uniform smoothing pattern applied. All units are in ppb.

2.3.1.2. Simplified tagging mechanism

Figure 2.2 illustrates the difference in total O_3 concentrations predicted at hour 12 of each day September 21-27, 2010 using source apportionment with simplified tagging mechanism (Simp) and without simplified mechanism (NoSimp). Concentration differences are shown as box and whisker plots across all grid cells in the model domain as a function of simulation date. Four source apportionment configurations are tested: (NO_x SA or VOC SA) $\times$ (NoSimp or Simp). Detailed statistical comparisons are presented in Table S2.2 and Table S2.3, with mean bias varying from -0.0731 to 0.1654 ppb and mean error varying from 0.0178 to 0.1660 ppb. All the source-apportionment configurations have similar accuracy compared to results generated without source apportionment. These findings suggest that the simplified tagging mechanisms can be adopted to achieve improved computational efficiency with little loss of overall accuracy.

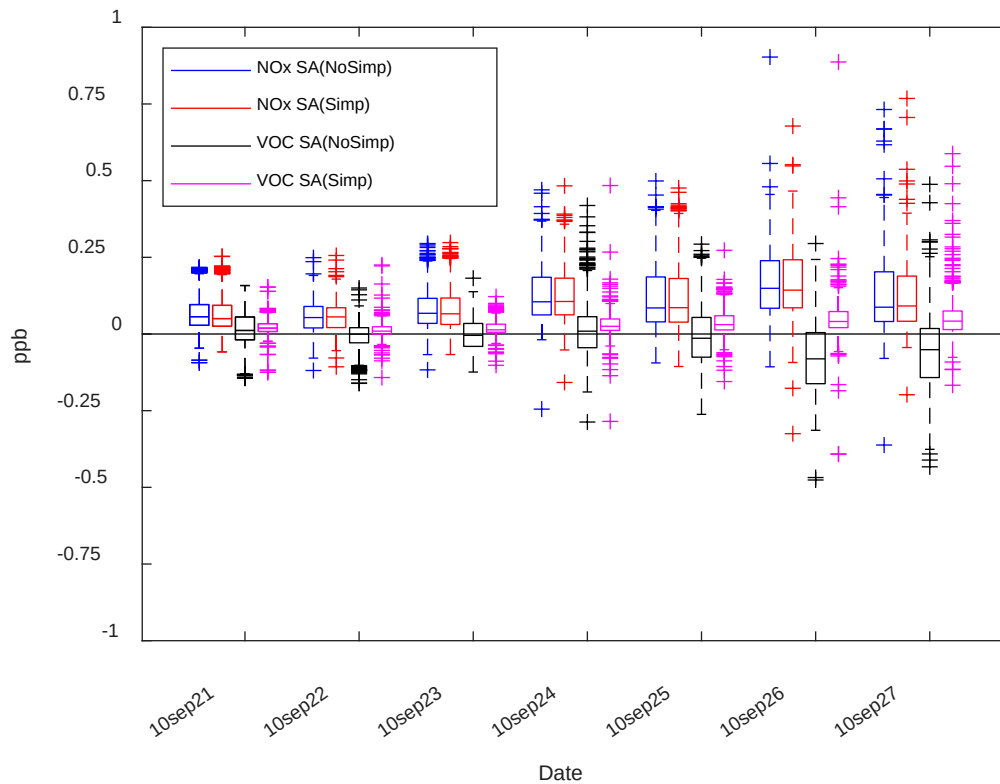


Figure 2.2: Total O₃ differences between results with SA and results without SA across the whole domain at hour 12 for the indicated days in September 2010.

Figure S2.2 and Figure S2.3 show the field plots comparing O₃ contributions from different sources for hour 12 of the last simulation day. For both NO_x SA and VOC SA, the source apportionment results have negligible change, indicating that the simplified method changes neither the total O₃ concentrations nor the source contributions to O₃. For VOC SA, we separate gasoline, diesel, and woodsmoke and food cooking emission sectors into six emission sectors, giving more details of source apportionment information.

2.3.2. Evaluation of ozone source apportionment technique in UCD/CIT model

2.3.2.1. Model results without SA technique

Table 2.3 part (a) presents the model performance statistics for CMAQ and UCD model predictions compared to measured concentrations. The locations of the four measurement sites used for the analysis

are shown in Figure S2.1. When comparing the daily maximum 8-hour average O₃ at the four sites, NMB values are 0.1184 for CMAQ and 0.0819 for UCD/CIT, and NME values are 0.1954 for CMAQ and 0.2020 for UCD/CIT, which meet the performance criteria typically used for CTM calculations (Emery et al., 2017). Correlation coefficients (r) are 0.7633 for CMAQ and 0.8567 for UCD/CIT, which meets the performance goals. Further analysis of performance statistics using 1-hour O₃ is shown in Table S2.4. In general, both CMAQ and the UCD/CIT model predicted O₃ concentrations with reasonable accuracy. Figure S2.4 illustrates the time series plots of O₃ predictions and measurements at individual monitoring sites.

Table 2.3: Model performance statistics for daily maximum 8-hour average O₃ at different sites in (a) CMAQ and UCD/CIT evaluation runs in September 2010; (b) UCD/CIT source apportionment runs in September 2010; (c) UCD/CIT source apportionment runs in July 2005; (d) UCD/CIT source apportionment runs in August 2015.

		NMB	NME	r
(a) 12KM runs using NEI2011 in September 2010	CMAQ	0.1184	0.1954	0.7633
	UCD/CIT	0.0819	0.2020	0.8567
(b) 4KM UCD/CIT SA runs using CARB emission inventory in September 2010	NO _x SA	0.0430	0.1097	0.9310
	VOC SA	0.0372	0.1086	0.9307
(c) 4KM UCD/CIT SA runs in July 2005	NO _x SA	-0.1211	0.1489	0.9058
	VOC SA	-0.1136	0.1454	0.9059
(d) 4KM UCD/CIT SA runs in August 2015	NO _x SA	0.1871	0.2137	0.4882
	VOC SA	0.1828	0.2102	0.4901

Note: For model performance of daily maximum 8-hour average O₃, “Goals” are NMB<±5%, NME<15%, r>0.75, which should be viewed as the best a model can be expected to achieve. “Criteria” are NMB<±15%, NME<25%, r>0.50, which should be viewed as what a majority of models have achieved (Emery et al., 2017).

2.3.2.2. Model results with SA technique

Figure 2.3 illustrates the source apportionment results of CMAQ-ISAM-O₃ and UCD/CIT SA at four monitoring sites. Ozone source contributions predicted using the same model are similar at all locations. Boundary conditions and initial conditions (BCIC) make the largest contributions to O₃ formation at all sites. The 30 – 50 ppb of background O₃ advected into California accounts for the majority of the BCIC contribution in both the NO_x and VOC source apportionment calculations. CMAQ-ISAM-O₃ results also identify BCIC as the single largest contributor to O₃ concentrations during the study period. For CMAQ-

ISAM-O₃ source apportionment results, off-road gasoline, off-road diesel, natural gas, biogenics, and other emission sectors make notable contributions to O₃ formation. On-road gasoline, on-road diesel, and wood smoke emission sectors make smaller contributions to the O₃ formation, while the food cooking sector makes negligible contributions to the O₃ formation.

For UCD/CIT-NO_x source apportionment results, NO_x emissions from the off-road diesel sector make the second largest contribution to the O₃ formation. NO_x emissions from off-road gasoline, natural gas, and other emission sectors also contribute to O₃ formation. NO_x emissions from on-road gasoline, on-road diesel, wood smoke, and food cooking make negligible contributions to the O₃ formation.

For UCD/CIT-VOC source apportionment results, VOC emissions from the biogenic sector contribute significantly to the O₃ formation. VOCs in off-road gasoline and other emissions sector make minor contributions to the O₃ formation. On-road gasoline, on-road diesel, off-road diesel, wood smoke, food cooking, and natural gas sources make negligible contributions to the O₃ formation.

CMAQ-ISAM-O₃ source apportionment calculations simultaneously track both NO_x and VOC contributions to O₃ formation, while the UCD/CIT model separately tracks NO_x and VOC contributions. The rank order of sources that contribute to O₃ formation is identical in the CMAQ-ISAM-O₃ results and the combined results from the UCD/CIT calculations (Figure S2.10). A further consistency check between the two models was carried out by configuring the CMAQ-ISAM model for separate NO_x and VOC tagging so that results could be directly compared to the UCD/CIT model for intermediate species, including NO, NO₂, and HCHO. The comparison illustrated in Figure S2.5 through Figure S2.7 show that the CMAQ-ISAM predictions are similar to the UCD/CIT model predictions, confirming that the model calculations are consistent. The different source apportionment perspectives illustrated in Figure 2.3 mainly result from the combined vs. separate approaches for NO_x and VOC source apportionment adopted in CMAQ and UCD/CIT, respectively.

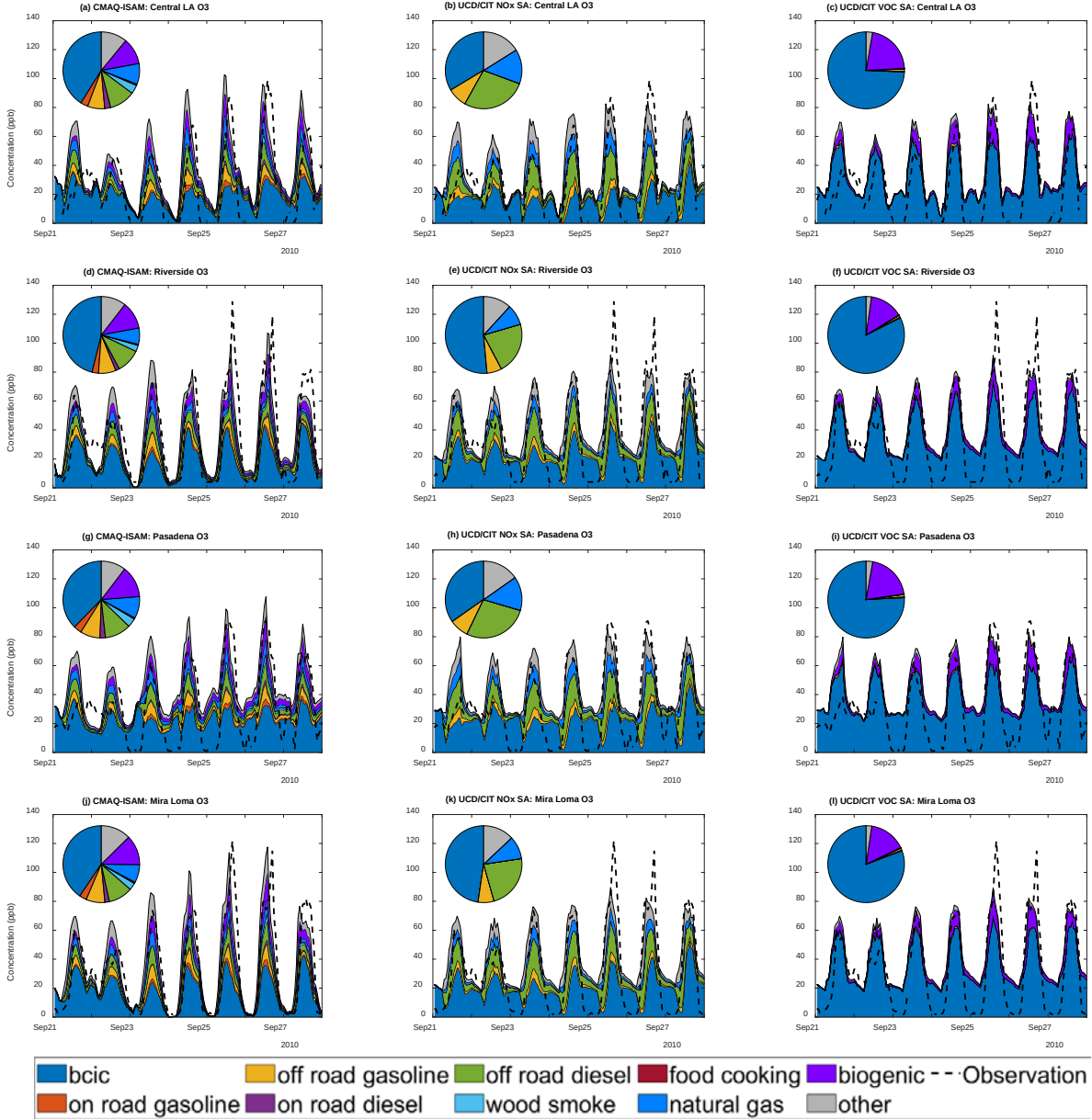


Figure 2.3: O_3 source contributions at different sites in 2010 September using the NEI2011 emissions. The left column presents the results of CMAQ-ISAM using O_3 as tagging class. The middle column presents the results of UCD/CIT using NOx SA. The right column presents the results of UCD/CIT using VOC SA. Pie charts are based on O_3 concentrations exceeding 70 ppb.

2.3.3. Ozone source apportionment

2.3.3.1 Model performance analysis

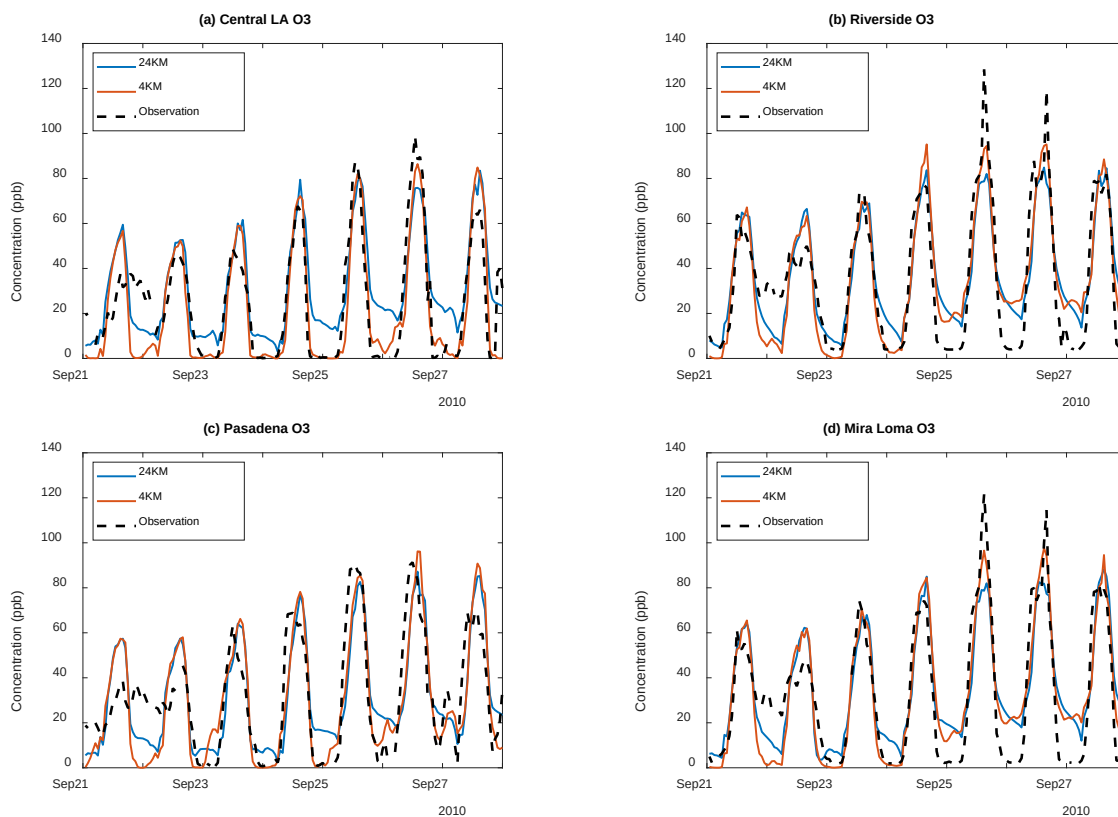


Figure 2.4: Time series plot of predicted and measured O_3 concentration in 2010 September at (a) central LA, (b) Riverside, (c) Pasadena, and (d) Mira Loma Van Buren at resolution of 24KM and 4KM using NO_x SA run results. All simulations use CARB emissions.

Figure 2.4 illustrates UCD/CIT predictions for O_3 concentrations carried out using spatial resolutions of 24KM and 4KM along with observations at four different sites in 2010 September. Simulations carried out at 4KM spatial resolution predict higher O_3 concentrations during the day and lower O_3 concentrations at night, which generally yields improved performance relative to simulations carried out at 24KM spatial resolution. Table 2.3 part (b) shows the model performance statistics for the 4KM simulations configured with both NO_x SA and VOC SA. NMB values are 0.0430 for NO_x SA and 0.0372 for VOC SA. NME values are 0.1097 for NO_x SA and 0.1086 for VOC SA, and r values are 0.9310 for NO_x SA and 0.9307 for VOC SA. Both NMB and NME meet the model performance criteria, and r meets the model

performance goals. The statistics indicate that O₃ concentrations predicted by the UCD/CIT model are reasonably accurate.

Figure S2.12 and Figure S2.13 show the UCD/CIT predictions for O₃ concentrations in 2005 July and 2015 August. Table 2.3 part (c) shows the model performance statistics for the 4KM simulations in 2005 July. The NMB values for both NO_x SA and VOC SA meet the performance criteria. The NME, and r values for both SA meet the performance goal. Table 2.3 part (d) shows the model performance statistics for the 4KM simulation in 2015 August. The NMB and r values for both NO_x SA and VOC SA slightly exceed the performance criteria. The NME values for both SA meet the performance criteria. Overall, both 2005 and 2015 simulations predict O₃ concentrations with acceptable accuracy.

2.3.3.2. Source apportionment

Figure 2.5(a)-(k) shows NO_x source contributions to O₃ concentrations at hour 12 on Sept 27, 2010. Boundary conditions and initial conditions (BCICs) contribute significantly to O₃ concentrations around the edges of the domain but have decreasing significance at interior locations. NO_x emitted from on-road gasoline, off-road gasoline, on-road diesel, and off-road diesel mainly contributes to O₃ formation in urban areas, such as San Francisco and Los Angeles. NO_x emitted from wood smoke and food cooking only contributes a very small amount to O₃ formation in the Central Valley of California. NO_x emitted from fertilized soils makes widespread contributions to O₃ formation, with a maximum contribution of 55.6 ppb in the Central Valley. NO_x emitted from aircraft only contribute to O₃ formation near major airports such as San Francisco International Airport (SFO), Los Angeles International Airport (LAX), and San Diego International Airport (SAN). NO_x emitted from natural gas combustion contributes a small amount to O₃ formation in highly urbanized areas.

Figure 2.6(a)-(k) shows VOC source contributions to O₃ concentrations at hour 12 on Sept 27, 2010. O₃ present in BCICs combined with O₃ formed from VOCs contained in BCICs account for a significant fraction of total O₃ concentrations across the entire state of California. Biogenic emissions also contribute

significantly to O₃ formation over the whole domain. VOCs emitted from on-road gasoline, off-road gasoline, on-road diesel, off-road diesel, wood smoke and food cooking, aircraft, and natural gas combustion make smaller contributions to O₃ formation. Volatile chemical products (VCPs) included in the ninth source category labelled “other” in Figure 2.6 contribute to approximately 4.44 ppb of O₃ formation over Los Angeles with lower contributions in other regions. The implications of potential biases in the VCP inventory (McDonald et al., 2018) are discussed in Section 3.4.2 below.

Figure 2.5(l) and Figure 2.6(l) show the O₃ sensitivity regimes for the September 2010 episode using a formaldehyde-to-NO₂ ratio (FNR) (Jin and Holloway, 2015; Jingwei Liu et al., 2021; Sillman, 1995). A FNR value of 4.6 is used as the transition between the NO_x-limited regime and the VOC-limited regime based on the smog chamber experiments conducted by Wu et al. (2022). Figure 2.5(l) and Figure 2.6(l) display FNR minus 4.6 so that negative values (blue) indicate VOC-limited conditions and positive values (red) indicate NO_x-limited conditions. Most areas of California are VOC-limited during the September 2010 episode.

Figure S2.14 and Figure S2.15 show the NO_x and VOC source contributions to O₃ concentrations at hour 12 on Jul. 19, 2005. Figure S2.17 and Figure S2.18 show the NO_x and VOC source contributions to O₃ concentrations at hour 12 on Aug. 21, 2015. The spatial pattern of the source contributions in these two years are very similar to the spatial pattern in 2010. The FNR results show that major urban areas and the Central Valley are VOC limited, similar to the patterns observed in Figure 2.5(l) for conditions in 2010.

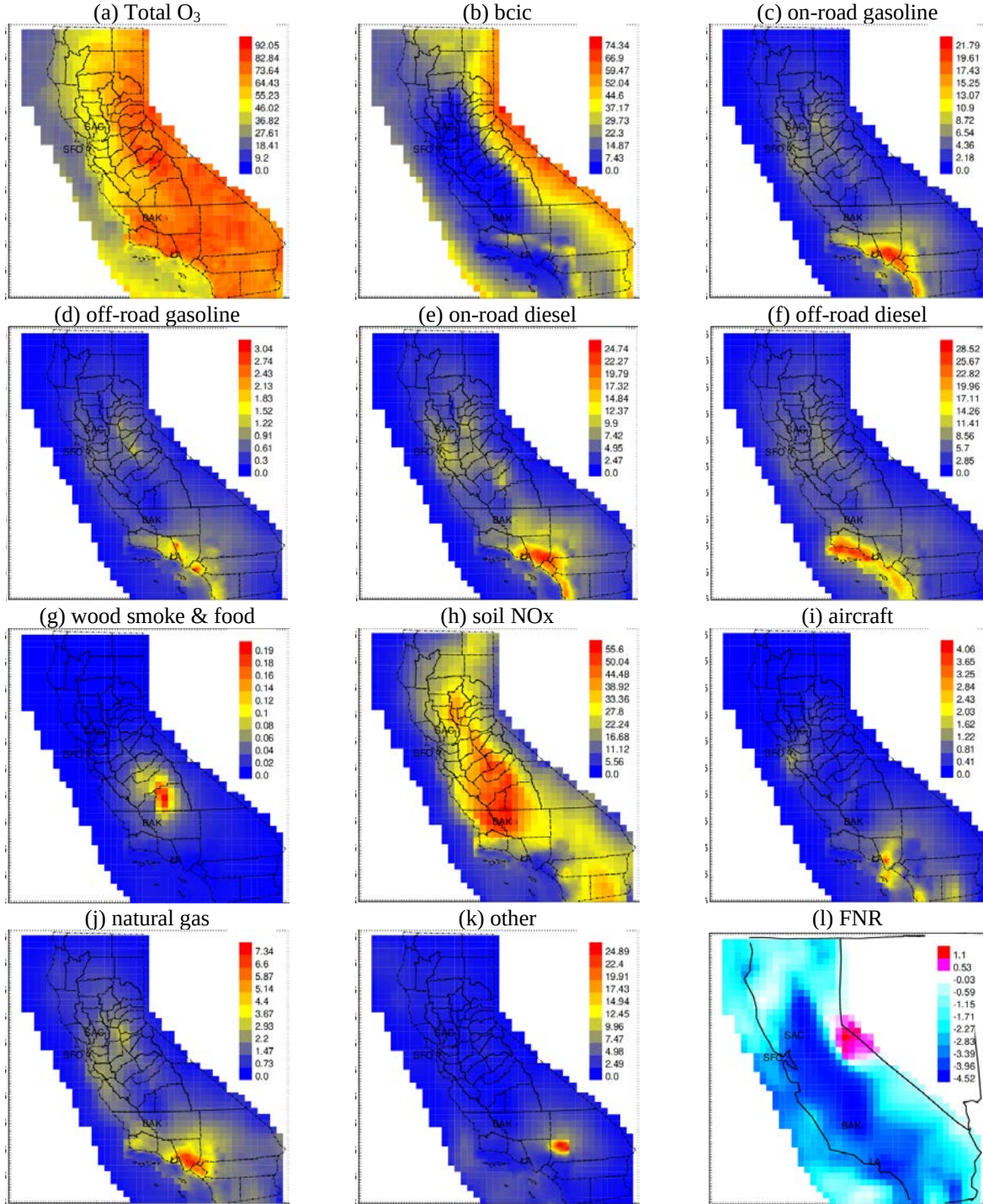


Figure 2.5: (a-k) Predicted NO_x source contributions to O₃ concentrations (ppb) and (l) FNR minus 4.6 at hour 12, Sep 27, 2010. All simulations use CARB emissions. Noting that each plot has different maximum values.

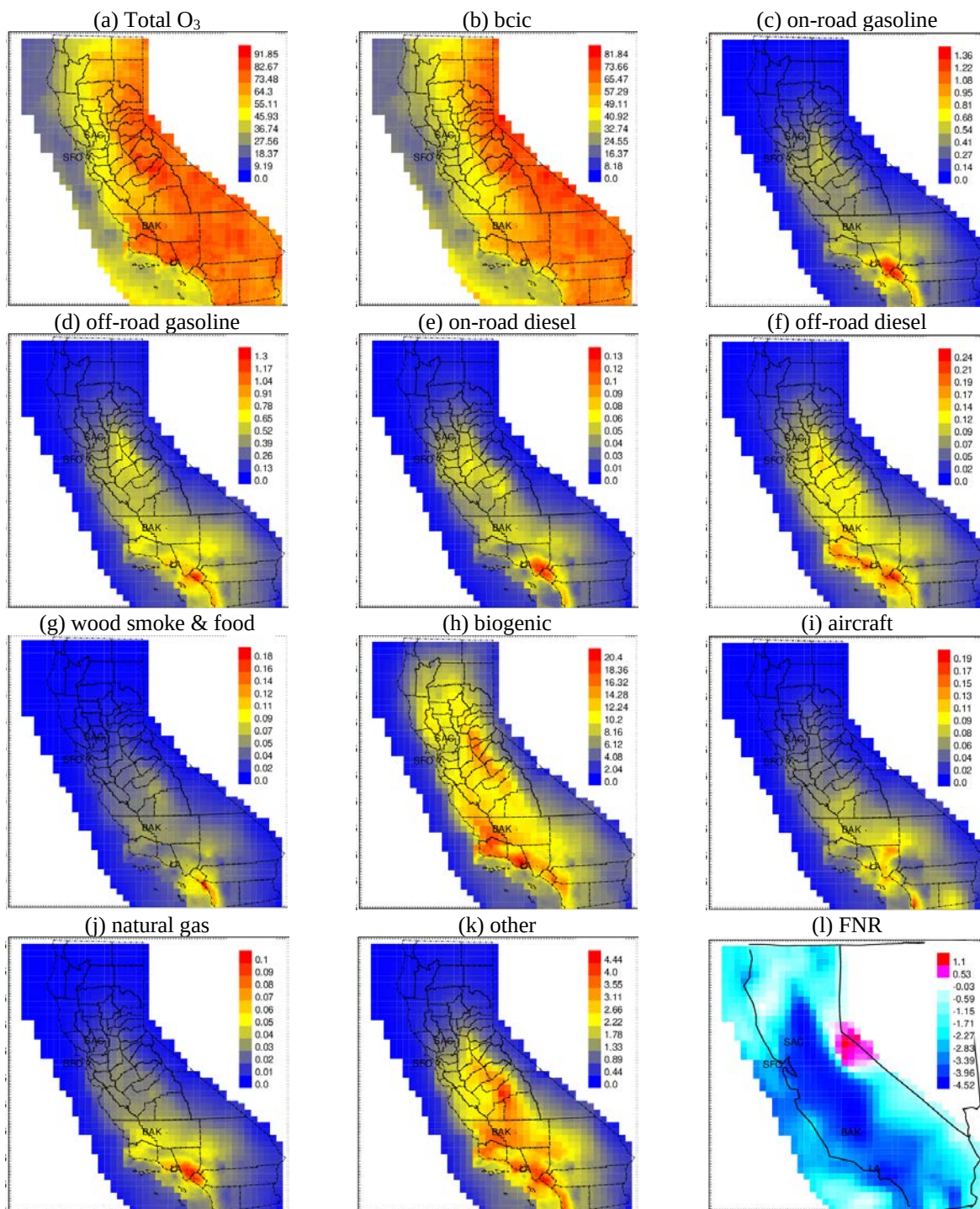


Figure 2.6: (a-k) Predicted VOC source contributions to O₃ concentrations (ppb) and (l) FNR minus 4.6 at hour 12, Sep 27, 2010. All simulations use CARB emissions. Noting that each plot has different maximum values.

2.3.3.3. Ozone time series plots

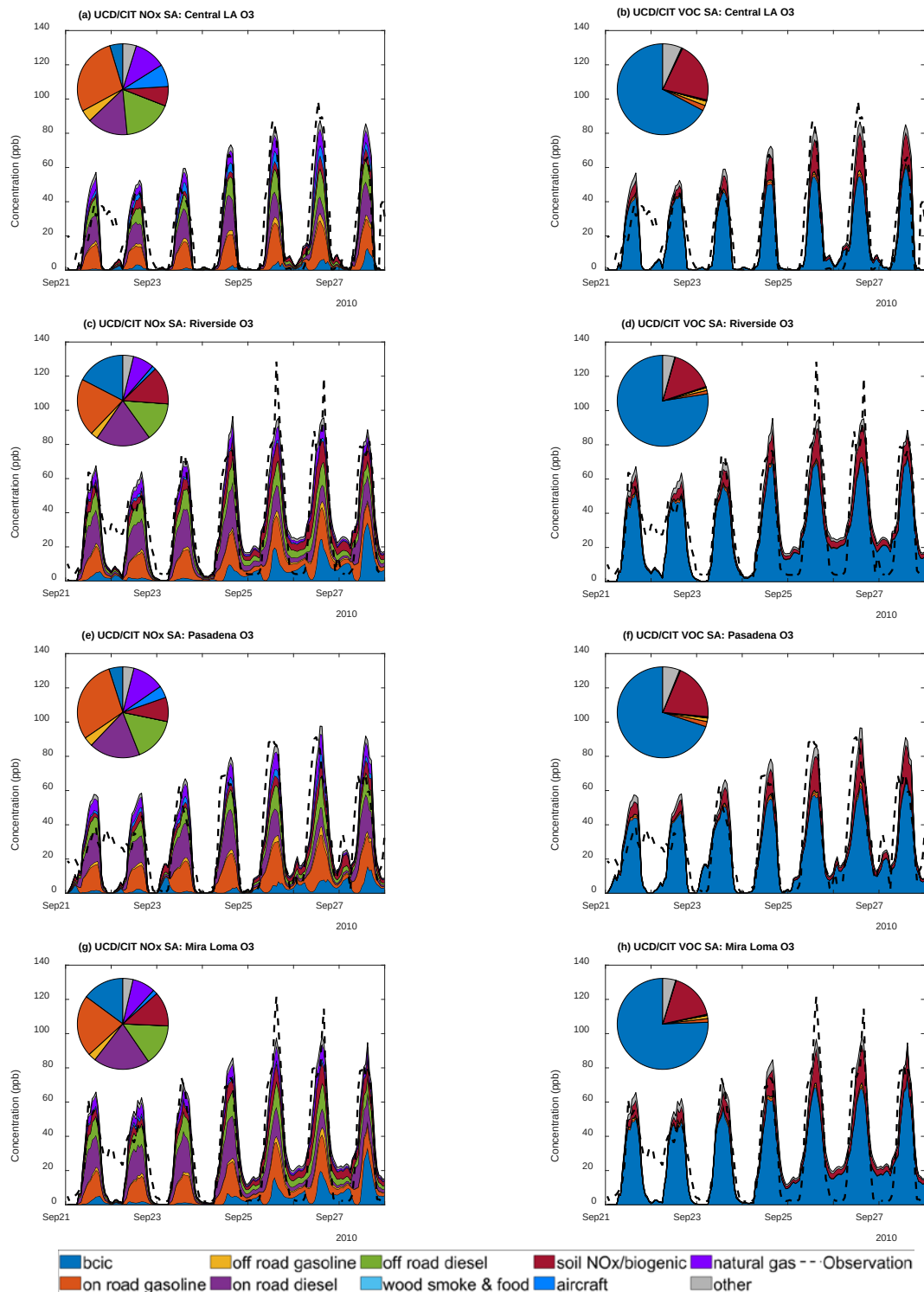


Figure 2.7: O₃ source contributions in 2010 September at central LA (a, b), Riverside (c, d), Pasadena (e, f), and Mira Loma Van Buren (g, h) at resolution of 4KM. Pie charts are based on O₃ concentrations exceeding 70 ppb. All simulations use CARB emissions.

Figure 2.7(a), (c), (e), (g) show the time-series of NO_x source apportionment results for O₃ concentrations in 2010 September at four different sites in the South Coast Air Basin (SoCAB) surrounding Los Angeles. On-road gasoline, on-road diesel, off-road diesel and soil NO_x are the dominant NO_x sources contributing to O₃ at all sites. NO_x contributions from BCICs are important in Riverside and Mira Loma, but less important in Los Angeles and Pasadena because these sites have higher emissions from anthropogenic sources. NO_x emitted from on-road gasoline, off-road diesel and on-road diesel sources account for over 50% of the O₃ formation at the monitoring sites, making NO_x from transportation the largest contributor to O₃ formation. Soil NO_x was previously identified as a major source of NO_x pollution in California (Almaraz et al., 2018). Soil NO_x accounts for 7% to 13% of the O₃ formation at the monitoring sites in the current study (see Section 4 for an in-depth analysis). NO_x contributions from additional sources, including off-road gasoline combustion, natural gas combustion, and aircraft increase peak daytime O₃ concentrations. All of the NO_x source contributions to O₃ formation follow a similar time pattern, with minimum contributions at night and maximum contributions at midday.

Figure 2.7(b), (d), (f), (h) show the VOC source contributions to O₃ concentrations in 2010 September at Los Angeles, Riverside, Pasadena, and Mira Loma. Source apportionment patterns are similar at all four sites. VOCs contained in BCICs make the largest contribution to O₃ formation, followed next by VOC emissions from biogenic sources. VOCs emitted from on-road gasoline and off-road gasoline make smaller contributions (approximated 1% each) to O₃ formation, and remaining sources are even less significant. Implications for potential under-estimates of VCP emissions on these results are discussed in Section 3.4.2 below.

Figure S2.16 shows the NO_x and VOC source contributions to O₃ concentrations in 2005 July at Los Angeles, Riverside, and Pasadena. The three sites show similar patterns. On-road gasoline, off-road gasoline, and on-road diesel are the three largest NO_x source contributors. BCICs and biogenic emissions are the main VOC source contributors. In 2015 August (Figure S2.19), the major NO_x source contributors

are on-road gasoline, on-road diesel, off-road diesel, and soil NO_x, while the major VOC source contributors are still BCICs and biogenic emissions.

Figure 2.8 illustrates the trend in NO_x and VOC source contributions to O₃ formation at Riverside in different time periods. NO_x emitted from on-road gasoline and on-road diesel engines make significant contributions to O₃ formation across all time periods. The contribution from off-road gasoline is significant in 2005, but not significant in 2010 and 2015, reflecting the large reduction in emissions from this category (Table S2.5). Relative contributions from off-road diesel and soil NO_x become more important over time as these emissions stay relatively constant while emissions from other sources are reduced. Upwind sources (BCICs) and biogenic emissions are consistently the two major VOC contributors to O₃ formation across all time periods. Off-road gasoline contributes ~ 6% to O₃ formation in 2005 but has much smaller contributions in later years due to emissions reductions in this category. All the other anthropogenic VOC sources make smaller contributions to O₃ formation in the current simulations. Implications for possible biases in VOC emissions estimates are discussed in Section 3.4.2. Similar trends for O₃ source contributions at other sites in the study domain are shown in Figure S2.20.

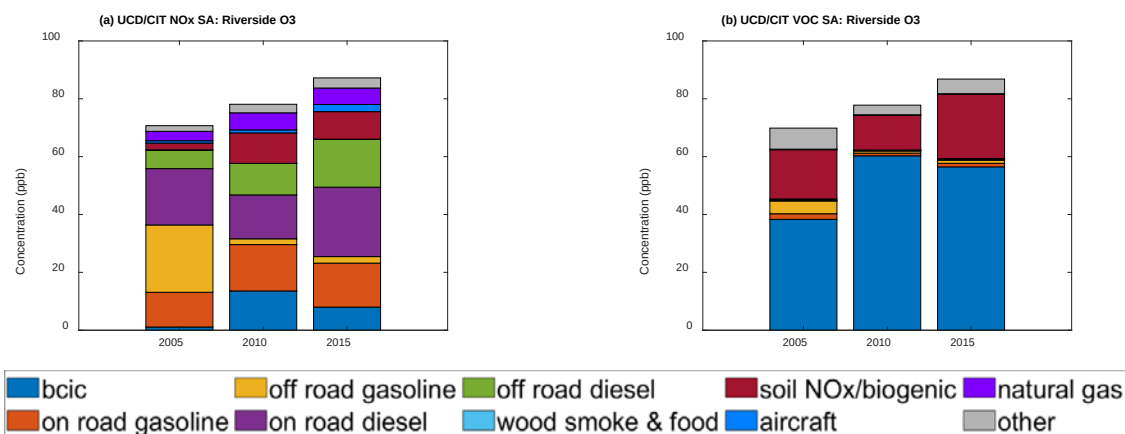


Figure 2.8: Trend of O₃ source contributions for (a)NO_x SA and (b)VOC SA at Riverside in different episodes when O₃ concentrations exceed 70 ppb.

2.3.4. Uncertainty analysis

2.3.4.1. Impact of minor formation channels

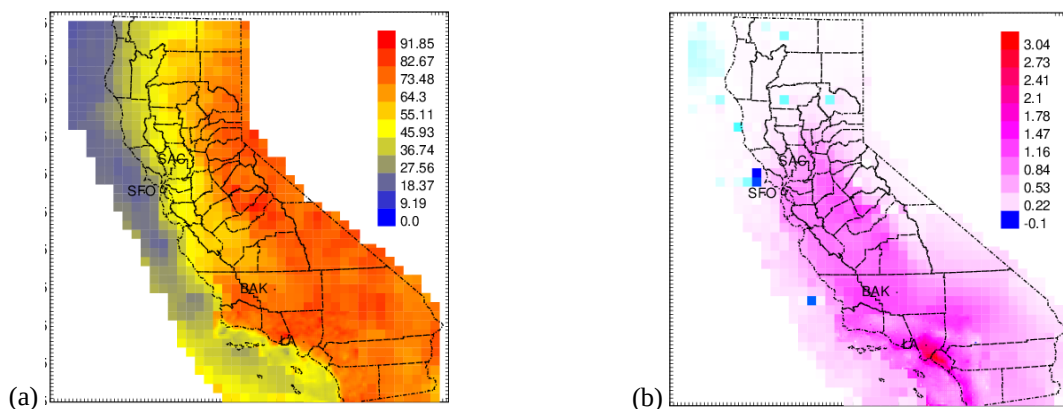


Figure 2.9: (a) field plot of original O₃ concentrations at hour 12 of sep27 2010. (b) increased O₃ concentrations when the CO emissions were increased by a factor of five. All simulations use CARB emissions.

The VOC source apportionment results shown in Figure 2.6 and Figure 2.7 indicate that upwind boundary conditions contribute strongly to O₃ formation. This may reflect upwind VOCs or it may reflect upwind O₃ and NO₂ that formed due to the influence of those upwind VOCs. CO has also been identified as an important precursor for O₃ formation under relatively low-concentration conditions (Pusede et al., 2014). This formation channel was assumed to be minor in the current study. CO was not tagged and the O₃ formed through the CO reaction channel was assigned to the untagged (i.e. ICBC) source. In order to confirm that this approximate treatment of the CO reaction pathway does not bias the source apportionment results, a separate set of calculations was performed that applied source tags to CO and all of the reaction products involved in this pathway. The predicted spatial distribution of O₃ concentrations associated with individual source types (Figure S2.9) is virtually unchanged compared to the results generated without source tagging in the CO formation channel (Figure 2.6). This finding did not change when the CO emission inventory was increased by a factor of five, suggesting that the CO formation pathway does not contribute strongly to O₃ concentrations in Los Angeles. Figure 2.9 shows the original O₃ concentrations (Figure 2.9(a)) and the O₃ concentrations when the CO emissions were increased by a factor of five (Figure 2.9(b)). The increased CO emissions only caused a maximum O₃ concentration increase of 3.04 ppb, once again confirming that this formation channel is relatively minor.

2.3.4.2. Perturbation analysis for VCP emissions

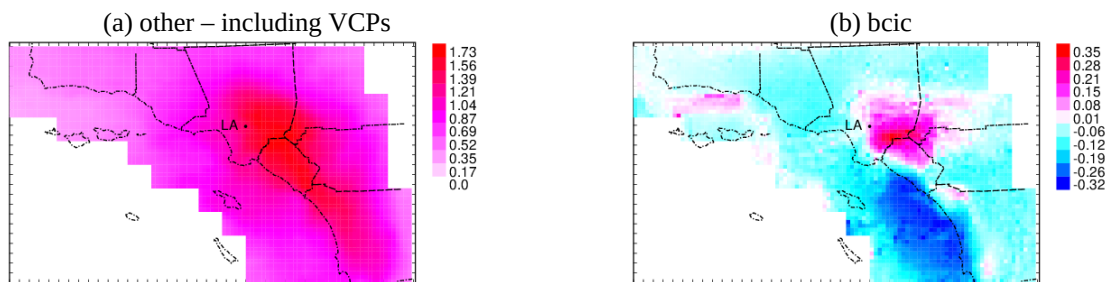


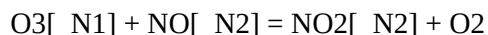
Figure 2.10: field plots of O_3 VOC source contribution differences between 3xVCP and 1xVCP by averaging hour 15 results from 10sep24 to 10sep27. All simulations use CARB emissions.

McDonald et al. (2018) measured high concentrations of volatile chemical products (VCPs) in the Los Angeles atmosphere and suggested that emissions inventories for VCPs may be under-estimated by a factor of approximately three. A perturbation analysis was carried out in the current study by tripling the VCP emissions (3xVCP) in “other” sources that contain VCPs to examine how this potential bias would influence the O_3 source apportionment results. Figure 2.10(a) shows the change in O_3 concentrations associated with source category 9 “other sources” that included contributions from VCPs caused by the adoption of the 3xVCP emissions. Figure 2.10(b) shows the change in untagged O_3 concentrations associated with boundary conditions caused by the adoption of the 3xVCP emissions. All other source contributions were approximately unchanged. Increasing VCP emissions by a factor of three increased the O_3 concentrations directly produced by VCP emissions by approximately 1.73 ppb. The increased reactivity of the atmosphere also had the indirect effects of increasing O_3 concentrations associated with BCICs by 0.35 ppb over south-east Los Angeles and decreasing O_3 concentrations associated with BCICs by approximately 0.2-0.3 ppb at other locations. All these changes are relatively minor compared to the dominance of VOC contributions to O_3 formation from biogenic sources and BCICs illustrated in Figure 2.6 above.

2.3.4.3. Impact of modified tagging mechanism

It should be noted that the source apportionment results discussed in the previous sections depend on the rules enforced in the tagging mechanism, which may be open to interpretation depending on the desired

information. For example, a perturbation analysis was conducted by modifying the following tagged reaction template in NO_x SA:



to



in order to better preserve information describing the impacts of upwind sources contributing to the local O₃ in the presence of the primary photolytic cycle. Figure 2.11 shows the modified NO_x SA result (right) compared to the original NO_x SA result (left) in Los Angeles. O₃ contribution from BCICs are greater than 75% in the modified NO_x SA result, dominating over all the other sources even though NO_x concentrations in the upwind atmosphere are relatively minor. The modified NO_x tagging mechanism effectively weights the identity of the NO_x source that contributed to O₃ formation towards the initial NO_x source instead of the most recent NO_x source. The choice of which approach provides more useful NO_x source apportionment information will depend on the preferences of the researcher conducting the analysis. Similar conclusions are reached for source contributions at other sites using the modified NO_x tagging mechanism (see Figure S2.11).

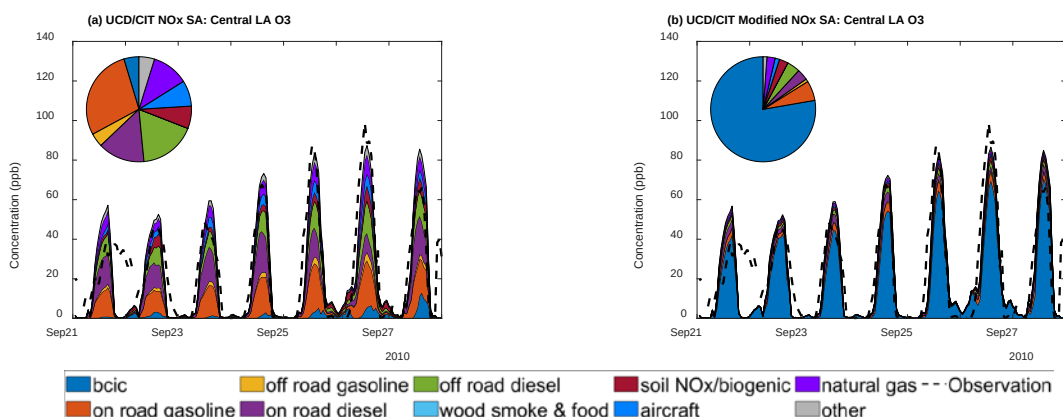


Figure 2.11: O₃ NO_x source contributions at central LA (a,b) at resolution of 4KM. Pie charts are based on O₃ concentrations exceeding 70 ppb. All simulations use CARB emissions.

2.4. Discussion

The lack of anthropogenic VOC sources that contribute to O₃ formation in the current study may reflect biases in the base emissions inventory, but tripling the VCP emissions in the CARB2010 inventory over Los Angeles to account for potential biases had limited impact on O₃ formation during the time period Sept 21-27, 2010. These results are consistent with simulations conducted by Zhu et al. (2019), who found that base-case CMAQ O₃ predictions during the CalNex study period in July 2010 were in good agreement with measurements, and increasing VCP emissions threefold had limited impact on predicted O₃ concentrations (approximately +3ppb averaged over the SoCAB). Predicted O₃ concentrations did increase (+15 ppb for peak maximum 8-hr O₃ concentrations) when all anthropogenic VOC emissions were scaled upwards, but the resulting concentrations were significantly higher than measured O₃ concentrations, emphasizing the unrealistic nature of this scenario.

The O₃ source apportionment results predicted by the UCD/CIT model and the CMAQ-ISAM model are in good agreement, but the insight gained from the UCD/CIT calculations about the lack of controllable VOC sources within the study domain is helpful when designing practical emissions control programs. The FNR plots show that the Los Angeles area is VOC-limited during each of the three O₃ episodes considered in the present study. Conventional approaches dictate that reducing VOC emissions will provide the most efficient path to control O₃, but the detailed results from the current analysis show that most of the VOCs contributing to O₃ formation over Los Angeles across all time periods originated from upwind boundary conditions outside of the study domain or biogenic emissions within the study domain. Anthropogenic VOC emissions contributed very little to O₃ formation, indicating that reducing anthropogenic VOC emissions might not be an effective O₃ control strategy. In contrast, most of the NO_x that contributed to O₃ formation was emitted from anthropogenic sources. Controlling NO_x emissions may therefore be the only practical strategy to control O₃ concentrations in the region even though the O₃ formation is VOC limited. Chamber experiments conducted by Wu et al. (2022) in Sacramento between April 2020 and December 2020 also found significant biogenic contributions to O₃ formation in the

summer. These measurements also suggest that the most practical strategy to control extreme O₃ concentrations over most of California is to reduce NO_x emissions until the atmospheric chemical regime becomes NO_x-limited.

It should be noted that the NO_x source contributions to O₃ concentrations in the VOC-limited regime are not a literal prediction of the amount of O₃ reduction that would be expected per unit of NO_x reduction.

The non-linear nature of the photochemical reaction system may even cause O₃ concentrations to increase when NO_x emissions from a prevalent source are slightly reduced when conditions are VOC-limited.

Two brute force tests were conducted by zeroing out either soil NO_x or biogenic emissions. The effects of the brute force are compared with the source contribution from soil NO_x in NO_x SA and biogenic emissions in VOC SA, respectively (Figure 2.12 and Figure S2.21). Figure 2.12 shows that in Central LA, and Riverside, when soil NO_x emissions are zeroed out, O₃ concentrations can either decrease or increase depending on the final chemical regime. In contrast, O₃ concentration reductions due to zeroing out the biogenic emissions are proportional to the VOC source contributions by biogenic emissions. Plots for Pasadena and Mira Loma Van Buren are shown as Figure S2.21. For the best interpretation of the SA results, both NO_x and VOC SA results should be reviewed together with the chemical regime for further control strategy analysis. Overall, the NO_x source apportionment results provide useful information about which NO_x sources should be targeted in order to achieve major emissions reductions that would shift the chemical regime to NO_x-limited conditions. Once the chemistry has become NO_x-limited, the NO_x source contributions to O₃ concentrations will be more proportional to the expected O₃ response to NO_x emissions reductions.

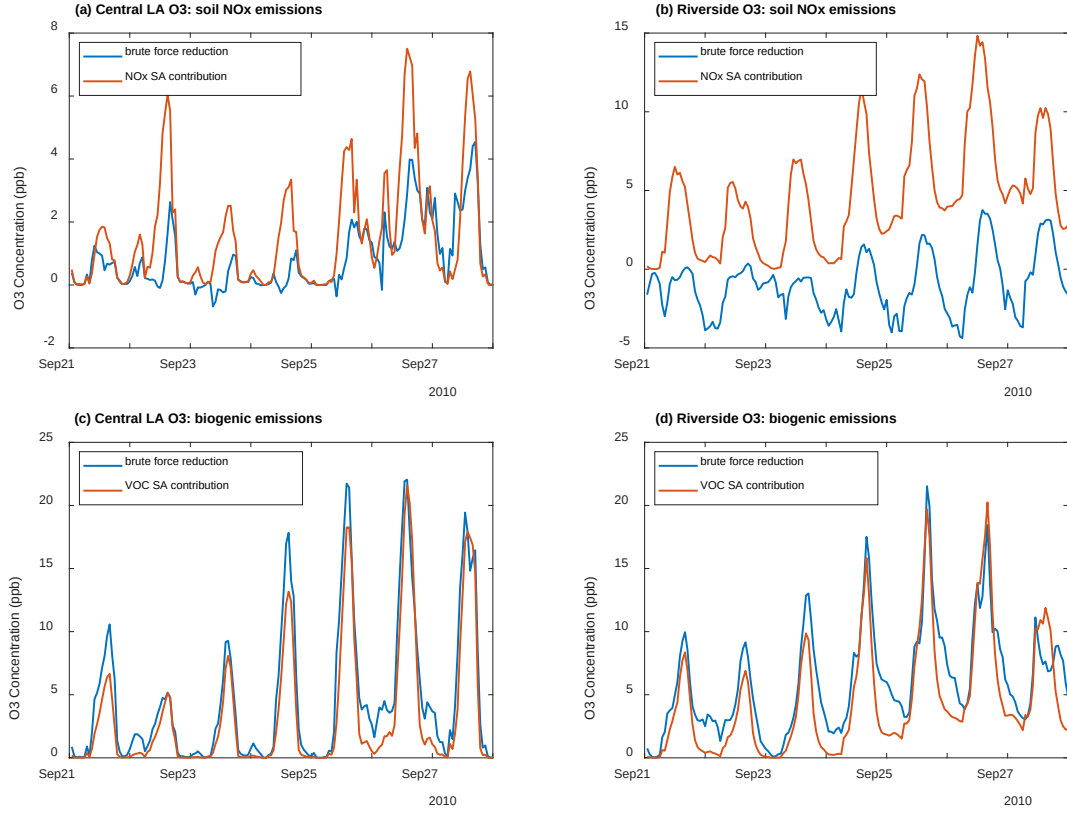


Figure 2.12: Comparison of (a, b) the O₃ reductions due to zeroing out soil NO_x and the O₃ contribution from soil NO_x in the NO_x SA results; (c,d) the O₃ reductions due to zeroing out biogenic emissions and the O₃ contribution from biogenic in the VOC SA results. Spatial resolution for all simulations is 4km.

2.5. Implications

A new O₃ source apportionment method has been developed to separately resolve NO_x source contributions and VOC source contributions to O₃ formation within the framework of a chemical transport model (CTM). The new method explicitly tags all molecules that carry odd oxygen within the chemical mechanism rather than making simplifying approximations that follow only a subset of tagged species. Explicitly tracking source-oriented species through the advection calculation required the development of a new Forester filter algorithm to reduce the computational noise induced by sharp wave fronts associated with individual sources. A new algorithm was also developed to efficiently represent reactions involving molecules that contain more than one source of odd oxygen within the source apportionment calculations.

The new source apportionment method was demonstrated using the SAPRC11 chemical mechanism within the UCD/CIT CTM applied to the peak O₃ episodes that occurred in Los Angeles during the years 2005, 2010, and 2015. Total O₃ concentrations and combined NO_x+VOC source contributions predicted by the new technique were consistent with results predicted by the CMAQ-ISAM results, but new insights were provided by separately resolving NO_x source contributions and VOC source contributions. The three case studies in 2005, 2010, and 2015 over Los Angeles suggest that most of the VOC emissions that contributed to O₃ formation were not controllable, indicating that NO_x emissions controls provided the best approach to reducing O₃ concentrations as recently as the year 2015 even though Los Angeles was in the VOC-limited O₃ formation regime. Gasoline-powered vehicles, diesel-powered engines, soil NO_x and natural gas combustion are identified as major sources that emit NO_x that contribute to O₃ formation. Missing sources of Volatile Chemical Products (VCPs) may influence the results of this case study, but the overall results of the new source apportionment algorithm are shown to be accurate subject to the uncertainties in the emissions inventory used to support the calculations. This new O₃ source apportionment technique should be useful for current and future simulations that seek to design effective emissions control programs.

2.6. Appendix

Table S2.1: Comparison of UCD/CIT and CMAQ model inputs.

	UCD/CIT	CMAQ
Meteorology	WRFv3.4	WRFv3.4
Initial condition	MOZART	MOZART
Boundary condition	MOZART	MOZART
Anthropogenic emissions	SMOKEv3.7	SMOKEv3.7
Biogenic emissions	MEGANv2.1	MEGANv2.1
Gas-phase chemical mechanism	SAPRC11	SAPRC07
Aerosol-phase chemical mechanism	ISSOROPIA for inorganics and n-product model for SOA	AERO7

Table S2.2: Statistics of comparison of SA runs without simplified (NoSimp) and simplified (Simp) NO_x SA with NonSA runs for predicted NonSA concentrations over 40 ppb in September 2010.

		Mean Bias (ppb)	Mean Error (ppb)	MFB (%)	MFE (%)	RMSE (ppb)
Sep21	NoSimp-NonSA	0.0649	0.0651	0.1602	0.1602	0.0807
	Simp- NonSA	0.0626	0.0634	0.1568	0.1572	0.0818
Sep22	NoSimp- NonSA	0.0589	0.0595	0.1380	0.1388	0.0732
	Simp- NonSA	0.0595	0.0599	0.1396	0.1399	0.0744
Sep23	NoSimp- NonSA	0.0724	0.0743	0.1606	0.1613	0.0928
	Simp- NonSA	0.0728	0.0749	0.1626	0.1635	0.0939
Sep24	NoSimp- NonSA	0.1109	0.1112	0.2287	0.2291	0.1320
	Simp- NonSA	0.1102	0.1105	0.2230	0.2237	0.1334
Sep25	NoSimp- NonSA	0.1085	0.1091	0.2131	0.2142	0.1459
	Simp- NonSA	0.1051	0.1054	0.2060	0.2066	0.1401
Sep26	NoSimp- NonSA	0.1473	0.1479	0.2418	0.2425	0.1737
	Simp- NonSA	0.1460	0.1477	0.2382	0.2410	0.1714
Sep27	NoSimp- NonSA	0.1042	0.1069	0.1865	0.1934	0.1402
	Simp- NonSA	0.0990	0.1010	0.1819	0.1865	0.1344

Table S2.3: Statistics of comparison of SA runs without simplified (NoSimp) and simplified (Simp) VOC SA with NonSA runs for predicted NonSA concentrations over 40 ppb in September 2010.

		Mean Bias (ppb)	Mean Error (ppb)	MFB (%)	MFE (%)	RMSE (ppb)
Sep21	NoSimp- NonSA	0.0055	0.0436	-0.0116	0.1027	0.0574
	Simp- NonSA	0.0196	0.0215	0.0455	0.0473	0.0290
Sep22	NoSimp- NonSA	-0.0026	0.0318	-0.0091	0.0732	0.0428
	Simp- NonSA	0.0182	0.0203	0.0420	0.0451	0.0266
Sep23	NoSimp- NonSA	-0.0040	0.0389	-0.0154	0.0802	0.0482
	Simp- NonSA	0.0170	0.0227	0.0382	0.0420	0.0311
Sep24	NoSimp- NonSA	0.0013	0.0602	-0.0044	0.1195	0.0808
	Simp- NonSA	0.0274	0.0299	0.0557	0.0584	0.0399
Sep25	NoSimp- NonSA	-0.0230	0.0774	-0.0372	0.1401	0.0986
	Simp- NonSA	0.0304	0.0340	0.0577	0.0644	0.0467
Sep26	NoSimp- NonSA	-0.0809	0.1139	-0.1545	0.1966	0.1364
	Simp- NonSA	0.0461	0.0513	0.0756	0.0813	0.0708
Sep27	NoSimp- NonSA	-0.0781	0.1211	-0.1558	0.2278	0.1543
	Simp- NonSA	0.0375	0.0411	0.0663	0.0734	0.0554

Table S2.4: Model performance statistics for 1-hour O₃ in four measurement sites in (a) CMAQ and UCD/CIT evaluation runs; (b) UCD/CIT source apportionment runs.

			NMB	NME	r
(a) 12KM runs using NEI2011 in September 2010	Central LA	CMAQ	0.0289	0.3214	0.6001
		UCD/CIT	0.0840	0.2192	0.8072
	Riverside	CMAQ	-0.0681	0.2472	0.7890
		UCD/CIT	-0.0571	0.1577	0.8675
	Pasadena	CMAQ	0.0462	0.2196	0.7410
		UCD/CIT	0.00006	0.1371	0.8454
	Mira Loma Van Buren	CMAQ	-0.0036	0.2834	0.8104
		UCD/CIT	-0.0287	0.1682	0.8801
(b) 4KM UCD/CIT SA runs using CARB emission inventory in September 2010	Central LA	NOx SA	0.0388	0.1785	0.7061
		VOC SA	0.0369	0.1774	0.7086
	Riverside	NOx SA	-0.0326	0.1423	0.7391
		VOC SA	-0.0347	0.1420	0.7408
	Pasadena	NOx SA	0.0109	0.1570	0.6948
		VOC SA	0.0091	0.1567	0.6959
	Mira Loma Van Buren	NOx SA	-0.0073	0.1428	0.7695
		VOC SA	-0.0096	0.1420	0.7712
(c) 4KM UCD/CIT SA runs using CARB emission inventory in July 2005	Central LA	NOx SA	0.0237	0.2259	0.8636
		VOC SA	0.0151	0.2256	0.8629
	Riverside	NOx SA	-0.2147	0.2847	0.9067
		VOC SA	-0.2236	0.2875	0.9068
	Pasadena	NOx SA	-0.1357	0.2794	0.8777
		VOC SA	-0.1484	0.2850	0.8761
(d) 4KM UCD/CIT SA runs using CARB emission inventory in August 2015	Central LA	NOx SA	0.1706	0.2933	0.8065
		VOC SA	0.1669	0.2909	0.8066
	Riverside	NOx SA	0.1305	0.1989	0.9223
		VOC SA	0.1266	0.1957	0.9221
	Pasadena	NOx SA	0.1998	0.3380	0.8275
		VOC SA	0.1951	0.3343	0.8272
	Mira Loma Van Buren	NOx SA	0.1169	0.2186	0.8971
		VOC SA	0.1128	0.2156	0.8968

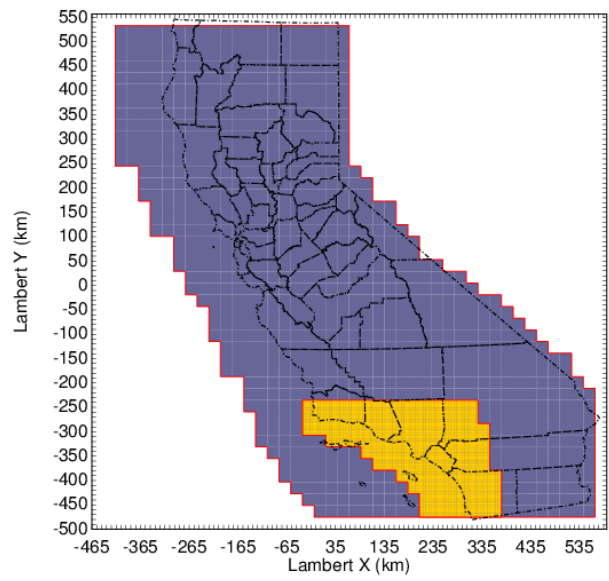
For model performance of 1-hour O₃, “Goals” are NMB<±5%, NME<15%, r>0.75, which should be viewed as the best a model can be expected to achieve. “Criteria” are NMB<±15%, NME<25%, r>0.50, which should be viewed as what a majority of models have achieved. The cutoff for NMB and NME are 40-ppb, while no cutoff for r (Emery et al., 2017).

Table S2.5: Summary of domain-wide emissions for a Wednesday in the different simulations.

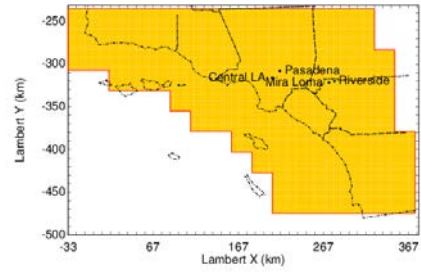
Source	NOx (kmol/day)			NMVOC (kmol/day)		
	2005	2010	2015	2005	2010	2015
on-road gasoline	13370	8249	4876	6354	3377	2051
off-road gasoline	23843	772	664	12511	1880	1933
on-road diesel	22769	12263	9795	802	680	620
off-road diesel	11320	11286	8879	2541	1224	975
wood smoke & food	198	32	27	2313	611	639
soil NOx /biogenic VOC	36240	42090	39997	281983	52514	194038
aircraft	1005	1055	1078	570	588	595
natural gas	3946	3298	2633	755	701	559
other	3967	5190	2500	44745	30839	16015
Total	116658	84235	70449	352574	92414	217425

Note: the biogenic VOC emissions on 9/22/2010 has less biogenic emissions than the summer months due to the cooler temperature.

Figure S2.1: Map of model domains and the locations of the four measurement sites



domain 1



domain 2

Figure S2.2: Ozone contribution by sources for hr12 on sep27. Sources with _NS suffix are results without simplified NOx SA. Sources with _S suffix are results with simplified NOx SA.

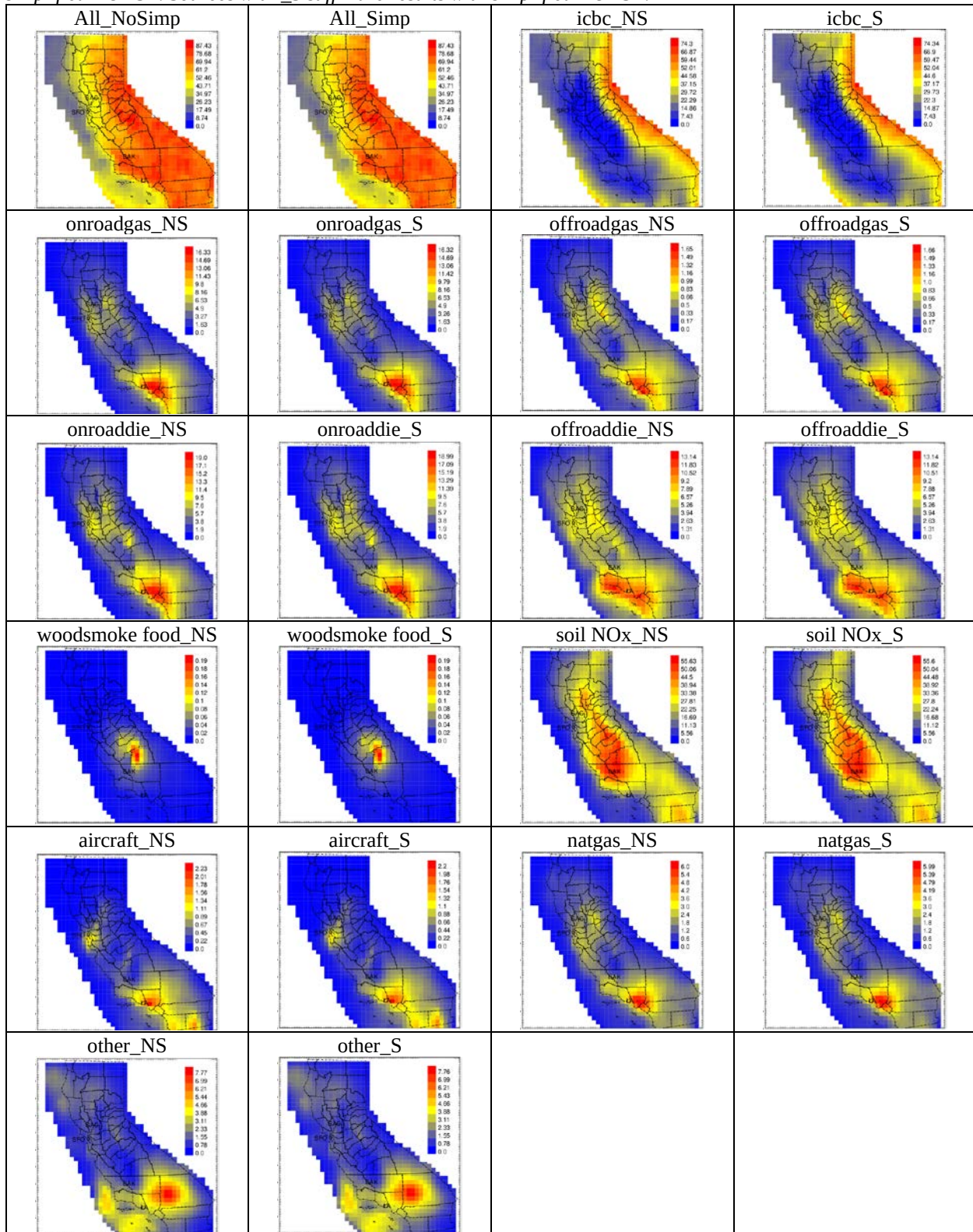


Figure S2.3: Ozone contribution by sources for hr12 on sep27. Sources with _NS suffix are results without simplified VOC SA. Sources with _S suffix are results with simplified VOC SA.

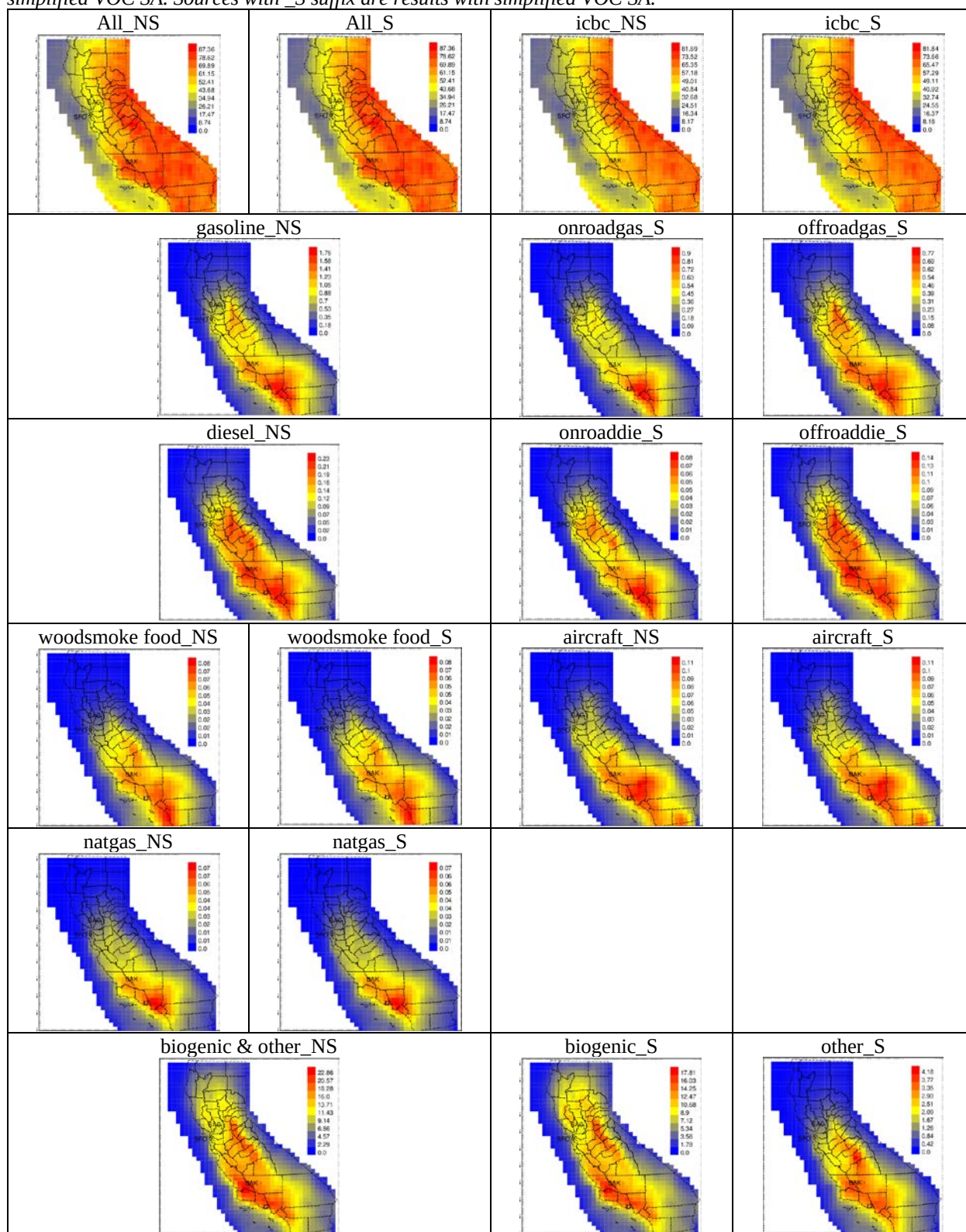


Figure S2.4: Ozone concentration of model results for UCD/CIT and CMAQ at four different sites.

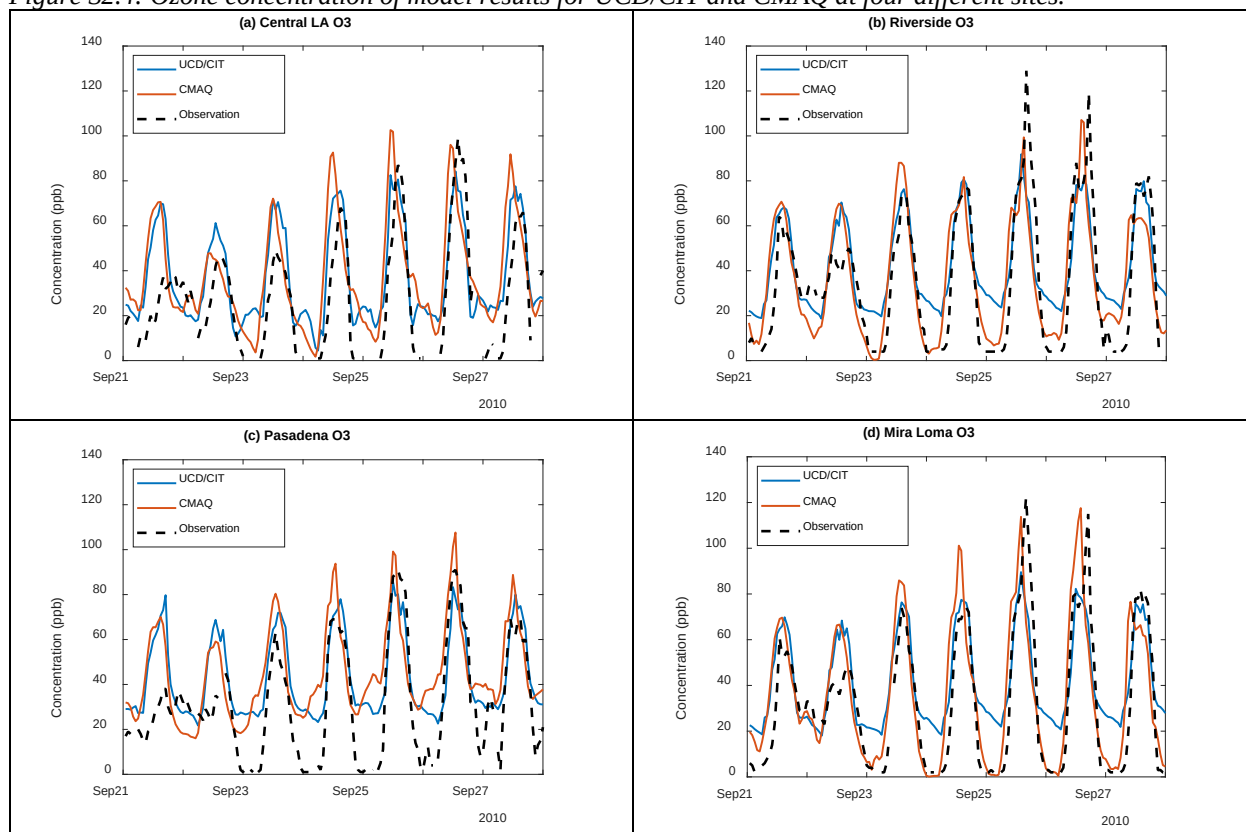


Figure S2.5: Time series plot of NO source contributions at different sites

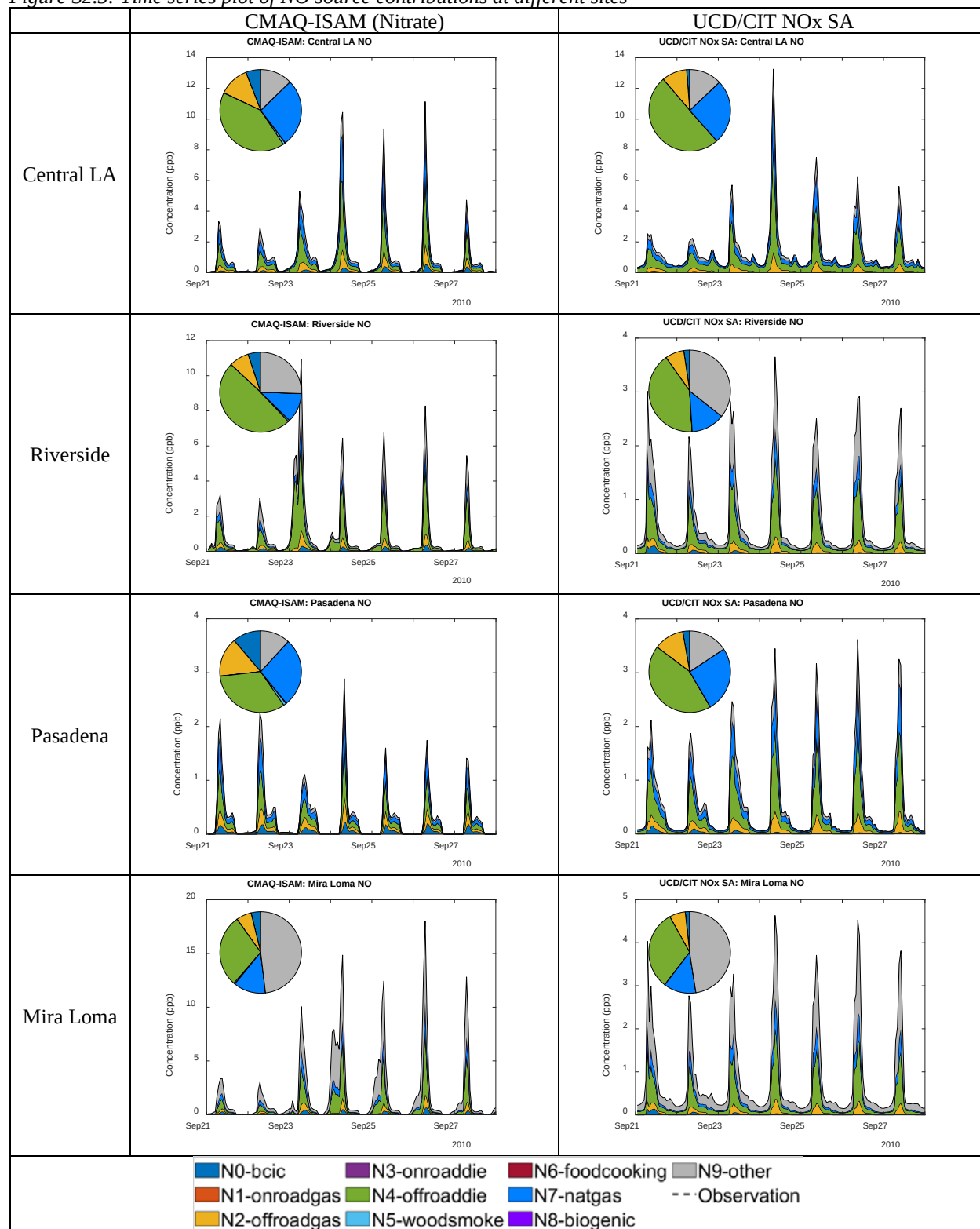


Figure S2.6: Time series plot of NO₂ source contributions at different sites

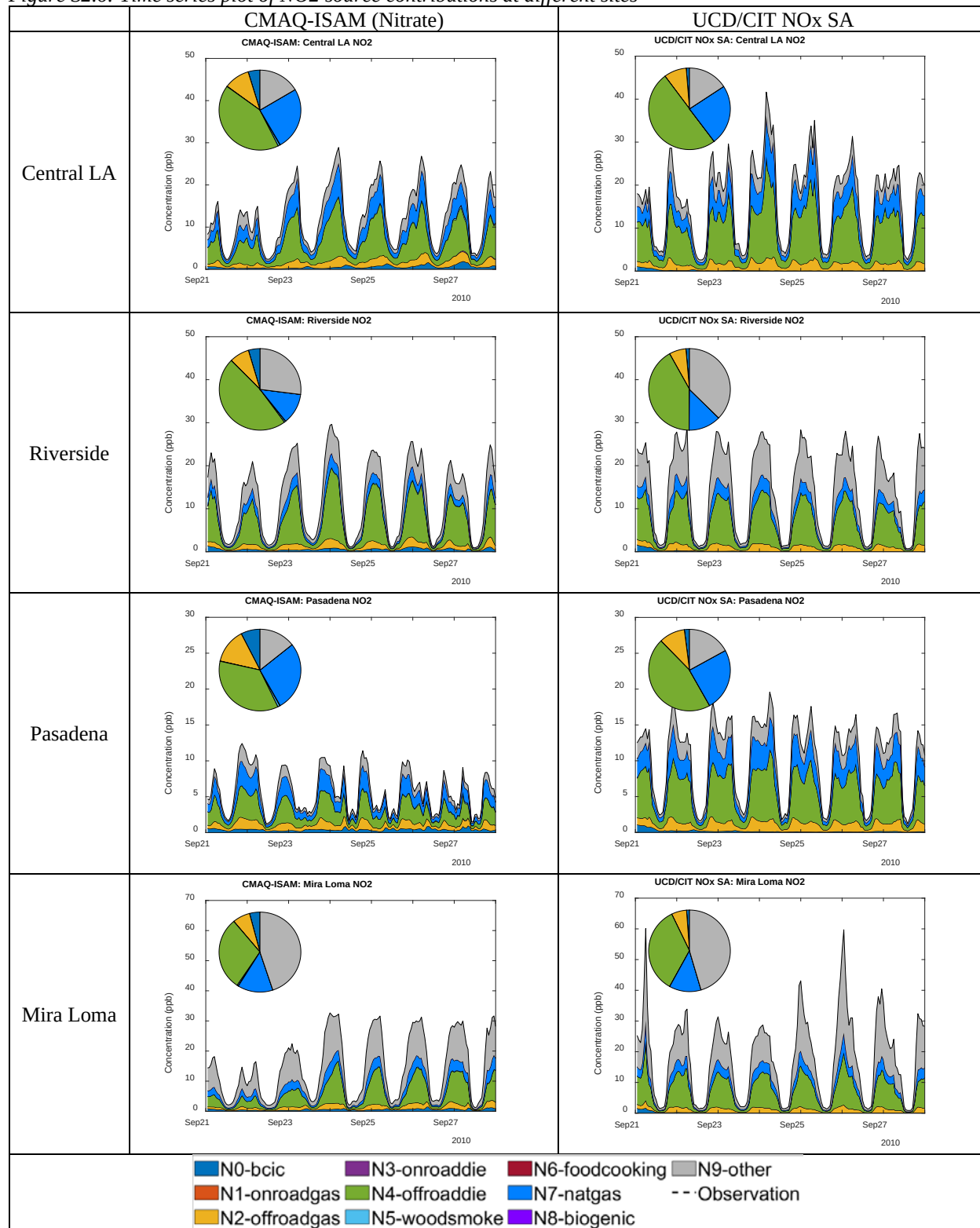


Figure S2.7: Time series plot of HCHO source contributions at different sites

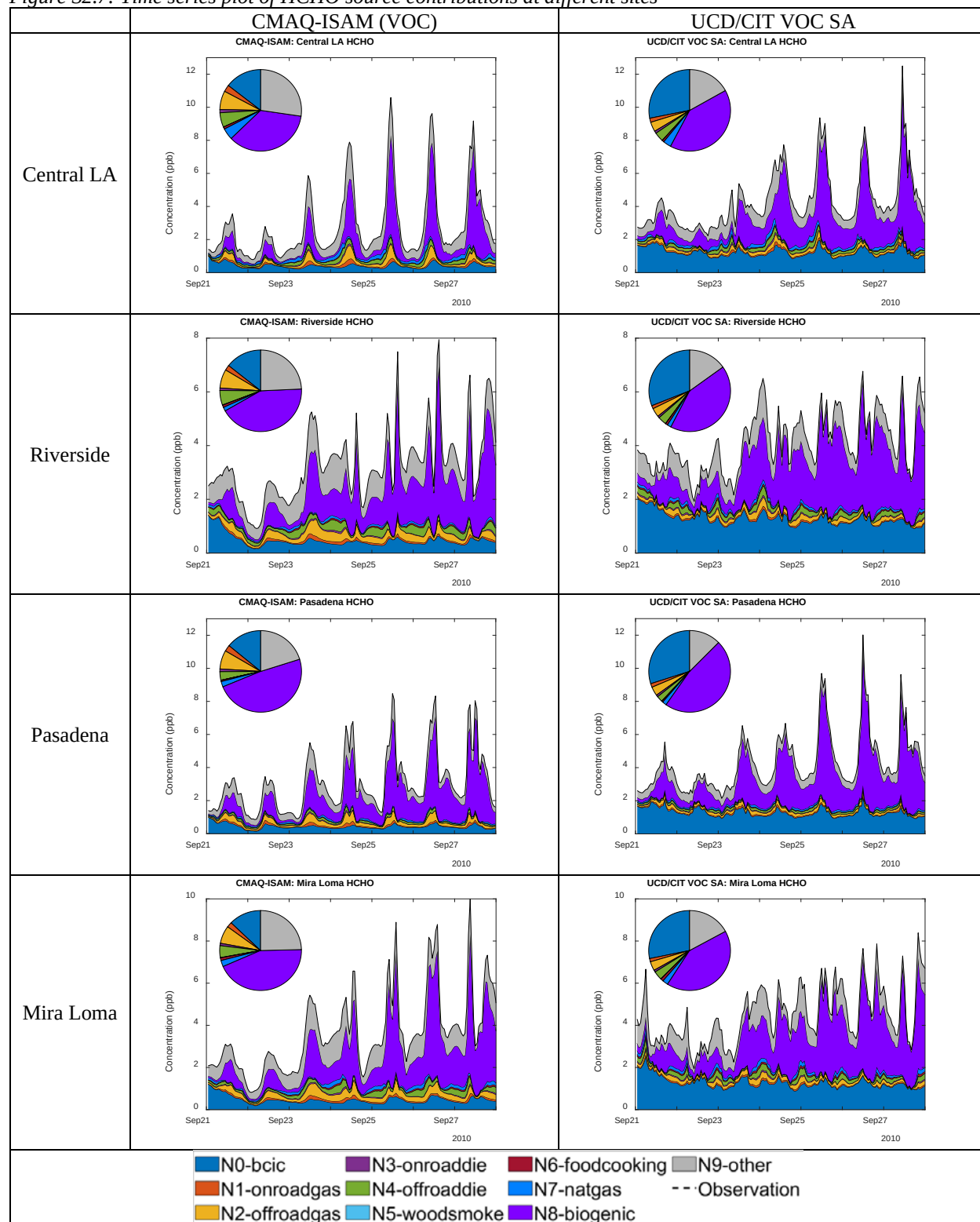
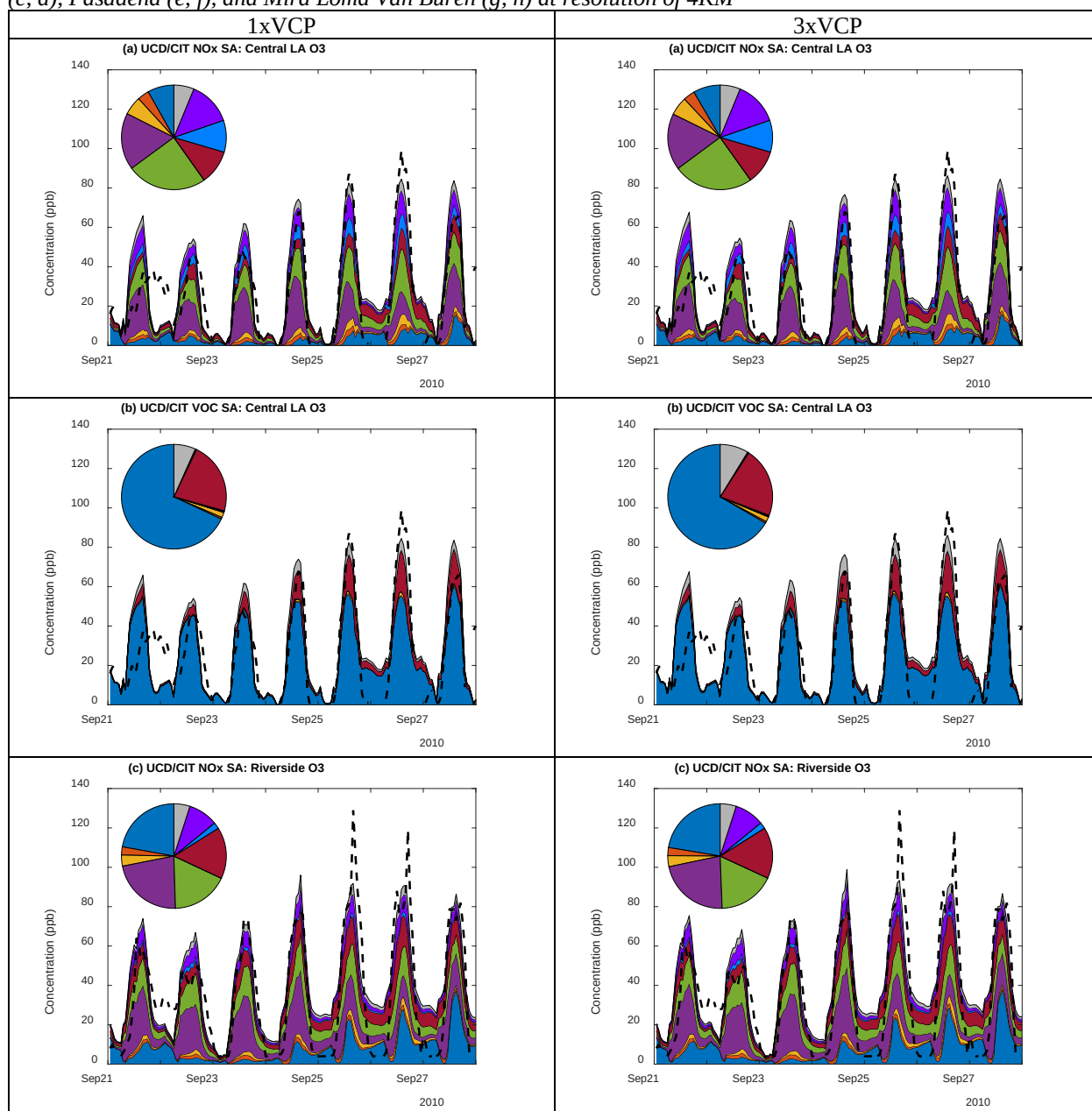
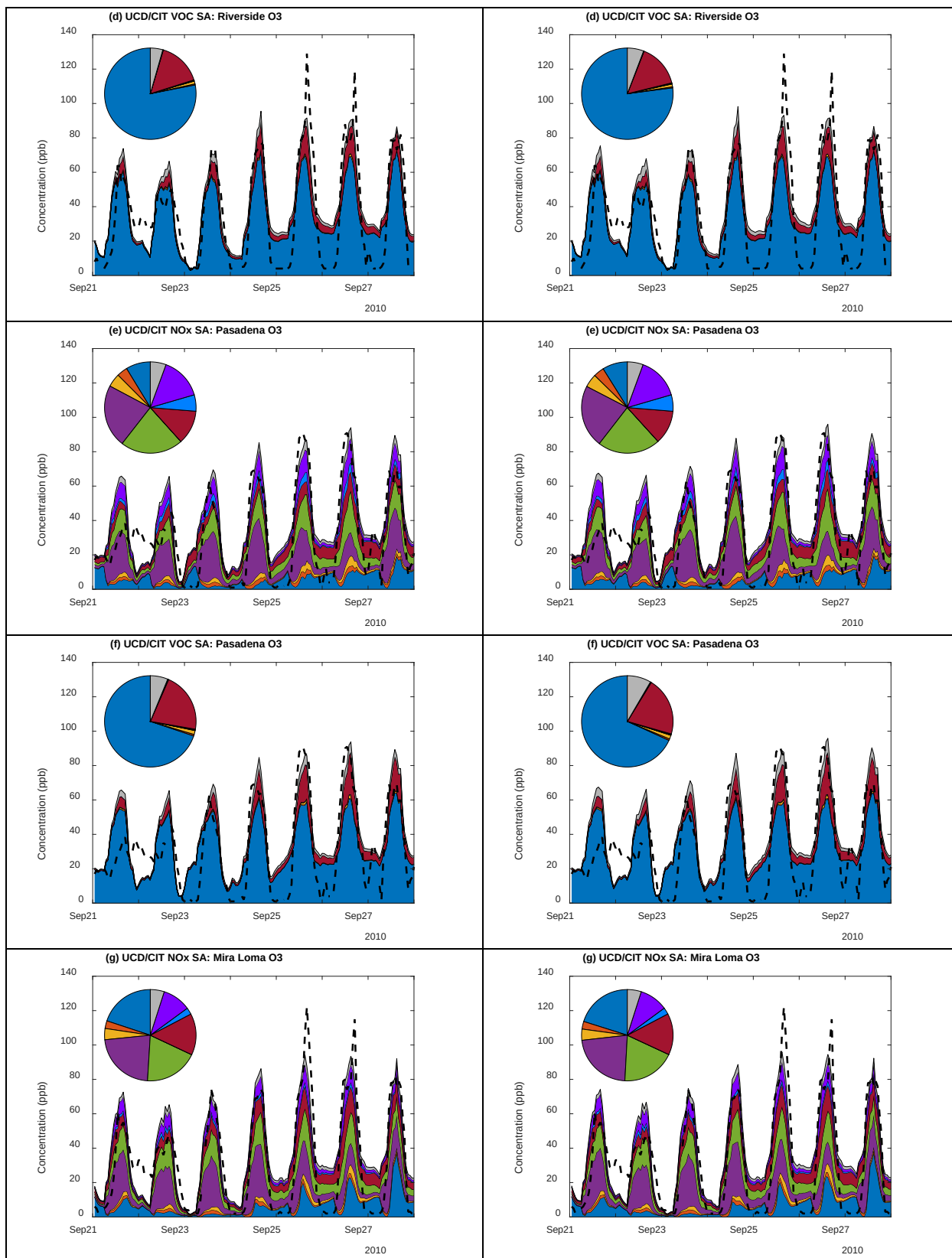


Figure S2.8: Time series plot of O3 source contributions with 3 times VCP emissions at central LA (a, b), Riverside (c, d), Pasadena (e, f), and Mira Loma Van Buren (g, h) at resolution of 4KM





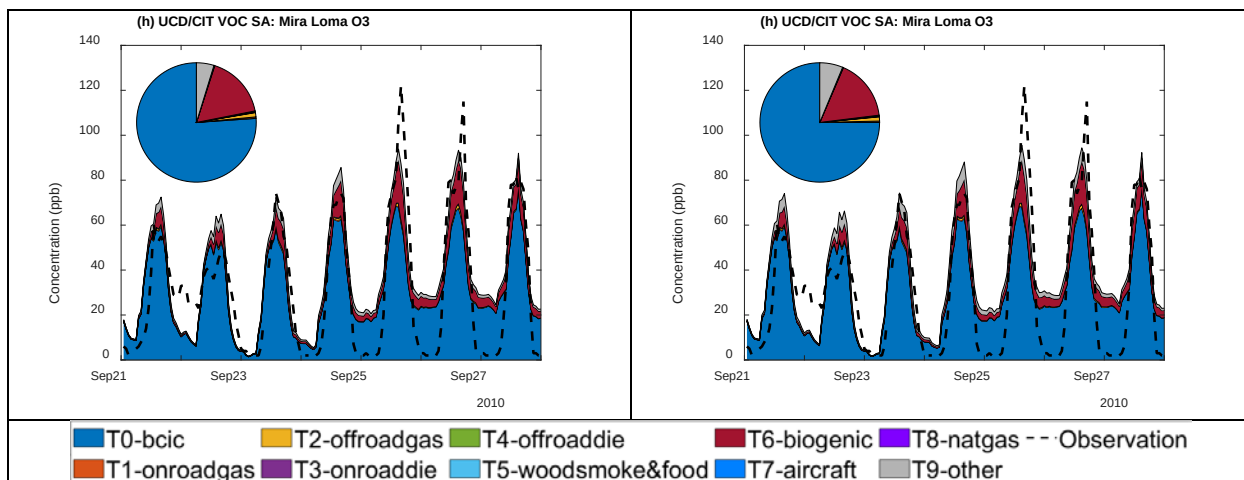


Figure S2.9: O_3 from different sources predicted by VOC source apportionment with CO tagged at hour 12, Sep 27, 2010

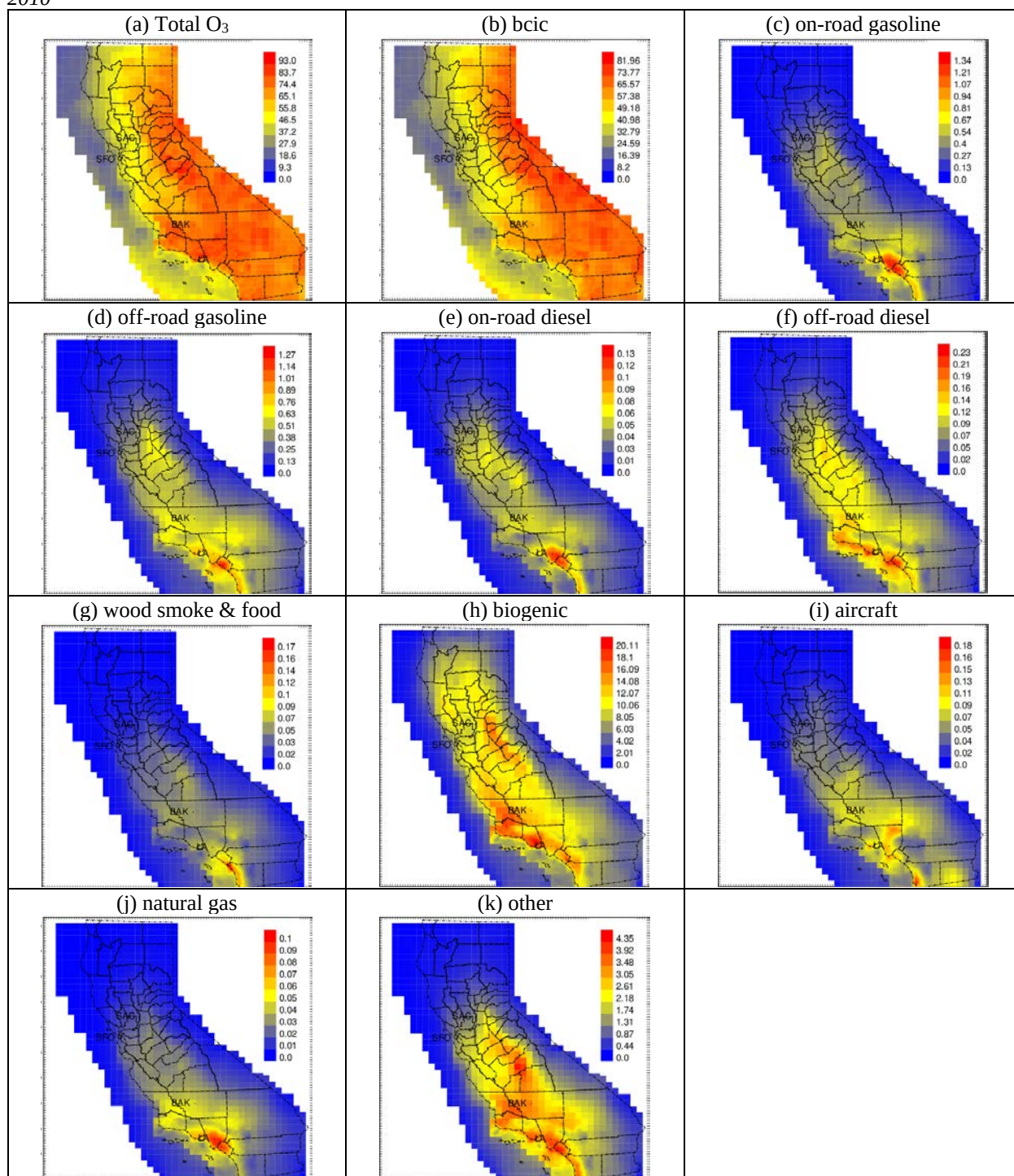
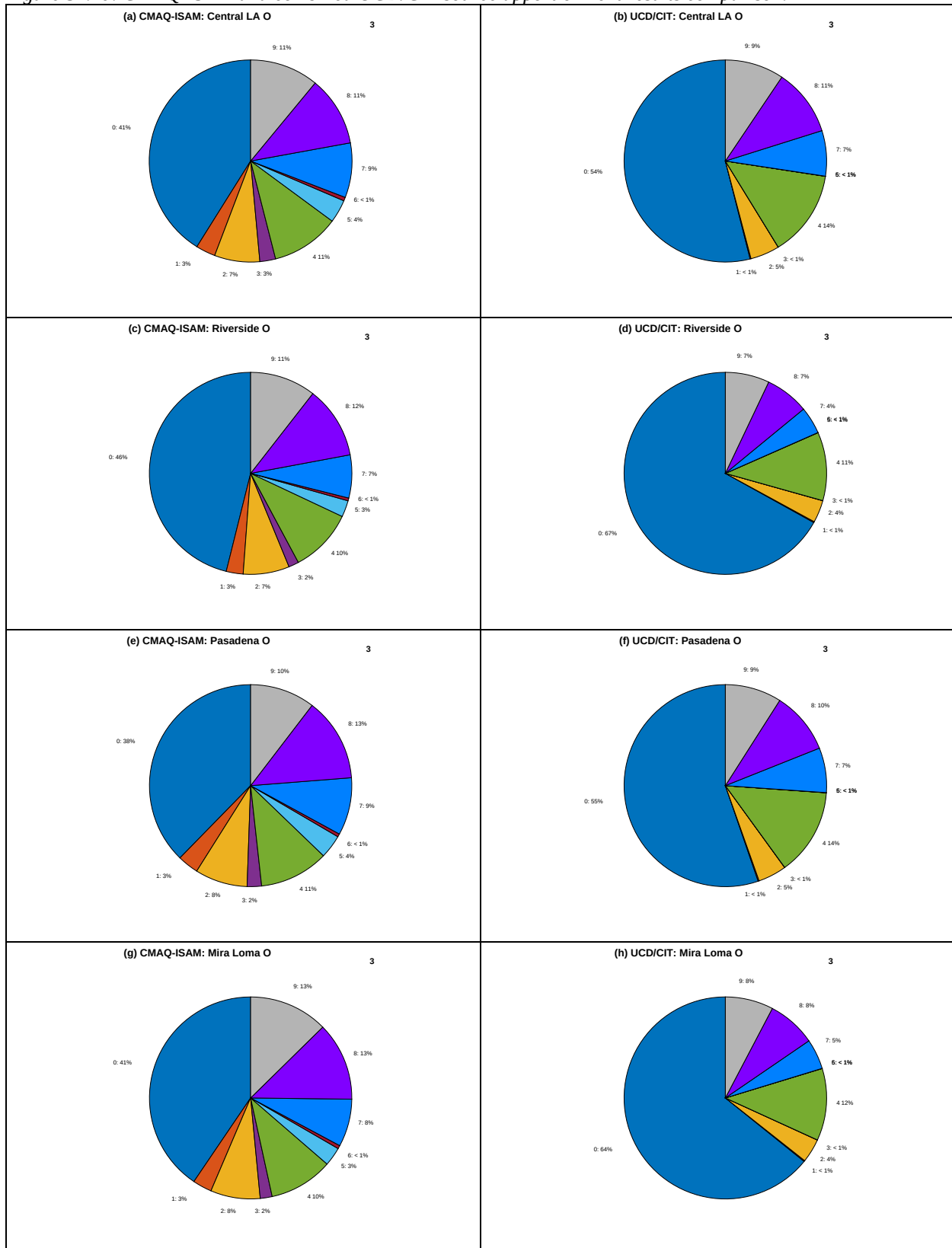


Figure S2.10: CMAQ-ISAM and combined UCD/CIT source apportionment results comparison.



UCD/CIT NO_x SA and VOC SA results are combined by averaging the contributions of each emission sector from both runs. The rankings of the emission contributions from different sectors are almost the same at each site for both CMAQ-ISAM results and UCD/CIT combined results.

Figure S2.11: O_3 NO_x source contributions at central LA (a,b), Riverside (c,d), Pasadena (e,f), and Mira Loma Van Buren (g,h) at resolution of 4KM. Left column is for the original tagging mechanism, and the right column is for the modified tagging mechanism. Pie charts are based on O_3 concentrations exceeding 70 ppb. All simulations use CARB emissions.

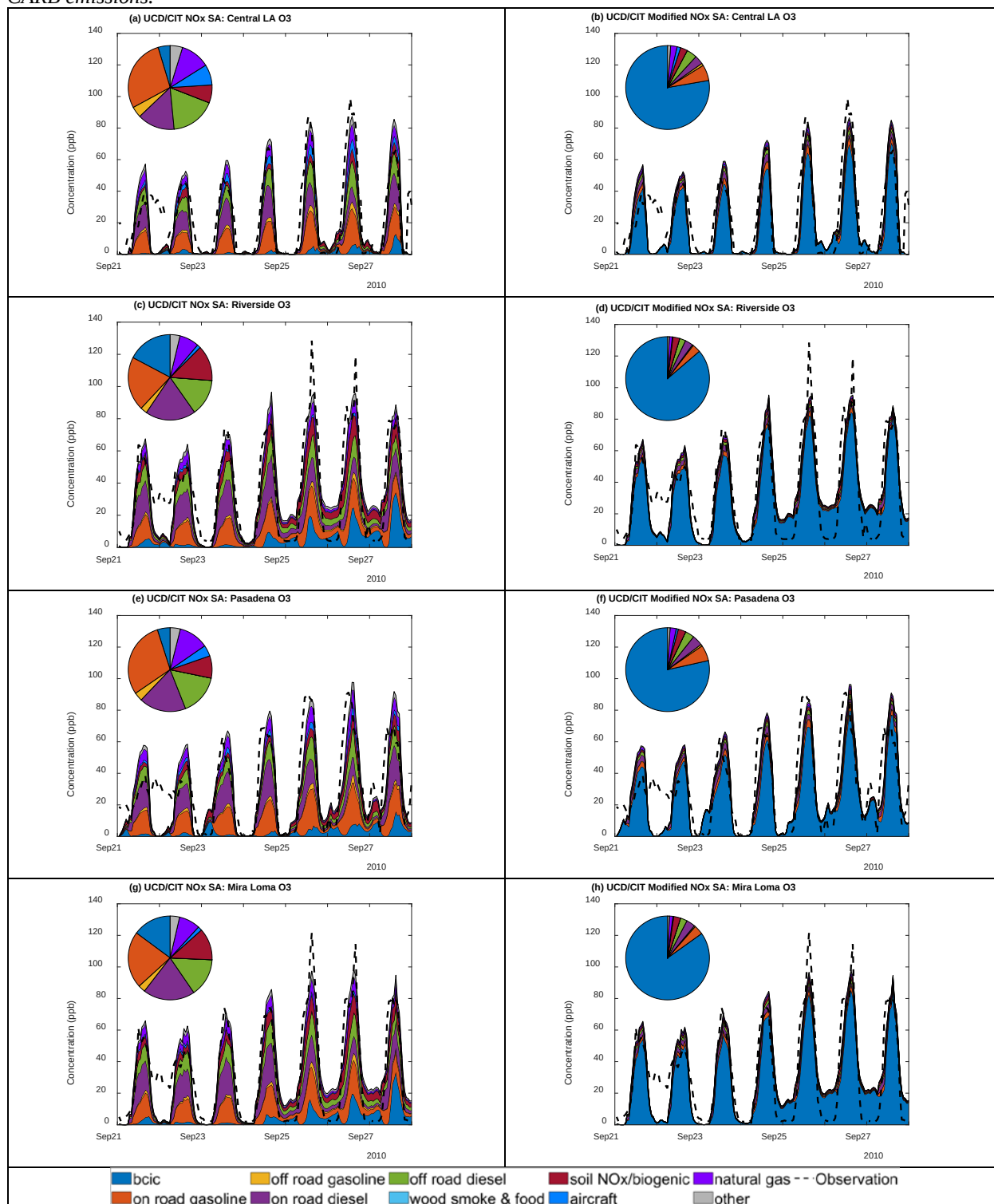


Figure S2.12: Time series plots of predicted and measured O_3 concentrations in 2005 July at (a)central LA, (b)Riverside, and (c)Pasadena at resolution of 24KM and 4KM. All simulations use CARB emissions.

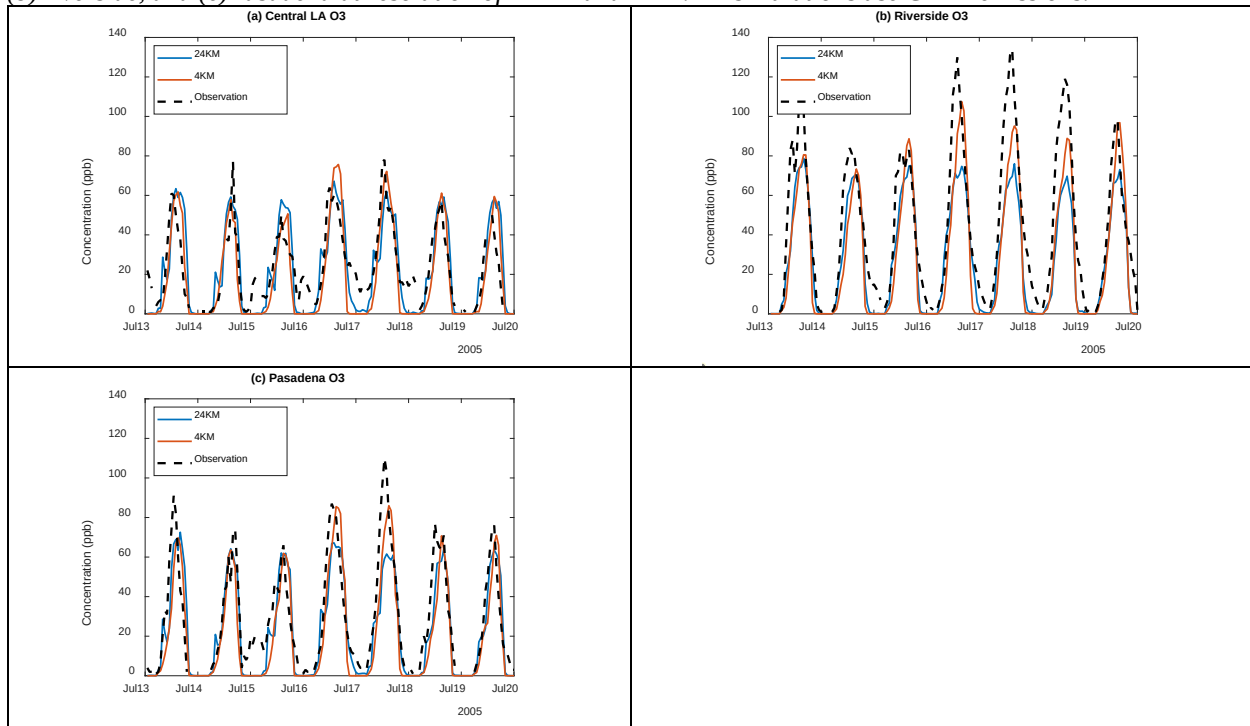


Figure S2.13: Time series plots of predicted and measured O_3 concentrations in 2015 August at (a)central LA, (b)Riverside, (c)Pasadena, and (d)Mira Loma Van Buren at resolution of 24KM and 4KM. All simulations use CARB emissions.

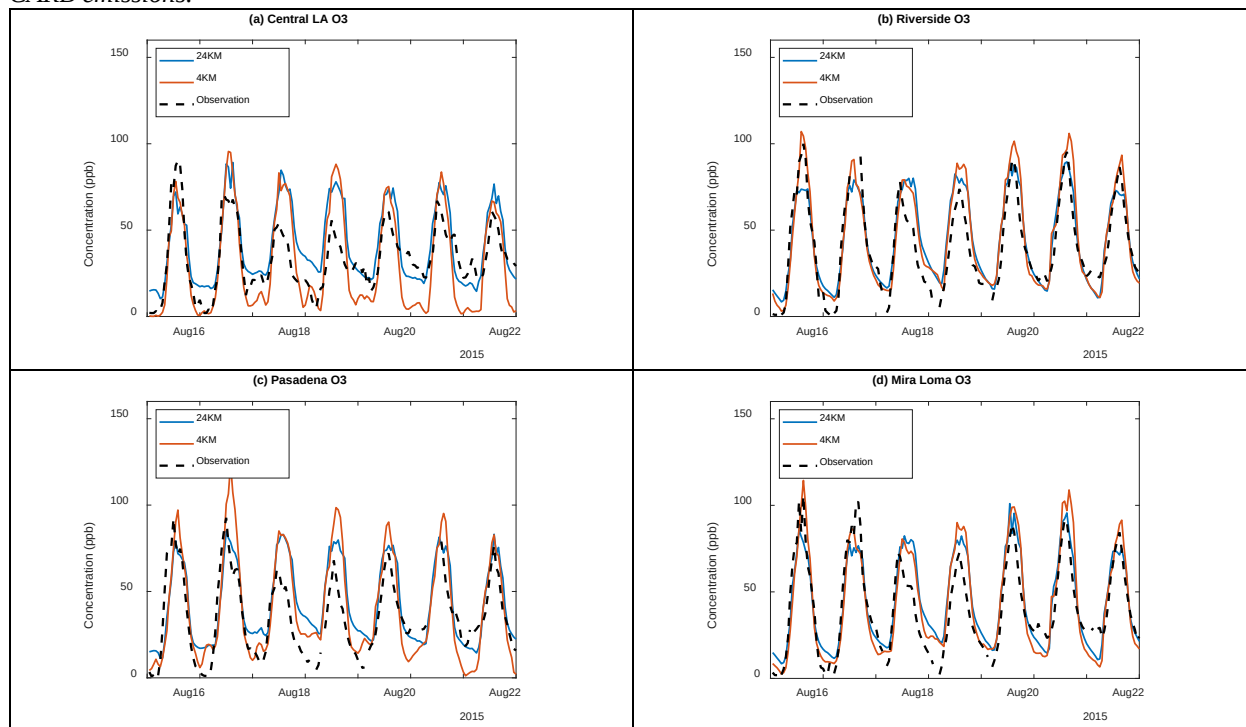


Figure S2.14: (a-k) Predicted NO_x source contributions to O₃ concentrations (ppb) and (l) FNR minus 4.6 at hour 12, Jul 19, 2005. All simulations use CARB emissions. Noting that each plot has different maximum values.

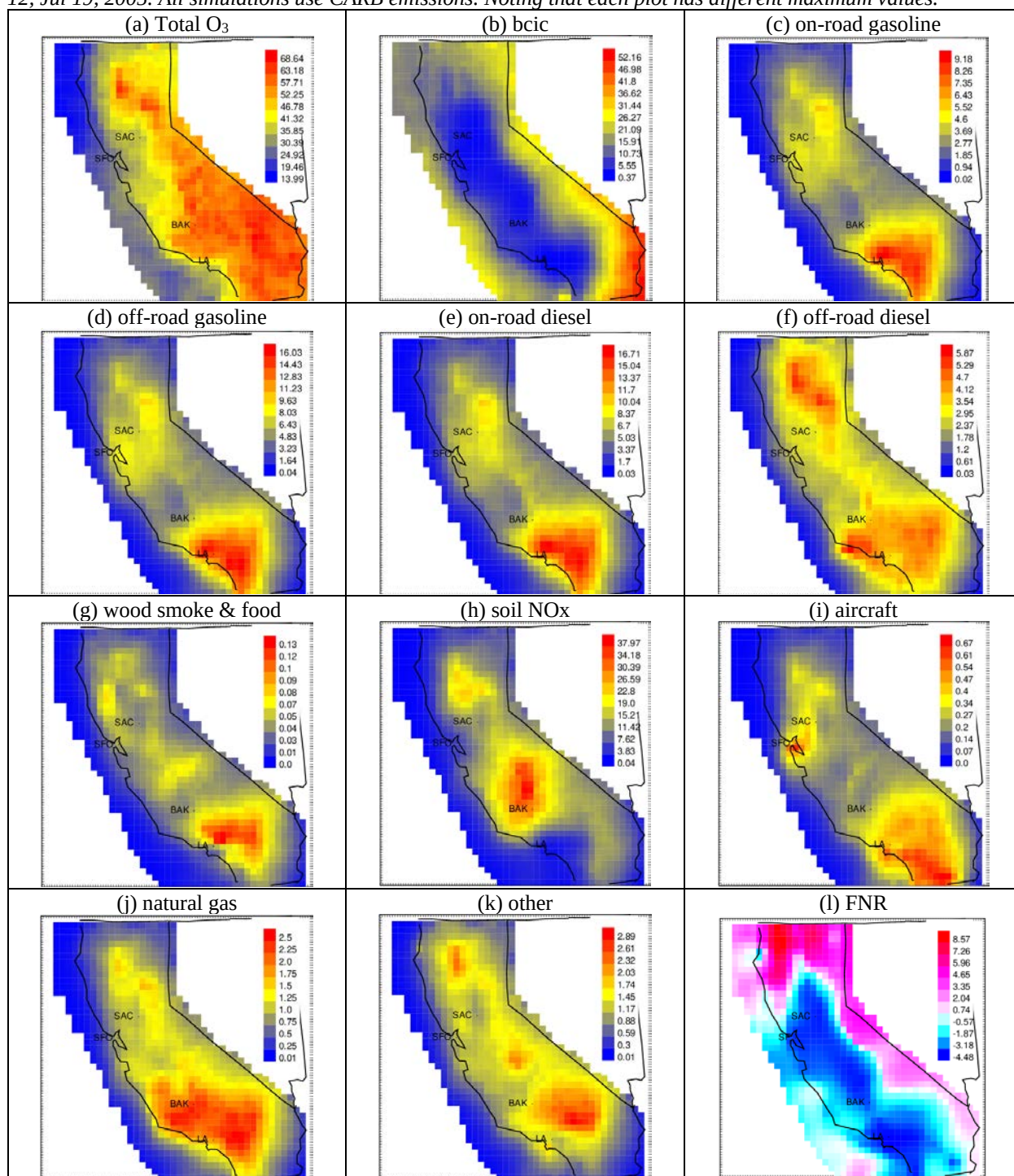


Figure S2.15: (a-k) Predicted VOC source contributions to O_3 concentrations (ppb) and (l) FNR minus 4.6 at hour 12, Jul 19, 2005. All simulations use CARB emissions. Noting that each plot has different maximum values.

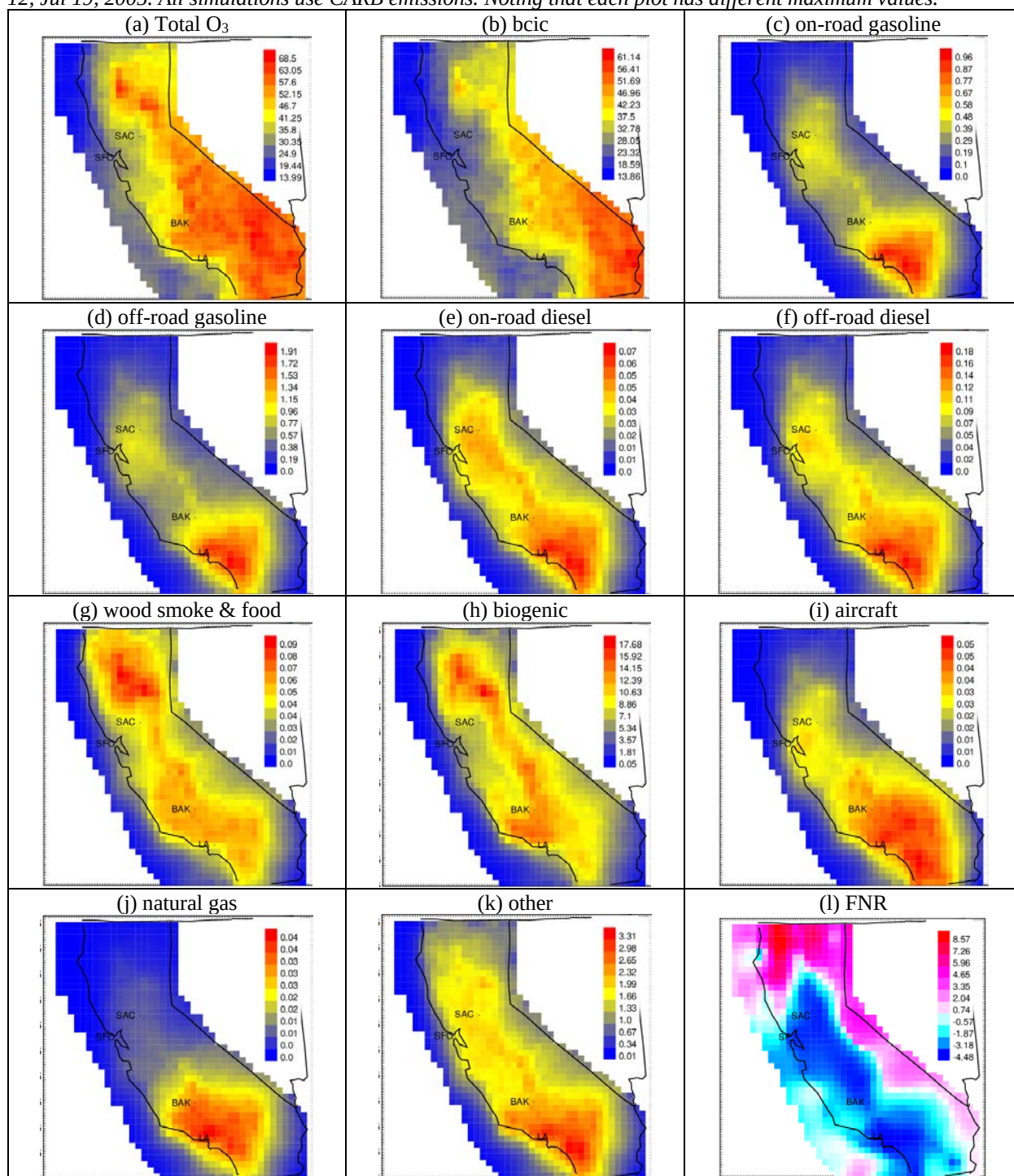


Figure S2.16: O_3 source contributions in 2005 July at central LA (a, b), Riverside (c, d), and Pasadena (e, f) at resolution of 4KM. Pie charts are based on O_3 concentrations exceeding 70 ppb. All simulations use CARB emissions.

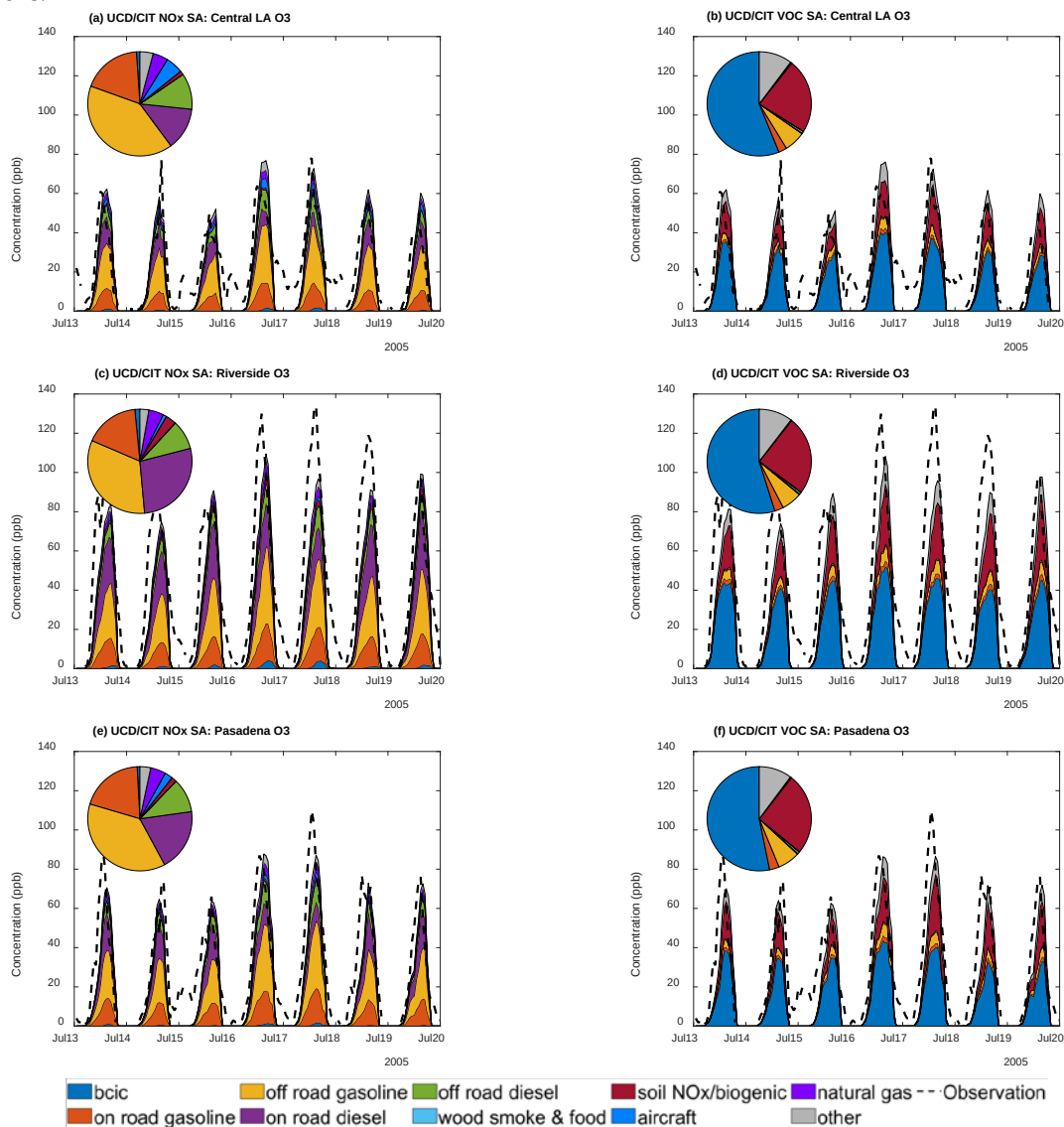


Figure S2.17: (a-k) Predicted NO_x source contributions to O₃ concentrations (ppb) and (l) FNR minus 4.6 at hour 12, Aug 21, 2015. All simulations use CARB emissions. Noting that each plot has different maximum values.

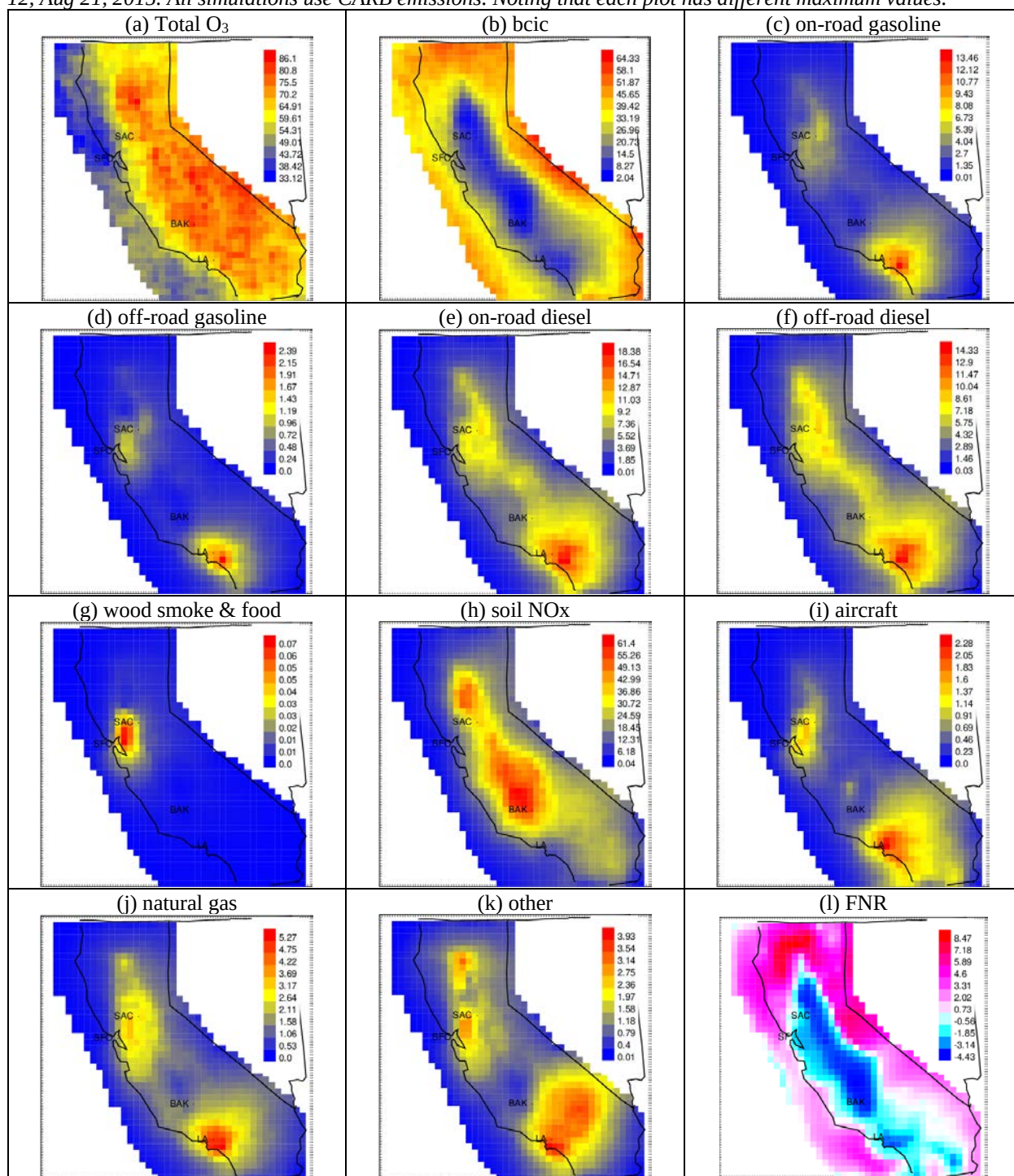


Figure S2.18: (a-k) Predicted NO_x source contributions to O₃ concentrations (ppb) and (l) FNR minus 4.6 at hour 12, Aug 21, 2015. All simulations use CARB emissions. Noting that each plot has different maximum values.

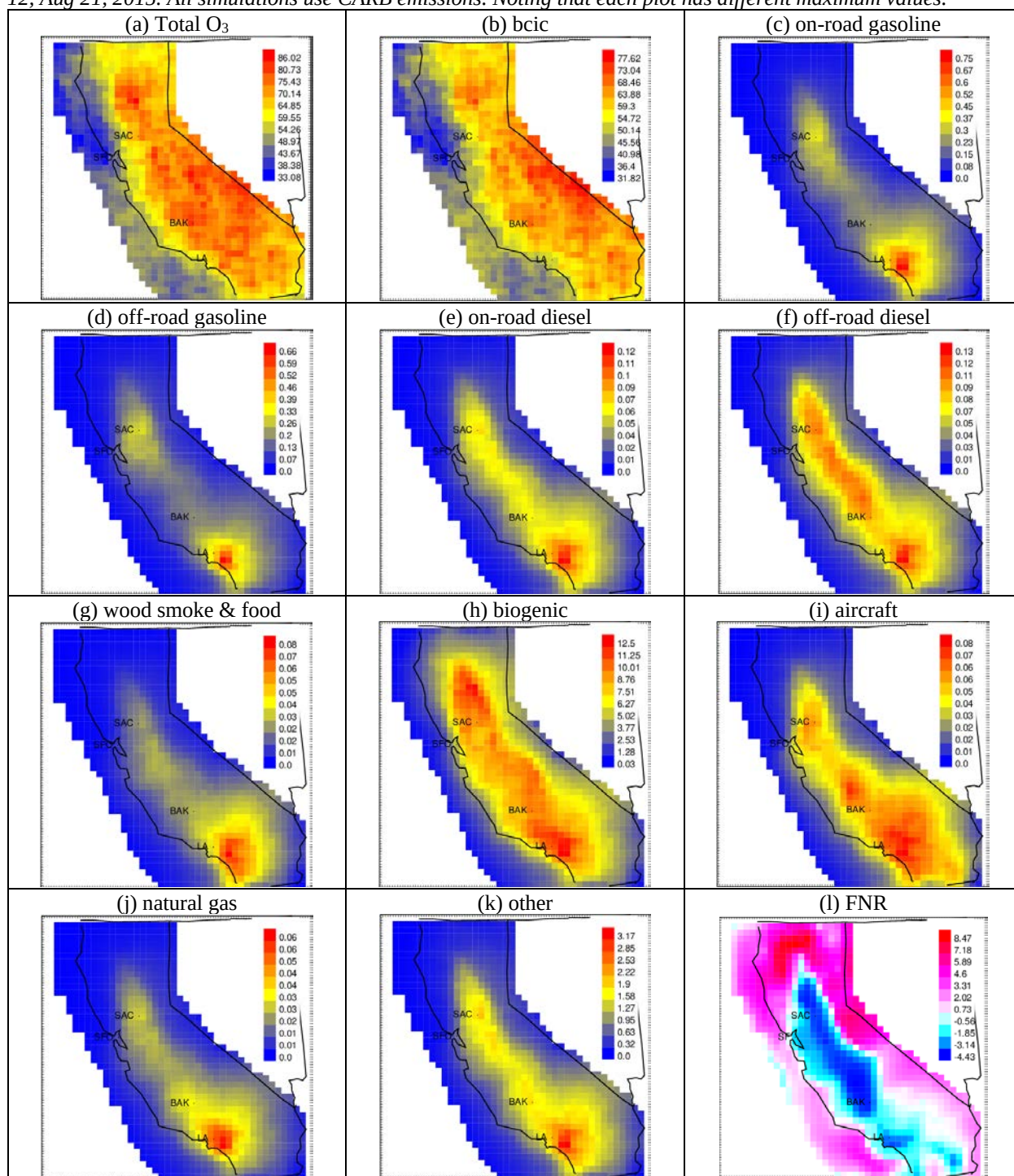


Figure S2.19: O_3 source contributions in 2015 August at central LA (a, b), Riverside (c, d), Pasadena (e, f), and Mira Loma Van Buren (g, h) at resolution of 4KM. Pie charts are based on O_3 concentrations exceeding 70 ppb. All simulations use CARB emissions.

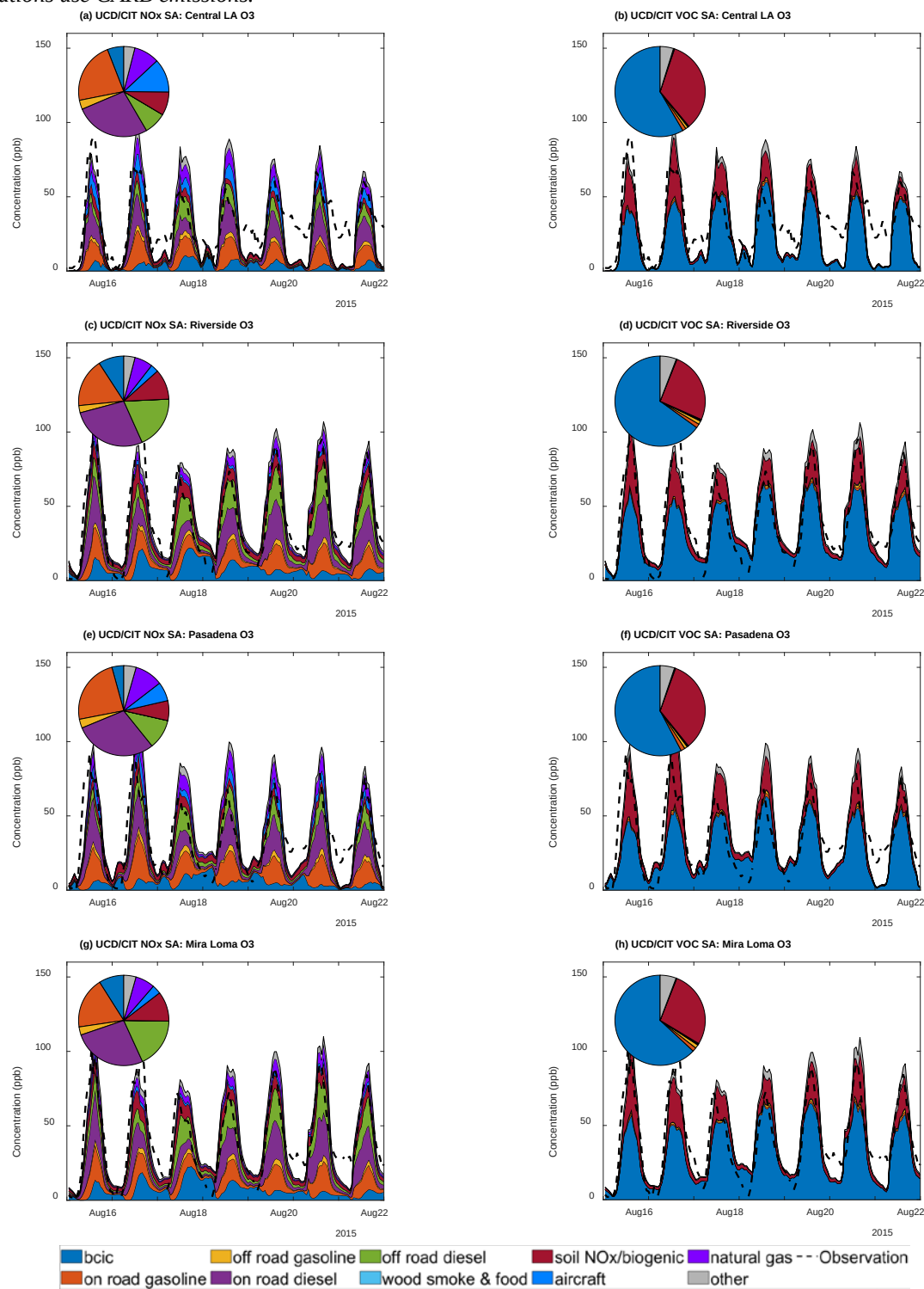


Figure S2.20: Trend of O_3 source contributions for NO_x SA and VOC SA at Central LA(a,b), Riverside(c,d), Pasadena(e,f), and Mira Loma Van Buren (g,h) in different episodes when O_3 concentrations exceed 70 ppb.

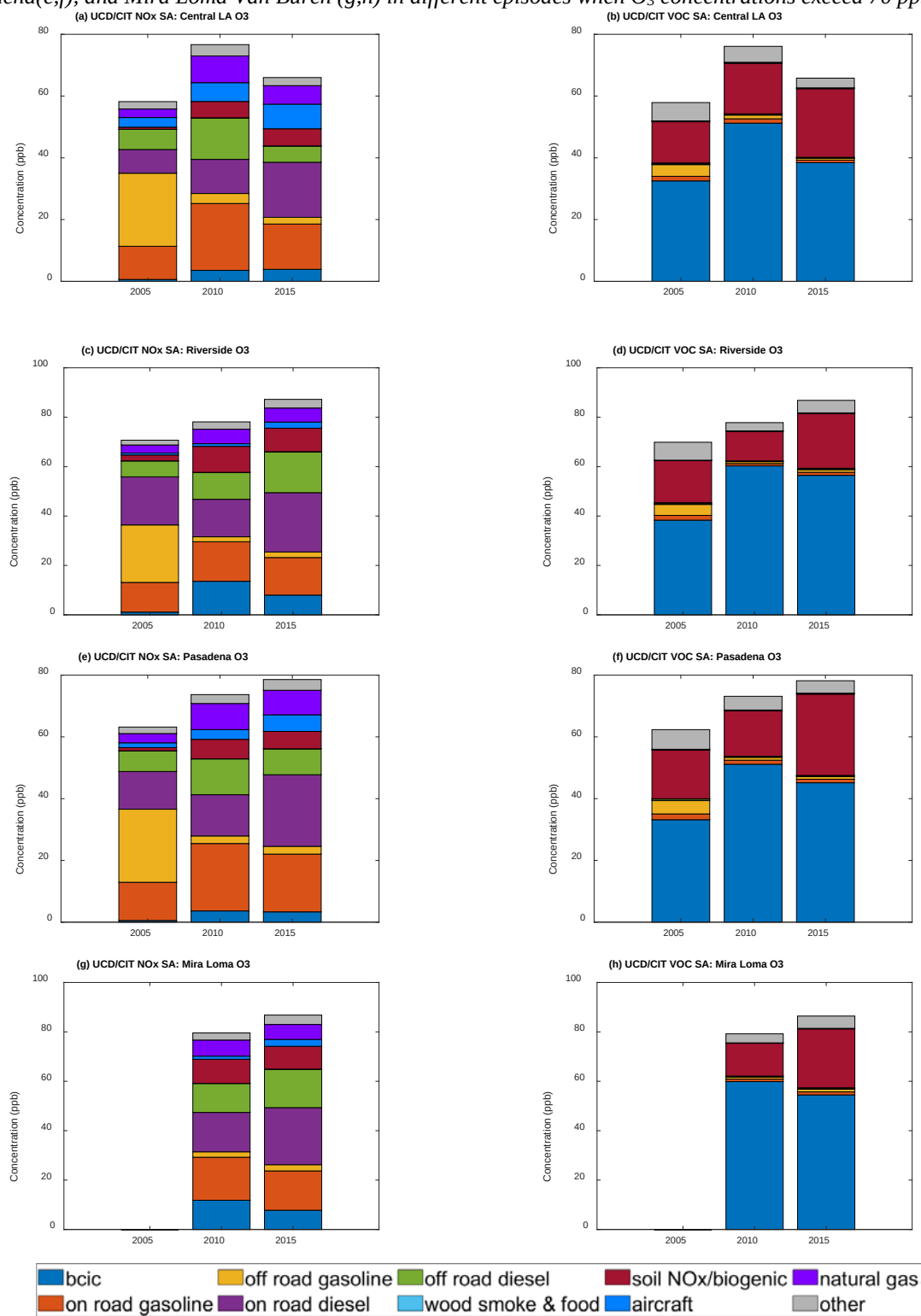
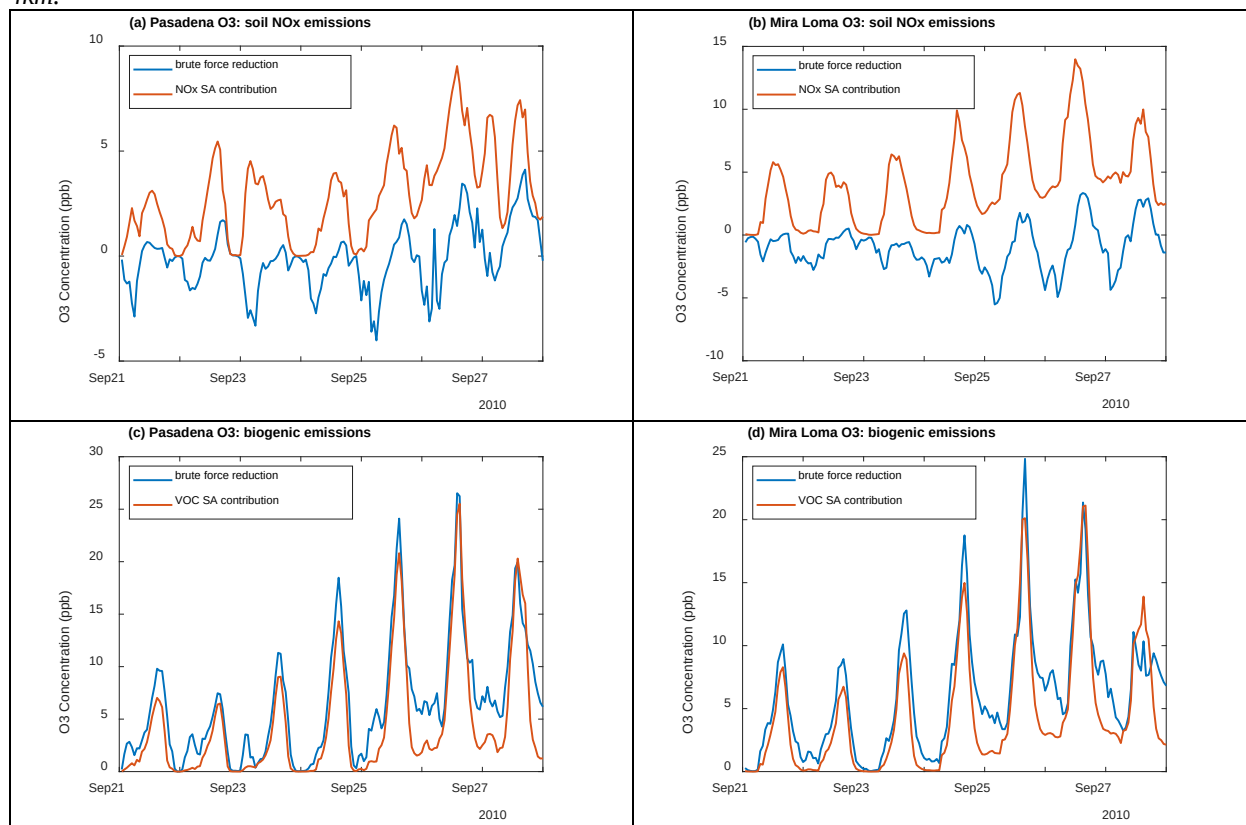


Figure S2.21: Comparison of (a, b) the O_3 reductions due to zeroing out soil NO_x and the O_3 contribution from soil NO_x in the NO_x SA results; (c,d) the O_3 reductions due to zeroing out biogenic emissions and the O_3 contribution from biogenic in the VOC SA results at Pasadena and Mira Loma Van Buren for 2010 Sep episode at resolution of 4km.



Chapter 3 Reducing southern California ozone concentrations in the year 2050 under a low carbon energy scenario

3.1. Introduction

Global efforts to mitigate the most harmful effects of climate change have gradually strengthened, with 196 parties of the United Nations Framework Convention on Climate Change (UNFCCC) agreeing to cut GHG emissions by 43% by 2030 (UNFCCC, 2015). Progressive cities and states with sufficient economic resources have also developed their own climate action plans. California has a long-standing commitment to a clean environment and a top 10 world economy. California therefore has both the motivation and the resources to take a leadership role on climate change. Assembly Bill 32 (passed in 2006) commits California to reducing GHG emissions by 80% of 1990 levels by the year 2050 (California Air Resources Board, 2006). Much of this reduction will be achieved through a transformation of the energy system towards renewable sources that emit little or no GHGs.

Transforming energy infrastructure is expensive, and many of the climate benefits will not be realized for decades. Immediate air quality co-benefits may make this transformation more attractive in the near term. Zapata et al. (2018a) and Li et al. (2022b) analyzed the air quality benefits associated with curbing GHG emissions in California and concluded that the immediate public health savings from reduced air pollution exceeded \$20B/yr, significantly offsetting the economic costs. Internal analysis conducted by staff at the California Air Resources Board confirms these findings (California Air Resources Board, 2022). Much of this public health saving is associated with reduced concentrations of airborne particulate matter (PM_{2.5}). The other major component of photochemical smog, ozone (O₃), does not respond as beneficially to programs that reduced GHG emissions due to the predicted increases of O₃ concentrations in urban areas. The South Coast Air Basin (SoCAB) in California is the only designated area in the United States where O₃ design values have exceeded 100 ppb for the past ten years (U.S. EPA, 2023). Anthropogenic emissions in the SoCAB have been significantly reduced over the past four decades (Wu et al., 2024)

leading to a long-term trend of declining O₃ concentrations, but recent progress has been more limited and O₃ design values started increasing again after 2016. Numerous measurement studies and model studies have analyzed the present-day trends (Perdigones et al., 2022; Wu et al., 2024, 2022; Zhu et al., 2019a) to support the creation of near-term control programs based on a weight of evidence approach. Similar efforts are needed for future scenarios that adopt low-carbon fuels.

Simulations of future conditions in the year 2050 with reduced GHG emissions predict that O₃ concentrations would continue to violate the National Ambient Air Quality Standards (NAAQS) in major California cities (Zapata et al., 2018a). Additional controls are therefore needed to address this future residual air quality problem. Here we conducted air quality simulations in California for the year 2050 using a chemical transport model (CTM) configured with a new O₃ source apportionment technique to assist in the development of future O₃ mitigation plans that are compatible with GHG emissions reduction goals. NO_x and volatile organic compound (VOC) source contributions to O₃ concentrations are quantified in the basecase scenario that focuses exclusively on GHG emissions reductions. Supplemental control programs are then designed that focus on the sources of NO_x and VOC that make the largest contributions to O₃ concentrations. Multiple control scenarios are analyzed with increasingly stringent controls to achieve compliance with the O₃ NAAQS. The public health benefits associated with each supplemental control program are estimated using established epidemiological relationships. The results of this study proactively develop solutions to anticipated air quality problems as California undertakes an energy transformation to address climate change.

3.2. Methodology

3.2.1. Model description

Air quality in the year 2050 was simulated using the University of California Davis/California Institute of Technology (UCD/CIT) air quality model configured with a new O₃ source apportionment technique. The UCD/CIT model is a 3-D source-oriented regional chemical transport model optimized for source tagging of primary and secondary air pollution (Kleeman and Cass, 2001; Yu et al., 2019). Performance statistics for O₃ and PM concentrations predicted by the UCD/CIT model meet the generally accepted criteria (Emery et al., 2017) for chemical transport models (Hu et al., 2015; Venecek et al., 2019, 2018b; Ying et al., 2008; Yu et al., 2019; Zhao et al., 2022). Most recently, Zhao et al. (2022) found that the O₃ performance of the UCD/CIT model is comparable to the performance of the CMAQ model developed by the US EPA. The UCD/CIT model has flexible solution algorithms that allow new chemical mechanisms to be tested with minimal effort. Two versions of the SAPRC11 chemical mechanism (Carter and Heo, 2013) were used to describe the gas-phase chemical reactions in the current study. The first version of the mechanism was configured to track NO_x source-contributions to O₃ while the second version was configured to track VOC source-contributions (Zhao et al., 2022).

UCD/CIT calculations were carried out over two domains in the current study (Figure S3.1). The outer domain covered the entire state of California with a resolution of 24 km, and the inner domain covered Southern California with a resolution of 4 km. The area with the bold outline in Figure S3.1 marks the boundary of the SoCAB, which is the primary focus area in the current study where O₃ concentrations exceed the standards designed to protect public health. The vertical domain extended 5km above the earth's surface using 16 telescoping layers with a height of 30m in the first layer. Multiple studies have demonstrated that this configuration is suitable for air quality predictions in California (Hu et al., 2015, 2014a, 2014b; Venecek et al., 2019; Yu et al., 2019).

Air quality simulations were conducted for 32 weeks randomly selected from 2046 to 2055 to properly represent inter-annual variability associated with the El Nino Southern Oscillation (ENSO) cycle. Eight (8) weeks were designated in each of the four seasons to ensure representative coverage throughout the year. This unbiased randomized sampling approach characterizes both the long-term average and the variability in pollutant concentrations without the computational expense of simulating every day in the 10-year window. Future meteorological fields were generated using the Weather Research and Forecasting model (WRFv3.4). Initial and boundary conditions for WRF simulations were generated using results from the Community Climate System Model (CCSM) under the representative concentration pathways (RCP) 8.5, which is a high GHG-emission (worst-case) scenario.

Future emissions for criteria air pollutants were generated by the CA-REMARQUE_v1.0 model, which will be discussed in detail in Section 2.2. Initial and boundary conditions for air quality simulations were based on predictions from the Model for Ozone and Related chemical Tracers (MOZART) for historical years, assuming that the initial and boundary conditions in 2050 will be fixed and similar to current conditions.

3.2.2. Future emissions

Future emission scenarios have been described in detail by Zapata et al. (2018a) and Li et al. (2022) and so only a brief summary is provided here. Two economically optimized energy scenarios were constructed for California in the year 2050 using the energy-economic optimization model, CA-TIMES. One scenario was a “business-as-usual” case (BAU) that incorporated current policy regulations to achieve the goals outlined in California Assembly Bill 32 (AB32). This scenario defines conditions when 2020 GHG emissions are limited to 1990 levels, but no extra efforts are taken to move toward a low-carbon society beyond 2020. The second scenario explored aggressive greenhouse gas mitigation strategies (GHGAi) that achieved an 80% reduction of GHG emissions relative to year 1990 by the year 2050 using deep penetration of advanced technologies and renewable energies. NO_x emissions in the GHGAi scenario are ~25% lower than the BAU scenario. The NO_x reductions are mainly from “off-road

equipment and railway”, and “residential and commercial buildings”. VOC emissions do not change significantly, with only 2.8% reduction from BAU to GHGAi.

Both energy scenarios were used as inputs to the CA-REMARQUE_v1.0 model to generate corresponding emissions for criteria air pollutants. Emissions were grouped into nine source sectors: tire and break wear, on road vehicles, off-road equipment and rail, marine vessels and aircraft, residential and commercial buildings, electricity generation, fuel supply, industrial and agricultural, and biogenic emissions (Li et al., 2022; Li et al., 2022b).

3.2.3. O₃ source apportionment technique

The O₃ source apportionment technique applied in the UCD/CIT model has been fully described by Zhao et al. (2022). The SAPRC11 chemical mechanism was expanded into two versions that tag O₃ precursors, intermediate products, and final O₃ concentrations. The first tagged version of the UCD/CIT model is a NO_x source apportionment (NO_x SA) method. This version tags the nitrogen atoms contained in NO_y species NO, NO₂, NO₃, N₂O₅, HNO₃, HNO₄, PAN, etc., and tracks NO_x source contributions to O₃ formation. In addition to the nitrogen atoms, O³P, O¹D, and O₃ are also tagged to pass the source apportionment information from NO_y species to O₃.

The second tagged version of the UCD/CIT model is a VOC source apportionment (VOC SA) method. This version tags odd-oxygen and tracks VOC source contributions to O₃ formation from different groups. Each VOC tag is then passed to the peroxy radicals and other compounds containing odd oxygen produced in the chemical reactions, which will finally go to O₃ and other sink species. It should be noted that tagging methods are purely an accounting exercise to track O₃ source contributions. The total concentrations (summed across all sources) of the species predicted by the NO_x SA and VOC SA variants of the UCD/CIT model are equivalent.

3.2.4. Emission reductions

Several emission reduction strategies are proposed based on the O₃ source apportionment results. Source sectors that contribute strongly to O₃ formation are prioritized for reductions. A formal cost analysis was not undertaken, but the cumulative emissions controls were generally configured in order of increasing reductions. We used the 3rd highest MD8H O₃ across the simulated 32 weeks (rank 3 out of 224 days) as criterion to assess O₃ violations. This percentile is approximately equivalent to the annual 4th highest MD8H O₃ in a year (rank 4 out of 365 days), known as the design value classified by the US EPA. The ambient O₃ concentrations predicted under each emissions control were evaluated before the next control stage was implemented.

3.2.5. Health benefits

The health benefits associated with O₃ reductions were calculated using the Environmental Benefits Mapping and Analysis Program – Community Edition (BenMAP-CE) v1.5.8.22 developed by the US EPA. The health functions used in the analysis are listed in Table S3.1, including Incidence of Asthma (Garcia et al., 2019), Incidence of Hay Fever/Rhinitis (Parker et al., 2009), and All-Cause Mortality (Turner et al., 2016). Average MD8H O₃ concentrations under the BAU scenario, the GHGAi scenario, and the Control Steps of the GHGAi scenario were used to calculate the health impacts associated with different scenarios and control strategies. This calculation uses the default BenMAP population data that is projected to 2050 by Woods & Poole (Woods & Poole Economics Inc, 2015).

3.3. Results and discussion

3.3.1. O₃ violation in future scenarios

Among the 32 simulated weeks (224 days), MD8H O₃ concentrations exceeded 70 ppb on 101 days under the BAU scenario and 71 days under the GHGAi scenario (see Table 3.1). The 3rd highest MD8H O₃ plots for the BAU and the GHGAi scenarios are shown in Figure 3.1. The 70 ppb O₃ standard is significantly exceeded in the SoCAB under both emissions scenarios, which is consistent with the findings in Zapata et al. (2018a). The maximum O₃ exceedance across all grid cells is 22.5 ppb in the BAU scenario, placing the SoCAB in the Moderate nonattainment category for the 2015 8-hour O₃ standard. The O₃ exceedance in the GHGAi scenario is 16.1 ppb, placing the SoCAB in the Moderate nonattainment category as well. O₃ violations occur in these future scenarios because reductions in NO_x emissions are insufficient to fully shift the atmosphere into the NO_x-limited chemical regime in the year 2050. More aggressive and targeted NO_x emissions controls are described in the following sections.

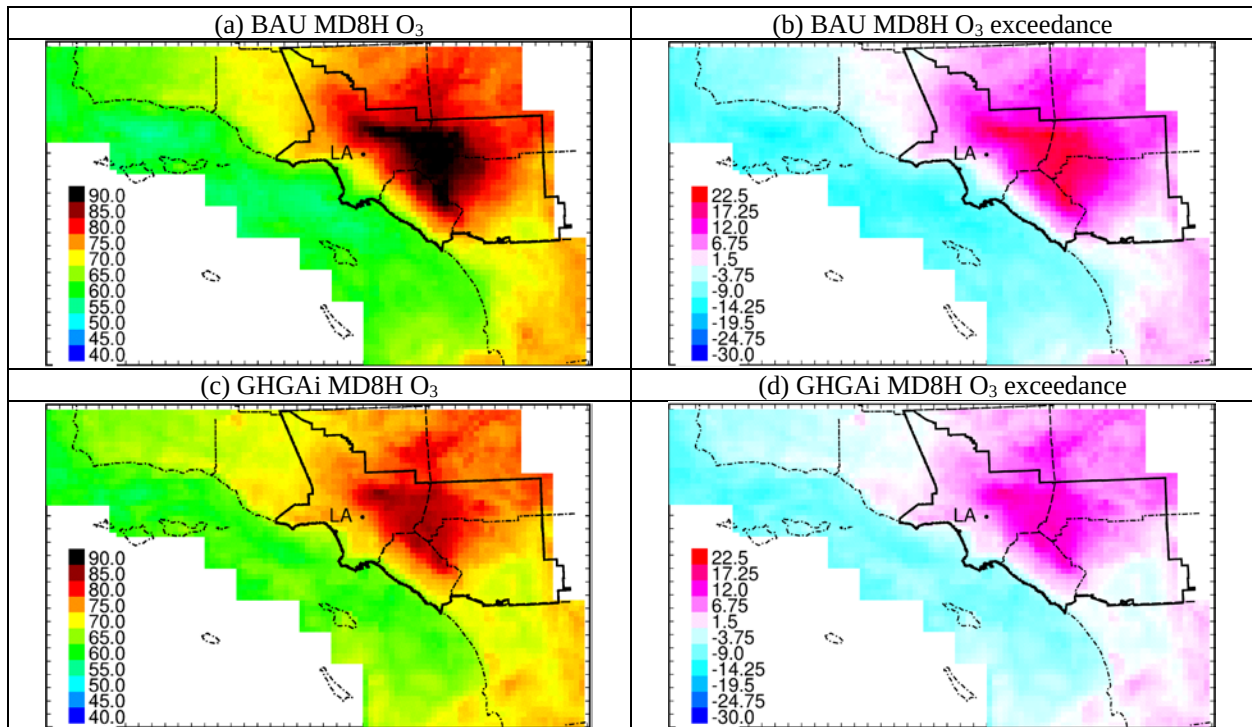


Figure 3.1: 3rd highest MD8H O₃ and exceedance (vs. 70 ppb), unit: ppb.

Table 3.1: Number of days with O₃ exceeding 70 ppb.

	BAU	GHGAi	GHGAi with Control Step I	GHGAi with Control Step II	GHGAi with Control Step III
Total days of simulation	224	224	140	56	35
Days of exceedance	101	71	26	21	13

3.3.2. O₃ source contributions under the GHGAi scenario

Source contributions to the 3rd highest MD8H O₃ concentrations under the GHGAi scenario are shown in Figure 3.2 and Figure 3.3. “Offroad equipment & rail”, and “marine vessels & aircraft” are the two major NO_x emission groups that contribute to O₃ violations (Figure 3.2). Emissions from “off-road equipment & rail” form 16-26.3 ppb of O₃. NO_x emissions from “marine vessels & aircraft” form 20-35 ppb of O₃. “Industrial & agricultural emissions” are the third largest O₃ contributor among the NO_x emission groups, forming 8-14 ppb of O₃ in the region. NO_x emissions from “residential & commercial buildings” and “electricity generation” each contribute to smaller amounts of O₃ formation (< 7 ppb each). NO_x emissions from on road vehicles and fuel supply make very small contributions to O₃ concentrations (<2.4 ppb each). It should be noted that “boundary & initial conditions (BCICs)” are a major source of O₃ in the NO_x source apportionment simulation in the San Diego region, but not in the SoCAB. This reflects the proximity of San Diego to the computational boundary.

VOC SA results (Figure 3.3) predict that BCICs play an important role in the central portion of the SoCAB with the 3rd highest O₃ concentration. Background O₃ and VOC concentrations contribute approximately 50 ppb of O₃ in the SoCAB, making BCICs the single largest O₃ “source” in the VOC SA calculations. BCIC contributions are even higher in the northeastern portion of the model domain, although this region has slightly lower total O₃ concentrations. Biogenic VOC emissions are the next most significant O₃ source, forming 10-21 ppb of O₃ in the central portion of the SoCAB. VOC emissions from “industrial & agricultural sources” contribute to approximately 10 ppb of O₃ formation. VOC emissions

from “off-road equipment & rail”, and “marine vessels & aircraft” contribute to 2.49-6.16 ppb and 1.4-4.63 ppb of O₃ formation, respectively. Contributions from the other VOC sources are very small and negligible.

The formaldehyde to NO₂ ratio (FNR) is often used as an indicator of the chemical regime for O₃ formation (NO_x-limited vs. VOC-limited). Figure 3.4 illustrates the FNR plots under the BAU and the GHGAi scenarios. A threshold of FNR=4.6 is used as the transition between the NO_x-limited and VOC-limited chemical regimes (Wu et al., 2022). Grid cells with positive values (red) are NO_x-limited, and grid cells with negative values (blue) are VOC-limited. In both scenarios, regions that violate the 70-ppb standard are mostly VOC-limited. O₃ chemistry in the SoCAB has historically been in the VOC-limited regime (Jin et al., 2020). Recent studies have stated that the basin is transitioning to NO_x-limited conditions, and may have been NO_x-limited on average during spring and summer of 2020 (Perdigones et al., 2022; Schroeder et al., 2022). Direct chamber measurements of ambient O₃ sensitivity present a more complex picture, with significant days still VOC-limited (Wu et al., 2024). However, considering that the major VOC sources that contribute to O₃ formation in the SoCAB are BCICs and biogenic emissions, it is more practical to reduce the anthropogenic emissions of the major NO_x sources.

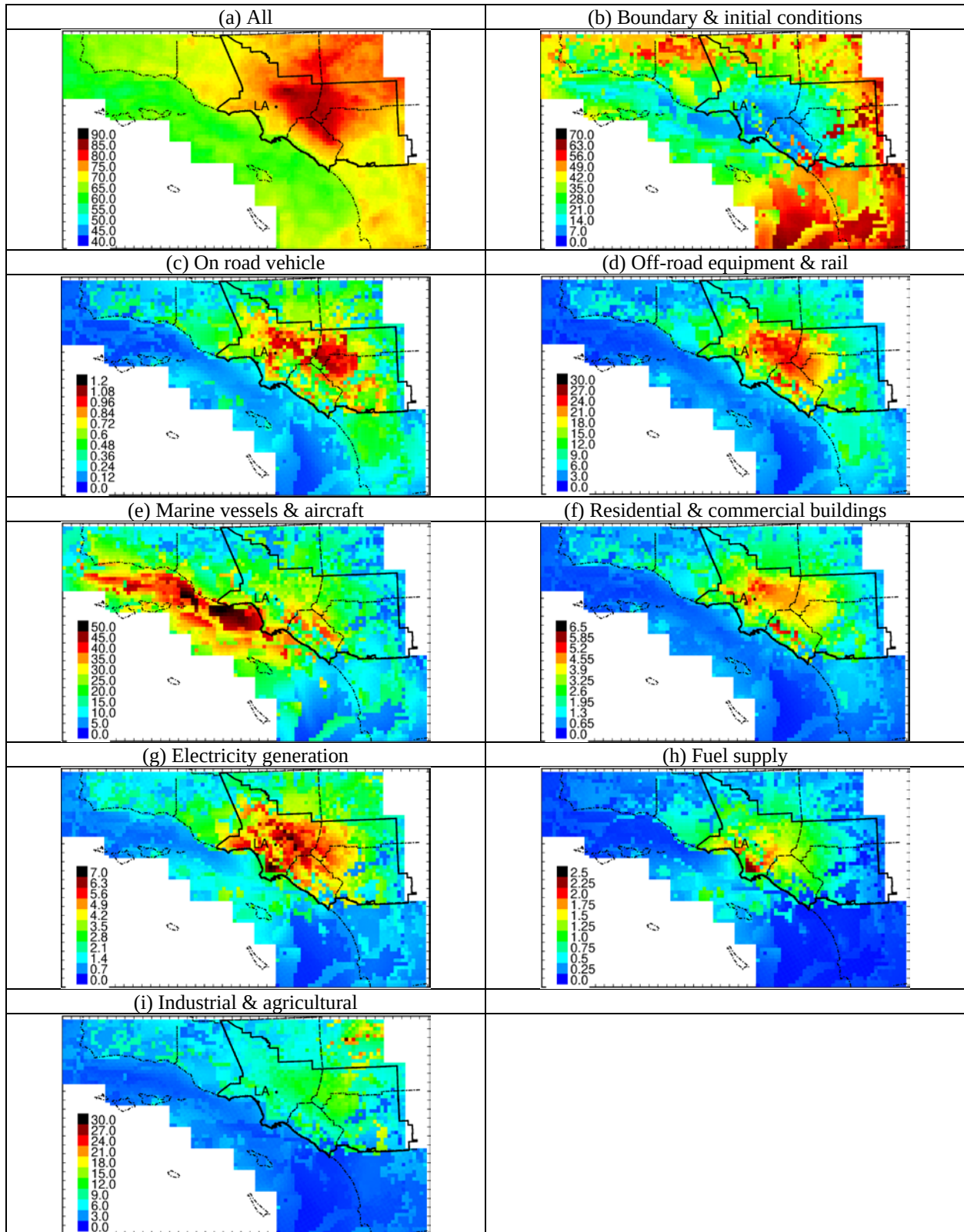


Figure 3.2: NOx Source Contributions to 3rd highest MD8H O₃ in GHGAI, unit: ppb.

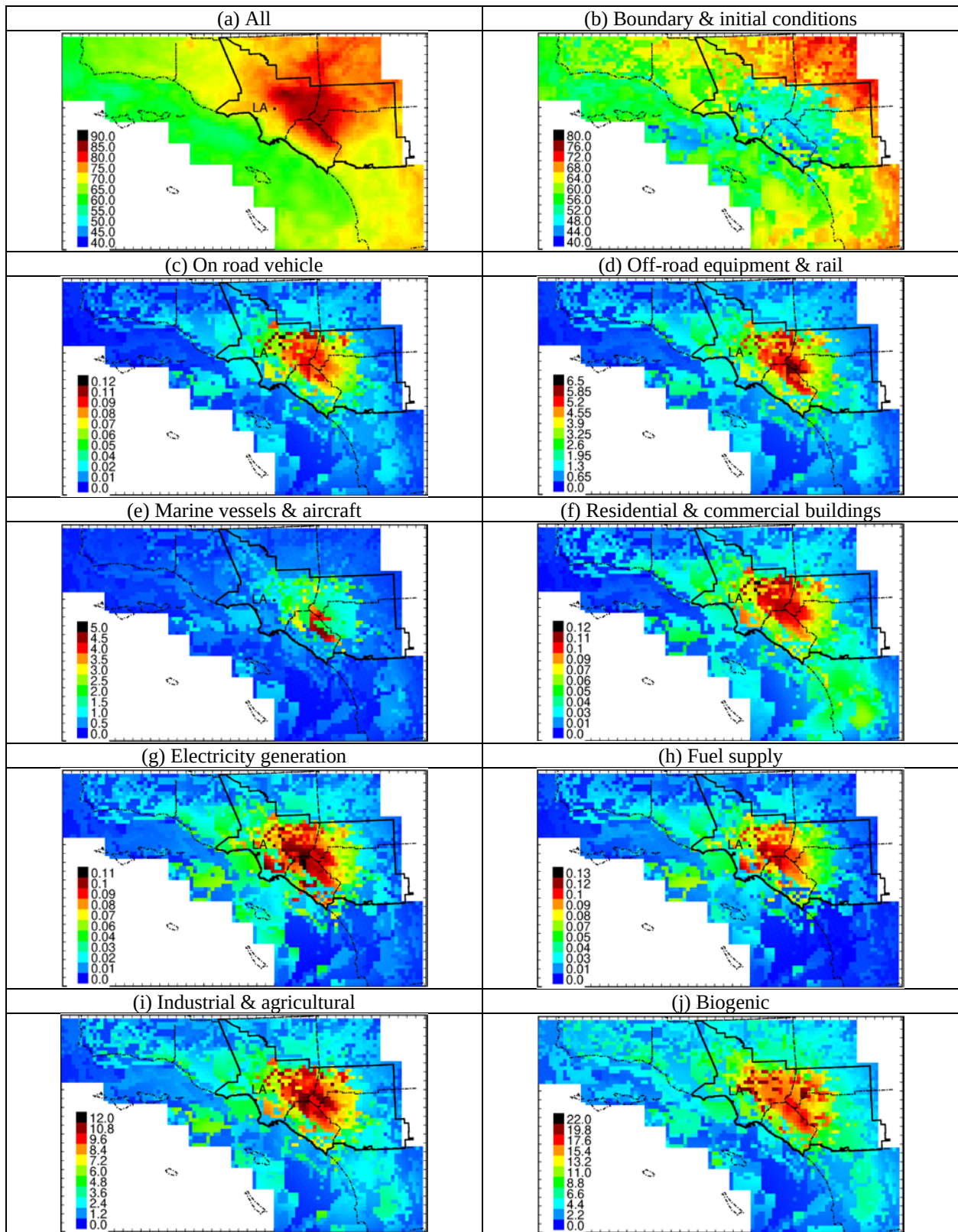


Figure 3.3: VOC Source Contributions to 3rd highest MD8H O₃ in GHGAi, unit: ppb.

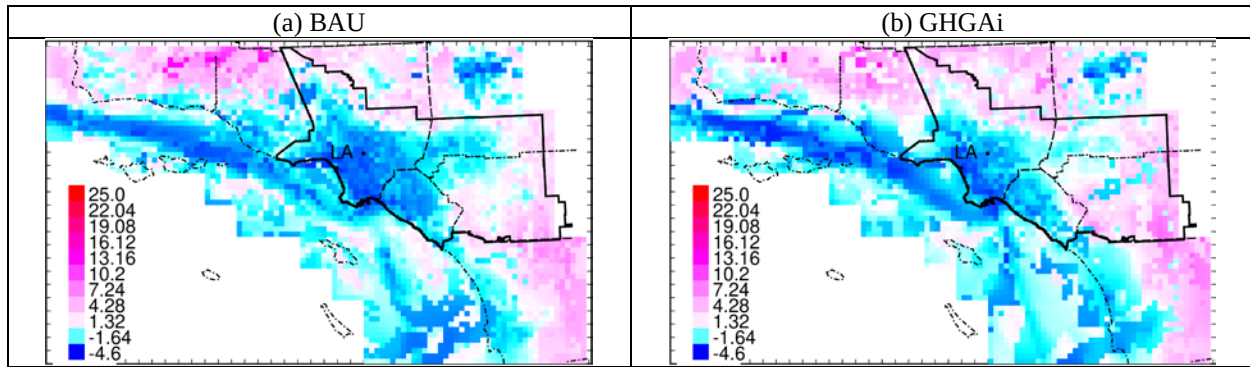


Figure 3.4: $HCHO/NO_2$ (FNR) for the corresponding 3rd highest MD8H O_3 days (The values are subtracted by the threshold).

3.3.3. Emissions reduction

Several emissions reduction strategies were investigated to reduce O_3 concentrations in future years.

Results from three cumulative levels of emissions controls are described in the following sections.

3.3.3.1. Emissions Control Step I

NO_x emissions controls were first applied to the two largest O_3 contributors: “off-road equipment & rail”, and “marine vessels & aircrafts”. In the “off-road equipment and railroad” emission sector, we assume adoption of electricity or some other power source that does not emit NO_x in future years. Emissions in this sector are therefore reduced to zero.

Future emissions of NO_x from marine vessels were reduced by 80% based on future compliance with the International Convention for the Prevention of Pollution from Ships (MARPOL) Annex VI Tier III standard. The original marine vessel emissions in the GHGAi scenario were based on 2010 levels (Zapata et al., 2018b) placing them in Annex VI Tier I. We assume an average lifespan for an ocean vessel is ≤ 30 years. Therefore, by the year of 2050, all in-use ocean vessels should comply with the Annex VI Tier III standard, with emissions reduced by 80% compared to Tier I. Total NO_x and None-Methane VOC (NMVOC) emissions in the SoCAB decrease by 65% and 15.5% relative to the GHGAi scenario, respectively.

Figure 3.5(a) and Figure 3.5(b) show the 3rd highest MD8H O₃ concentrations and O₃ exceedance under Emissions Control Step I. O₃ concentrations are significantly reduced across the SoCAB, and a large portion of the O₃ violation disappears under the enhanced emissions controls. O₃ concentrations are reduced by a maximum of 18.9 ppb in Control Step I (Figure S3.5(a)). The reductions in the 3rd highest O₃ concentrations under Control Step I are sufficient to move the SoCAB from Moderate to Marginal non-attainment status.

Figure S3.2 shows the NO_x SA results for the Control Step I. Emissions from “offroad equipment & rail” are reduced to zero in this scenario and so these sources no longer contribute to O₃ formation. NO_x emissions from marine vessels are reduced by 80%, greatly reducing their contribution to O₃ formation in coastal areas. Residual NO_x emissions from “marine vessels and aircraft” still contribute up to 30.2 ppb of O₃ formation in the inland regions of the SoCAB.

3.3.3.2. Emissions Control Step II

The remaining O₃ violations under Emissions Control Step I have significant source contributions from industrial and agricultural sources. Additional cumulative measures in Control Step II reduce emissions from industrial and agricultural sources by 50% through the adoption of low-NO_x engines similar to those used in the on-road fleet. Total NO_x and NMVOC emissions in the SoCAB decrease by 73.6% and 15.5% relative to the GHGAi scenario, respectively.

Figure 3.5(c) and Figure 3.5(d) show the 3rd highest MD8H O₃ plots and O₃ exceedance under Emissions Control Step II. The region that experiences O₃ violations inside the SoCAB shrinks under Control Step II, with one grid cell near Redlands and several grid cells at the northeastern boundary continuing to exceed 70 ppb. However, the region outside the SoCAB that experiences O₃ violations is relatively unchanged by these control measures. Figure S3.5(b) shows that the basin-wide O₃ reduction from Control Step I to Step II is less than 5 ppb. Some areas show very small O₃ increases (<0.2 ppb) due to decreased NO_x emissions in the NO_x-rich chemical regime that exists at those locations (Figure 3.6(b)).

3.3.3.3. Emissions Control Step III

Emissions Control Step III applies more aggressive controls in an attempt to further reduce ambient O₃ concentrations. NO_x emissions from marine vessels are reduced by 90% instead of 80%, and NO_x emissions from the industrial and agricultural sectors are completely removed with the assumption that these sources will be electrified. Offroad equipment and rail remain at zero emissions. Total NO_x and NMVOC emissions in the SoCAB decrease by 85.4% and 15.5% relative to the GHGAi scenario, respectively. The cost and feasibility of these emissions controls are not evaluated in the current study, but this case illustrates the limiting behavior of the system.

Figure 3.5(e) and Figure 3.5(f) show the 3rd highest MD8H O₃ and O₃ exceedance under Emissions Control Step III. With the more stringent control measures in the Control Step III, O₃ concentrations are basically below 70 ppb across the SoCAB. The remaining few grid cells with minor exceedance are located at non-populated wilderness areas, which should not represent a widespread public health risk. Similarly, the region with O₃ violations outside the SoCAB also shrinks under Emissions Control Step III.

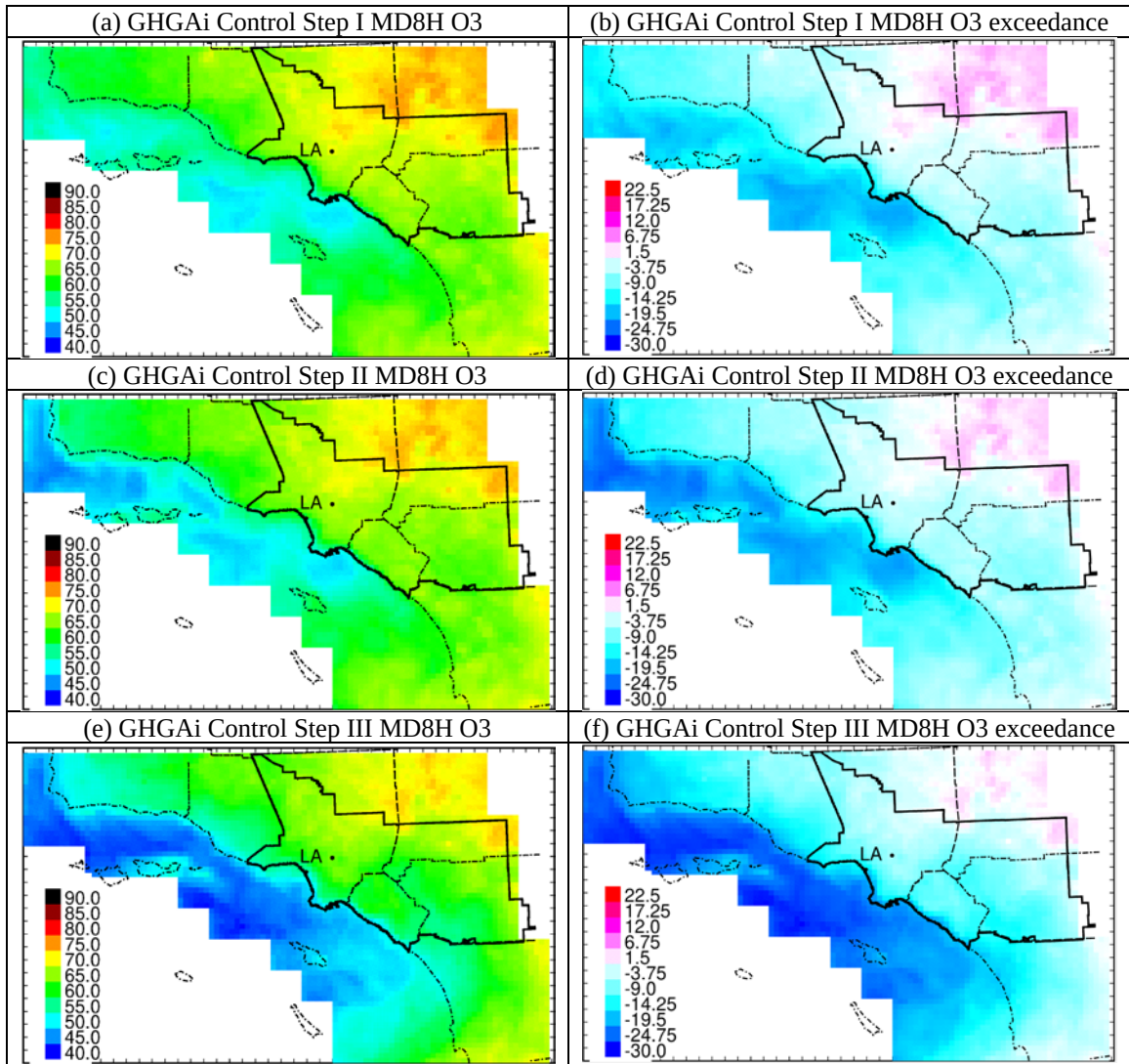


Figure 3.5: 3rd highest MD8H O₃ and exceedance (vs. 70 ppb) in different emission control steps, unit: ppb.

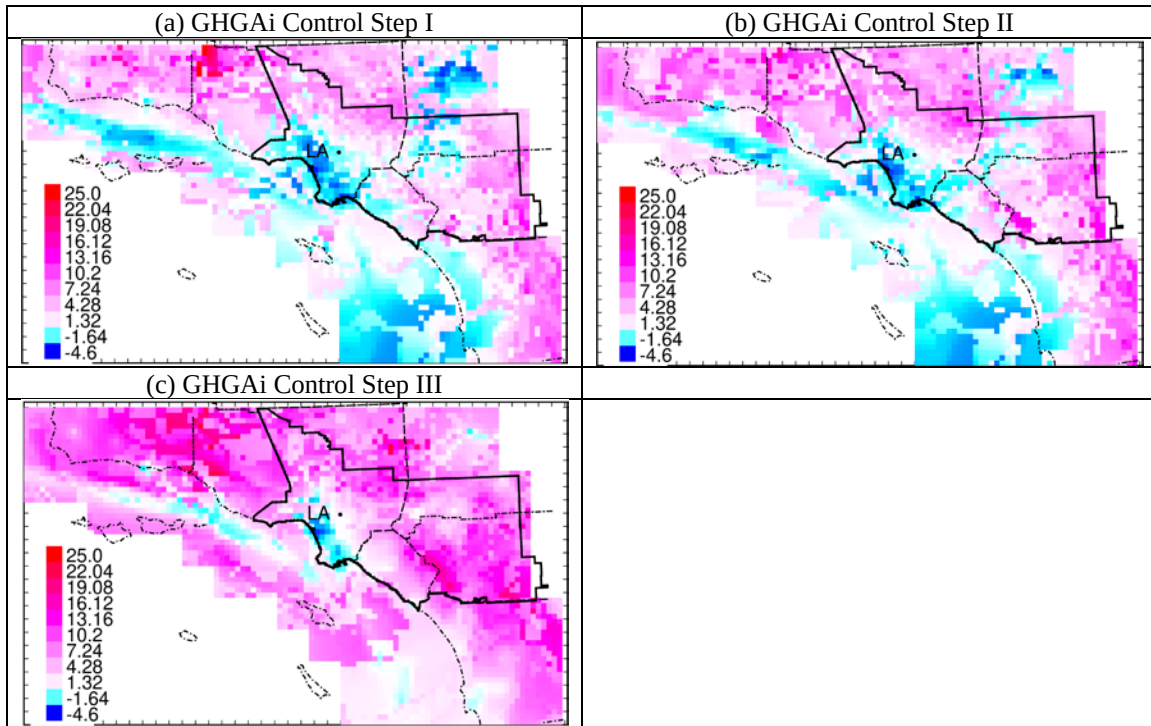


Figure 3.6: $HCHO/NO_2$ (FNR) for the corresponding 3rd highest MD8H O_3 days in different control steps (The values are subtracted by the threshold).

3.3.4. Health benefits

Figure 3.7 shows the 32-week average MD8H O_3 concentration predicted under the BAU, GHGAi, and the three GHGAi control step scenarios used in the BenMAP calculations. Domain-wide calculations of the health benefits based on the averaged MD8H O_3 in Southern California are shown in Figure 3.8 and Table S3.2. Each health benefit is expressed relative to a reference case. GHGAi-BAU uses the BAU scenario as the reference case. StepI-GHGAi, StepII-GHGAi, and StepIII-GHGAi each use the GHGAi scenario as the reference case. In Figure 3.8, the health benefits were shown as the percentage of the highest health benefits of the three controls. Each health benefit is proportional to the changes in O_3 concentrations, and so the distribution of benefits across scenarios looks similar. The baseline supplemental controls in Step I reduced incidence of hay fever/rhinitis and asthma by a factor of 8.2 and reduced total mortality by a factor of 11.4 relative to the GHGAi-BAU health benefits. The most stringent controls in Step III reduced the incidence of hay fever/rhinitis and asthma being a factor of 12.3 and the

reduced total mortality being a factor of 17.5 relative to the GHGAi-BAU health benefits. The public-health present-day value of these controls are estimated at \$19.70-30.36B/yr using a value of a statistical life equal to \$7.6M. These public health savings should be considered when weighing the costs of each control measure.

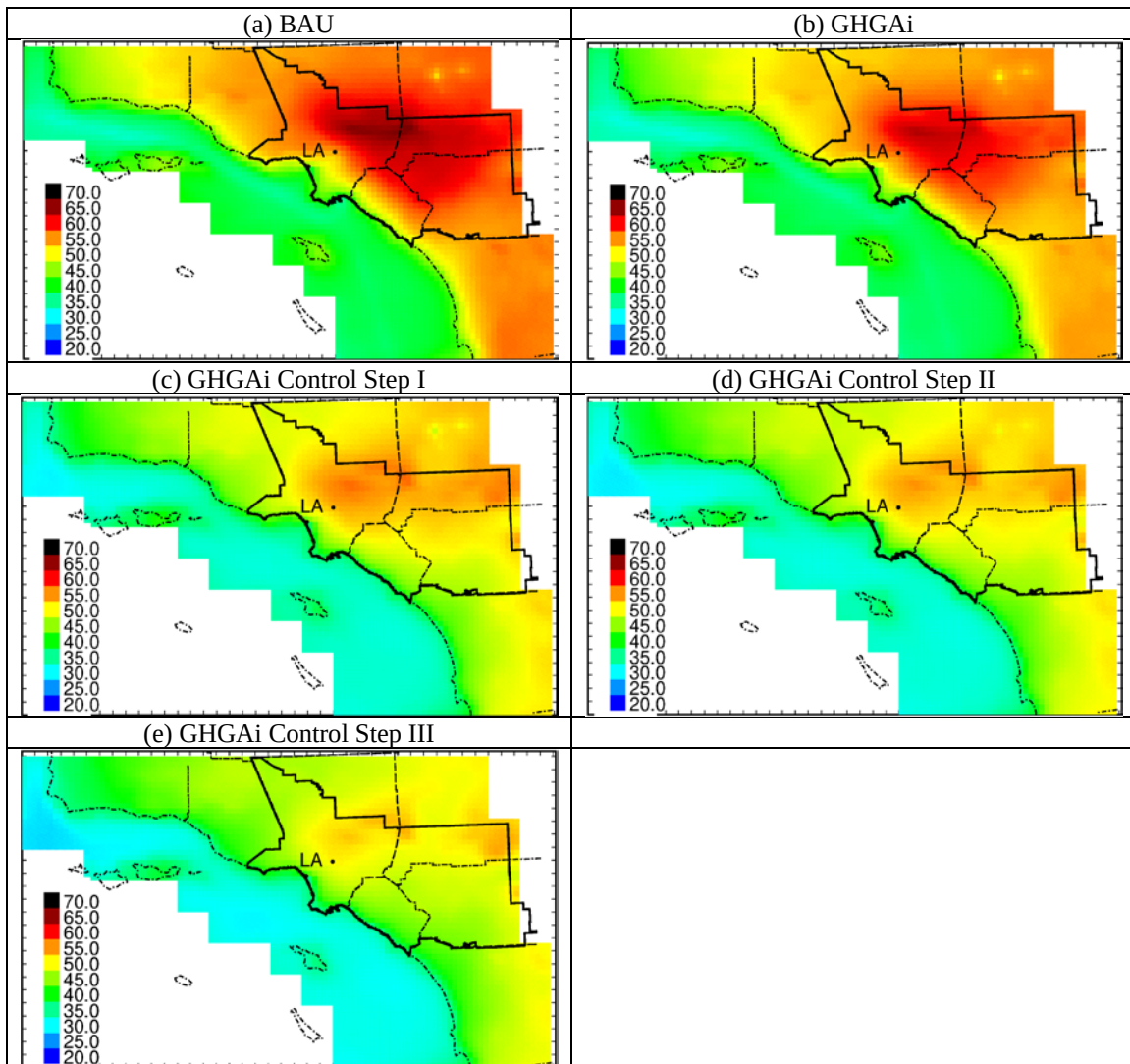


Figure 3.7: 32-week average MD8H O₃ plots in all scenarios, unit: ppb.

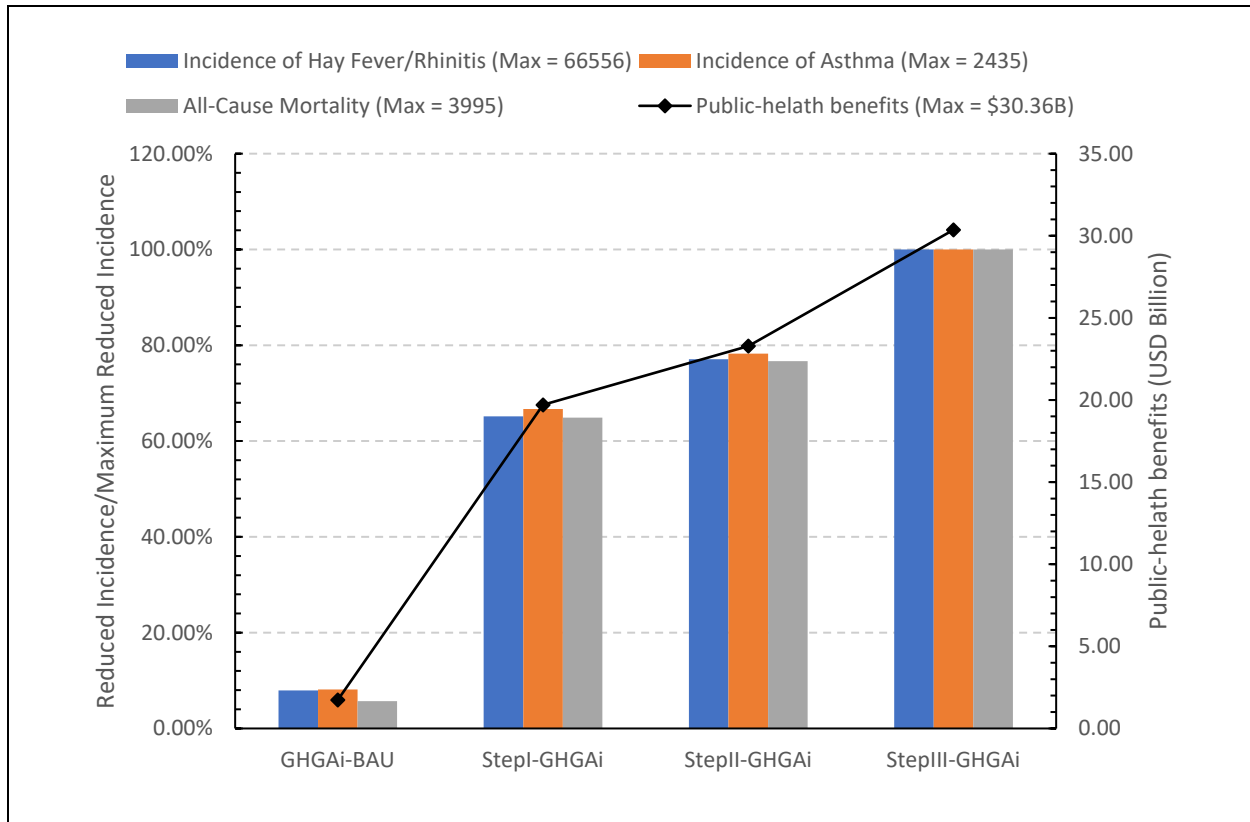


Figure 3.8: Health benefits in different scenarios. The reduced incidence is shown as the percentage compared to the maximum reduced incidence.

3.4. Implications

Air quality simulations for Southern California in the year 2050 under a Business as Usual (BAU) and GHG reduction (GHGAi) scenario previously predicted continued violations of the current 8-hour O₃ standard despite significant reductions in PM_{2.5} mass concentrations. These O₃ violations largely stem from persistent NO_x-rich chemistry in urban cores that produces higher O₃ concentrations as combustion sources are replaced by renewable energy sources. A new O₃ apportionment technique was used to identify emission sources that contribute to the high O₃ concentrations in the SoCAB in the year 2050. Major VOC sources that contribute to O₃ formation include biogenic emissions within the study area and upwind sources outside the study area, meaning that local VOC controls will not be effective at reducing high O₃ concentrations in the year 2050. Major NO_x sources that contribute to O₃ formation include “off-road equipment & rail”, “marine vessels & aircraft”, and “industrial & agricultural emissions”. Each of these sources could be controlled to reduce O₃ concentrations.

Three cumulative emission control strategies were designed to further reduce NO_x emissions that contribute to O₃ formation in the SoCAB in the year 2050 under a reduced GHG emissions case. Control Step I reduced emissions from “offroad equipment and rail” to zero and reduced emissions from marine vessels by 80% leading to a 53% reduction in regional NO_x emissions. The maximum O₃ exceedance for the 3rd highest MD8H O₃ decreased from 16.1 ppb to 5.1 ppb, shifting the non-attainment status of the basin from Moderate to Marginal. Control Step II reduced emissions from “industrial and agricultural sources” by 50% leading to a 64% reduction in regional NO_x emissions. O₃ violations near the city of Los Angeles disappeared under Control Step II, but exceedances still occurred near Redlands and at other locations to the northeast of Los Angeles. A more aggressive Control Step III was tested that reduced the NO_x emissions from marine vessels by 90% and eliminated the NO_x emissions from the industrial and agricultural sources (offroad equipment and rail emissions remain at zero) produced an 80% reduction in regional NO_x emissions. Control Step III reduced O₃ concentrations below 70 ppb throughout the SoCAB except for a few unpopulated mountainous locations.

The three control steps reduced hay fever/rhinitis, asthma, and all-cause mortality in the SoCAB. Control Step 1 improved health benefits by a factor of 9 relative to the reduced GHG emissions scenario, while Control Step III improved health benefits by a factor of 14.8 relative to the reduced GHG emissions scenario. The public health savings associated with these control measures are estimated to be \$19.70-30.36B/yr.

The sources identified for emissions reduction in Control Steps I, II, and III release emissions in California but the proposed emission controls are not necessarily subject to current California regulations. Controls on international and inter-state goods movement and agricultural engines will require planning and coordination with other governing agencies. Some of these emissions controls may also require the development or deployment of new power sources to replace traditional combustion system. Each of these efforts could take decades to implement. Identifying sources of O₃ formation now provides the necessary planning timeline to address this key element of photochemical smog formation in California.

3.5. Appendix

Table S3.1: Health Impact Functions used in BenMAP analysis.

Endpoint Group	Endpoint	Author	Start Age	End Age	Year
Incidence, Respiratory	Incidence, Hay Fever/Rhinitis	Parker et al.	3	17	2009
Incidence, Respiratory	Incidence, Asthma	Garcia et al.	9	18	2019
Mortality	Mortality, All Cause	Turner et al.	30	99	2016

Table S3.2: Health benefits results from BenMAP

	Incidence of Hay Fever/Rhinitis	Incidence of Asthma	All-Cause Mortality	Public-health benefits in USD (billion)
GHGAi-BAU	5274	198	228	1.73
ControlStepI-GHGAi	43368	1624	2592	19.70
ControlStepII-GHGAi	51295	1905	3064	23.28
ControlStepIII-GHGAi	66556	2435	3995	30.36

Note: the public-health benefits in USD are calculated using the value of a statistical life (VSL) equal to USD 7.6 million.

Figure S3.1: Model domain

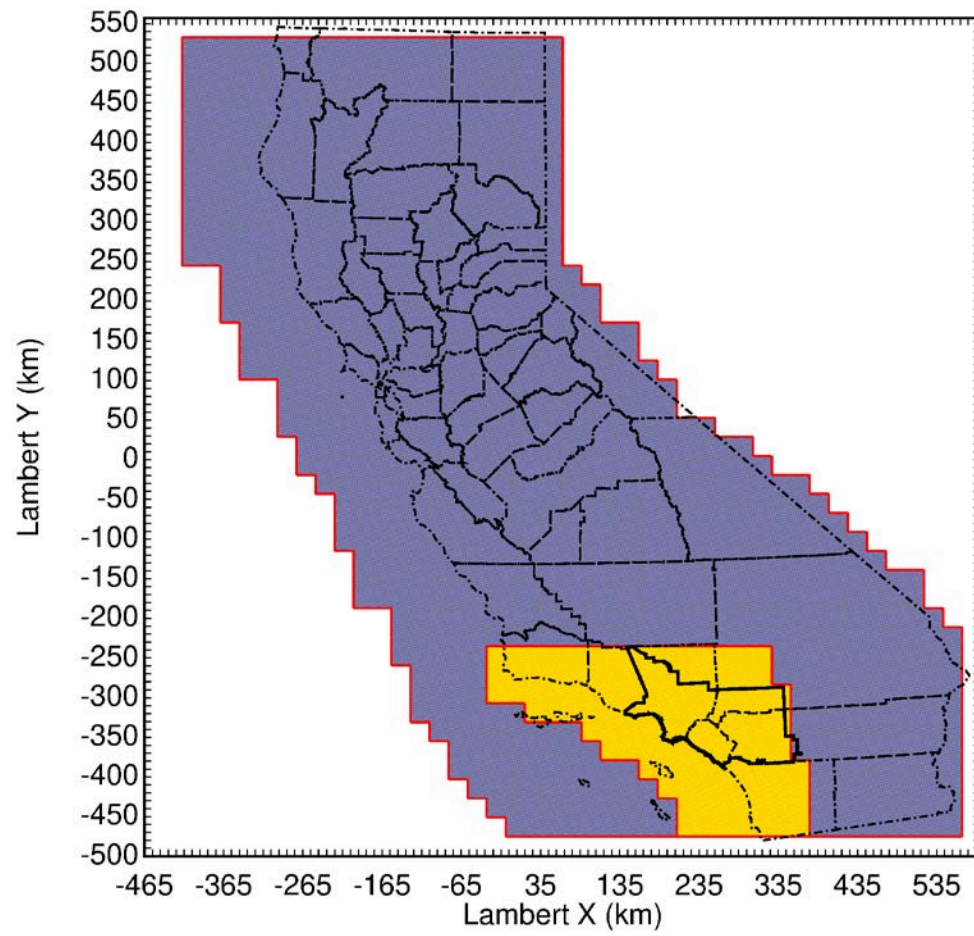


Figure S3.2: 3rd highest MD8H O_3 in GHGai Control Step I: NO_x SA, unit: ppb.

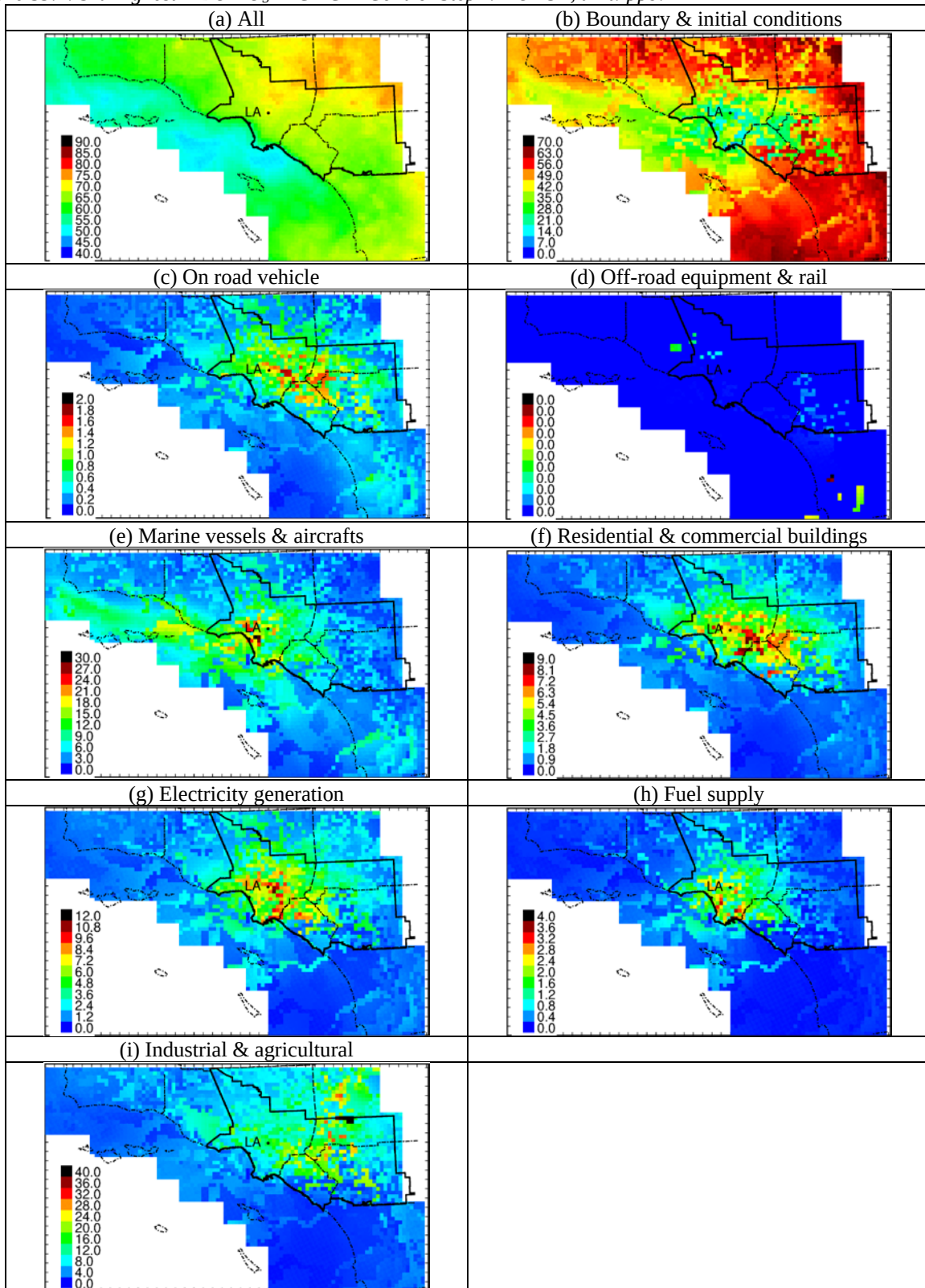


Figure S3.3: 3rd highest MD8H O_3 in GHGai Control Step II: NO_x SA, unit: ppb.

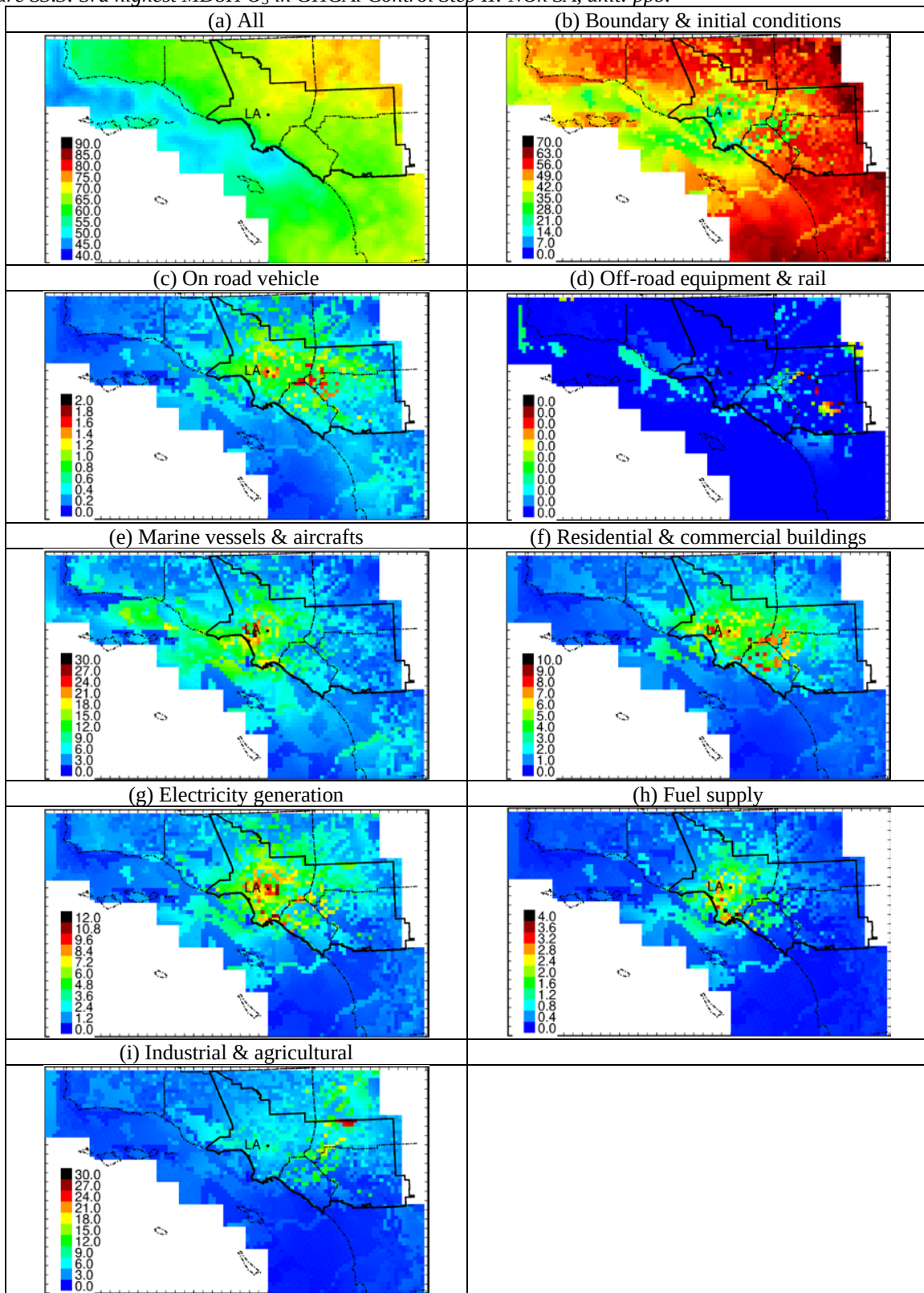


Figure S3.4: 3rd highest MD8H O₃ in GHGai Control Step III: NO_x SA, unit: ppb.

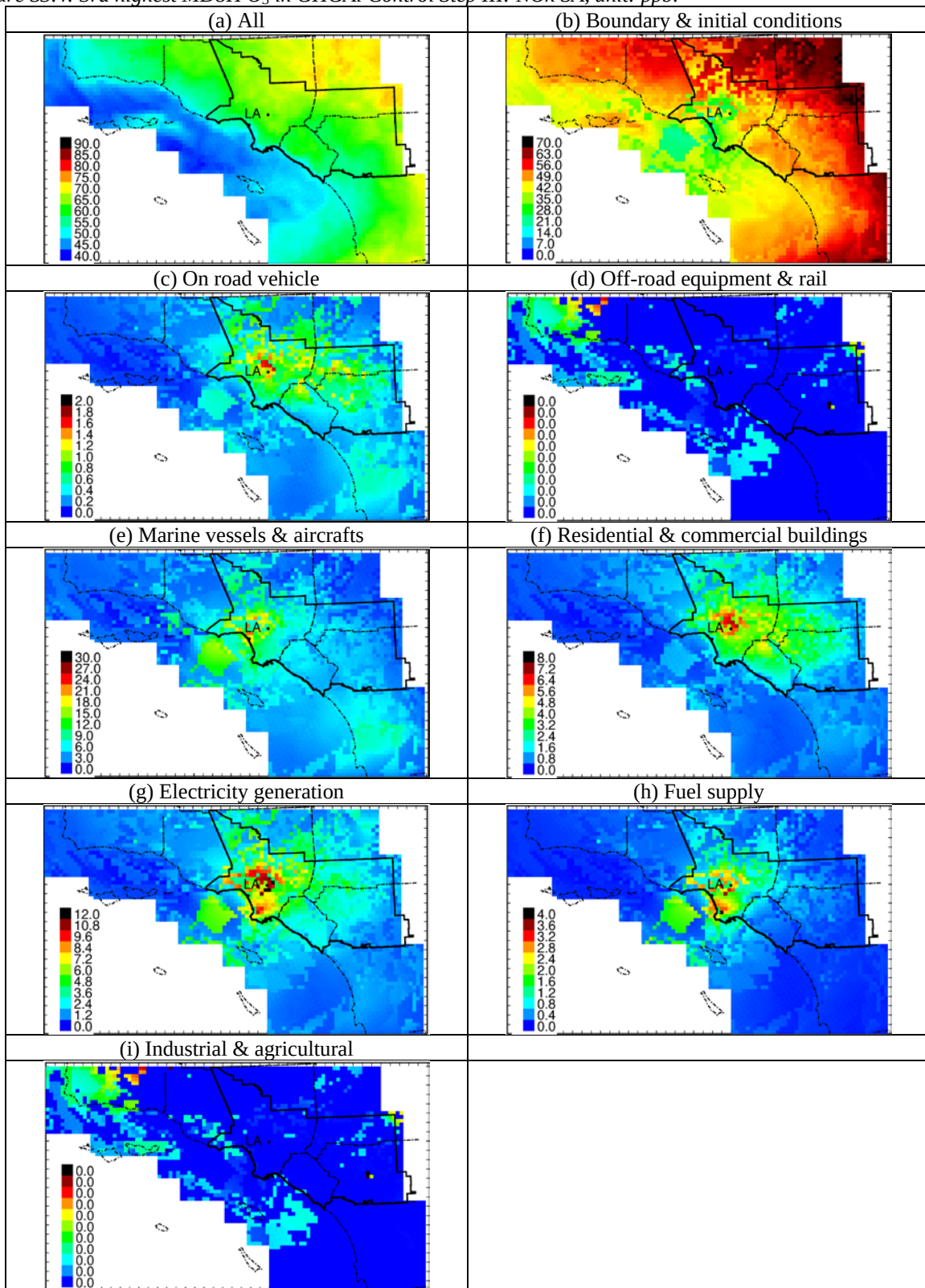


Figure S3.5: 3rd highest MD8H O₃ reductions in different Control Steps, unit: ppb.

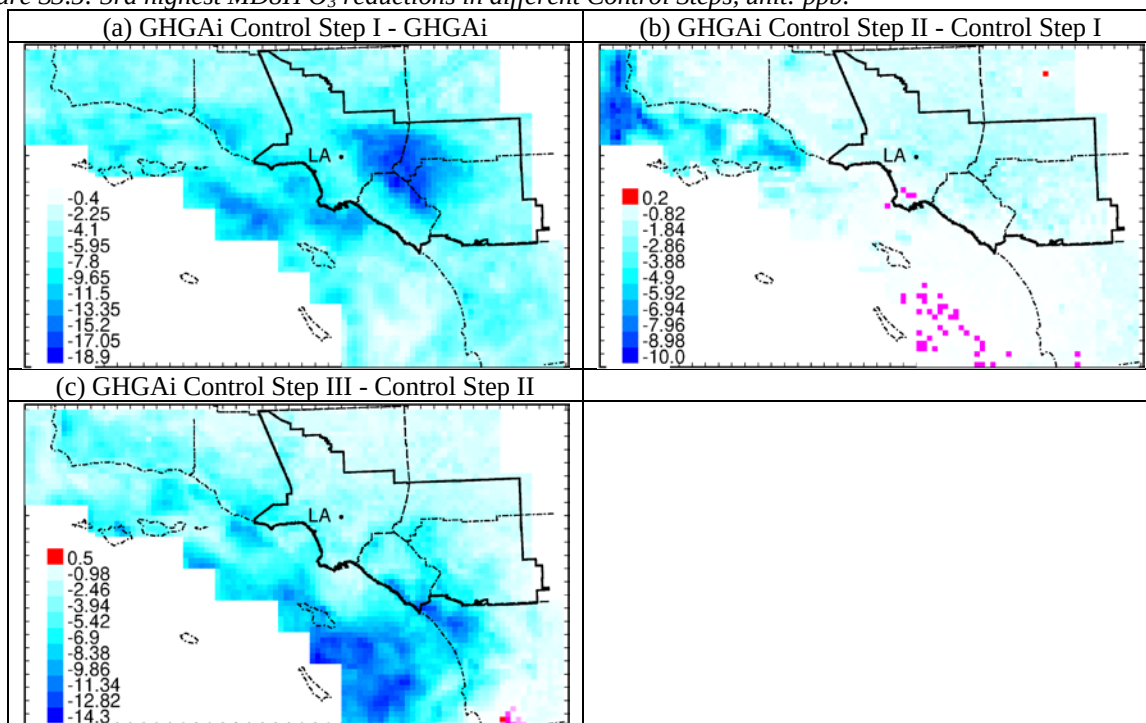


Figure S3.6: 32 weeks averaged MD8H O₃ reductions in different scenarios, unit: ppb.

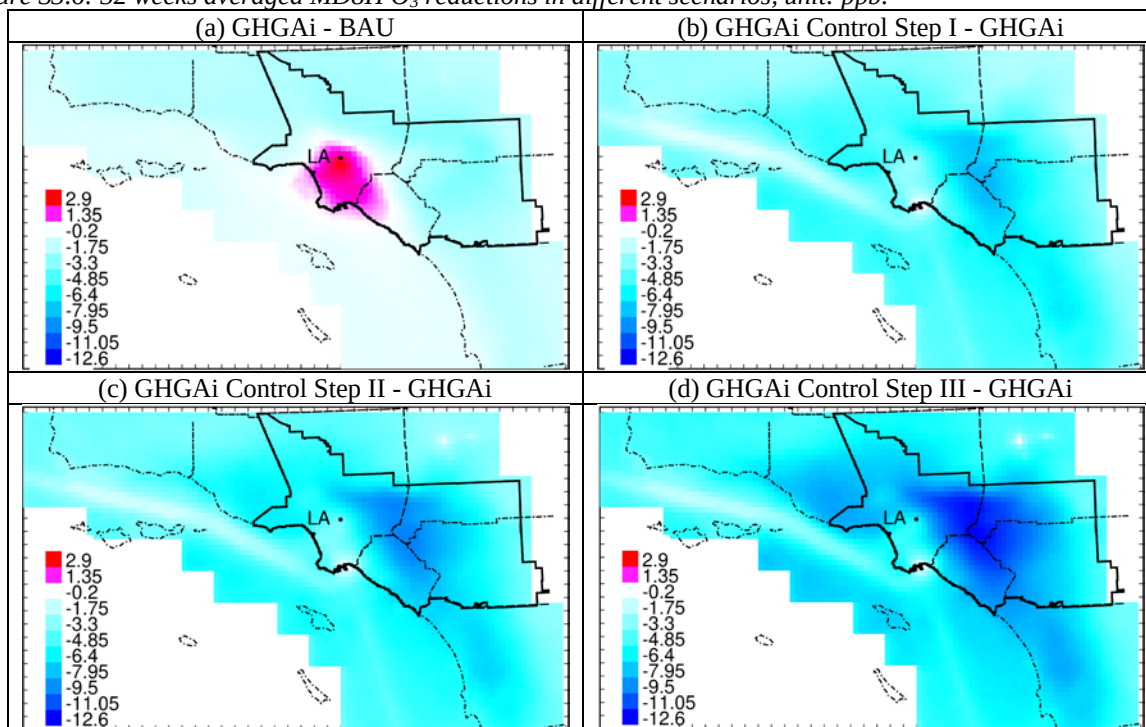
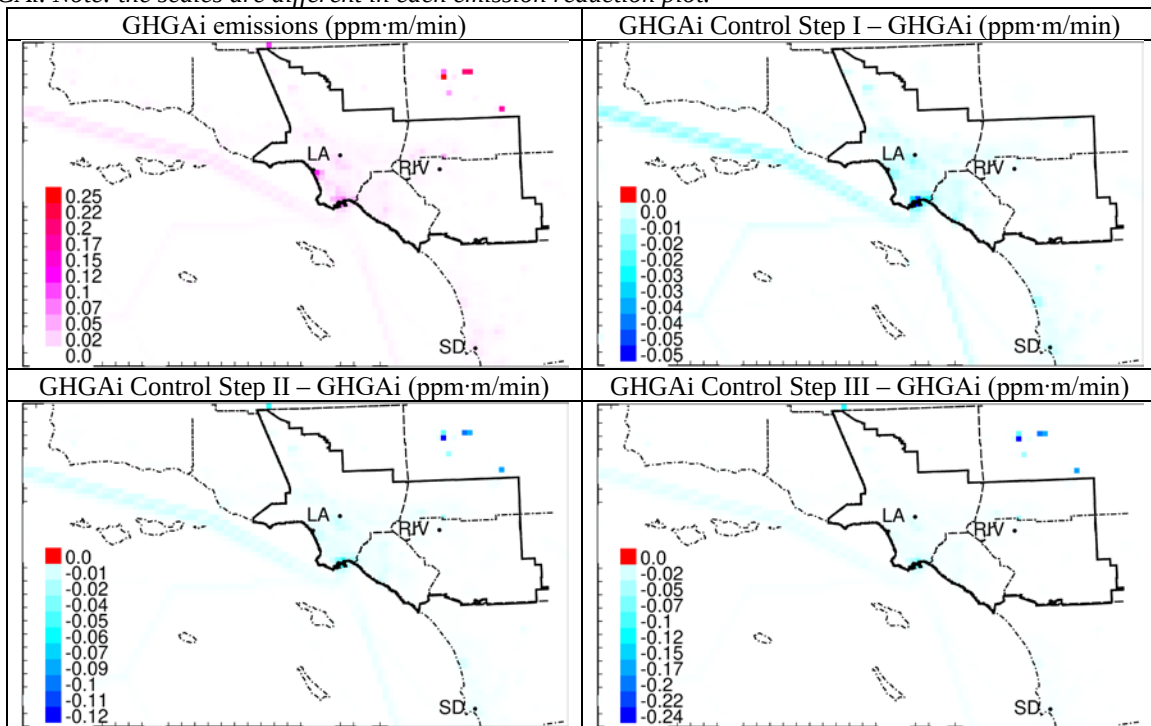


Figure S3.7: Spatial plots of NO_x emissions in GHGAi and the reductions in different Control Steps compared to GHGAi. Note: the scales are different in each emission reduction plot.



Chapter 4 Southern California Ozone Exposure Disparities under Different Emissions Control Strategies in a Low-Carbon Future

4.1. Introduction

Despite decades of control efforts, ambient air pollution persists as one of the greatest environmental threats to global human health, causing an estimated 4.2 million premature deaths in 2019 alone (World Health Organization, 2022). In the United States, concentrations of criteria air pollutants have declined significantly over the past five decades, bringing most of the U.S. territories into compliance with National Ambient Air Quality Standards (NAAQS). Despite this progress, residual air pollution problems exist, and they do not affect all U.S. residents equally, especially for ground-level ozone (O₃) (Collins et al., 2022; Miranda et al., 2011; Pope et al., 2016). In 2023, the national average of Fourth Daily Max 8-hour O₃ was 69 ppb among 484 national sites, with a maximum value of 107 ppb, and with 189 sites exceeding the 70-ppb NAAQS (U.S. EPA, 2024a). The spatial pattern of air pollution combined with historical housing practices and present-day socio-economic factors results in higher air pollution exposures in minority communities, causing environmental disparities including higher health risks (Anderson et al., 2018; Bluhm et al., 2022; Cushing et al., 2015; Lane et al., 2022; Jiawen Liu et al., 2021; Miranda et al., 2011; Morello-Frosch et al., 2002; Tessum et al., 2021).

Many studies have emphasized that environmental justice (EJ) must be considered when new air quality control strategies are designed (Anderson et al., 2018; Boyce and Pastor, 2013; Gallagher and Holloway, 2022; Mitchell et al., 2015; Morelli et al., 2019; Picciano et al., 2023; Yuzhou Wang et al., 2023). This is especially important for California, as a state with the second highest racial diversity index in the U.S. (U.S. Census Bureau, 2021). EJ has been defined by the United States Environmental Protection Agency (US EPA) as the fair treatment and meaningful engagement of all people, regardless of income, race, color, national origin, tribal affiliation, or disability, during the process of agency decision-making and any federal activities that could impact human health and the environment (U.S. EPA, 2024b). When EJ is

properly incorporated into environmental regulations, people will be fully protected from disproportionate and adverse human health and environment risks and hazards, and have equitable access to a healthy, sustainable, and resilient environment.

Previous studies have focused on EJ analysis of particulate matter (PM), O₃, and nitrogen dioxide (NO₂), but most of these studies focus on past years (Bravo et al., 2016; Colmer et al., 2020; Kheirbek et al., 2013; Li et al., 2022a; Mitchell and Dorling, 2003). A few studies look at the future EJ, but only for PM (Li et al., 2022b; Luo et al., 2022; Picciano et al., 2023). Meanwhile, many studies have analyzed the impact of certain emission sources and locations on EJ (Do et al., 2021; Goodkind et al., 2019; Houston et al., 2004; Li et al., 2022b; Nguyen and Marshall, 2018; Shah et al., 2020; Thind et al., 2019), but these studies generally didn't use source apportionment methods to identify sources of O₃ exposure disparities. Wang et al. (2022) used a source-receptor matrix in their model to estimate the optimized emission sectors for reduction to minimize the PM_{2.5} exposure disparities, but their model was not able to predict O₃ (Tessum et al., 2017). More studies are needed to explore future O₃ exposure disparities and disparity reduction strategies.

California is transitioning to low carbon fuels in direct response to climate change, but these measures will also influence concentrations of traditional air pollutants such as O₃. The regulations and bills designed to reduce greenhouse gas (GHG) emissions 80% below 1990 levels by the year 2050 (California Air Resources Board, 2006) will also reduce concentrations of NO+NO₂ (=NO_x), which is a precursor to O₃ formation. O₃ chemistry is complex and nonlinear, meaning that NO_x reductions in urban cores can lead to higher O₃ concentrations (Wu et al., 2024, 2022; Zapata et al., 2018a; Zhao et al., 2024). However, previous studies have shown that the majority of VOC emissions in Southern California that contribute to O₃ formation are biogenic emissions (Pfannerstill et al., 2024; Wu et al., 2024; Zhao et al., 2024), which makes it difficult to control O₃ by reducing VOC emissions. To avoid the increased O₃ due to NO_x reductions, a deep cut in NO_x emissions would be necessary, i.e. greater than 40% as suggested by Wu et

al. (2024). Supplemental controls were designed to offset this unintended increase in O₃ concentrations for the year 2050 (Zhao et al., 2024) but the EJ aspects of these strategies need further study.

Here we analyze the environmental disparities related to O₃ and NO₂ exposures for the year 2050 after the adoption of low carbon energy and supplemental measures (Li et al., 2022b; Zapata et al., 2018a) that were previously established in Zhao et al. (2024) to achieve compliance with the O₃ NAAQS in the South Coast Air Basin (SoCAB). We also analyze the environmental disparities for historical periods between 2000-2019 for comparison. We use a 3-D chemical transport model (CTM) to simulate the air quality for the past two decades and future scenarios with reduced GHG emissions (Li et al., 2022b; Zapata et al., 2018a). An O₃ source apportionment technique is applied to help design supplemental O₃ control strategies that can achieve compliance with the O₃ NAAQS in the future. Exposure disparities under each future scenario are analyzed for race/ethnicity groups defined by the American Community Survey (ACS). The issues that cause residual exposure disparities are discussed and future strategies to reach exposure equity for all race/ethnicity groups are explored.

4.2 Methodology

4.2.1 Air quality simulations

4.2.1.1 Model description

Air quality fields were simulated using the University of California Davis/California Institute of Technology (UCD/CIT) air quality model. The UCD/CIT model is a research CTM model that has robust model performance statistics (Hu et al., 2015; Venecek et al., 2019, 2018b; Ying et al., 2008; Yu et al., 2019; Zhao et al., 2022). In the current study, the UCD/CIT model was configured with a flexible O₃ source apportionment technique that enables O₃ tagging for NO_x and VOC sources (Zhao et al., 2022). The source tagging technique can quantify the contributions of emissions from different geographical regions to concentrations in other geographical regions (Ying and Kleeman, 2006) or emissions from different source sectors to the concentrations at receptor locations (Cohan and Napelenok, 2011; Ying et al., 2004). In this study, we only analyzed the contributions of emissions from different source sectors. The SAPRC11 chemical mechanism (Carter and Heo, 2013) was used to describe the gas-phase chemical reactions in the UCD/CIT model. Previous studies show that SAPRC11 has superior performance when predicting O₃ in California compared to SAPRC16 (Venecek et al., 2018a), which is very similar to the most recent SAPRC22 mechanism. The SAPRC11 chemical mechanism was configured two ways, one way enabling O₃ apportionment from NO_x sources (NO_x SA) and the second way enabling O₃ apportionment from VOC sources (VOC SA). NO_x SA tags the nitrogen atom in NO_x and NO_x reaction products, including NO₃, N₂O₅, HNO₃, HNO₄, PAN, etc. VOC SA tags the odd oxygen in all VOC species. Both methods tag the species involved in the primary photolytic cycle, including O³P, O¹D, and O₃.

4.2.1.2 Simulation domain and periods

Air quality was simulated for two domains that covered the state of California with a resolution of 24 km, and Southern California with a resolution of 4 km (Figure S4.1). This study focuses on the 4-km Southern

California domain. Simulations were conducted over three 10-year periods. The first two periods from 2000 to 2009 and 2010 to 2019 establish a historical context for air pollution exposure in California. The future 32-week period spans from 2046 to 2055 to analyze upcoming air quality issues and to develop effective control strategies. The sample subset of 32 weeks (Figure 4.1) was randomly selected from 2046 to 2055 to properly represent inter-annual variability associated with the El Nino Southern Oscillation (ENSO) cycle, which is the dominant mode of inter-annual climate variability that affects regional climate and air quality in California (Lin et al., 2015; Xu et al., 2017; Zhang et al., 2012). Eight weeks were selected in each of the four seasons to ensure representative coverage throughout the year, with each week having extra four days for spin-up time (total of 11 days simulated for each week). This sampling approach characterizes both the long-term average and the variability (Table S4.1) in pollutant concentrations, yielding standard deviations (std_devs) of BAU and GHGAI concentrations under RCP8.5 that are comparable with the std_devs of concentrations predicted for the years 2010-2019. The approach balances accuracy with computational efficiency that avoids simulating every day in the 10-year window. The uncertainty associated with this 32-week sampling approach is discussed in the following section.

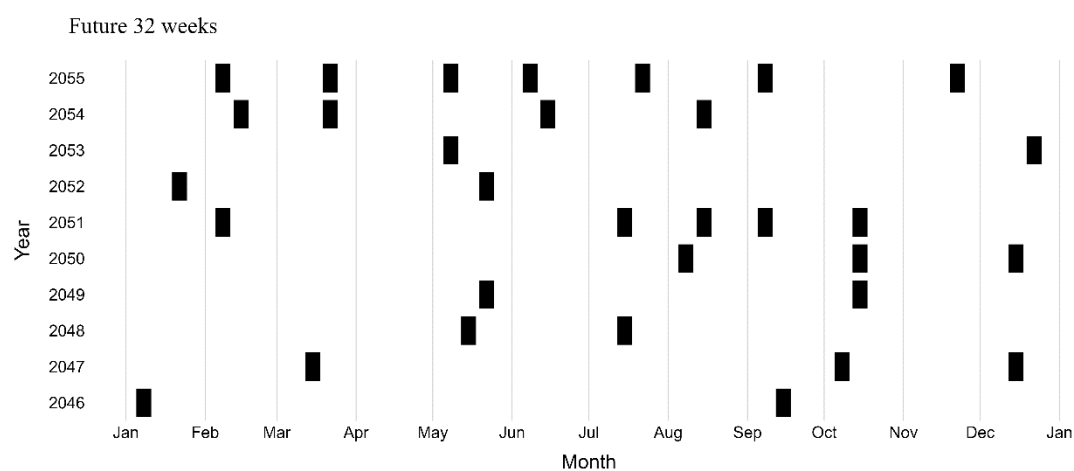


Figure 4.1: Selected 32 weeks during the 10-year period. Each black bar indicates a selected week.

4.2.1.3 Meteorological fields

Meteorology inputs for the CTM were generated by the Weather Research and Forecasting (WRFv3.4) model. The periods 2000-2009 and 2010-2019 used initial/boundary conditions from NCEP North American Regional Reanalysis (NARR) (National Centers for Environmental Prediction et al., 2005). The future 32-week period used initial/boundary conditions from the Community Earth System Model (CESM) (Research Data Archive et al., 2011) under the representative concentration pathway (RCP) 8.5, an upper-bound high GHG-emissions scenario, and the intermediate RCP4.5 scenario described by the Intergovernmental Panel on Climate Change (IPCC). The RCP8.5 was chosen as the focus of this study to analyze worst-case climate scenario for the feasibility of O₃ control strategies. A recent study has shown that RCP8.5 is the best match to the midcentury under current policies (Schwalm et al., 2020). The RCP4.5 sensitivity study was used in combination with two California emissions scenarios to analyze the impacts of alternative climate scenarios on EJ. Four-dimensional data assimilation (FDDA) was used in 2000-2009, and 2010-2019 periods, but not in the future 32-week period. The FDDA used the NCAR ADP observation database (National Centers for Environmental Prediction et al., 2004a, 2004b, 1980a, 1980b) with the global CFSR model data (Saha et al., 2014, 2010) quality control checked as background.

4.2.1.4 Emissions

Five future emission scenarios for criteria pollutants in the state of California were simulated in this study (see Table 4.1). Emissions in each scenario were grouped into nine source sectors: “tire and break wear”, “on road vehicles”, “off-road equipment and rail”, “marine vessels and aircraft”, “residential and commercial buildings”, “electricity generation”, “fuel supply”, “industrial and agricultural”, and “biogenic emissions”. Two emission scenarios, “business-as-usual” (BAU) scenario and “greenhouse gas reduction” (GHGAi) scenario were previously constructed using the energy-economic optimization model, CA-TIMES, combined with the California Regional Multisector Air Quality Emissions (CA-REMARQUE_v1.0) model (Li et al., 2022; Zapata et al., 2018b). In the BAU scenario, GHG emissions are reduced to 1990 levels. In the GHGAi scenario, GHG emissions are reduced 80% below 1990 levels

in the most economical manner possible in order to achieve California’s climate goal (California Air Resources Board, 2006). Each GHG emissions scenario was translated to a criteria pollutant emissions scenario using CA-REMARQUE. Three additional criteria pollutant control scenarios were constructed based on the GHGAi scenario in order to reduce O₃ concentrations in SoCAB in the year 2050 to comply with the O₃ NAAQS (Zhao et al., 2024). The three GHGAi control scenarios reduced the emissions cumulatively, with GHGAi_ControlStepI being least stringent and GHGAi_ControlStepIII being most stringent. GHGAi_ControlStepI reduced 100% of all pollutant emissions from “off-road equipment & rail” by assuming adoption of clean energy that has zero emissions, and 80% NO_x emissions from “marine vessels” in compliance with the International Convention for the Prevention of Pollution from Ships (MARPOL) Annex VI Tier III standard. In addition to the emission reductions in GHGAi_ControlStepI, GHGAi_ControlStepII further reduced 50% of the NO_x emissions from “industry and agriculture” through the adoption of low-NO_x engines. GHGAi_ControlStepIII used more clean energy and applied more aggressive controls than the previous two control measures, with 100% of all pollutant emissions eliminated from “off-road equipment & rail”, 90% of the NO_x emissions eliminated from “marine vessels”, and 100% of the NO_x emissions eliminated from “industry and agriculture”. All five future emission scenarios were analyzed under meteorology from the RCP8.5 scenario, while the BAU and GHGAi emission scenarios were additionally analyzed under the RCP4.5 climate scenario as a sensitivity study. Hereafter, all mention of “BAU” and “GHGAi” refers to the BAU and GHGAi scenarios coupled with RCP8.5 unless otherwise noted. Figure S4.2 and Figure S4.3 show the annual average NO_x and NMVOC emissions (tons per day) in GHGAi and the reductions in different Control Steps compared to GHGAi. Table S4.2 shows the population weighted annual total emissions (tons per year) in LA and SD under GHGAi and the percentage of change in different Control Steps compared to GHGAi. Anthropogenic emissions during the 2000-2009 and 2010-2019 historical periods were generated using the Sparse Matrix Operator Kernel Emissions (SMOKEv3.7) modeling system with the California Air Resource Board (CARB) emission inventories. Biogenic emissions for the three 10-year

periods were generated using the Model of Emissions of Gases and Aerosols from Nature (MEGANv2.1) based on daily meteorological inputs from WRF.

Table 4.1: Regulatory Compliance Future Emission Scenario description.

Scenario	Description
BAU	A “business-as-usual” case where greenhouse gas emissions in 2020 are reduced below 1990 levels but no more constraints beyond 2020 under current California’s regulations
GHGAi	A climate-friendly greenhouse gas reduction case that achieved California’s climate goal of 80% reduction of GHG emissions relative to 1990 levels by the year 2050 with adoption of advanced technologies and renewable energies
GHGAi_ControlStepI	An emission reduction scenario based on GHGAi scenario that reduced 100% of all pollutant emissions from “off-road equipment & rail” and 80% NOx emissions from “marine vessels”
GHGAi_ControlStepII	An emission reduction scenario based on GHGAi scenario that reduced 100% of all pollutant emissions from “off-road equipment & rail”, 80% NOx emissions from “marine vessels”, and 50% NOx emissions from “industry and agriculture”
GHGAi_ControlStepIII	An aggressive emission reduction scenario based on GHGAi scenario that reduced 100% of all pollutant emissions from “off-road equipment & rail”, 90% NOx emissions from “marine vessels”, and 100% NOx emissions from “industry and agriculture”

4.2.1.5 Initial and boundary conditions

Predictions from the Model for Ozone and Related chemical Tracers (MOZART) for 2000-2015 and the Community Atmosphere Model with Chemistry (CAM-chem) for 2016-2019 were used as the initial and boundary conditions for air quality simulations from 2000-2019. For the year 2050, we assumed that the initial and boundary conditions would be similar to current conditions adjusted for seasonality. Therefore, initial and boundary conditions for 2046-2055 used MOZART predictions for the same day of the year in the range 2000-2009.

4.2.2 Environmental disparity

Race and ethnicity information was obtained from the American Community Survey (ACS) 2012-2016 dataset (U.S. Census Bureau, 2020) that includes Black and African Americans (Black), Hispanic or Latino (Hispanic), Asian, and non-Hispanic or non-Latino White (White) people at the census tract level. Figure S4.4 shows the two geographic regions in Southern California used in this calculation: Los Angeles (LA) and San Diego (SD). The population data by race/ethnicity group in the LA and SD regions is shown in Table S4.3. Estimates of changing future demographics are highly uncertain, and so present-day population demographics are used for all calculations.

Environmental disparity was calculated using population weighted average concentrations for 4KM results for two air pollutants: maximum daily 8-hour average (MD8H) O₃ and 24 hour-averaged (24hr-avg) NO₂. The population weighted average is a good proxy for the exposure for a whole race/ethnicity group and enables racial equity comparison (Gallagher and Holloway, 2022; Lane et al., 2022; Li et al., 2022b; Liu et al., 2021; Picciano et al., 2023; Tessum et al., 2021; Yifan Wang et al., 2023). This approach does not consider the total numbers of exposed people in each race/ethnicity group since each race/ethnicity group should be treated fairly, regardless of size. Both pollutants were averaged across 2000-2009 (2000-2009_avg), 2010-2019 (2010-2019_avg), and future 32 weeks under different emission scenarios. Average pollutant exposures for each race/ethnicity group were calculated using the equation:

$$C_{pop-wgtd}^k = \frac{\sum_{(i,j)=(1,1)}^{(imax,jmax)} C_{i,j} P_{i,j}^k}{\sum_{(i,j)=(1,1)}^{(imax,jmax)} P_{i,j}^k}$$

Where: $C_{pop-wgtd}^k$ is the population weighted concentration for race k . $C_{i,j}$ is the average pollutant concentration at grid location (i,j) . $P_{i,j}^k$ is the population data at grid location (i,j) for race k .

$(imax,jmax)$ is the maximum value for grid location (i,j) . Based on historical simulations conducted for the 10-year window between 2010-2019, the uncertainty (Table S4.4) in predicted population-weighted concentrations of O₃ and NO₂ associated with the 32-week simulation strategy in Los Angeles

would be ± 1.8 ppb and ± 0.71 ppb, respectively. As discussed below, the actual uncertainty in the disparity calculations is even smaller than this value.

Once population-weighted concentrations were tabulated, the relative environmental disparity for each race/ethnicity group was then calculated as:

$$RD^k = \frac{C_{pop-wgtd}^k - C_{pop-wgtd}^{All}}{C_{pop-wgtd}^{All}} \times 100\%$$

Where: RD^k is the relative disparity for race k . $C_{pop-wgtd}^k$ is the population weighted concentration for race k . $C_{pop-wgtd}^{All}$ is the population weighted concentration for all race/ethnicity groups combined. The uncertainty introduced by the 32-week simulation strategy in Los Angeles is minor because all race/ethnicity groups are affected approximately equally by the meteorological variability that affects total population exposures. The maximum exposure disparities associated with the 32-week simulation approach for O_3 and NO_2 are estimated to have an uncertainty of 0.11 ppb and 0.12 ppb, respectively, based on historical simulations between 2010-2019 over Los Angeles.

4.2.3 Threshold for healthy air

In addition to the environmental disparities, we also analyzed the percentage of people living in each study area that experienced unhealthy O_3 or NO_2 concentrations. The O_3 health threshold was set to 35 ppb based on a statistical analysis for respiratory mortality ($P=0.002$) and circulatory mortality ($P=0.07$) (Turner et al., 2016). The NO_2 health threshold was set to 4.6 ppb as suggested by the latest World Health Organization (WHO) global air quality guidelines (AQG) (World Health Organization, 2021). The AQG level is the long-term concentration of the pollutant that will generate minimal relevant health outcome. The WHO determined the lowest level of exposure based on the 5th percentile of the exposure distribution from previous studies. The average of the five lowest 5th percentile levels were used as the NO_2 AQG level ($8.8 \mu\text{g}/\text{m}^3 = 4.6$ ppb for NO_2 at 1 atm and 273.15 K).

The percentage of people experiencing unhealthy air quality was calculated as the number of people exposed to O₃ or NO₂ concentrations above the healthy limit divided by the total number of people in the study region.

4.2.4 Additional experiments to reduce disparity

Residual O₃ and NO₂ exposure disparities under the three GHGAi+control scenarios will be further explored using “brute force” reductions targeted at dominant sources upwind of the affected populations. During this process, the feasibility of the “brute force” reductions will not be discussed, as the main purpose is to verify the effectiveness of the O₃ source apportionment tool for disparity reduction.

4.3 Results and discussion

4.3.1 Model performance for 2000-2009 and 2010-2019 periods

The performance of the WRF model for temperature, wind, and relative humidity (Table S4.5) is consistent with a previous long-term air pollution modeling study in California (Hu et al., 2014a). Mean fractional bias (MFB) of temperature and wind are generally within ± 0.15 . root mean square errors (RMSE) of temperature are generally lower than 4 °C, and RMSE of wind are generally lower than 2 m/s.

Table 4.2: Model performance statistics of MD8H O₃ at selected EPA sites for 2000-2009 and 2010-2019 periods.

	2000-2009			2010-2019		
	NMB	NME	r	NMB	NME	r
060371103 Los Angeles	5.12%	25.76%	0.778	7.58%	24.44%	0.650
060658001 Riverside	-1.76%	19.95%	0.809	-0.11%	20.28%	0.688
060372005 Pasadena	3.29%	23.89%	0.786	8.18%	20.88%	0.667
060714003 Redlands	2.43%	19.53%	0.829	-1.33%	17.95%	0.756

Table 4.2 summarizes the CTM performance statistics for MD8H O₃ predictions at four selected urban EPA monitoring sites in Figure S4.1 with continuous data for 2000-2009 and 2010-2019 periods. Figure S4.5 and Figure S4.6 show the time series of simulated and observed MD8H O₃ at these monitoring sites for 2000-2009 and 2010-2019 periods. Recommended benchmarks for air quality model performance statistics of MD8H O₃ were taken from Emery et al. (2017). The performance statistics “goals” are Normalized Mean Bias (NMB) < $\pm 5\%$, Normalized Mean Error (NME) < 15%, and Correlation Coefficient (r) > 0.75, which should be viewed as the best a CTM can be expected to achieve. The performance statistics “criteria” are NMB < $\pm 15\%$, NME < 25%, r > 0.50, which should be viewed as the skill that most CTMs routinely achieve. The formulas of these performance statistics are provided in Table S4.4. Of the 24 performance statistics, 10 meet the most stringent “goals” and 13 meet the “criteria”. The only performance statistic that slightly exceeds the criteria is the NME value at Los

Angeles during the 2000-2009 period. Sharp spatial gradients around the Los Angeles monitoring site associated with fresh NO_x emissions may not be fully resolved with the 4km grid resolution used in the current study. The performance statistics for 2010-2019 are slightly degraded compared to the statistics for 2000-2009, possibly because the lower O₃ concentrations in 2010-2019 could cause larger percentage error even if the value of absolute error didn't change. Note that O₃ concentrations are overestimated in 2013 at Los Angeles and Pasadena due to a wildfire event near the two sites. The model calculations might not accurately represent the details of the wildfire plume dynamics or the microscale meteorology during this isolated event, resulting in an overestimation of O₃ concentrations. However, future simulations will not include random and unpredictable wildfire events and so this issue will not influence calculated exposure disparities. Overall, the performance statistics indicate that simulated O₃ concentrations over the historical time period 2000-2019 are accurate, increasing confidence in the future predictions.

NO₂ predictions are in good agreement with observations for the time period 2000-2009 (Figure S4.7) and 2010-2019 (Figure S4.8) with both average values and seasonal trends captured. VOC predictions and measurements for formaldehyde, isoprene, benzene, and toluene in Los Angeles for 2000-2019 (Figure S4.9 and Figure S4.10) also have similar average values and seasonal trends, but VOC measurements have greater variability about the averaged concentrations than model predictions, suggesting that VOC emissions inventories do not fully capture the short-term variability of sources. This issue will not affect calculated exposure disparity for NO₂ and O₃. Further details of the VOC comparison are discussed in SI.

4.3.2 Averaged air quality exposure

Figure 4.2 and Figure 4.3 show the MD8H O₃ and 24hr-avg NO₂ concentrations in Southern California averaged across 2000-2009, 2010-2019, and the 32-week simulation period in 2046-2054 under different future RCP8.5 GHG emission scenarios. MD8H O₃ concentrations significantly increase in the BAU scenario compared to 2000-2009_avg and 2010-2019_avg, while 24hr-avg NO₂ concentrations significantly decrease. For the five future scenarios, both MD8H O₃ and 24hr-avg NO₂ concentrations are

significantly reduced in the three increasingly stringent control strategies. The three GHGAi control steps reduced MD8H O₃ concentrations by as much as 8.6 ppb to 12.6 ppb and 24hr-avg NO₂ concentrations by as much as 13.94 ppb to 35.54 ppb compared to the GHGAi scenario (Figure S4.11 and Figure S4.12). Table S4.6 shows the population weighted O₃ concentration decreases by 9-15% in LA and 12-15% in SD under the GHGAi scenario. The population weighted NO₂ decreases by more than 50% in both LA and SD regions in three supplemental GHGAi control steps. Averaged MD8H O₃ concentrations mainly peak in the north and east portions of SoCAB outside the urban core (Figure 4.2). NO₂ concentrations are elevated across the central SoCAB region compared to the outlying regions in 2000-2009 and 2010-2019, but concentrations decrease for future scenarios, with urban hotspots remaining at the port of Long Beach, port of Los Angeles, and Los Angeles International Airport (LAX) (Figure 4.3).

Figure 4.4 shows the hour 13 Pacific Time HCHO / NO₂ ratio (FNR), corresponding to the typical peak in O₃ concentrations, averaged over 2000-2009, 2010-2019, and the future 32-week simulation periods under a range of RCP8.5 emissions scenarios. The hour 13 FNR value was also used to determine the transition between NO_x-limited and VOC-limited chemical regimes in California (Wu et al., 2022). A transition value of 4.6 has been subtracted from the FNR values and the color key has been adjusted so that VOC-limited regions are blue, NO_x-limited regions are red, and regions in the transition zone between NO_x-limited and VOC-limited chemistry are in white. Both 2000-2009_avg and 2010-2019_avg are VOC-limited across the entire SoCAB. NO_x-limited regions start to appear outside the major urban area in the future emissions scenarios as NO_x emissions are reduced. The VOC-limited regions in the future scenarios shrink significantly as increasingly stringent emissions controls are applied, but the region between downtown LA and the Port of LA remains VOC-limited under all future emission scenarios.

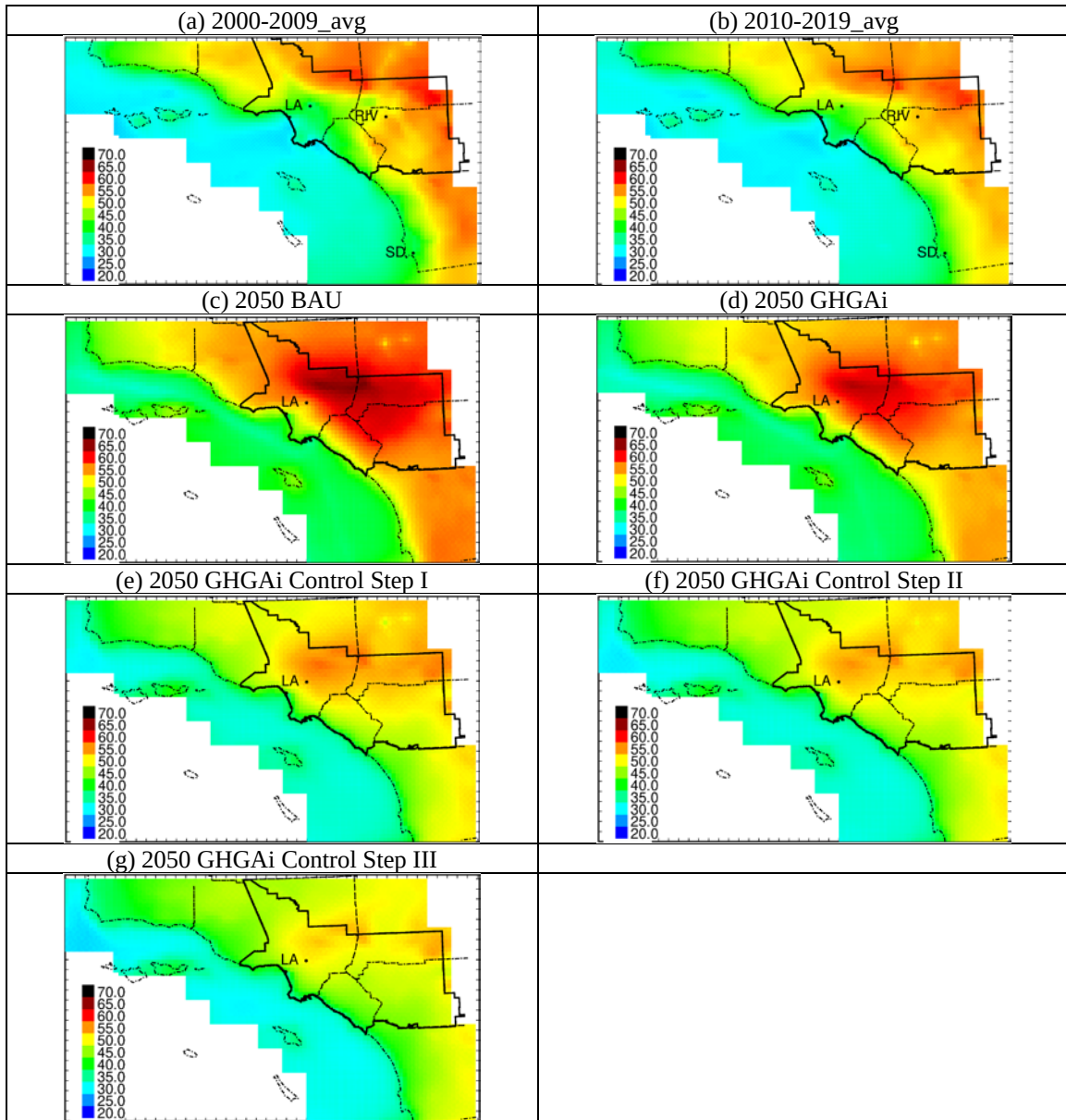


Figure 4.2: MD8H O₃ concentrations averaged across 2000-2009, 2010-2019, and the future 32-week simulation period under RCP8.5. Bold line indicates border of the SoCAB. (All concentrations in units of ppb)

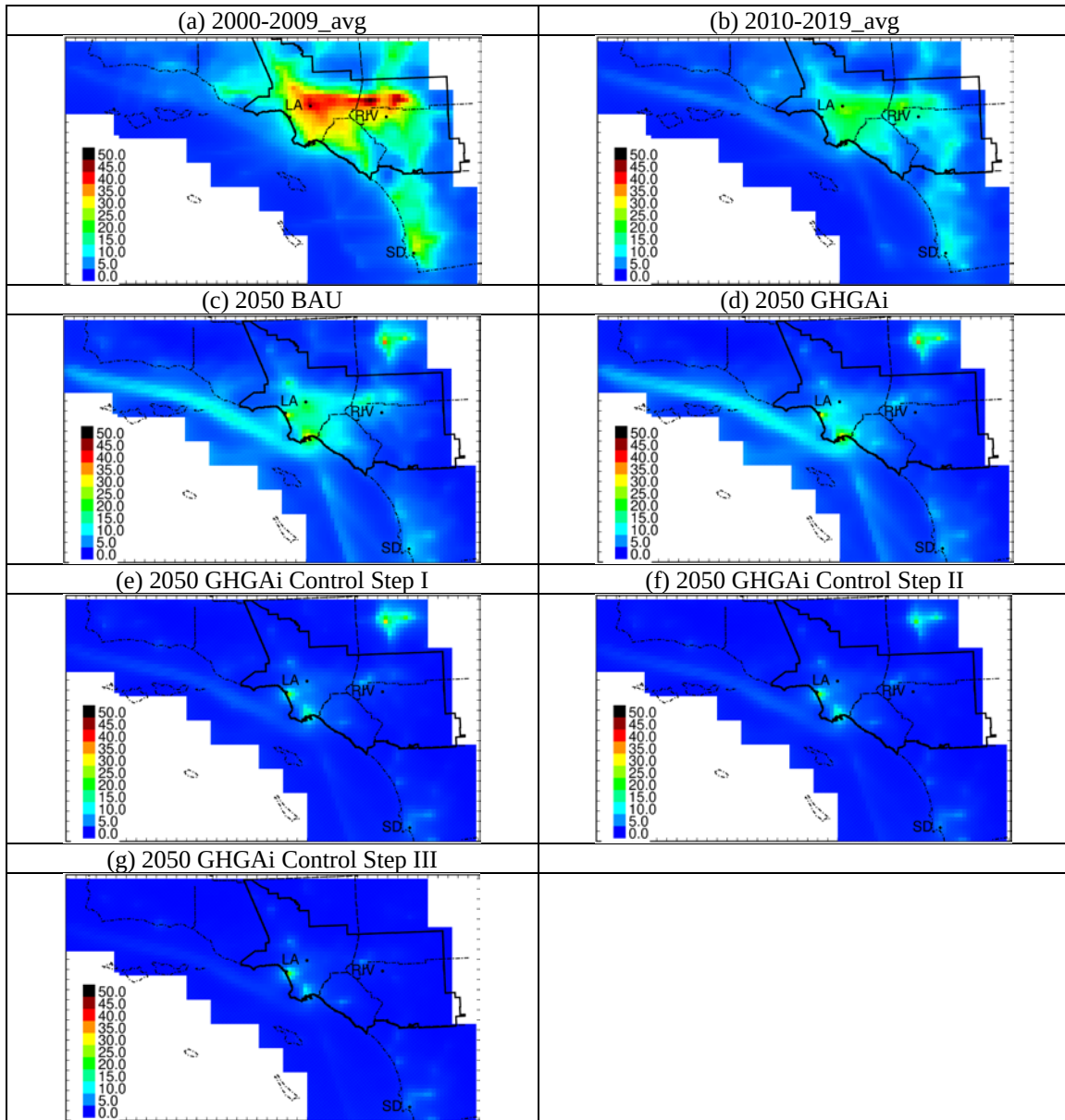


Figure 4.3: 24hr-avg NO_2 concentrations averaged across 2000-2009, 2010-2019, and the future 32-week simulation period under RCP8.5. Bold line indicates border of the SoCAB. (All concentrations in units of ppb)

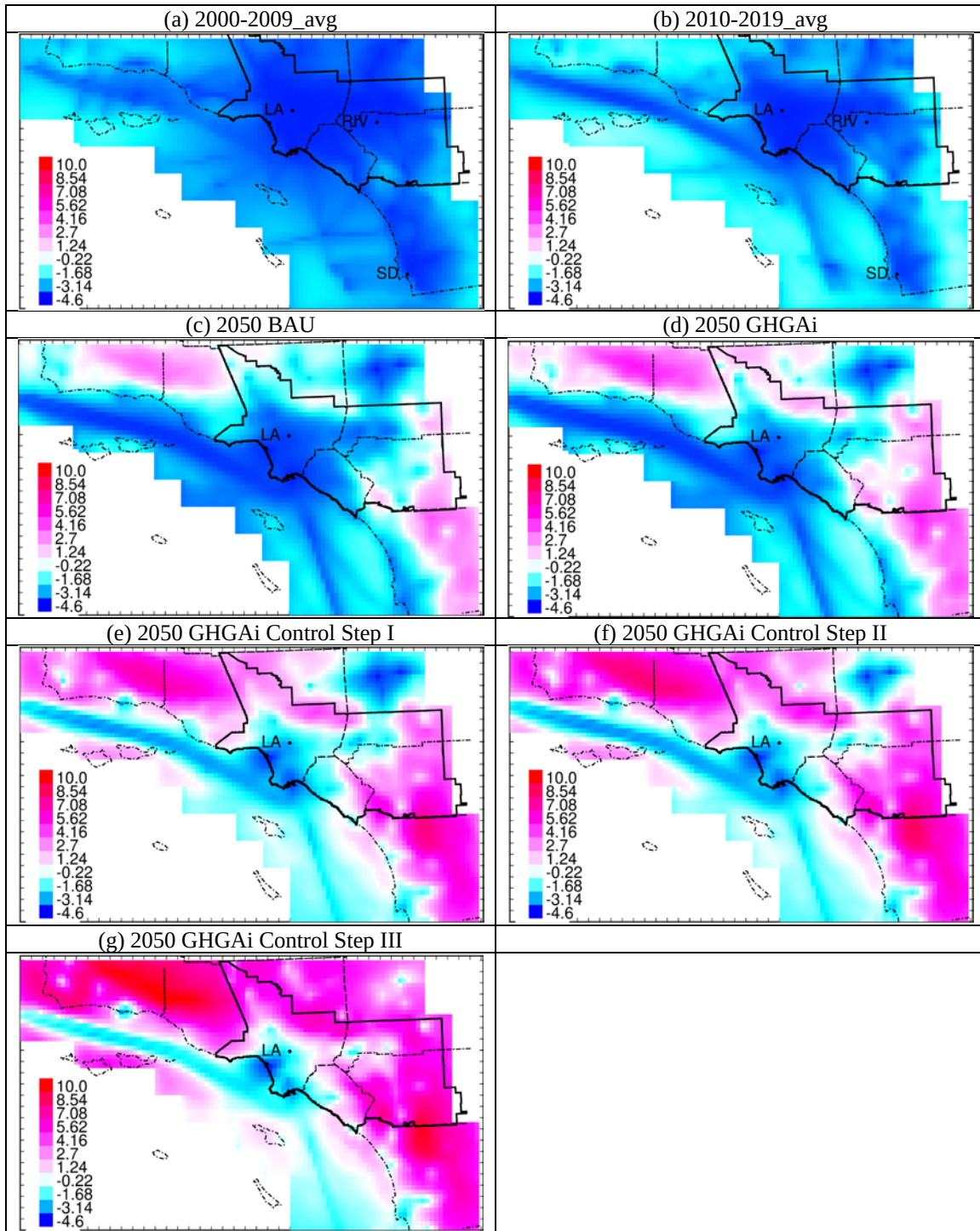


Figure 4.4: Formaldehyde to NO_2 (FNR) ratio at hour 13 averaged across 2000-2009, 2010-2019, and the future 32-week simulation period under RCP8.5. Transition value of 4.6 is subtracted from all values. Blue indicates VOC-limited, red indicates NO_x -limited.

Figure S4.13 shows the population weighted MD8H O_3 , 24hr-avg NO_2 concentrations, and the hour 13

FNR values in LA and SD. Population weighted MD8H O_3 in LA and SD increases 7-11 ppb (~16-27%)

in RCP8.5 BAU and RCP8.5 GHGAI scenarios compared to the 2000-2009_avg and 2010-2019_avg period. MD8H O₃ is reduced by less than 8 ppb (~15%) compared to the GHGAI concentrations in the three future supplemental control scenarios under RCP8.5. The population weighted 24hr-avg NO₂ concentrations in LA are reduced from 29.1 ppb in 2000-2009_avg to 10.2 ppb under RCP8.5 BAU, and then to 1.93 ppb under the GHGAI_ControlStepIII scenario. The population weighted 24hr-avg NO₂ concentrations in SD are reduced from 16.6 ppb in 2000-2009_avg to 5.0 ppb under RCP8.5 BAU, and then to 1.6 ppb under the GHGAI_ControlStepIII scenario. The population weighted FNR values increase, and the chemical regimes become less VOC-limited as the emissions are reduced. However, using a transition FNR of 4.6, the average resident in the LA and SD regions still lives in the VOC-limited chemical regime under all scenarios analyzed in the current study.

Since O₃ concentrations may also be affected by different climate conditions, we compare the MD8H O₃ changes associated with meteorological conditions under constant emissions to MD8H O₃ changes associated with changing emissions under constant meteorological conditions (Figure 4.5). Under the same emission condition, changing from RCP8.5 to RCP4.5 results in MD8H O₃ changes from -2.2 ppb to +2.1 ppb (Figure 4.5(a) and (b)). Under the same meteorological conditions, changing from BAU to GHGAI emissions results in MD8H O₃ changes from -3.9 ppb to +2.9 ppb (Figure 4.5(c) and (d)). Thus, emission changes have an equal or greater impact on ozone concentrations than meteorological changes in Southern California. These results are in agreement with the findings from previous studies that also showed that changes in anthropogenic emissions have greater effect on ozone than climate change (Moghani and Archer, 2020; Steiner et al., 2006; Stowell et al., 2017; Tagaris et al., 2007; Wu et al., 2008).

The relative importance of emissions vs. meteorology depends on the analysis time period, since emissions are in continual decline over time whereas climate change strengthens over time. The current study focuses on the mid-century time period when meteorological conditions under different climate scenarios are still somewhat similar to each other. In our simulations, the 32-week average temperatures

increase by 0.5-1.1 °C across California from RCP4.5 to RCP8.5. It has been reported that the projected global mean surface air temperature for the mid-21st century would increase by 1.0-2.0 °C in average from RCP2.6 to RCP8.5 (IPCC, 2013), which is consistent with our simulations. Therefore, we would expect small perturbations in O₃ concentrations within such small temperature variations in the near future. Meanwhile, predicted reductions in anthropogenic emissions are big enough to surpass the effects of climate change. A similar analysis conducted in the year 2100 would likely show that meteorological conditions under diverging climate pathways will more significantly influence O₃ concentrations, but this analysis is beyond the scope of the current study.

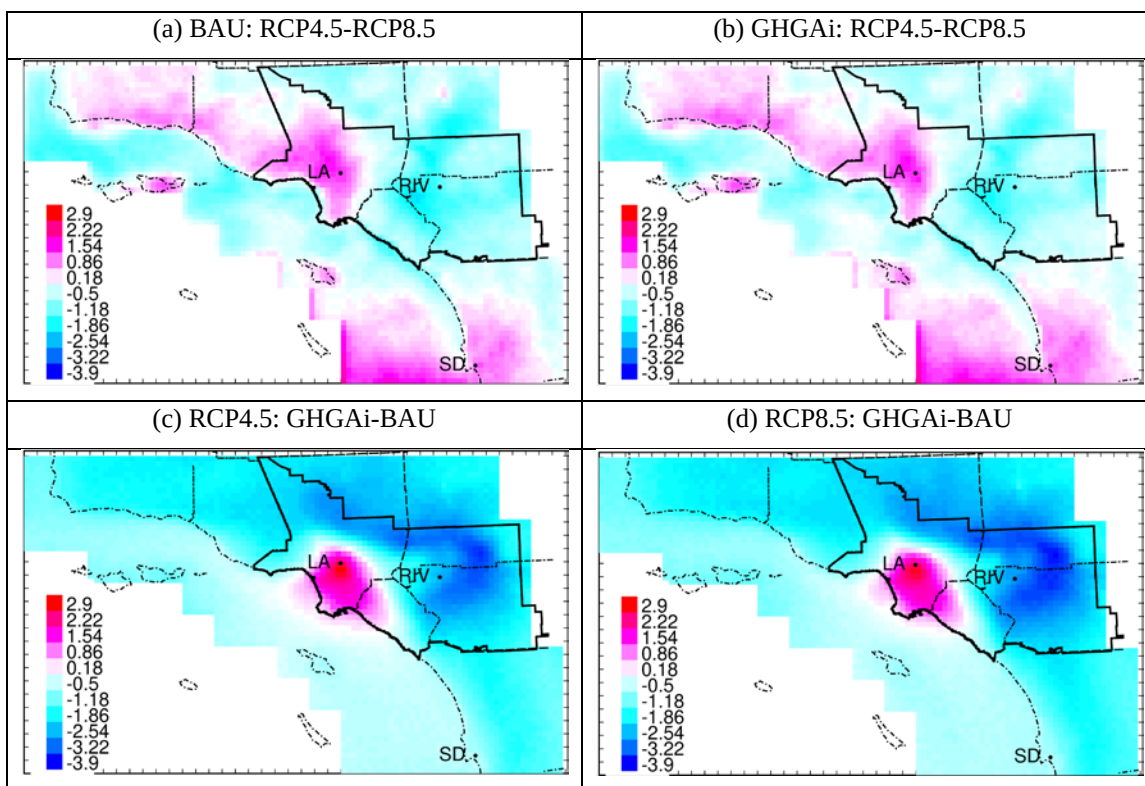


Figure 4.5: Impacts of meteorological and emissions changes on 32-week averaged MD8H O₃ under RCP4.5 and RCP8.5 with BAU and GHGAI emission scenarios.

4.3.3 Environmental disparities

Table S4.7 and Table S4.8 tabulate the calculated population weighted O₃ and NO₂ concentrations and their std_devs for difference race/ethnicity groups under different scenarios. The BAU_avg indicates the average of BAU scenarios under RCP8.5 and RCP4.5, and the GHGAi_avg indicates the average of GHGAi scenarios under RCP8.5 and RCP4.5. The std_devs of future scenarios are comparable to the std_devs of 2000-2009_avg and 2010-2019_avg, with std_devs decreasing with increasingly strict emissions controls. Figure 4.6(a) and Figure 4.7(a) show the relative exposure disparity of MD8H O₃ (left) and the percentage of population that is exposed to healthy/unhealthy levels of O₃ concentrations (right) in the LA and SD regions averaged for different scenarios. Positive disparity values indicate that the race/ethnicity group is exposed to O₃ concentrations above the population average, while negative disparity values indicate that the group is exposed to O₃ concentrations below the population average. Figure 4.6(a) shows that Hispanic or Latino residents in Los Angeles are exposed to above-average O₃ concentrations under all scenarios except 2000-2009_avg (-0.2%), with exposure disparities ranging from 0.5% in 2010-2019_avg to 2.0% under the GHGAi_ControlStepIII. Black and African American residents experience the lowest O₃ concentrations in 2000-2009_avg, 2010-2019_avg, and the BAU_avg scenario, with exposures of 5.1%, 3.8%, and 3.4% below the average, respectively. However, the absolute value of relative O₃ exposure disparity for Black residents decreases under the control scenarios, falling to 2.2% below the average under GHGAi_avg and to 0.1% above the average under GHGAi_ControlStepIII. Asian residents in Los Angeles consistently have absolute values of relative O₃ exposure disparities within 1% of the population average across all scenarios. White residents are exposed to higher-than-average O₃ concentrations in 2000-2009_avg and 2010-2019_avg scenarios, with disparities of 1.7% and 0.3%, respectively. However, White residents are exposed to lower-than-average O₃ concentrations under all future scenarios, with a maximum disparity of -2.5% under the strictest emissions controls. In 2000-2009_avg, 21.6% of Black residents in LA are exposed to MD8H O₃ below 35 ppb, while the ratios for other race/ethnicity groups are approximately 10%. In 2010-2019_avg, 6.4% of White residents in LA

live in areas with MD8H O₃ below 35 ppb, while the ratios for other race/ethnicity groups are approximately 2%. Under all future scenarios, less than 5% of residents in LA from each race/ethnicity group are exposed to MD8H O₃ below 35 ppb.

O₃ exposure disparities are generally smaller in SD compared to LA (Figure 4.7(a) vs. Figure 4.6(a)). Black residents in San Diego are exposed to below-average O₃ concentrations in 2000-2009_avg, but above-average O₃ concentrations in other scenarios. The Black residents always experience the highest absolute values of relative exposure disparities under all scenarios, from 0.5% to 2.1%. Hispanic residents are always exposed to above-average O₃ concentrations. Hispanic residents have the highest O₃ exposure in 2000-2009, but second highest O₃ exposure with disparities ranging from 0.6% to 1.0% in other scenarios. Asian residents are exposed to below-average O₃ concentrations in 2000-2009_avg and 2010-2019_avg, but above-average O₃ concentrations in all future scenarios. Asian residents have the same exposure disparity as Black residents in 2000-2009_avg (-1.1%), but very little O₃ exposure disparity in other scenarios. White residents are exposed to slightly above-average O₃ concentrations in 2000-2009_avg with disparity of 0.1%, but below-average O₃ concentrations in other scenarios with disparities ranging from -0.6% to -0.9% as emissions are reduced under different scenarios. None of the residents of different race/ethnicity groups in SD are exposed to MD8H O₃ below 35 ppb in 2000-2009_avg, 2010-2019_avg, BAU_avg or GHGAi_avg. Under the three GHGAi control scenarios, the percentage of residents exposed to low O₃ concentrations increase from less than 1% to 7%.

Figure 4.6(b) and Figure 4.7(b) show the 24hr-avg NO₂ exposure disparity (left) and the percentage of population that is exposed to healthy/unhealthy levels of NO₂ concentrations (right) in the LA and SD regions averaged for different scenarios. In both LA and SD regions, Black and Hispanic residents are consistently exposed to above-average NO₂ concentrations, while White residents are consistently exposed to below-average NO₂ concentrations. Asian residents are exposed to above-average NO₂ concentrations in 2000-2009_avg and 2010-2019_avg, and below-average NO₂ concentrations in the future GHGAi control scenarios in both LA and SD. For BAU_avg and GHGAi_avg scenarios, the 24hr-

avg NO₂ concentrations for Asian residents are slightly below the average in LA but slightly above the average in SD.

In the LA region, the relative exposure disparities for Black residents increase significantly as the future control strategies to achieve regulatory compliance reduce emissions from off-road sources in outlying areas. The traditional approach that targets the precursors contributing to the highest regional O₃ concentrations are not optimal for reducing exposure disparities in the LA region. Such traditional control measures reduce NO₂ concentrations more slowly for Black residents compared to the regional average reduction. In both LA and SD, the percentages of Black residents exposed to unhealthy 24hr-avg NO₂ concentrations above 4.6 ppb under all scenarios are always highest, followed by Hispanic, Asian, and then White residents. In SD, all the residents are exposed to NO₂ concentrations below 4.6 ppb under the three future traditional control scenarios, indicating that any residual NO₂ exposure disparity will not affect public health.

In both Figure 4.6 and Figure 4.7, the relative disparities under the RCP4.5 BAU and RCP4.5 GHGAI scenarios are very similar to the RCP8.5 BAU and RCP8.5 GHGAI scenarios, respectively. Using the difference between the RCP4.5 and RCP8.5 results, the uncertainties of relative exposure disparities of MD8H O₃ range from 0.03% to 0.17% for Black, 0.05% to 0.22% for Hispanic, 0.07% to 0.65% for Asian, and 0.0003% to 0.08% for White. The uncertainties of relative exposure disparities of 24hr-avg NO₂ range from 0.17 % to 0.53 % for Black, 0.08 % to 0.40 % for Hispanic, 0.21 % to 0.34 % for Asian, and 0.003 % to 0.41 % for White. All the uncertainties of the relative disparities are less than 0.7%. The fractional error for the relative exposure disparities (length of the error bar from the center divided by the absolute mean relative disparity) for the highest exposed groups is less than 18% for MD8H O₃ and 15% for 24hr-avg NO₂. Note that fractional errors cannot be calculated for groups with extremely low (~0) exposure disparities.

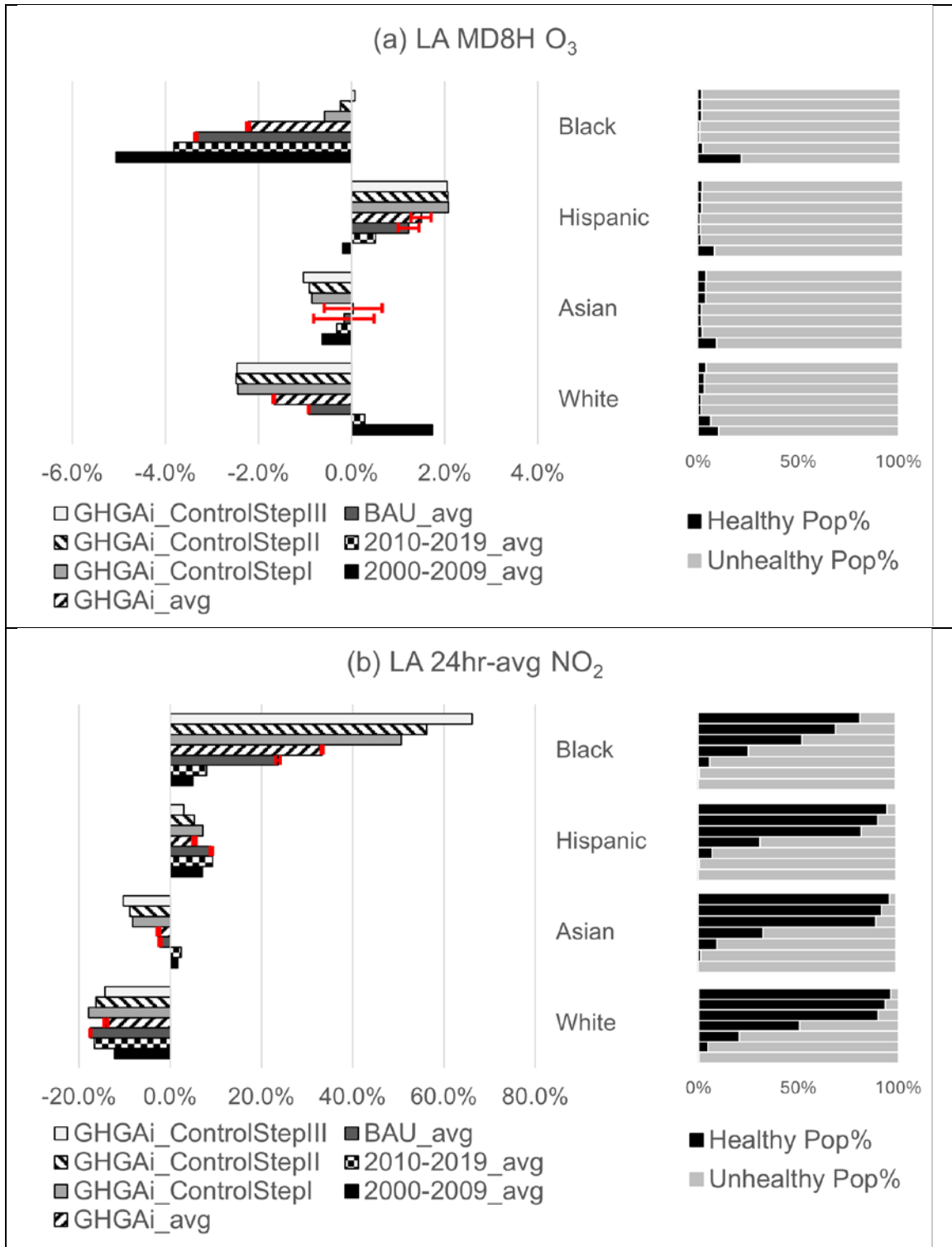


Figure 4.6: Relative disparity of population weighted averaged MD8H O₃ and 24hr-avg NO₂ exposure (left) and percentage of population exposed to healthy/unhealthy concentration levels (right) for different race/ethnicity groups at LA. The red error bars of the BAU_avg and GHGAI_avg indicate the disparities under RCP8.5 and RCP4.5 scenarios.

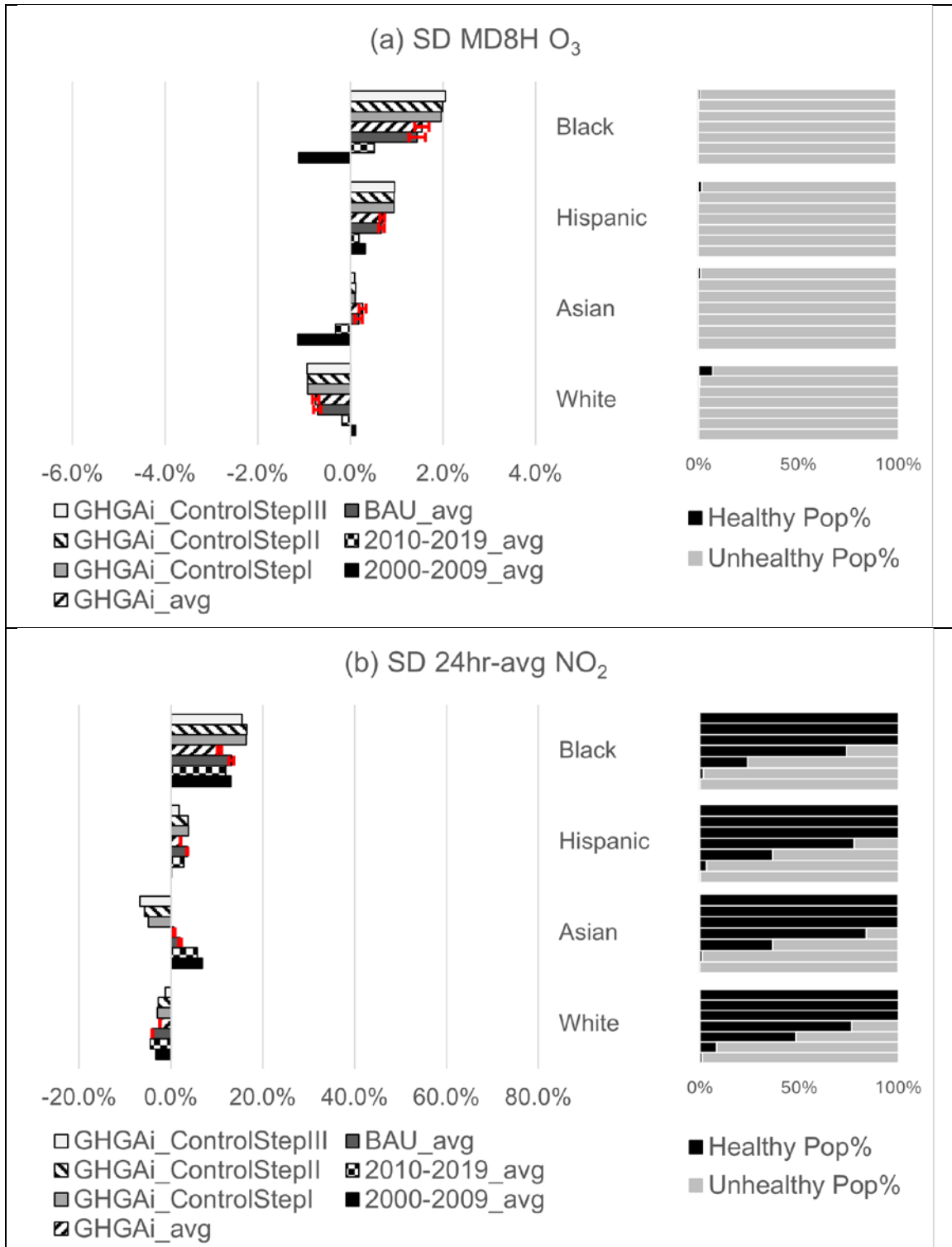


Figure 4.7: Relative disparity of population weighted averaged MD8H O₃ and 24hr-avg NO₂ exposure (left) and percentage of population exposed to healthy/unhealthy concentration levels (right) for different race/ethnicity groups at SD. The red error bars of the BAU_avg and GHGAi_avg indicate the disparities under RCP8.5 and RCP4.5 scenarios.

Table 4.3 shows the maximum relative disparity differences between race/ethnicity groups that have highest and lowest exposure under RCP8.5 and RCP4.5 with BAU and GHGAi emission scenarios. The changes from RCP8.5 to RCP4.5 range from -0.5% to 1.0%, which are relatively small. Overall, the largest relative exposure disparities are not sensitive to the choice of RCP8.5 vs. RCP4.5 climate scenarios.

Table 4.3: Maximum relative disparity differences of MD8H O₃ and 24hr-avg NO₂ exposure between race/ethnicity groups that have highest and lowest exposure under RCP8.5 and RCP4.5 with BAU and GHGAi emission scenarios.

Pollutants	Emission Scenario	Max disparity difference under RCP8.5	Max disparity difference under RCP4.5	Change from RCP8.5 to RCP4.5
LA O ₃	BAU	4.8%	4.4%	-0.4%
	GHGAi	3.9%	3.5%	-0.4%
LA NO ₂	BAU	40.7%	41.6%	-0.9%
	GHGAi	47.7%	47.2%	0.5%
SD O ₃	BAU	1.9%	2.4%	0.5%
	GHGAi	2.1%	2.5%	0.4%
SD NO ₂	BAU	16.7%	17.7%	1.0%
	GHGAi	12.7%	13.5%	0.9%
Note: $Change\ from\ RCP8.5\ to\ RCP4.5 = Max\ Difference_{RCP4.5} - Max\ Difference_{RCP8.5}$				

Figure 4.8, Figure 4.9, and Figure S4.14 through Figure S4.16 illustrate the population maps for different race/ethnicity groups in Southern California overlaid on contour lines for O₃ formation chemical regimes under different future RCP8.5 scenarios. These maps show that Black residents are clustered in urban core regions with lower FNR regions (NOx-rich), while the other race/ethnicity groups live in outlying regions with higher FNR due to lower NOx concentrations. These spatial patterns explain why NOx emissions reductions have different effects on different race/ethnicity groups. Under the RCP8.5 GHGAi scenario, all race/ethnicity groups live in a NOx-rich atmosphere (Figure 4.8). Under the RCP8.5 GHGAi_ControlStepIII scenario, some fraction of the region where Hispanic, Asian, and White residents live transitions to a NOx-limited chemical regime, but the Black residents living between central LA and Long Beach remain in a NOx-rich region (Figure 4.9). Figure S4.17 shows the population weighted FNR centered on 4.6 for different race/ethnicity groups in the LA and SD regions. All race/ethnicity groups

live in VOC-limited regions on average under all control scenarios, with the exception that Asian residents live in NO_x-limited regions on average under the RCP8.5 GHGAI_ControlStepIII scenario. Black and African American residents always live in the most VOC-limited regions under all control scenarios. Figure S4.18 shows the relative disparity of FNR at hour 13 in the LA and SD regions. Black and African American residents are always exposed to below-average FNR values in both LA and SD under all scenarios.

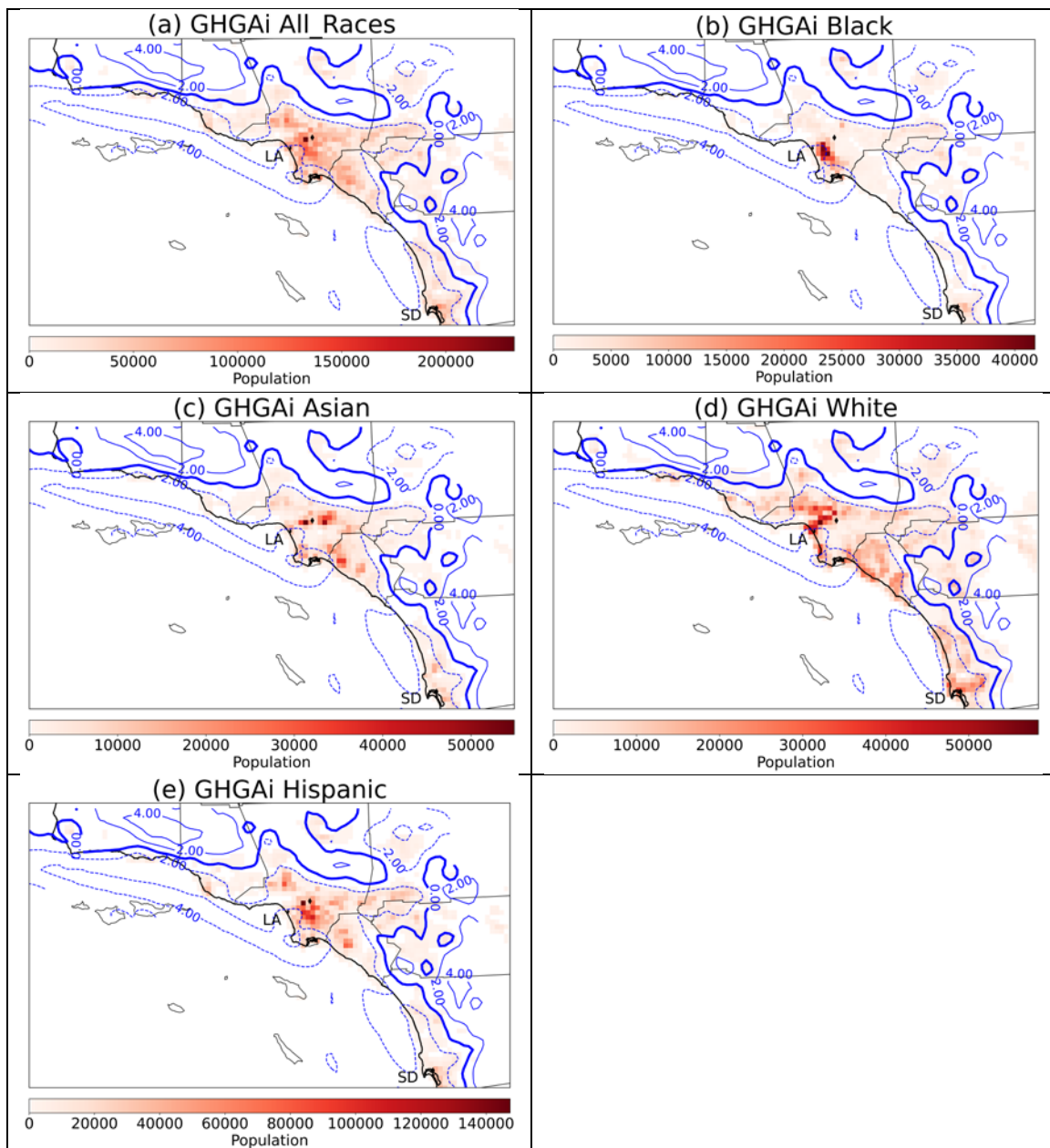


Figure 4.8: Population map for different race/ethnicity groups with chemical regimes indicated by FNR under the RCP8.5 GHGai scenario (blue contour lines are the values of FNR-4.6). Bold contour line indicates transition from NOx-limited chemistry (solid contour lines) to VOC-limited chemistry (dashed contour lines).

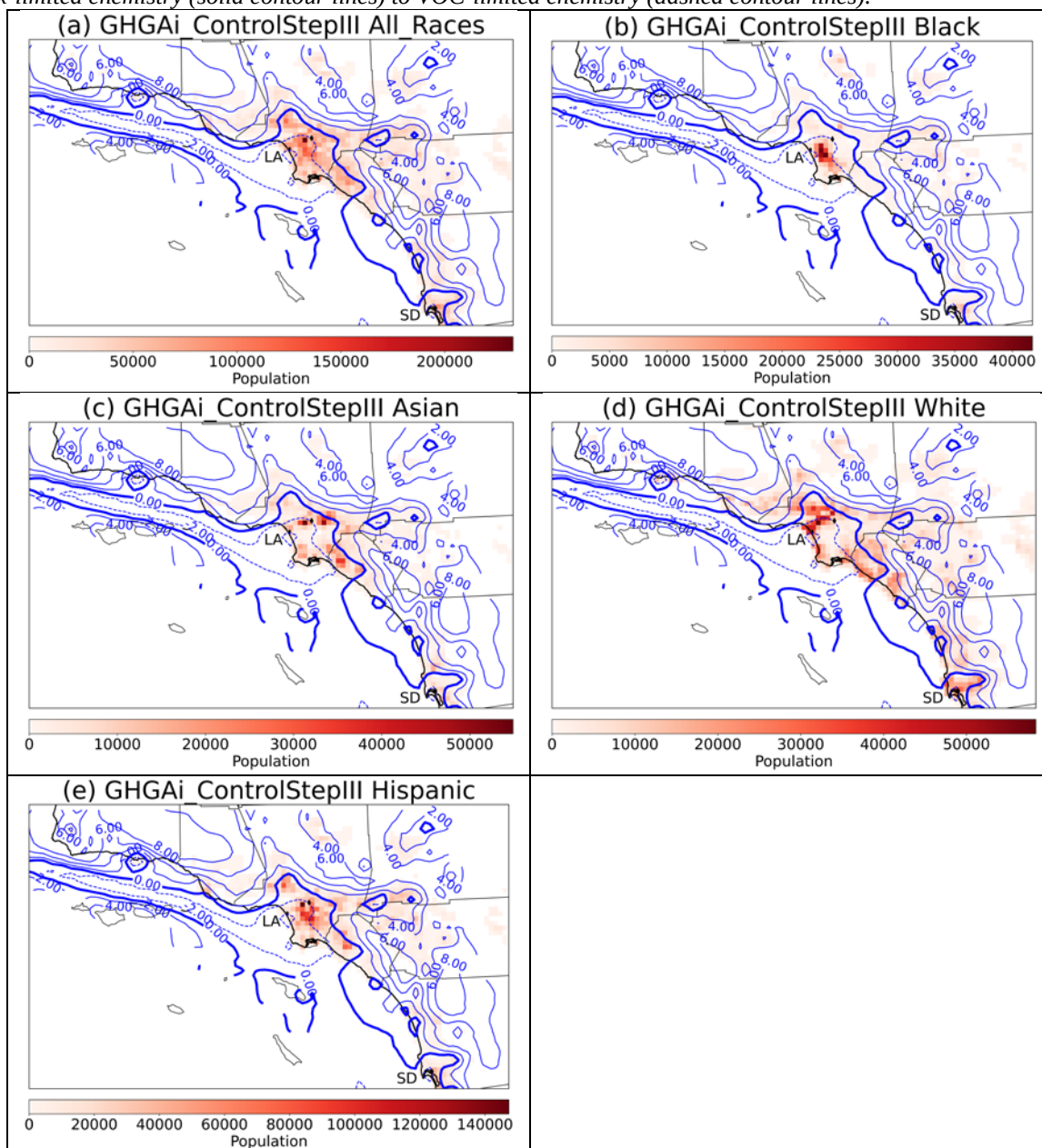


Figure 4.9: Population map for different race/ethnicity groups with chemical regimes indicated by FNR under the RCP8.5 GHGai Control Step III scenario (blue contour lines are the values of FNR-4.6). Bold contour line indicates transition from NOx-limited chemistry (solid contour lines) to VOC-limited chemistry (dashed contour lines).

4.3.4 Disparity reduction strategies for future scenarios

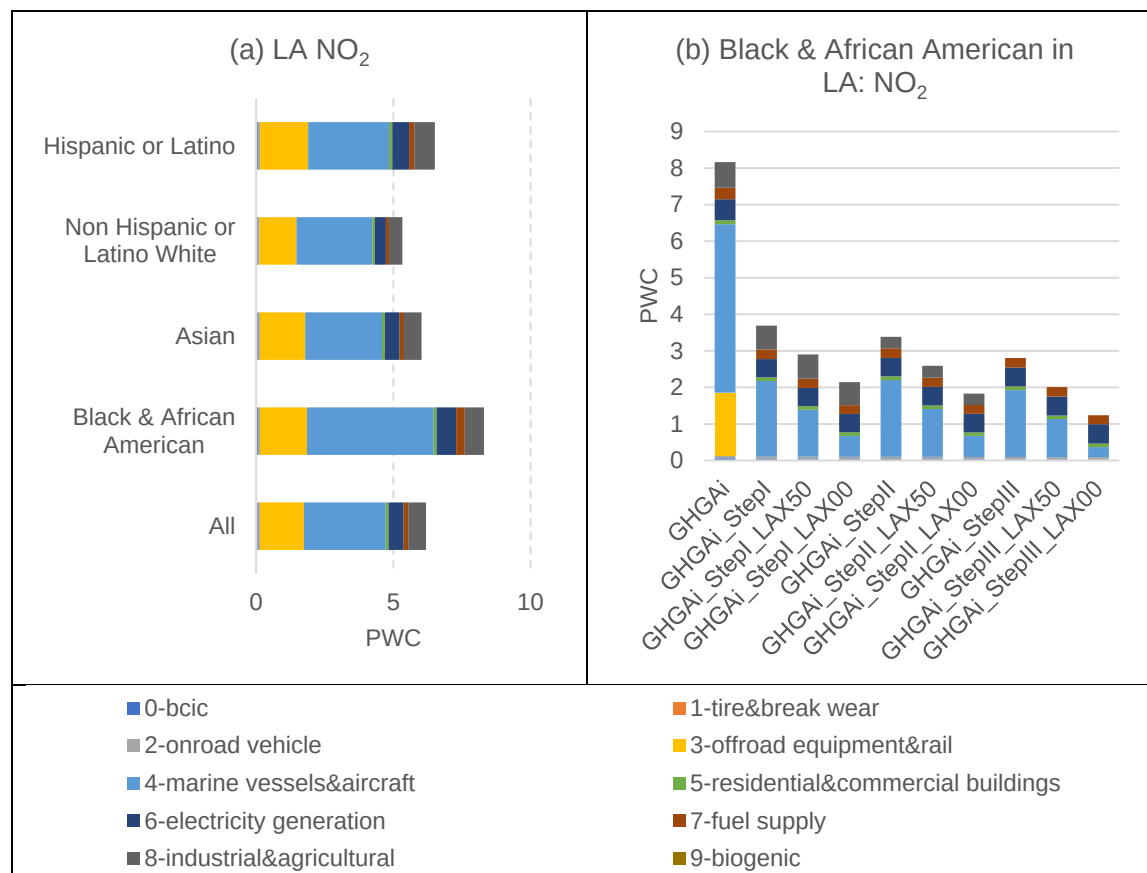


Figure 4.10: Population weighted concentrations (PWC) of summertime NO₂ from NO_x source apportionment in LA for (a) different race/ethnicity groups under RCP8.5 GHGAi and (b) Black & African Americans under different RCP8.5 scenarios (unit: ppb). BCIC refers to boundary and initial conditions.

In order to reduce the exposure disparities for Black residents under future scenarios, future sources that contribute to 24hr-avg NO₂ and MD8H O₃ across different race/ethnicity groups were analyzed (Figure 4.10 and Figure S4.19). Figure 4.10(a) and Figure S4.19(a) illustrate the NO_x source apportionment results of population weighted 24hr-avg NO₂ and MD8H O₃ for different race/ethnicity groups in LA under the RCP8.5 GHGAi scenario. Source contributions to MD8H O₃ are similar across race/ethnicity groups (Figure S4.19), while marine vessel and aircraft contributions to 24hr-avg NO₂ are elevated for Black and African American residents in LA (Figure 4.10(a)). Boundary and initial conditions (BCICs) contribute more strongly to O₃ in the control scenarios in both LA and SD but background O₃ is not a dominant source of O₃ exposure disparity. BCICs remain unchanged as emissions are reduced and less background O₃ reacts with local-emitted NO_x, causing BCICs to contribute more to relative and absolute

concentrations of the residual air pollution in these cleaner scenarios. Biogenic NO emissions in the LA and SD regions are very low relative to anthropogenic NO emissions. Biogenic sources therefore show little to no contributions to NO₂ concentrations in Figure 4.10 and Figure S4.19. Biogenic VOC emissions do contribute significantly to O₃ formation in Southern California (Zhao et al., 2024).

Table 4.4: Additional future emission scenarios for exposure disparity reduction.

Scenario	Description
GHGAi_ControlStepI_LAX50	An emission reduction scenario based on GHGAi_ControlStepI scenario that further reduced 50% NOx emissions from LAX airport
GHGAi_ControlStepII_LAX50	An emission reduction scenario based on GHGAi_ControlStepII scenario that further reduced 50% NOx emissions from LAX airport
GHGAi_ControlStepIII_LAX50	An emission reduction scenario based on GHGAi_ControlStepIII scenario that further reduced 50% NOx emissions from LAX airport
GHGAi_ControlStepI_LAX00	An aggressive emission reduction scenario based on GHGAi_ControlStepI scenario that further reduced 100% NOx emissions from LAX airport
GHGAi_ControlStepII_LAX00	An aggressive emission reduction scenario based on GHGAi_ControlStepII scenario that further reduced 100% NOx emissions from LAX airport
GHGAi_ControlStepIII_LAX00	An aggressive emission reduction scenario based on GHGAi_ControlStepIII scenario that further reduced 100% NOx emissions from LAX airport

Figure 4.10(b) and Figure S4.19(b) show evolving source contributions to 24hr-avg NO₂ and MD8H O₃ for Black & African American residents under future traditional emissions control scenarios. Marine vessels & aircraft remain as significant sources of NO₂ for Black and African American residents under all control scenarios. Considering that 80-90% of NOx emissions from marine vessels have been reduced, the majority of the remaining emissions are released by aircraft. As Los Angeles International Airport (LAX) is the largest airport in the LA region, two additional disparity reduction scenarios/sensitivity tests with brute-force method were analyzed to explore the effects of reducing local emissions from LAX under each traditional control step. One sensitivity test reduced LAX emissions by 50% (LAX50) while the second sensitivity test reduced LAX emissions by 100% (LAX00) under GHGAi StepI, StepII, and

Step III (six additional sensitivity test scenarios – see Table 4.4). All the sensitivity tests were performed during summer months (June, July & August), when O₃ exceedances are most common (Zhao et al., 2024). The values discussed in the remainder of this analysis all correspond to summer days. Figure S4.20 and Figure S4.21 show the relative disparities for summertime, which have similar patterns as the 32-week average disparity plots. Such similarity also exists for the winter months (December, January & February) (not shown). Therefore, we should expect similar effects of reducing LAX emissions on the relative disparities for summer months to the 32-week average.

Figure 4.11, Figure 4.12, Figure S4.20 and Figure S4.21 show the relative disparities for population weighted summertime MD8H O₃ and 24hr-avg NO₂ (left), and percentage of population exposed to healthy/unhealthy concentration levels (right) under the six LAX test scenarios alongside the original control scenarios. Changes to MD8H O₃ exposure disparities for Black and African American residents induced by the additional NO_x controls at LAX are minor. However, the relative NO₂ exposure disparities for Black and African American residents in LA are reduced significantly as NO_x at LAX is controlled. Reducing LAX emissions by 50% reduces the NO₂ exposure disparity for Black and African American residents from 53.1% to 40.9 % for Control Step I, from 59.3% to 45.8% for Control Step II, and from 71.3% to 55.3% for Control Step III. The total removal of LAX emissions reduces the NO₂ exposure disparity for Black and African American residents from 53.1% to 23.9 % for Control Step I, 59.3% to 26.8% for Control Step II, and 71.3% to 29.6% for Control Step III. The percentage of Black and African American residents who are exposed to unhealthy 24hr-avg NO₂ concentrations (≥ 4.6 ppb) decreases significantly, from greater than 22% under original control scenarios to less than 10% after LAX emissions scenarios are eliminated. Reductions in LAX emissions have minor effect on the NO₂ exposure disparities for other race/ethnicity groups since they are not concentrated in regions immediately downwind of the airport.

It should be noted that all the sensitivity tests for LAX emissions are unrealistic based on current technology. Elimination of NO_x emissions from jet aircraft would require new control technology that

does not yet exist. The main purpose of the sensitivity analysis conducted here is to verify the source tagging results that identify LAX emissions as a major source of NO_x exposure for downwind residents.

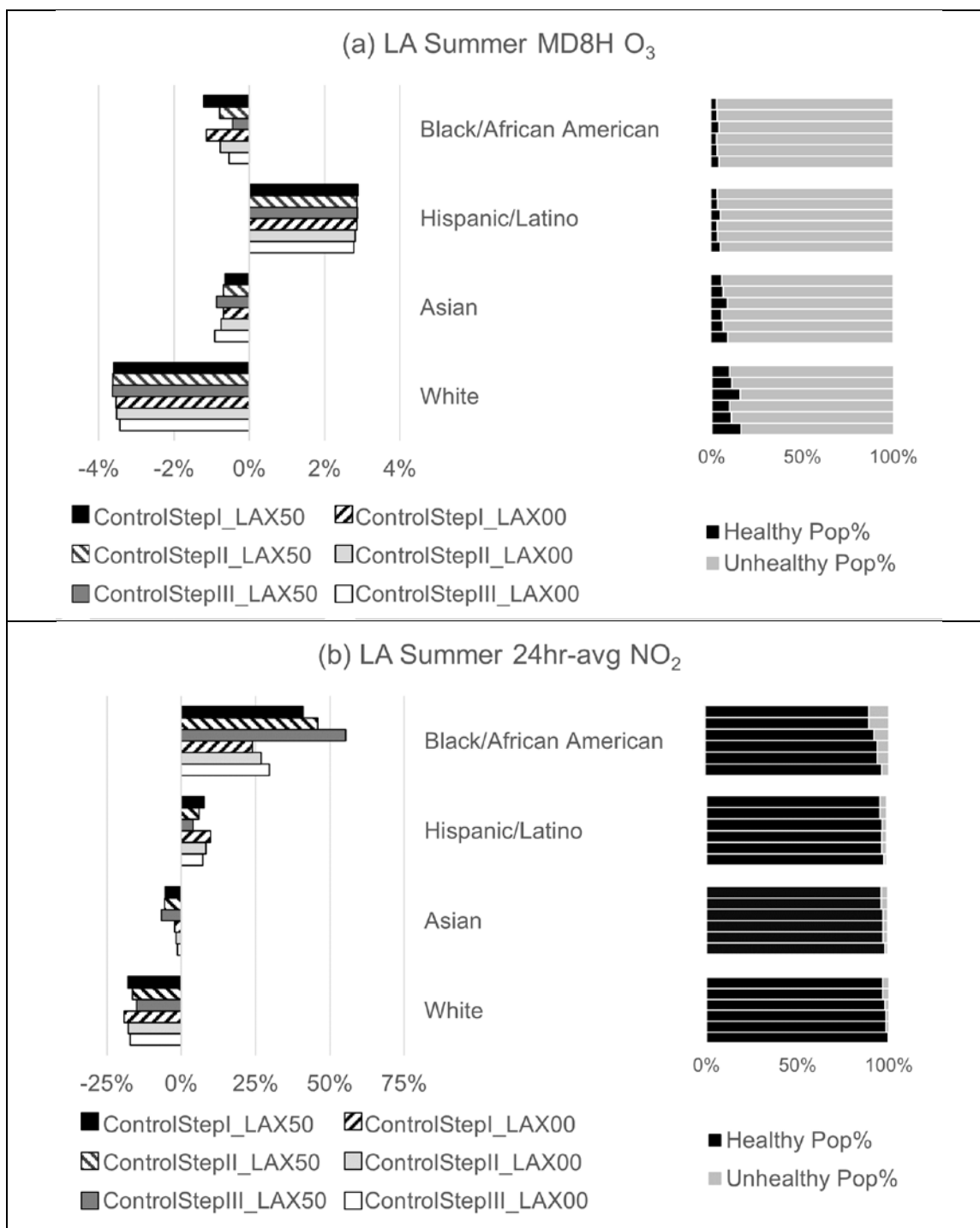


Figure 4.11: Relative disparity of population weighted summertime MD8H O₃ and 24hr-avg NO₂ exposure (left) and percentage of population exposed to healthy/unhealthy concentration levels (right) for different race/ethnicity groups under the three control steps with different levels of reduced LAX emissions at LA under RCP8.5.

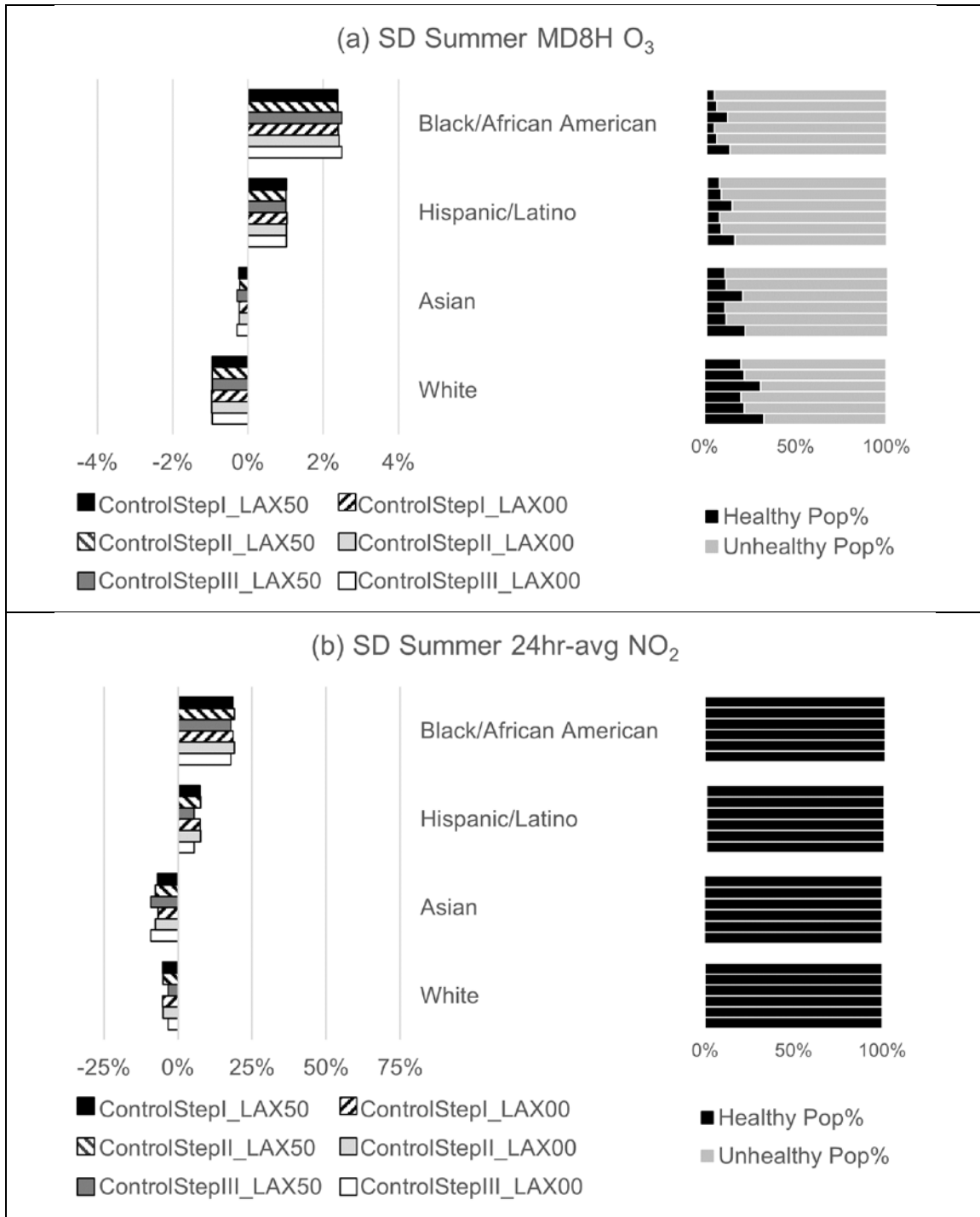


Figure 4.12: Relative disparity of population weighted summertime MD8H O₃ and 24hr-avg NO₂ exposure (left) and percentage of population exposed to healthy/unhealthy concentration levels (right) for different race/ethnicity groups under the three control steps with different levels of reduced LAX emissions at SD under RCP8.5.

4.4 Implications

This study has focused on the future EJ analysis of O₃ and NO₂ exposure disparities under different emissions reduction scenarios. Previous studies show that biogenic VOC emissions would prevent attainment of O₃ standards in Southern California, making NO_x control the only viable long-term strategy. While controlling NO_x emissions, policy makers should keep in mind that small reductions in NO_x emissions may cause increases in O₃ concentrations, and only a deep cut in NO_x emissions can avoid such disbenefits. Future emissions control programs can be developed to reduce O₃ concentrations in Southern California after the adoption of low-carbon energy scenarios through reductions targeting residual sources of precursor NO_x emissions. However, these traditional control strategies do not reduce environmental disparities for O₃ and NO₂ across different race and ethnicity groups in the Los Angeles region. Relative exposure disparities of MD8H O₃ and 24hr-avg NO₂ even increase for the Black and African American communities under the future emissions control strategies studied here. Black and African American residents live in the urban core of LA that has higher NO_x concentrations compared to outlying regions. Controls targeting NO_x sources reduce NO_x concentrations for the Black residents, but the O₃ chemistry does not transition fully to NO_x-limited conditions in the urban core region, resulting in slower MD8H O₃ reductions for Black residents compared to the general population. Meanwhile, as the absolute 24hr-avg NO₂ concentrations are much lower for the general population than for the Black residents, the relative exposure disparities for Black residents respond more slowly than for other residents. This finding emphasizes the need to consider environmental justice as a main objective when beginning the design of emissions control strategies.

This study demonstrates a novel method to develop controls optimized to reduce exposure disparity, using the source-apportionment capabilities of the CTMs that were used to design emissions controls. Emissions from the Los Angeles International Airport (LAX) were identified as a significant contributor to NO₂ exposure disparities for Black and African American residents in Los Angeles. Sensitivity tests were conducted by reducing the LAX emissions by 50% and 100% under each of the three traditional

control scenarios to confirm this finding. The sensitivity tests significantly reduced the relative disparities of 24hr-avg NO₂ exposures for Black residents by up to 50%. The feasibility of reducing emissions from major airports is beyond the scope of the current analysis, but the results demonstrate that the same tools (O₃ source apportionment technique) used to develop control strategies for compliance with regional air pollution regulations can also be used to develop effective control strategies to reduce exposure disparities to photochemical pollutants even in the presence of non-linear chemical reactions that change response factors across regions. Note that the O₃ source apportionment technique can also identify emissions contributions by geographical regions, but these results are not discussed in the current study. Future studies should take advantage of these capabilities to design emissions control programs to reduce exposure disparities.

The choice of background climate scenario did not strongly influence the projected O₃ and NO₂ exposure disparities. Results generated under the RCP4.5 scenario coupled with BAU and GHGAI emission scenarios were similar to the results from the RCP8.5 BAU and GHGAI scenarios. As the future period of this study is 2050, the changes to mean surface air temperature under different climate scenarios are modest, which limits the impact on O₃ concentrations. Studies that look at disparities in the year 2100 will need to more comprehensively consider background climate effects on O₃ concentrations.

The current study considered criteria pollutant emissions reductions across the entire state of California with a focus on impacts in the Southern California region. Changes to criteria pollutant emissions outside of California were not considered. Emissions reductions outside California can affect upwind concentrations of pollutants but these generally have minor influence in Southern California (represented as the BCIC in the current study). Local emissions sources are the dominant factor that affects the exposure disparities in Los Angeles under the BAU and GHGAI scenarios. Assuming that BCICs will not change by an order of magnitude between present day and 2050, the conclusions about the sources of O₃ and NO₂ exposure disparity are not sensitive to the choice of upwind boundary conditions. Simulations conducted further into the future (~year 2100) may need to consider these changes to upwind boundary

conditions when calculating contributions to exposure disparities, but this analysis is beyond the scope of the current study.

4.5 Appendix

Table S4.1: Standard deviation (std_dev) of daily MD8H O₃ for 2010-2019, BAU, and GHGAi scenarios under RCP8.5.

	LA	SD
2010-2019	11.6	10.6
BAU	9.8	7.1
GHGAi	7.8	6.6

Note: The std_dev of BAU (7.1-9.8 ppb) and GHGAi (6.6-7.8 ppb) scenarios are similar to the std of 2010-2019 period (10.6-11.6 ppb), with a slight reduction over time due to the reductions in emissions. Therefore, the std_dev values of future BAU and GHGAi are comparable with the std_dev of 2010-2019, meaning that the 32-week simulation period captures the variability of O₃ for the 10-year period.

Table S4.2: Population weighted emissions in LA and SD under GHGAi and the percentage of change in different Control Steps compared to GHGAi.

Scenario	Species	LA		SD	
		Pop-wgt Emis (tons/year)	Change in %	Pop-wgt Emis (tons/year)	Change in %
GHGAi	NOx	79.74		41.84	
	VOC	589.19		438.58	
GHGAi_ControlStepI	NOx	37.38	-53.13%	18.41	-56.01%
	VOC	452.41	-23.21%	361.45	-17.59%
GHGAi_ControlStepII	NOx	30.55	-61.69%	17.18	-58.95%
	VOC	452.41	-23.21%	361.45	-17.59%
GHGAi_ControlStepIII	NOx	22.78	-71.45%	15.19	-63.70%
	VOC	452.41	-23.21%	361.45	-17.59%

Table S4.3: Population of difference race/ethnicity groups in the selected LA and SD regions.

Region	Non-Hispanic White	Asian	Hispanic/Latino	Black/African
LA	4,270,607	2,141,542	6,690,133	920,808
SD	1,420,956	357,288	934,465	146,401

Table S4.4: Statistics formulas

Statistic	Formula
Sample standard deviation (s)	$\sqrt{\frac{\sum (C_i - \bar{C})^2}{(n - 1)}}$
Uncertainty in population-weighted concentrations	$\frac{s}{\sqrt{n}}$
Normalized mean bias (NMB)	$\frac{\sum (M_j - O_j)}{\sum O_j} \times 100\%$
Normalized mean error (NME)	$\frac{\sum M_j - O_j }{\sum O_j} \times 100\%$
Correlation coefficient (r)	$\frac{\sum [(M_j - \bar{M}) \times (O_j - \bar{O})]}{\sqrt{\sum (M_j - \bar{M})^2 \times \sum (O_j - \bar{O})^2}}$
Mean Fractional Bias (MFB)	$\frac{2}{N} \sum \frac{M_j - O_j}{M_j + O_j}$
Mean Fractional Error (MFE)	$\frac{2}{N} \sum \frac{ M_j - O_j }{M_j + O_j}$
Root Mean Square Error (RMSE)	$\sqrt{\frac{\sum (M_j - O_j)^2}{N}}$

where:

C_i - population-weighted concentration of day i ,

$\bar{C}$ - population-weighted concentration averaged over the target time period (10 years for historical simulations in this study),

n - the total number of records used over the target time period,

M_j - model concentration for record j ,

O_j - observed concentration for record j ,

$\bar{M}$ - average model concentration over all records that match with observations,

$\bar{O}$ - average observed concentrations over all records that match with model results,

N - number of observations.

Table S4.5: Basin-wide meteorological evaluation metrics for 2010 (middle year of 2000-2019) in California air basins, including average observed values (AveObs), average model predicted values (AveSim), mean fractional bias (MFB), mean fractional error (MFE), and root mean square error (RMSE).

	Temperature					Wind					Relative Humidity				
Basin	AveObs °C	AveSim °C	MFB -	MFE -	RMSE °C	AveObs m/s	AveSim m/s	MFB -	MFE -	RMSE m/s	AveObs %	AveSim %	MFB -	MFE -	RMSE %
GBV	12.95	11.97	-0.03	0.21	3.83	2.94	2.02	-0.26	0.68	2.50	39.92	38.65	-0.01	0.32	16.23
LC	12.73	12.13	0.04	0.29	3.98	3.34	1.84	-0.44	0.66	2.53	64.99	66.03	0.06	0.27	19.45
LT	6.87	6.71	0.20	0.30	4.19	1.44	2.64	0.53	0.70	1.89	58.73	63.63	0.11	0.32	21.69
NC	11.67	10.60	0.01	0.29	3.85	2.48	1.65	-0.24	0.69	2.17	70.09	72.66	0.07	0.23	18.67
NCC	13.33	13.52	0.05	0.22	3.31	2.19	1.87	-0.10	0.62	1.81	72.05	71.74	0.02	0.20	15.93
NEP	9.05	8.12	-0.05	0.27	3.38	2.65	1.78	-0.31	0.64	1.96	59.22	63.14	0.09	0.25	17.16
MD	16.85	15.83	-0.04	0.20	3.01	3.20	2.32	-0.19	0.62	2.41	43.32	44.73	0.05	0.27	14.40
MC	12.17	11.27	-0.03	0.25	3.77	2.30	1.82	-0.09	0.59	1.79	61.01	61.92	0.05	0.25	17.59
SC	16.12	15.13	-0.03	0.17	3.16	2.44	1.77	-0.24	0.60	1.92	60.38	61.60	0.03	0.21	15.03
SCC	14.20	13.62	-0.01	0.19	3.26	2.39	1.93	-0.08	0.59	1.91	65.39	69.58	0.09	0.23	17.93
SD	15.59	15.19	0.01	0.19	3.05	1.99	2.00	0.04	0.53	1.35	62.69	62.67	0.03	0.22	15.14
SFB	13.56	13.03	-0.01	0.18	2.98	2.57	1.74	-0.17	0.65	2.20	72.16	75.68	0.07	0.20	17.46
SJV	15.15	15.01	0.06	0.20	3.05	2.03	1.47	-0.23	0.57	1.50	62.44	59.89	-0.02	0.23	16.91
SS	22.59	22.45	0.03	0.17	4.12	2.23	1.71	-0.19	0.62	1.73	46.08	39.34	-0.16	0.31	17.19
SV	14.73	14.23	0.01	0.18	2.61	2.29	1.66	-0.20	0.59	1.75	62.93	62.26	-0.01	0.19	13.76
CA	14.42	13.82	0.00	0.21	3.29	2.38	1.78	-0.17	0.61	1.89	61.39	62.04	0.03	0.23	16.59

Table S4.6: Percentile change in population weighted concentrations of MD8H O₃ and 24hr-avg NO₂ for LA and SD regions under RCP8.5.

Scenario	LA		SD	
	O ₃	NO ₂	O ₃	NO ₂
GHGAI - BAU	1%	-39%	-2%	-24%
GHGAI_ControlStepI - GHGAI	-9%	-52%	-12%	-51%
GHGAI_ControlStepII - GHGAI	-11%	-59%	-13%	-53%
GHGAI_ControlStepIII - GHGAI	-15%	-69%	-15%	-58%

Table S4.7: Population weighted O₃ concentration (PWC) and the standard deviation (std_dev) for different scenarios.

O ₃	All		Black		Asian		White		Hispanic	
LA	PWC	std_d ev	PWC	std_d ev	PWC	std_d ev	PWC	std_d ev	PWC	std_d ev
2000-2009_avg	41.72	5.48	39.61	5.93	41.46	4.72	42.45	5.58	41.64	5.46
2010-2019_avg	44.44	5.41	42.75	5.66	44.29	4.79	44.56	5.84	44.67	5.20
BAU_avg	53.79	8.36	51.99	8.40	53.70	8.15	53.29	9.04	54.44	7.80
GHGAi_avg	54.04	7.25	52.84	6.77	54.06	7.38	53.14	8.11	54.84	6.44
GHGAi_ControlStepI	48.26	4.44	47.97	3.75	47.84	4.63	47.08	5.16	49.26	3.75
GHGAi_ControlStepI I	47.28	4.15	47.16	3.43	46.85	4.34	46.11	4.85	48.26	3.47
GHGAi_ControlStepI II	45.25	3.84	45.28	3.12	44.78	4.02	44.14	4.53	46.18	3.18
SD	PWC	std_d ev	PWC	std_d ev	PWC	std_d ev	PWC	std_d ev	PWC	std_d ev
2000-2009_avg	42.48	3.95	42.01	3.25	42.00	3.22	42.53	4.36	42.62	3.61
2010-2019_avg	43.26	3.46	43.48	2.66	43.11	2.66	43.18	3.90	43.33	3.10
BAU_avg	50.55	5.44	51.27	4.15	50.64	4.49	50.19	6.17	50.89	4.62
GHGAi_avg	49.35	5.01	50.11	3.82	49.48	4.13	48.98	5.68	49.69	4.23
GHGAi_ControlStepI	43.31	3.35	44.16	2.58	43.36	2.78	42.91	3.78	43.72	2.84
GHGAi_ControlStepI I	42.75	3.30	43.60	2.54	42.80	2.73	42.36	3.72	43.15	2.79
GHGAi_ControlStepI II	41.61	3.26	42.46	2.53	41.64	2.70	41.22	3.68	42.01	2.77

Note: BAU_avg is the average of BAU scenarios under RCP8.5 and RCP4.5. GHGAi_avg is the average of GHGAi scenarios under RCP8.5 and RCP4.5.

Table S4.8: Population weighted NO₂ concentration (PWC) and the standard deviation (std_dev) for different scenarios.

NO ₂	All		Black		Asian		White		Hispanic	
LA	PWC	std_d ev	PWC	std_d ev	PWC	std_d ev	PWC	std_d ev	PWC	std_d ev
2000-2009_avg	29.14	8.22	30.57	5.85	29.62	8.09	25.58	9.35	31.18	6.84
2010-2019_avg	13.89	4.46	15.00	3.34	14.22	4.30	11.57	4.31	15.18	4.13
BAU_avg	9.94	6.24	12.29	6.63	9.72	5.43	8.20	5.91	10.84	6.04
GHGAi_avg	6.01	5.15	8.01	6.22	5.85	4.52	5.16	5.08	6.33	4.97
GHGAi_ControlStepI	2.99	2.35	4.50	2.95	2.74	2.08	2.45	2.32	3.20	2.21
GHGAi_ControlStepI I	2.55	2.25	3.98	2.89	2.32	1.99	2.13	2.27	2.68	2.11
GHGAi_ControlStepI II	1.93	1.95	3.21	2.60	1.73	1.69	1.65	2.06	1.99	1.74
SD	PWC	std_d ev	PWC	std_d ev	PWC	std_d ev	PWC	std_d ev	PWC	std_d ev
2000-2009_avg	16.63	4.94	18.79	4.63	17.77	4.33	16.09	5.14	16.64	4.72
2010-2019_avg	7.78	2.07	8.70	1.96	8.22	1.74	7.43	2.13	7.99	2.00
BAU_avg	4.84	2.39	5.47	2.24	4.94	1.93	4.64	2.47	5.01	2.41
GHGAi_avg	3.67	1.97	4.06	1.83	3.69	1.57	3.58	2.07	3.75	1.95
GHGAi_ControlStepI	1.86	1.00	2.16	0.91	1.76	0.87	1.80	1.06	1.93	0.93
GHGAi_ControlStepI I	1.76	0.98	2.06	0.90	1.66	0.86	1.72	1.05	1.83	0.92
GHGAi_ControlStepI II	1.59	0.93	1.84	0.84	1.48	0.81	1.57	1.00	1.62	0.85

Note: BAU_avg is the average of BAU scenarios under RCP8.5 and RCP4.5. GHGAi_avg is the average of GHGAi scenarios under RCP8.5 and RCP4.5.

Figure S4.1: Air quality model domain for 24KM (in grey) and 4KM (in yellow), with locations of four monitoring sites that were used in the model performance calculation.

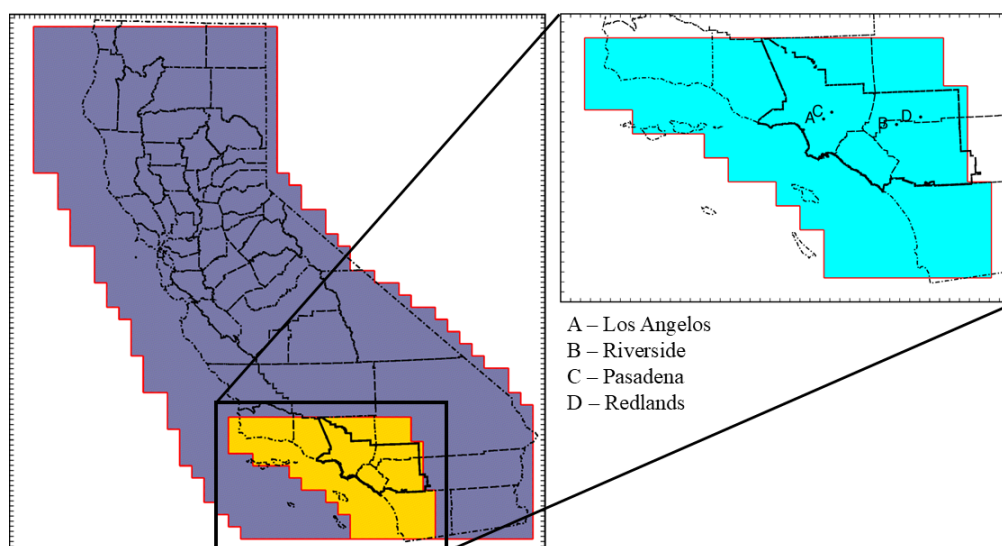


Figure S4.2: Spatial plots of NO_x emissions in GHGAI and the reductions in different Control Steps compared to GHGAI. Note: the scales are different in each emission reduction plot.

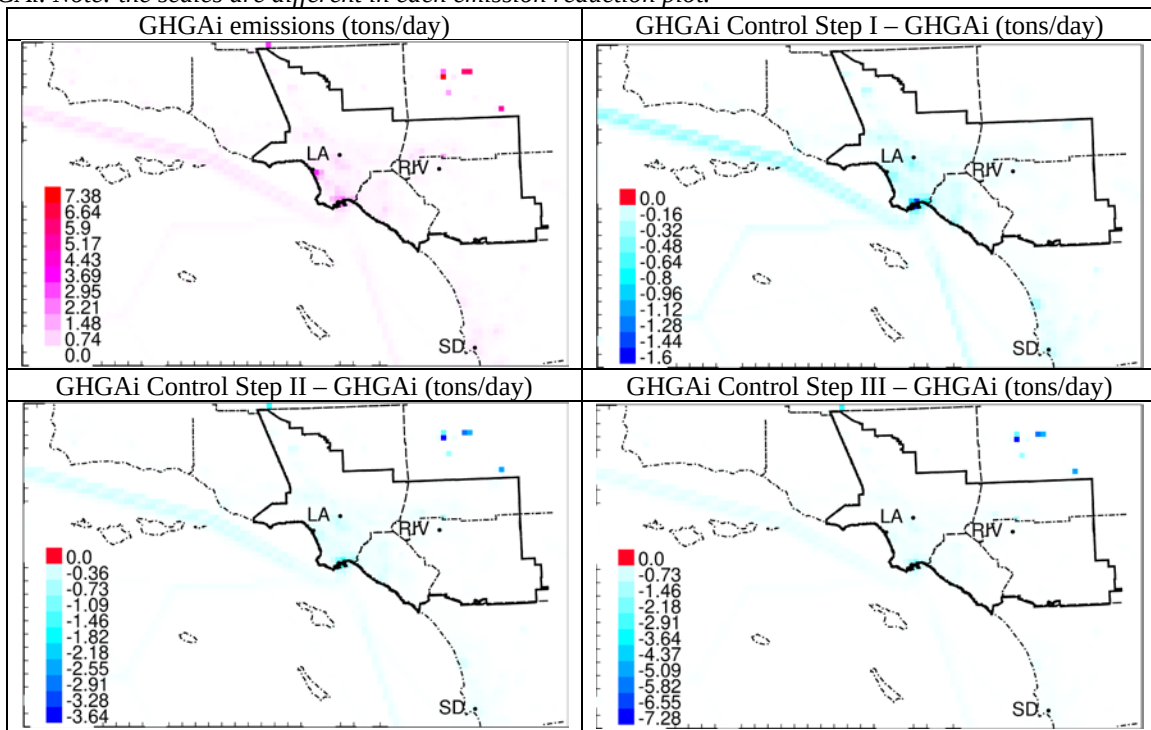


Figure S4.3: Spatial plots of NMVOC emissions in GHGAi and the reduction in different Control Steps compared to GHGAi.

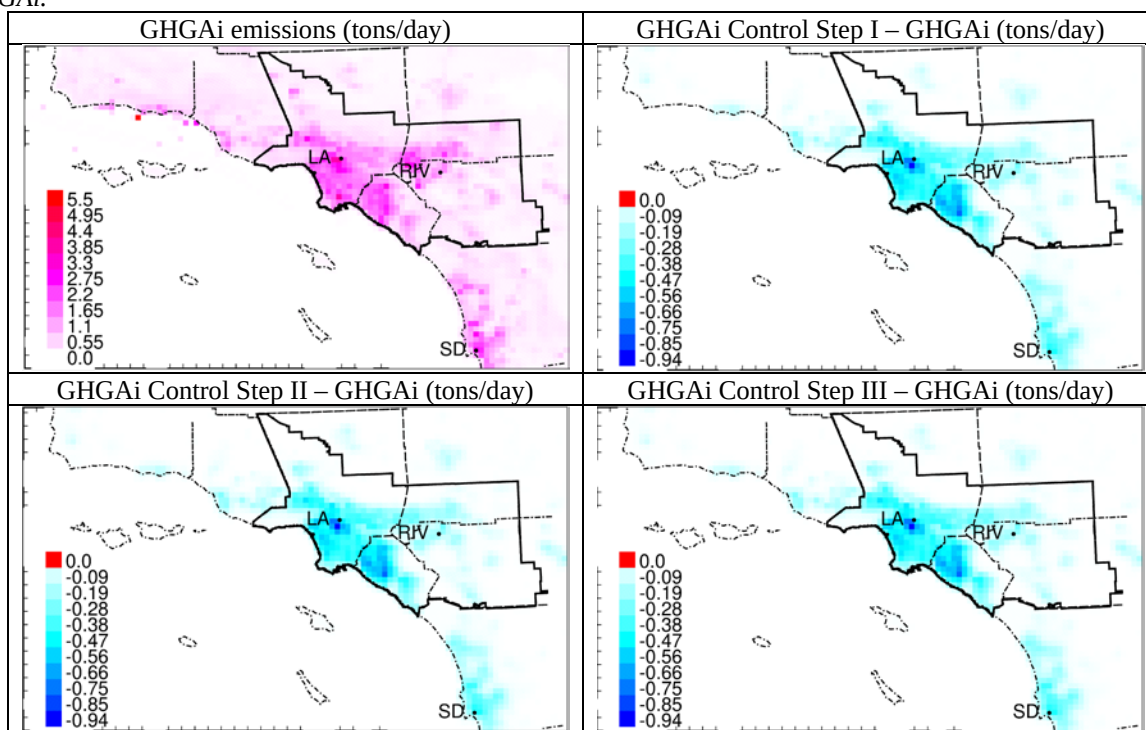


Figure S4.4: Domains for Environmental Disparity calculation.

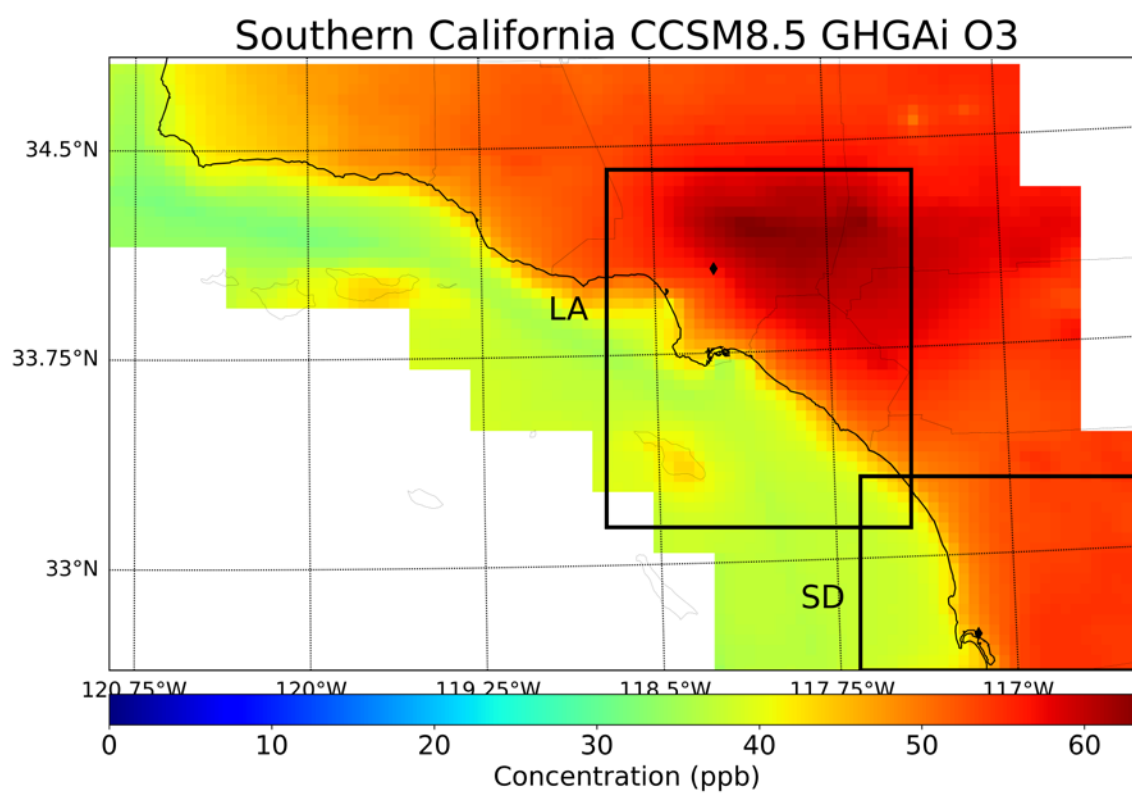


Figure S4.5: Simulated and observed MD8H O₃ at selected EPA sites for 2000-2009.

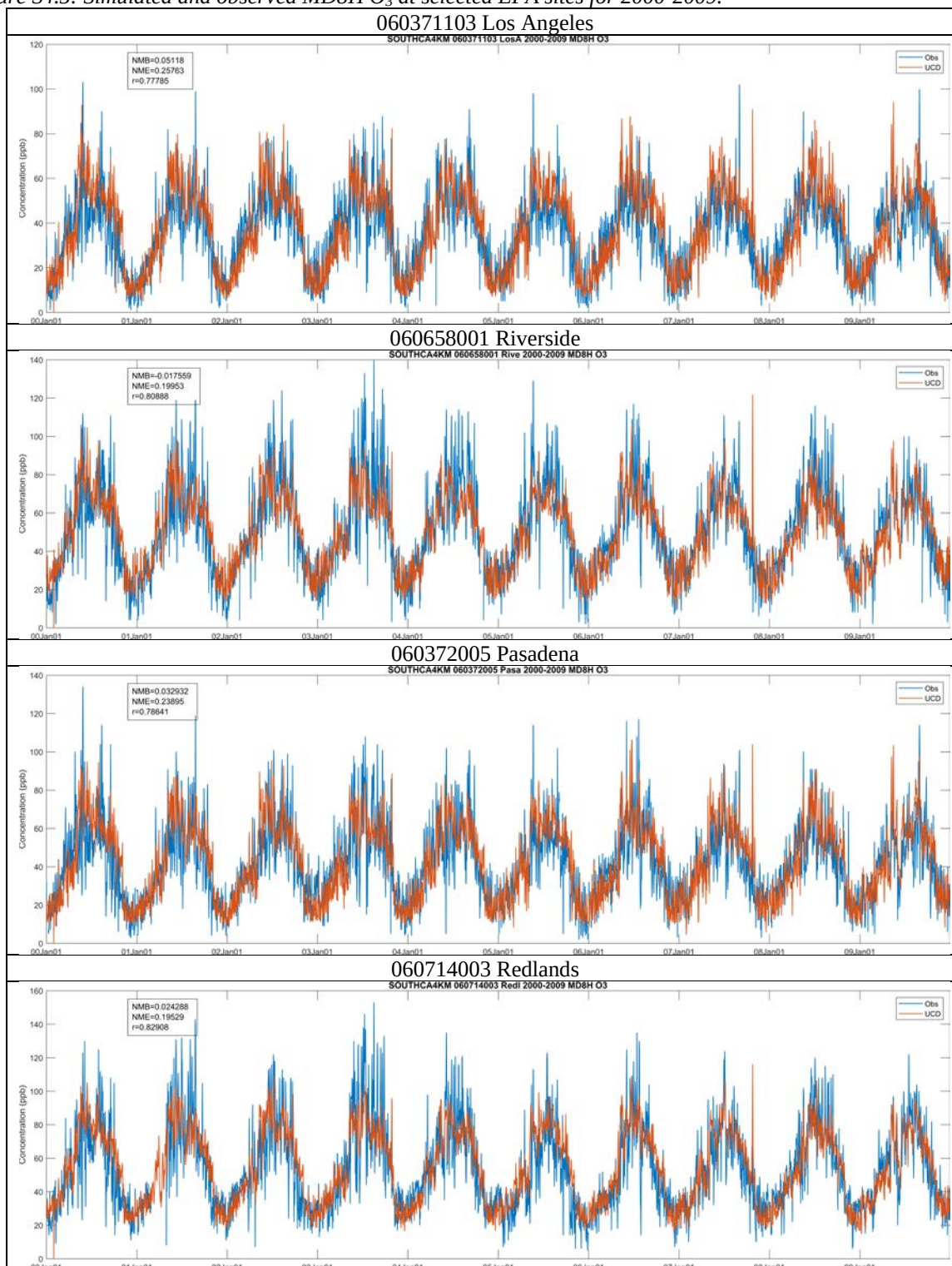


Figure S4.6: Simulated and observed MD8H O₃ at selected EPA sites for 2010-2019.

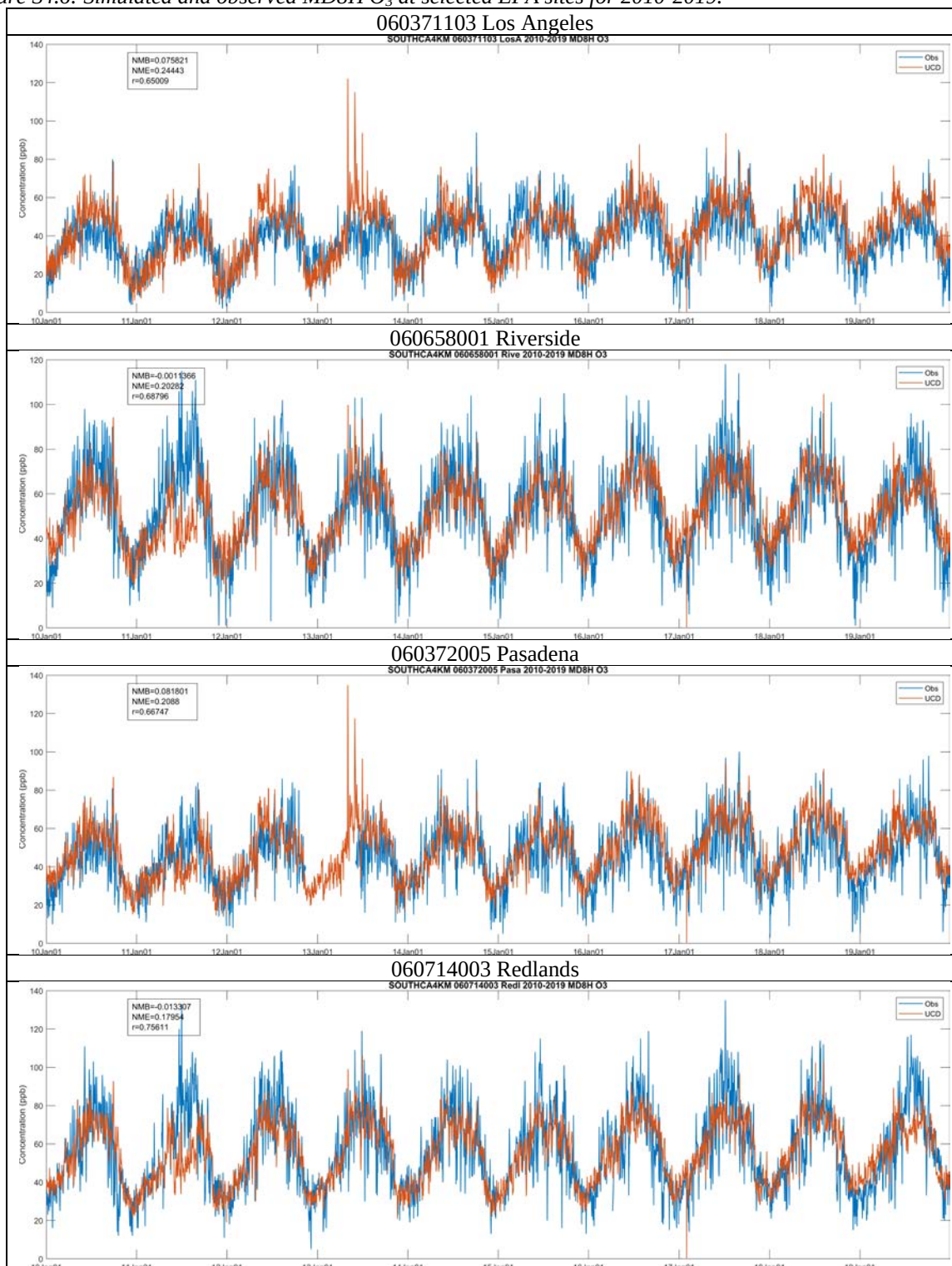


Figure S4.7: Simulated and observed daily average NO_2 at selected EPA sites for 2000-2009.

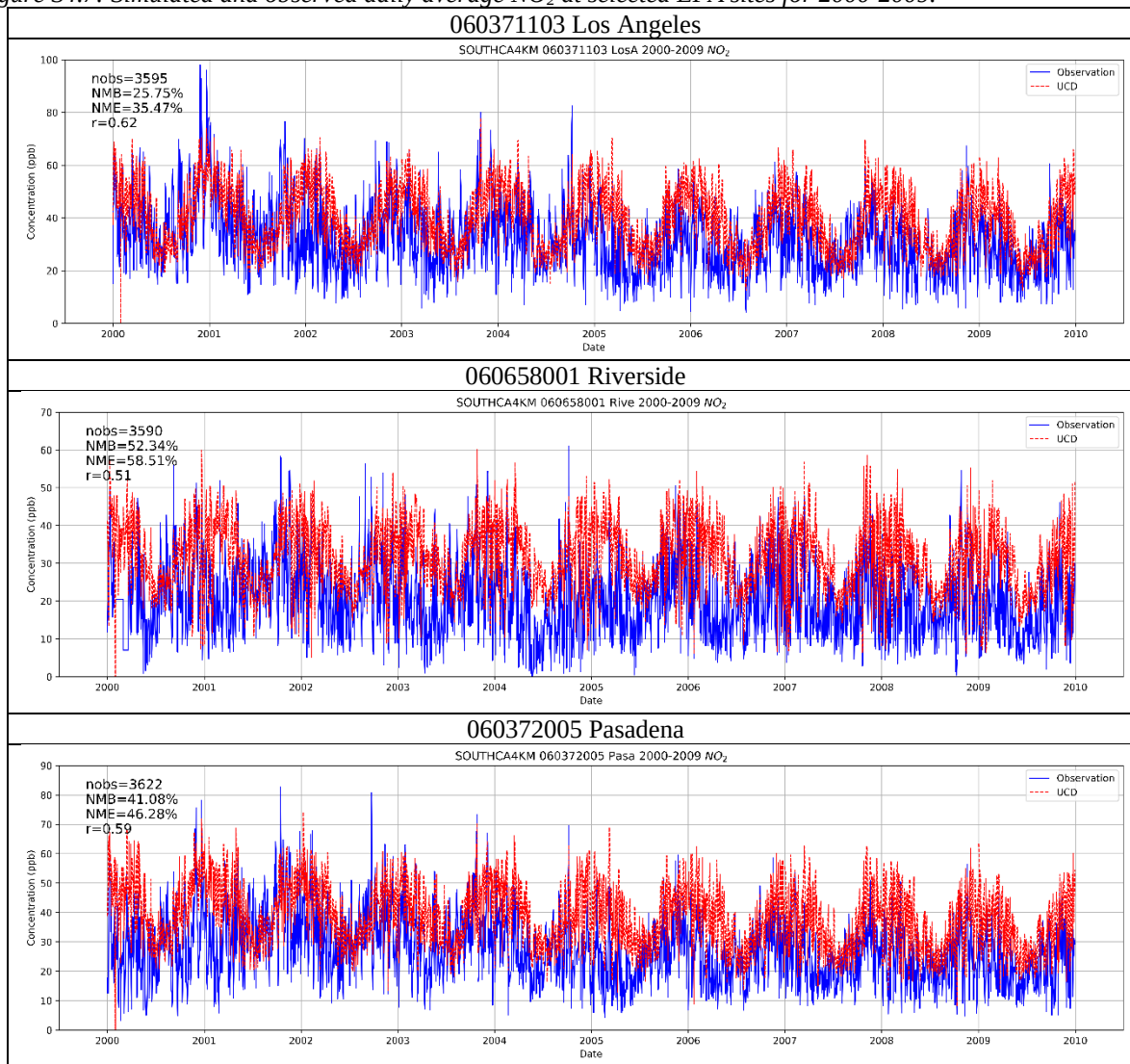
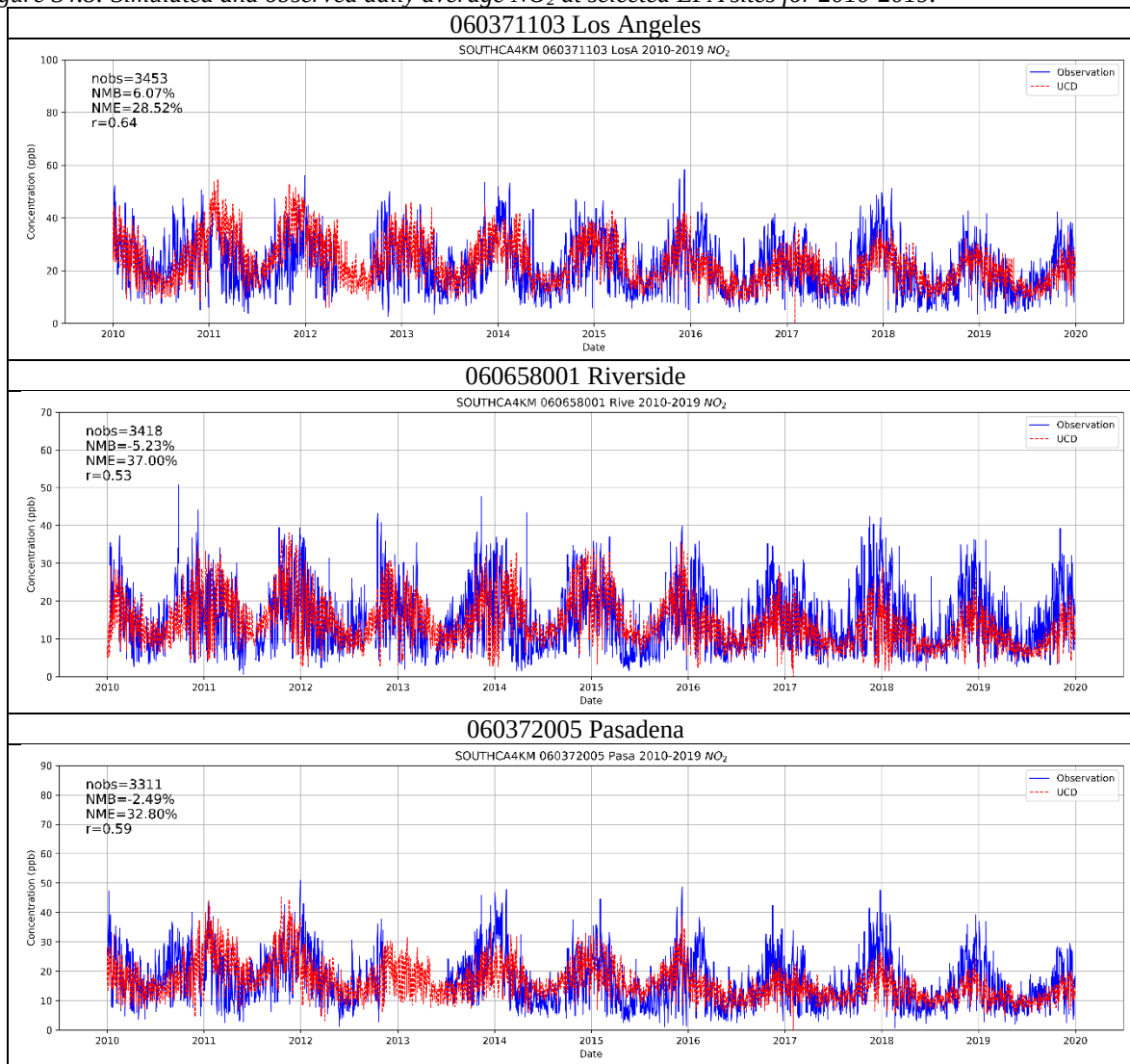


Figure S4.8: Simulated and observed daily average NO_2 at selected EPA sites for 2010-2019.



Predicted and measured VOC concentrations (formaldehyde, isoprene, benzene, toluene) are shown in Figure S4.9 and Figure S4.10. Note that isoprene measurements are only available starting in the year 2010 and so isoprene is not shown in Figure S4.9. Very few chemical transport models compare predicted concentrations of individual VOC species to measurements and so there are no published metrics for model performance. In the current study, the predicted VOC concentrations and measurements have similar average values, and the predicted seasonal trends are similar to the measured seasonal trends. VOC measurements have greater variability about the averaged concentrations than model predictions, suggesting that VOC emissions inventories do not fully capture the short-term variability of sources. The performance of predicted benzene and toluene concentrations are better than HCHO and isoprene. This is probably because HCHO and isoprene are reactive, with atmospheric lifetimes of only a few hours, while benzene and toluene have lifetimes of around 10 days and 2.4 days, respectively. Therefore, concentrations of longer-lived VOCs are relatively more stable, and their model performance would be better. Overall, the comparison between predicted and measured O₃, NO₂, and VOC concentrations indicates that the chemical transport model captures the dominant features of the O₃ formation system in Southern California.

Figure S4.9: Simulated and observed weekly averaged VOC species at the Los Angeles site for 2000-2009. UCD sampled dots correspond to the dates that have observations. (No isoprene due to lack of observations).

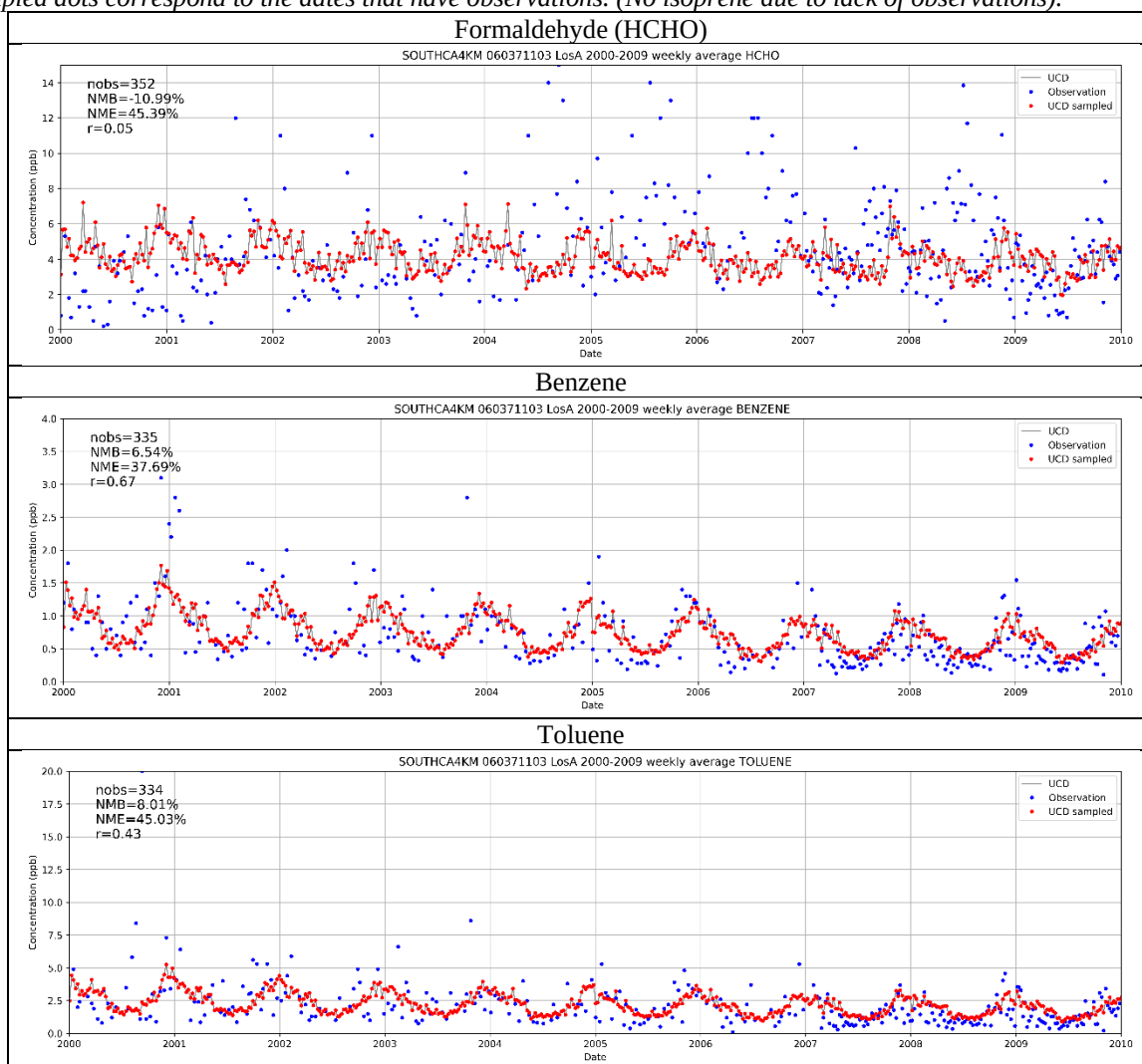


Figure S4.10: Simulated and observed weekly averaged VOC species at the Los Angeles site for 2010-2019. UCD sampled dots correspond to the dates that have observations.

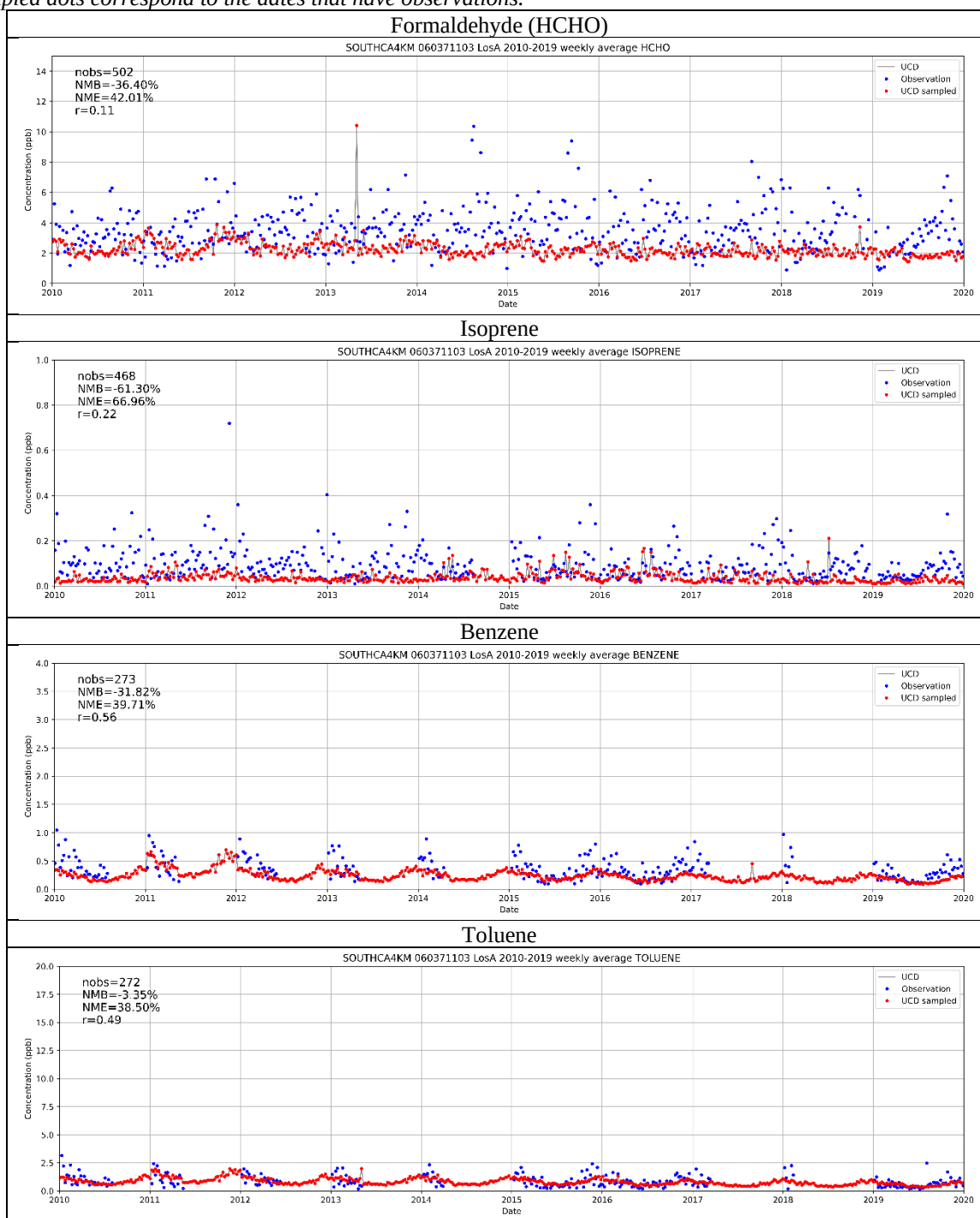


Figure S4.11: 32 weeks averaged MD8H O₃ reductions in different emission scenarios under RCP8.5, unit: ppb.

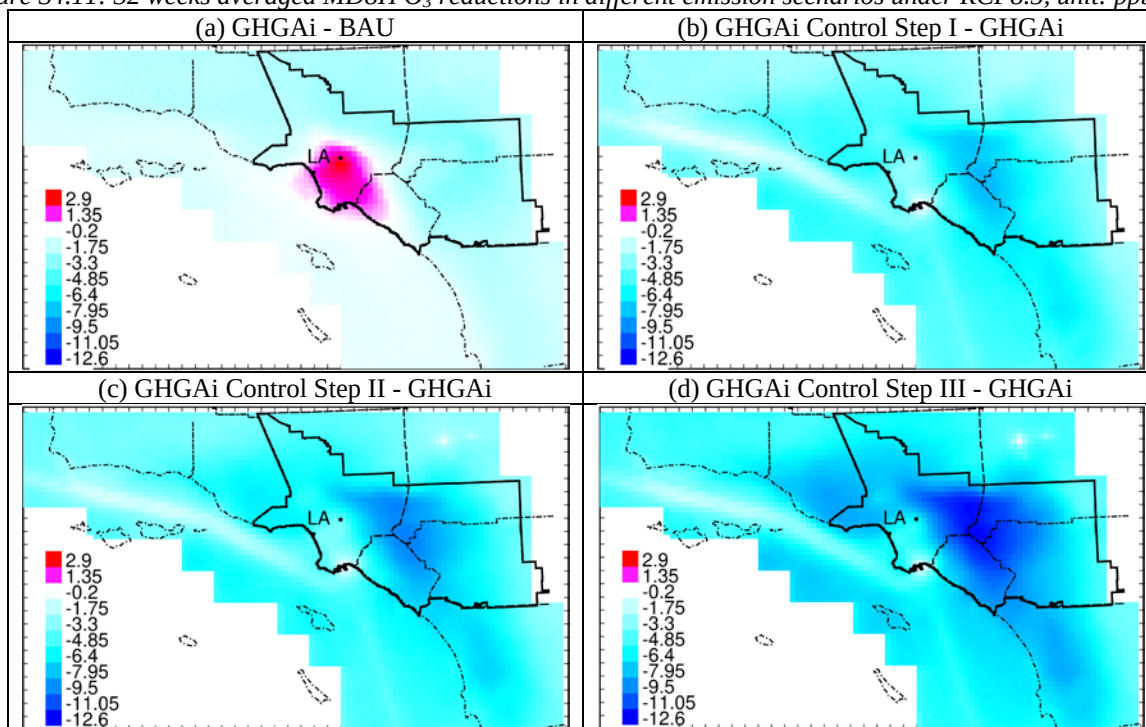


Figure S4.12: 32 weeks averaged 24hr-avg NO_2 reductions in different emission scenarios under RCP8.5, unit: ppb.

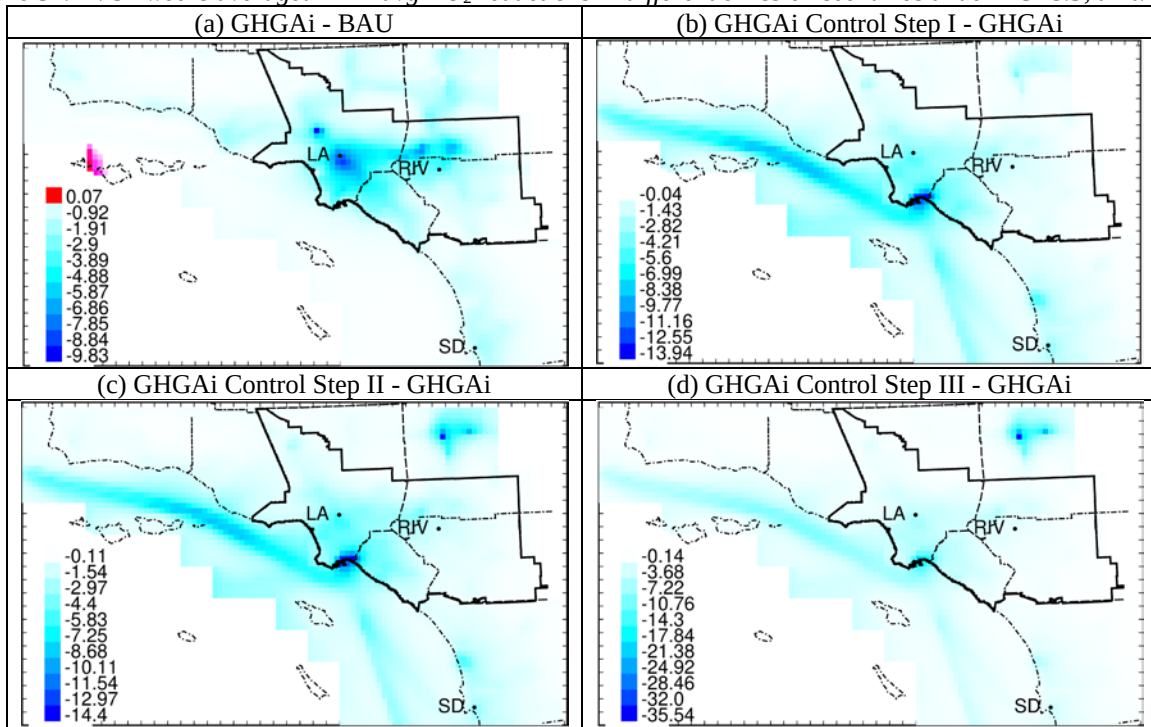


Figure S4.13: Population weighted averaged MD8H O₃, 24hr-avg NO₂ concentrations, and FNR at hour 13 for all race/ethnicity groups. (All BAU and GHGAi related scenarios in this figure are under RCP8.5.)

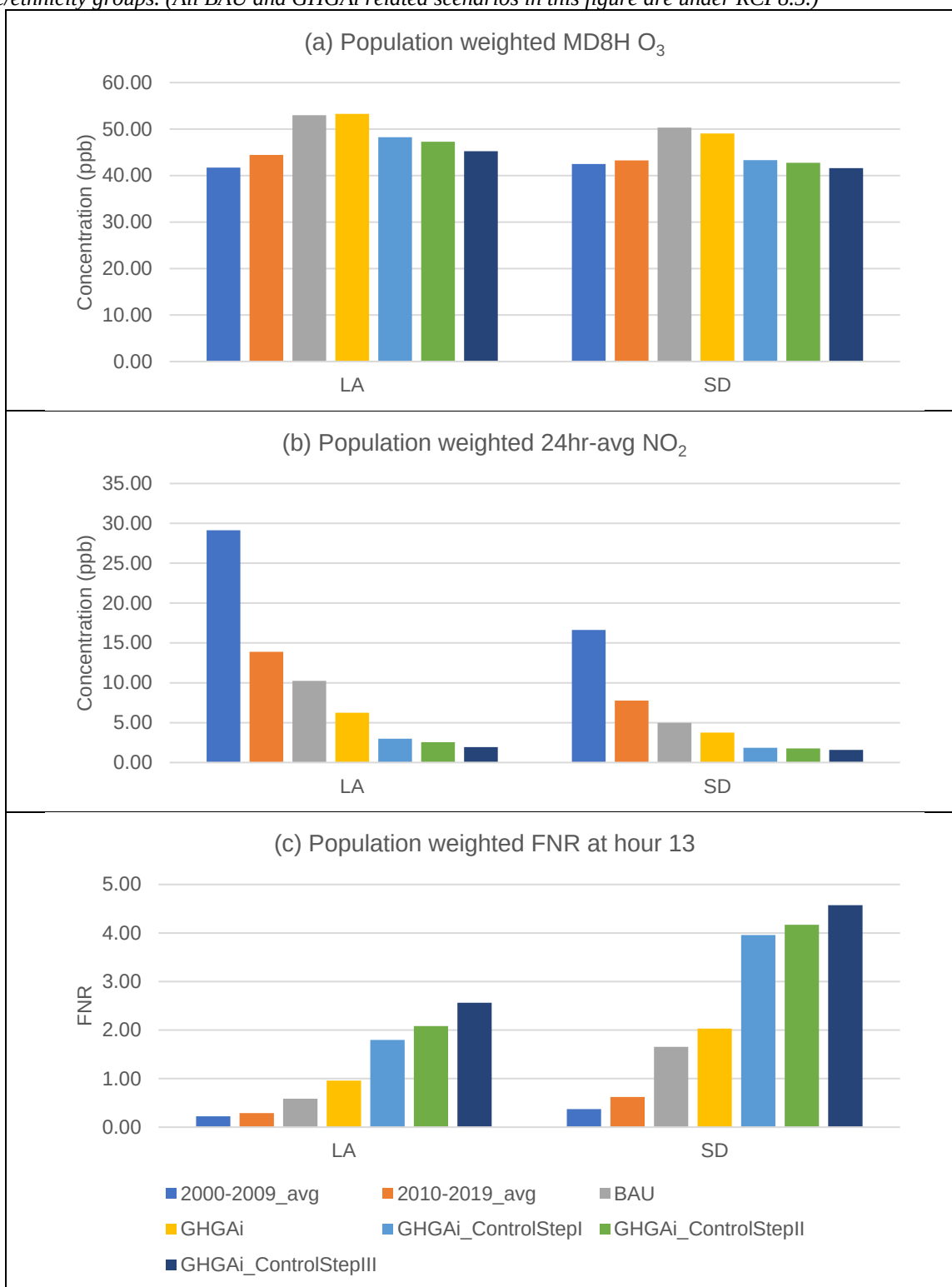


Figure S4.14: Population map for different race/ethnicity groups with chemical regimes indicated by FNR under the RCP8.5 BAU scenario (blue contour lines are the values of FNR-4.6). Bold contour line indicates transition from NO_x-limited chemistry (solid contour lines) to VOC-limited chemistry (dashed contour lines).

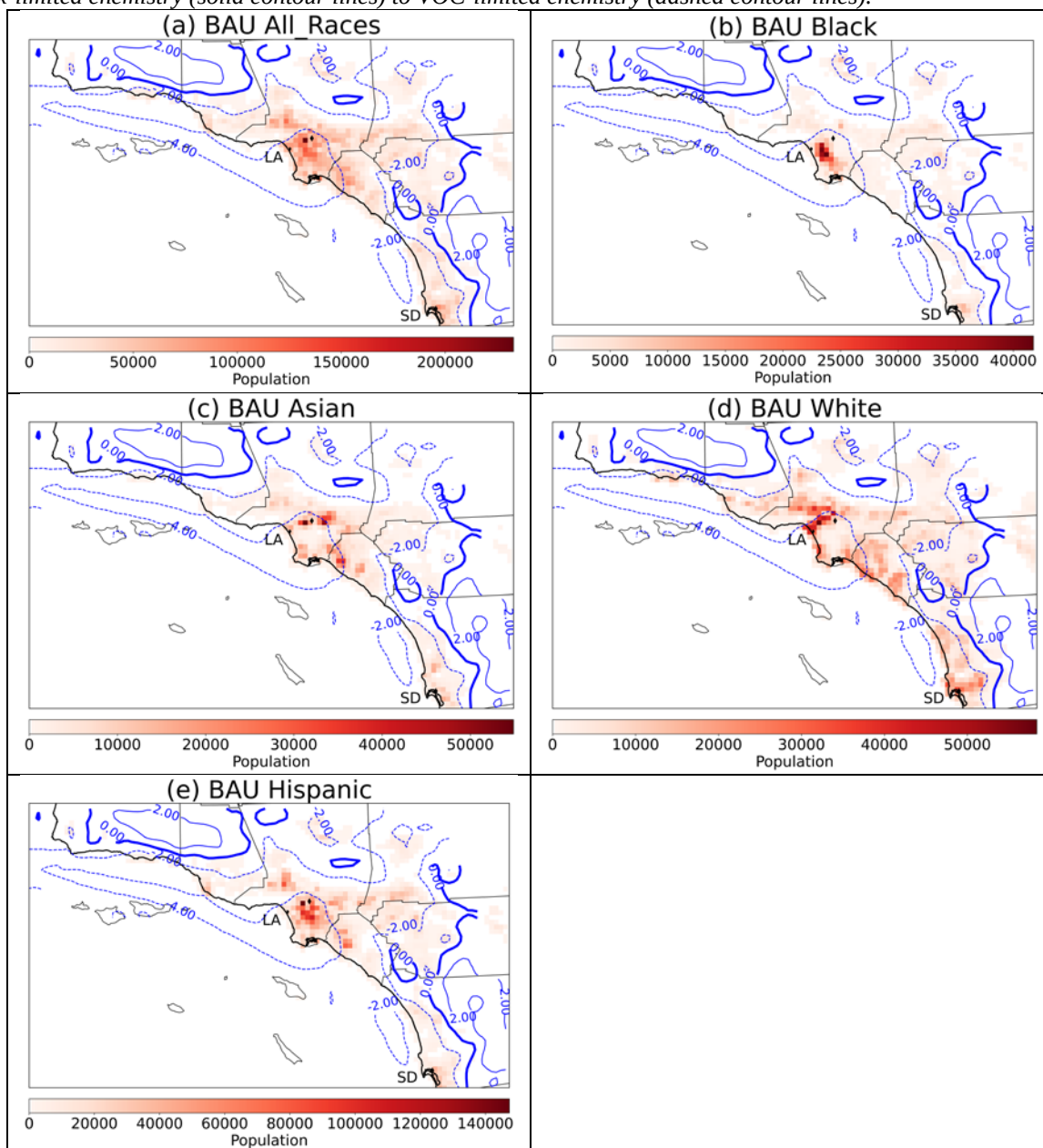


Figure S4.15: Population map for different race/ethnicity groups with chemical regimes indicated by FNR under the RCP8.5 GHGai Control Step I scenario (blue contour lines are the values of FNR-4.6). Bold contour line indicates transition from NOx-limited chemistry (solid contour lines) to VOC-limited chemistry (dashed contour lines).

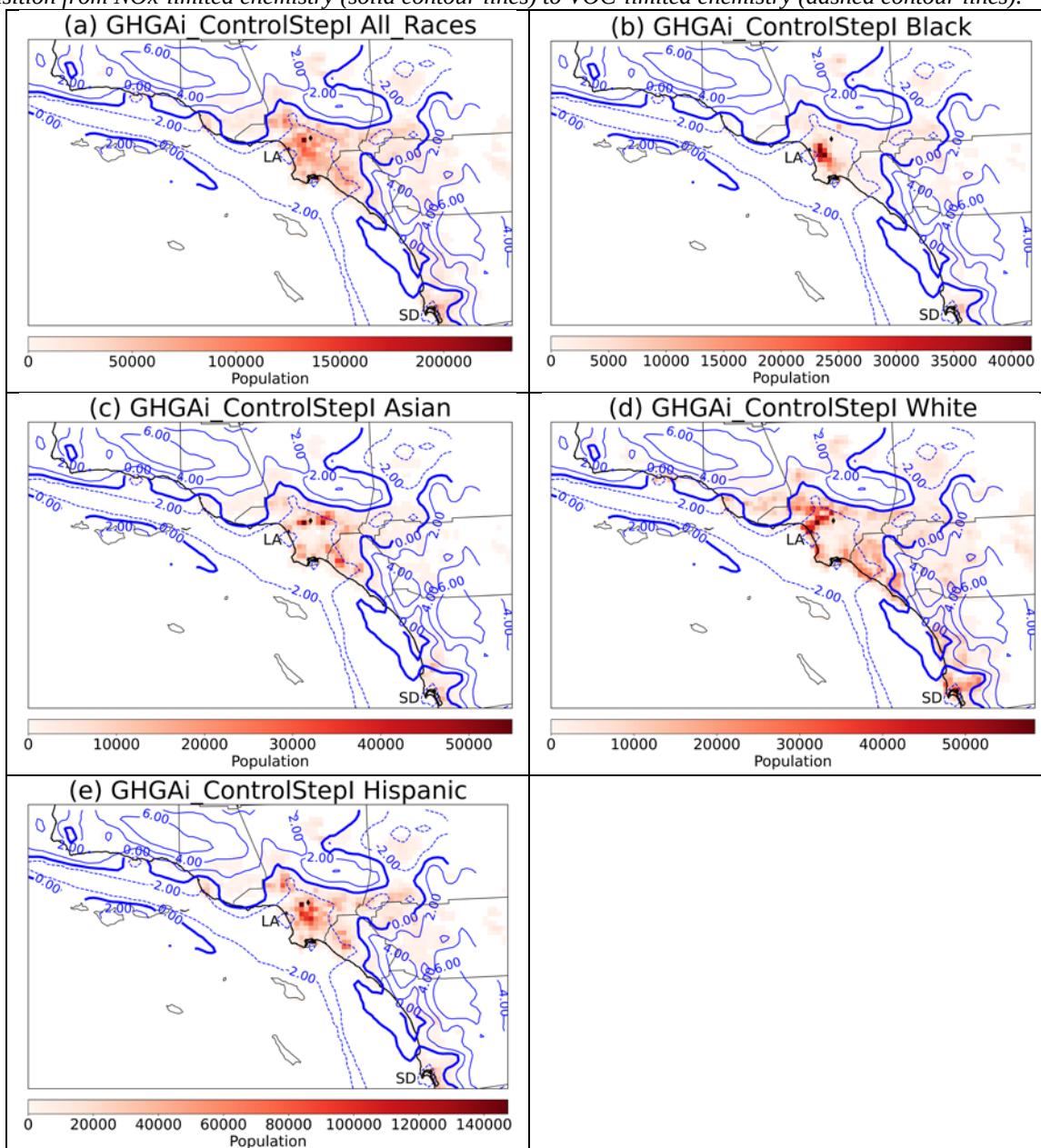


Figure S4.16: Population map for different race/ethnicity groups with chemical regimes indicated by FNR under the RCP8.5 GHGai Control Step II scenario (blue contour lines are the values of FNR-4.6). Bold contour line indicates transition from NOx-limited chemistry (solid contour lines) to VOC-limited chemistry (dashed contour lines).

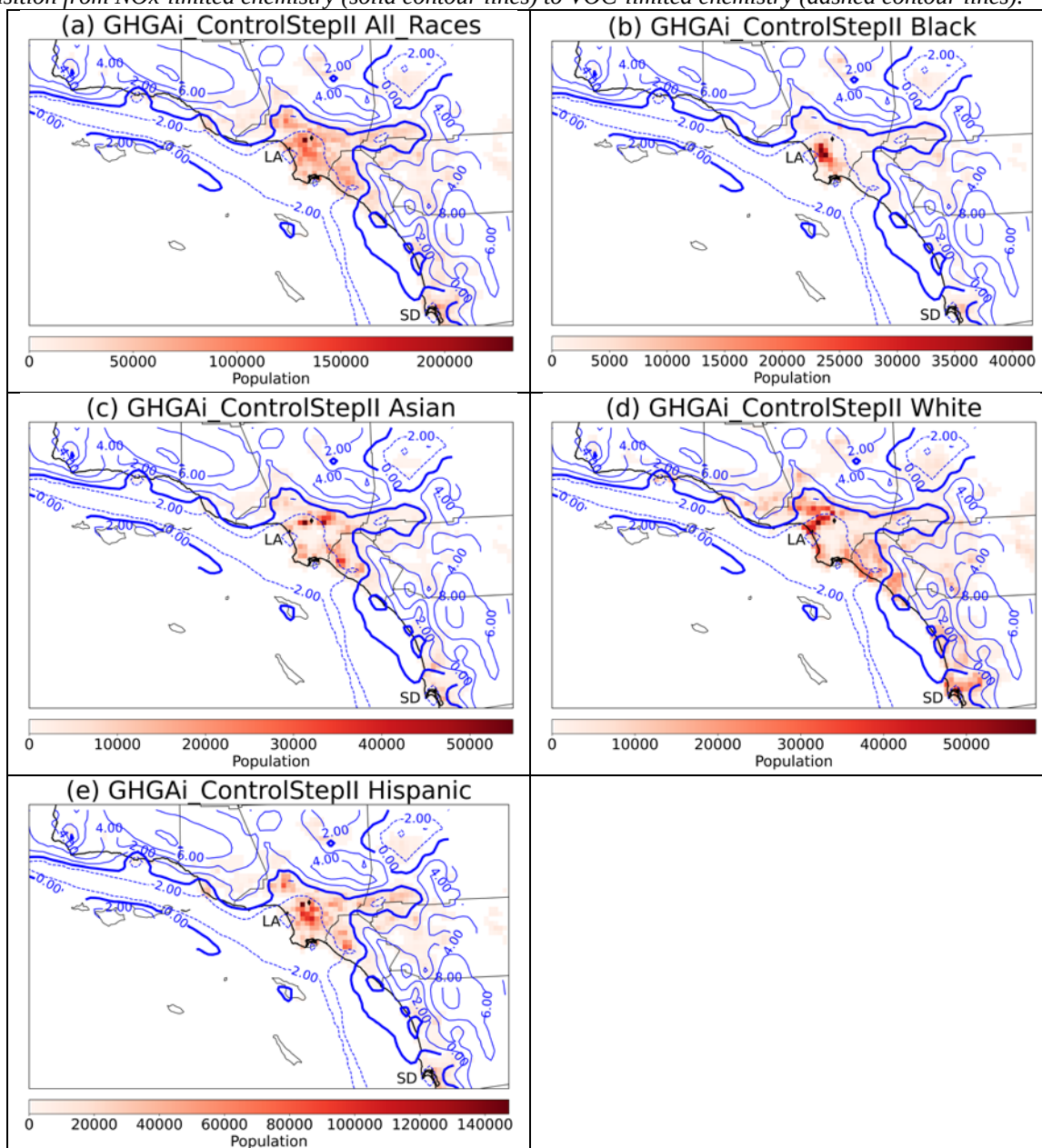


Figure S4.17: Population weighted averaged FNR-4.6 at hour 13 for different race/ethnicity groups. (All BAU and GHGAi related scenarios in this figure are under RCP8.5.)

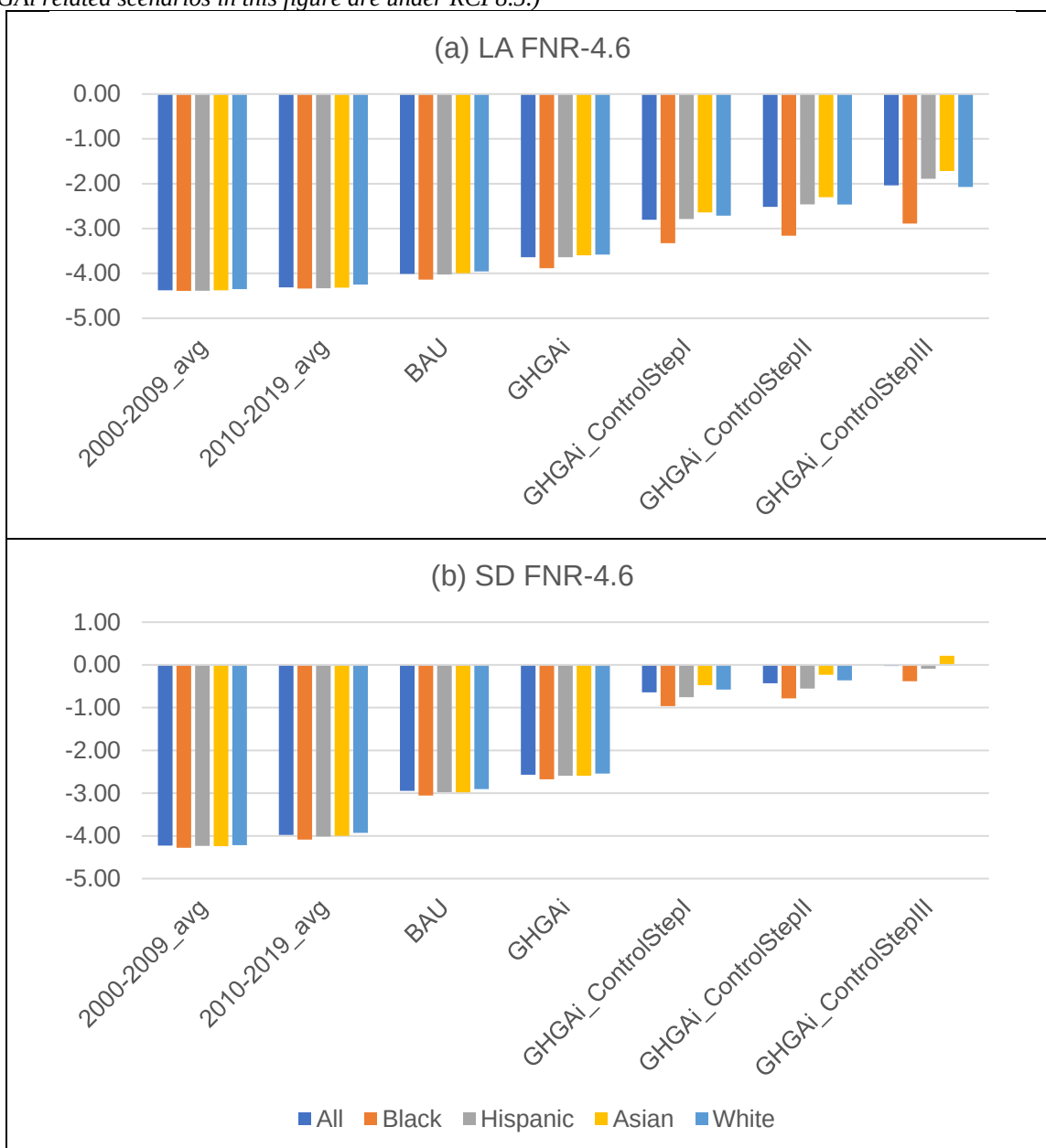


Figure S4.18: Relative disparity of population weighted FNR at hour 13 for different race/ethnicity groups. (All BAU and GHGAi related scenarios in this figure are under RCP8.5.)

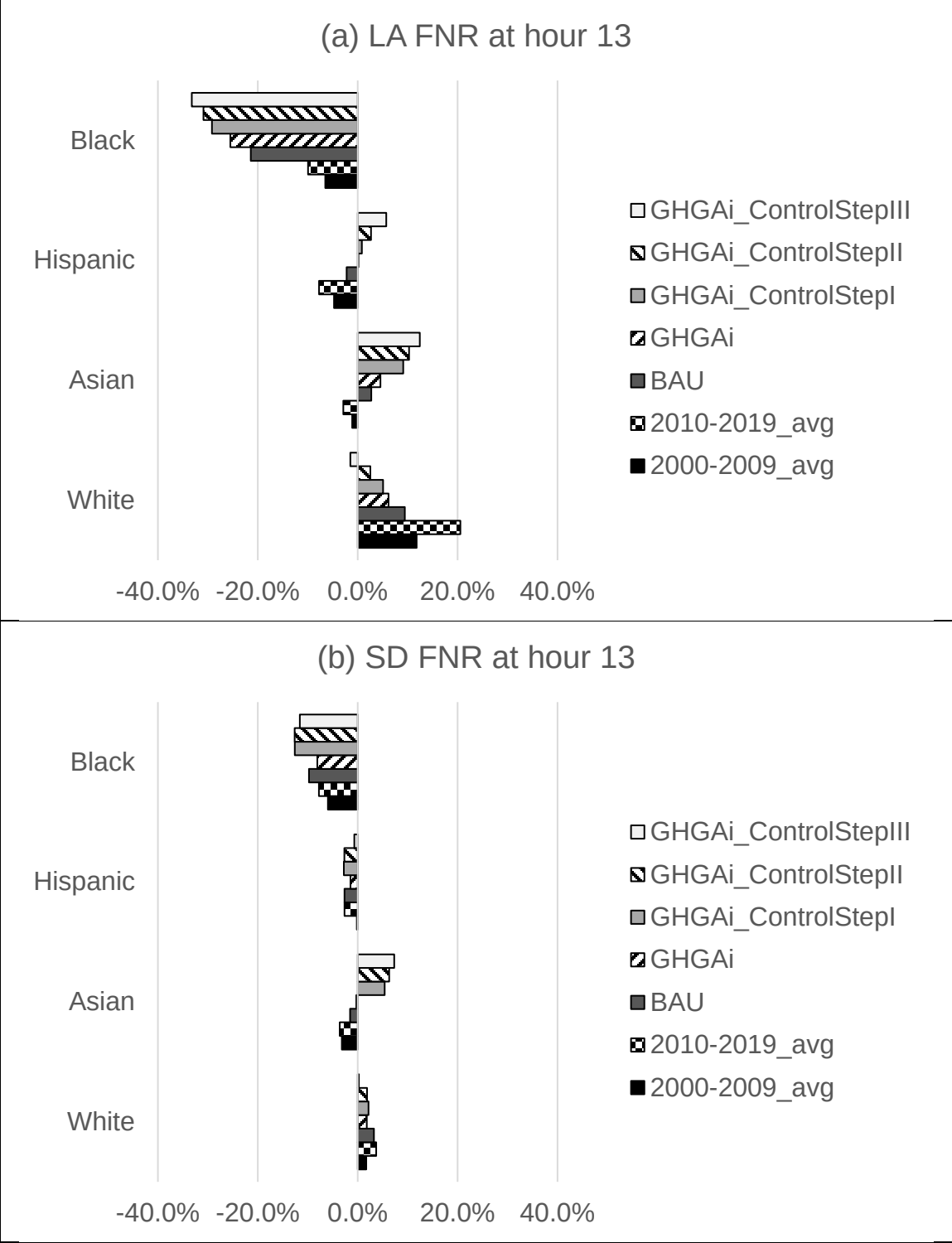


Figure S4.19: Population weighted concentrations (PWC) of summertime O_3 and NO_2 from NO_x source apportionment results for (a,c,e) different race/ethnicity groups under RCP8.5 GHGAI and (b,d,f) Black & African Americans under different RCP8.5 scenarios (unit: ppb).

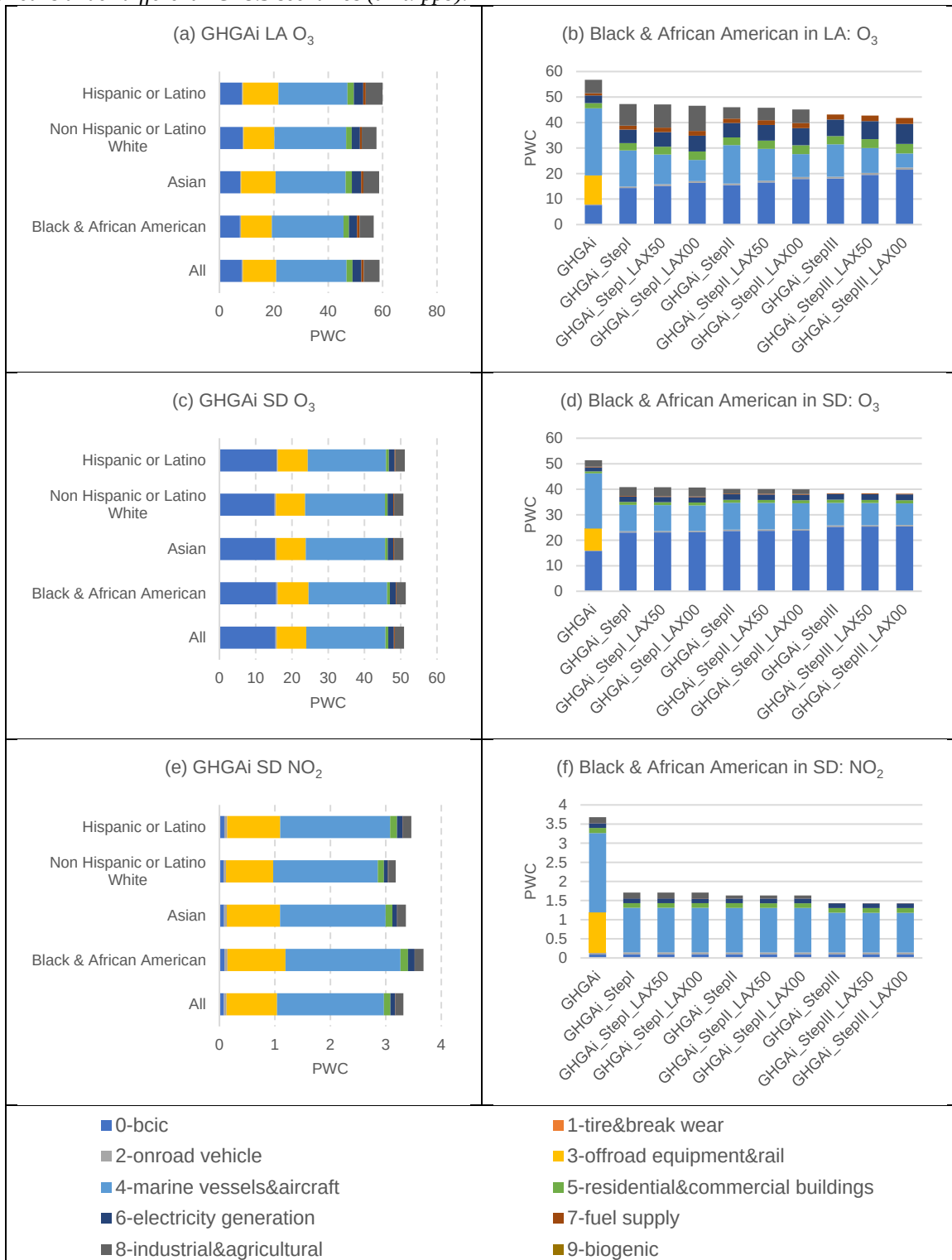


Figure S4.20: Relative disparity of population weighted summertime MD8H O₃ and 24hr-avg NO₂ exposure (left) and percentage of population exposed to healthy/unhealthy concentration levels (right) for different race/ethnicity groups at LA under RCP8.5.

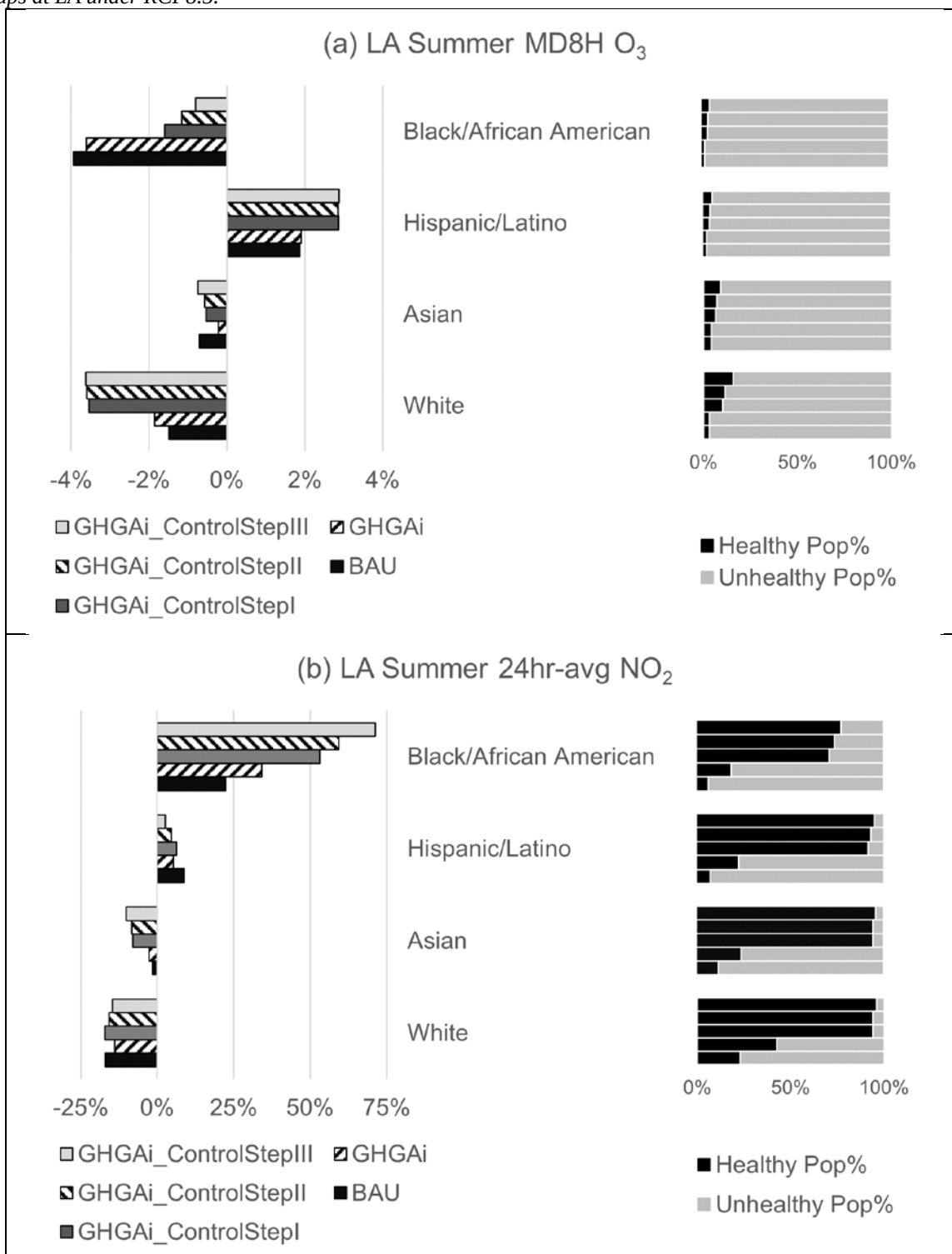
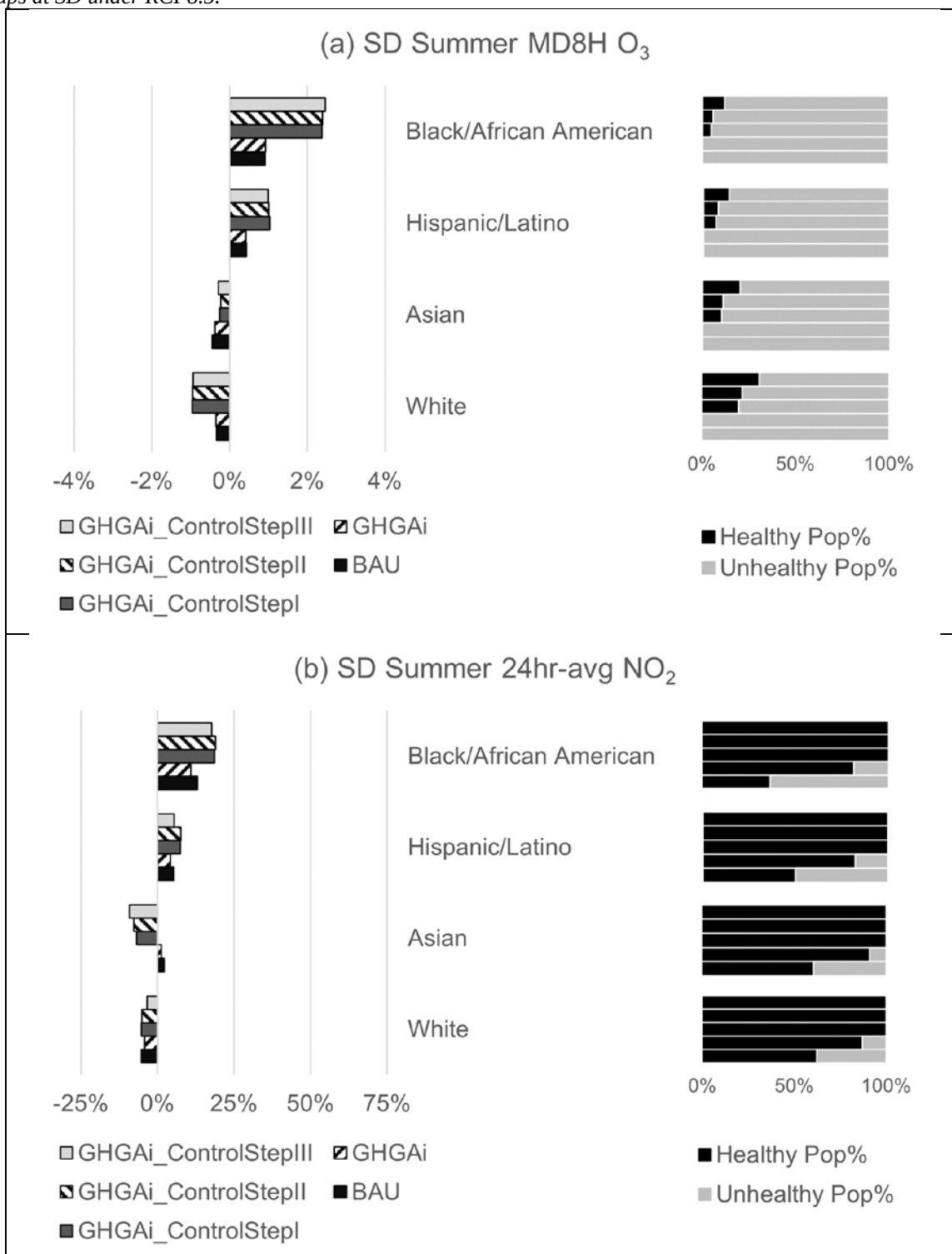


Figure S4.21: Relative disparity of population weighted summertime MD8H O₃ and 24hr-avg NO₂ exposure (left) and percentage of population exposed to healthy/unhealthy concentration levels (right) for different race/ethnicity groups at SD under RCP8.5.



Chapter 5 Conclusions

O₃ source apportionment technique is a powerful tool to quantify the contributions to O₃ formation from different emission sources. The source apportionment technique is very useful for designing effective emissions control strategies and addressing environmental justice problems. The work in this thesis establishes a complete framework for the development and implementation of a new O₃ source apportionment technique, which can be used for future research.

In the early stage of the research, a novel O₃ source apportionment technique is developed and serves as the research foundation of this thesis. The new O₃ source apportionment technique can separately resolve the contributions to O₃ formation from NO_x sources and VOC sources by explicitly tagging all molecules that carry odd oxygen within the chemical mechanism, providing a more detailed view of O₃ source origins. A simplification algorithm is also used in the tagging method to efficiently represent reactions involving molecules that contain more than one source of odd oxygen within the source apportionment calculations, while the information of source contributions and accuracy are preserved. By demonstrating the new source apportionment method in the UCD/CIT model using the peak O₃ episodes in Los Angeles, we show that the source apportionment results in UCD/CIT are consistent with the CMAQ-ISAM results, while the new O₃ source apportionment in UCD/CIT can provide new insights and better understanding of the roles of NO_x and VOCs in O₃ formation. Although missing sources of VCPs may affect the results of the case study, the overall results are still accurate considering the uncertainties.

By simulating the air quality for southern California in the year 2050, we find that the O₃ violations are largely due to the persistent VOC-limited chemistry in urban cores, where replacing combustion sources with renewable energy sources can produce higher O₃ concentrations. With the implementation of the new O₃ source apportionment technique, major emission sources that contribute to the high O₃ concentrations in the SoCAB are identified. While urban cores are VOC-limited, the major VOC sources are biogenic emissions within the study region and upwind sources outside the study region, making it not

effective at reducing O₃ concentrations by controlling local VOCs. The major NO_x sources include “off-road equipment & rail”, “marine vessels & aircraft”, and “industrial & agricultural emissions”, which become the target emission sources to control for O₃ reduction. Three cumulative emission Control Steps are designed under the GHGAi scenario. As the Control Steps become more and more stringent, the high O₃ concentrations are successfully reduced below 70 ppb in urban areas. The three Control Steps also result in significant public health benefits, with factors ranging from 9.3 to 14.1 relative to the GHGAi scenario. The public health savings due to the reduced O₃ concentrations under these Control Steps are estimated to be \$19.70-30.36B/yr.

A more comprehensive analysis is conducted on the results of previous Control Steps by analyzing their environmental justice for different race/ethnicity groups. O₃ and NO₂ exposure disparities under different scenarios are calculated. While the Control Steps reduced O₃ concentrations successfully, the exposure disparities for O₃ and NO₂ are not reduced. Relative exposure disparities of MD8H O₃ and 24hr-avg NO₂ even increase for the Black and African American communities in Los Angeles under the Control Steps. Black and African American residents live in the urban core of Los Angeles that has higher NO_x concentrations than outlying regions. While the higher NO_x concentrations mean a larger NO_x concentration reduction, the O₃ chemistry does not change fully to NO_x-limited conditions in the urban core, which results in slower MD8H O₃ reductions for Black residents compared to everyone else. Meanwhile, the 24hr-avg NO₂ concentrations are much lower for the general population than for the Black residents, which cause the relative exposure disparities for Black residents to also respond more slowly than everyone else. To reduce the exposure disparities for Black residents, we analyze the sources that significantly contribute to such disparities by using the O₃ source apportionment again. We find that emissions from the Los Angeles International Airport (LAX) are one of the significant contributors. By reducing the LAX emissions in the sensitivity tests, we are able to reduce the relative disparities of NO₂ by up to 50%. Although the feasibility of reducing LAX emissions is not analyzed, the reduced relative

disparities demonstrate that the O₃ source apportionment technique can also be used for the purpose of environmental justice.

All the control strategies above are not necessarily subject to current California regulations. Future studies may also need to consider different boundary and initial conditions, or a further future that have very different meteorology. Overall, the new O₃ source apportionment technique developed in this thesis proves to be a novel and useful tool for future research and designing effective emissions control programs.

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