

ABSTRACT

Title of Dissertation: CHARACTERIZING NEAR-SURFACE
OZONE ACROSS THE UNITED STATES:
PRODUCTION REGIMES, PRECURSOR
MONITORING AND MODEL EVALUATION

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Exposure to elevated concentrations of surface ozone poses significant risks to human health, contributes to premature mortality, and disproportionately impacts socioeconomically disadvantaged communities. Identifying factors influencing surface ozone formation is complicated because ozone photochemical production rates are non-linearly dependent on concentrations of precursors such as nitrogen oxides (NO_x) and volatile organic compounds (VOCs). Surface ozone regulation policies rely heavily on air quality models, such as CAMx and CMAQ, for guidance. Comparison with observations is crucial to evaluating a model's ability to represent ozone production chemistry and predict exceedance events. This work analyses ozone production regimes (OPRs) identified from satellite observations and model simulations. CAMx simulations for the summer of 2016 over the Contiguous United States (CONUS) are compared against OMI NO_2 and formaldehyde (HCHO) retrievals, exploiting the model's hourly and vertically

resolved output to examine the diurnal and vertical evolution of OPR. A new metric is developed to highlight areas where satellite measurements of OPR may not accurately represent near-surface chemistry and where additional ground-based or aircraft measurements are needed. To further assess model capabilities, CMAQ ozone predictions across CONUS from 2003-2019 are evaluated, focusing on exceedance detection capability above the National Ambient Air Quality Standards (NAAQS) threshold. Using a quadrant-based framework, regional and seasonal patterns in model performance are assessed, revealing significant disparities in hit rates across regions. To address monitoring coverage gaps, TEMPO satellite observations were integrated with the US EPA's Environmental Justice Screening and Mapping Tool (EJScreen). A flexible framework for optimal Air Quality System (AQS) sites placement is developed that integrates socioeconomic variables, population density, and satellite retrieved concentrations of NO₂ and HCHO. These findings underscore the necessity for targeted policies and interventions to address environmental justice concerns and expand monitoring coverage in underserved areas. This thesis enhances our understanding of ozone production chemistry, model performance limitations and monitoring network gaps, demonstrating the value of integrating air quality models with satellite observations, surface monitors and socioeconomic data to inform equitable and effective air quality management strategies.

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by

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List of Abbreviations

ACET	Acetone
ACS	American Community Survey
ADHD	Attention Deficit/Hyperactive Disorder
AK	Averaging Kernal
AMF	Air Mass Factor
AOD	Aerosol Optical Depth
AQ	Air Quality
AQS	Air Quality System
BEIS	Biogenic Emission Inventory System
BELD	Biogenic Emissions Landuse Database
BIRA-IASB	Belgian Institute for Space Aeronomy
CAA	Clean Air Act
CAAA	Clean Air Act Amendments
CAMx	Comprehensive Air Quality Model with Extensions
CASAC	Clean Air Scientific Advisory Committee
CASTNET	Clean Air Status and Trends Network
CB6r5	Carbon Bond 6 revision 5
CBSA	Core Based Statistical Area
CF	Cloud Fraction
CFR	Code of Federal Regulations
CHOCHO	Glyoxal
CMAQ	Community Multiscale Air Quality Modeling System
CO	Carbon Monoxide
CO ₂	Carbon Dioxide
CONUS	Contiguous United States
CPU	Central Processing unit
CSAPR	Cross-State Air Pollution Rule
DENS	Density
DISCOVER-AQ	Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality
DNPH	2,4-dinitrophenylhydrazine
DOMINO	Dutch OMI NO
EBI	Euler Backward Iterative
EGU	Electrical Generating Units
EJ	Environmental Justice
EOS	Earth Observing System
EPA	Environmental Protection Agency
EPIC	Environmental Policy Integrated Climate Model
EQUATES	EPA's Air QUALity Time Series
FACD	Formic Acid
FIA	Forest Inventory and Analysis
FNR	Formaldehyde to NO ₂ Ratio
FORM	Formaldehyde
GEMS	Geostationary Environmental Monitoring Spectrometer

GEOS CHEM	Goddard Earth Observing System - Chemistry
GLY	Glyoxal
GLYD	Glycolaldehyde
GOME	Global Ozone Monitoring Experiment
GSFC	NASA Goddard Space Flight Center
HCHO	Formaldehyde
HOX	Hypohalous Acids
HPC	High Performance Computing
HPLD	Hydroperoxyaldehyde
HPMS	Highway Performance Monitoring System
I _{IAP}	Integrated AQS Placement Index
IMPROVE	Interagency Monitoring of Protected Visual Environments
INTEXA	Intercontinental Chemical Transport Experiment
ISPD	Isoprene Product
IUPB	Institute of Environmental Physics, University of Bremen
JJA	June July August
KNMI	Koninklijk Nederlands Meteorologisch Instituut
LISTOS	Long Island Sound Tropospheric Ozone Study
LT	Local Time
MACR	Methacrolein
MDA8	Maximum Daily Average 8-hour Ozone
MGLY	Methylglyoxal
MOVES	Motor Vehicle Emissions Simulator
MPIC	Max Planck Institute for Chemistry
MSA	Metropolitan Statistical Area
NAAQS	National Ambient Air Quality Standards
NASA	National Aeronautics and Space Administration
NATTS	National Air Toxics Trends Stations
NBP	NO _x Budget Training Program
NEI	National Emissions Inventory
NESCAUM	Northeast States for Coordinated Air Use Management
NMB	Normalized Mean Bias
NO	Nitric Oxide
NO _x	Nitrogen Oxides
O ₃	Ozone
OH	Hydroxyl Radical
OMI	Ozone Monitoring Instrument
OPR	Ozone Production Regime
OTC	Ozone Transport Commission
OZIE	Ozarks Isoprene Experiment
PAMS	Photochemical Assessment Monitoring Stations
PAN	Peroxyacetyl Nitrate
PANX	C3 and Higher Peroxyacyl Nitrate
PAR	Paraffin Carbon Bond (C-C)
PBL	Planetary Boundary Layer
PCTL	Percentile

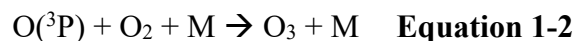
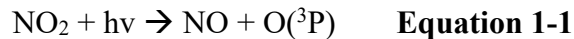
PPM	Parts Per Million
PRES	Pressure
QA4ECV	Quality Assurance for Essential Climate Variables
QF	Quality Flag
RMSE	Root Mean Squared Error
SAO	Smithsonian Astrophysical Observatory
SASS	Subsonics Assessment
SEAC ⁴ RS	Studies of Emissions, Atmospheric Composition, Clouds and Climate Coupling by Regional Surveys
SIP	State Implementation Program
SLAMS	State and Local Air Monitoring Stations
SMOKE	Sparse Matrix Operator Kernel Emissions
SONEX	SASS (Subsonics Assessment) Ozone and NO _x Experiment
SW	Scattering Weight
SZA	Solar Zenith Angle
TEMPO	Tropospheric Emissions: Monitoring Pollution
TIGER	Topologically Integrated Geographic Encoding and Referencing
TROPOMI	TROPOspheric Monitoring Instrument
TSD	Technical Support Documentation
TUV	Tropospheric Ultraviolet and Visible Radiation Model.
UC	Uncertainty
USDA-USFS	United States Department of Agriculture - United States Forest Service
UV	Ultraviolet Radiation
VCD	Vertical Column Density
VCP	Volatile Chemical Products
VOC	Volatile Organic Compounds
WRF	Weather Research and Forecasting Model
WUR	Wageningen University & Research

1. Introduction

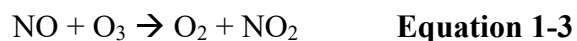
Tropospheric ozone is an important secondary atmospheric pollutant produced in situ through photochemical reactions or transported from the stratosphere. Tropospheric ozone primarily acts as a hydroxyl (OH) precursor without anthropogenic pollution. OH is one of the most important oxidants in the troposphere as it is responsible for the termination reactions of volatile organic compounds (VOCs), methane, and CO, among other important species. The oxidation of VOCs, CO and methane eventually forms CO₂. Tropospheric ozone is also a greenhouse gas, and its radiative forcing between 1750 to 2019 is almost equivalent to CH₄ (0.54 W/m² for CH₄ and 0.47 W/m² for ozone). However, since tropospheric ozone is not well mixed in the atmosphere owing to its shorter lifetime, local radiative forcings can be higher than global estimates, causing tropospheric ozone in the tropics to have a higher impact on the global temperature budget than in the mid-latitudes (Hansen et al., 1997; Stevenson et al., 2013). Therefore, ozone directly and indirectly (through its relationship with OH) can impact global warming.

1.1. Tropospheric ozone chemistry

Tropospheric ozone is formed via photochemical reactions and is nonlinearly dependent on its two major precursors: nitrogen oxides (NO_x) and VOCs (Crutzen, 1974; Finlayson-Pitts and Pitts, 1999; Seinfeld and Pandis, 2006). An overview of tropospheric ozone photochemistry begins with the photolysis of NO₂ at wavelengths <424 nm leads to the production of O(³P) (**Equation 1-1**) which undergoes a termolecular reaction with O₂ to form ozone (**Equation 1-2**) (Atkinson, 2000; Lu et al., 2019; Seinfeld and Pandis, 2006).



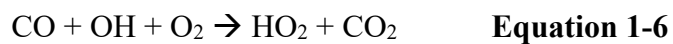
Ozone reacts with NO to regenerate NO₂ (**Equation 1-3**). Equations 1-1 to 1-3 lead to null production of ozone.

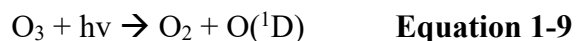
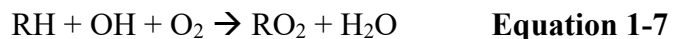


The presence of radicals (hydroperoxyl (HO₂) and peroxy (RO₂)) provides alternative pathways for NO to react instead of with ozone (**Equation 1-4 and 1-5**).

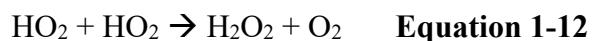
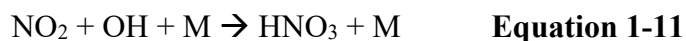


Oxidation of CO (**Equation 1-6**), hydrocarbons (**Equation 1-7**) and alkoxy radicals (**Equation 1-8**) leads to the formation of RO₂ and HO₂. The hydroxyl radicals (OH) used are generated from photolysis of ozone and subsequent reaction with water vapour (**Equation 1-9 and 1-10**).





Equations 1.1 to 1.10 represent the production of tropospheric ozone through a chain of photochemical oxidations of CO and hydrocarbons (VOCs) in the presence of NO_x. Chain termination reactions are shown in **Equation 1-11 and 1-12** by the loss of HO_x radicals. H₂O₂ and HNO₃ are then removed by wet deposition.



1.2. Tropospheric ozone production regimes

Atmospheric chemists categorize the interaction between ozone and its key anthropogenic precursors into NO_x-limited, transition, and VOC-limited regimes. Ozone production is considered NO_x-limited when the loss of hydrogen oxide radicals (HO_x) primarily occurs due to the self-reaction of peroxy radicals, and is considered VOC-limited when the loss of HO_x primarily occurs due to reactions between OH and NO₂ (Sillman, 1999, 1995). Ozone production is in the transition regime when loss of HO_x by both self-

reaction and reaction with NO_2 is important. These regimes are shown in **Figure 1-1** where blue dashed line separates the VOC-limited and NO_x -limited regimes of tropospheric ozone formation.

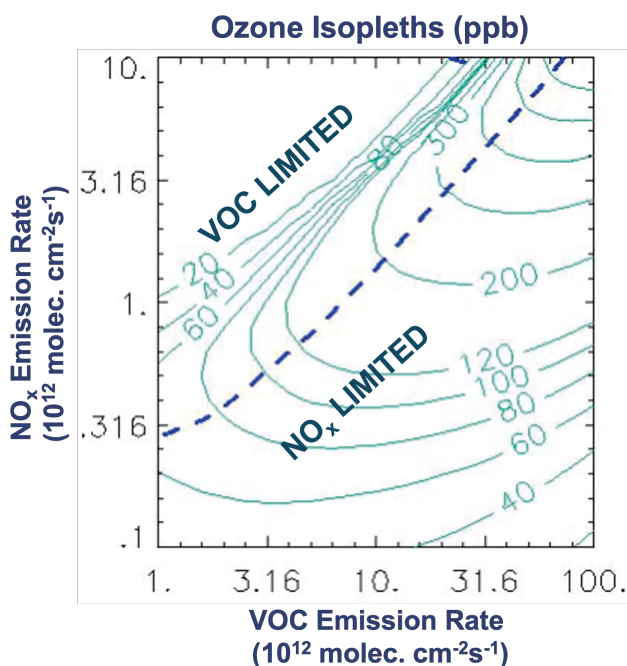


Figure 1-1: Ozone isopleths (ppb) as a function of the average emission rate for NO_x and VOC (10^{12} molec. $\text{cm}^{-2}\text{s}^{-1}$) in chemical box model calculations. The isopleths (solid green lines) represent conditions during the afternoon following 3-day calculations with a constant emission rate, at the hour corresponding to maximum ozone. The short blue dashed line represents the transition from VOC-limited to NO_x -limited conditions. Image adopted from (Sillman and He, 2002)

One of the most common methods for describing ozone production regimes (OPRs) uses the ratio of HCHO/NO_2 (formaldehyde to nitrogen dioxide ratio, or FNR) (Acđan et al., 2023; Duncan et al., 2010; Martin et al., 2004; Schroeder et al., 2017; Tonnesen and Dennis, 2000). Although other metrics may be more accurate, FNR is a useful indicator of ozone sensitivity since both HCHO and NO_2 have similar lifetimes, and consequently their

ratio can represent local ozone production. FNR is also a useful indicator since both HCHO and NO₂ are readily measured from space using satellites. In the absence of a rich dataset of hydrocarbon concentrations and their rate constants and products, HCHO is an effective analogue as many commonly found VOCs such as isoprene breakdown to form HCHO. Before the development of FNR, ratios of H₂O₂/HNO₃, H₂O₂/([O₃]+[NO₂]), O₃/NO_x, O₃/(NO_y-NO_x) and HCHO/NO_y were proposed and tested as a means to assess whether tropospheric ozone production was NO_x or VOC-limited (Jacob et al., 1995; Kleinman et al., 2001; Sillman, 1995; Sillman and He, 2002; Tonnesen and Dennis, 2000). A preferred indicator of ozone production regimes is H₂O₂/HNO₃, however these species are not observed from orbital platforms and are not routinely measured or monitored (Sillman, 1995). The ratio of LRO_x (radical loss rates of self-reaction) to LNO_x (reaction rate loss of OH with NO₂) is a good indicator of OPR, although the transition point between regimes is still debated (Kleinman et al., 2001; Roberts et al., 2022; Schroeder et al., 2017; Sebol et al., 2024; Xiong et al., 2023).

1.3. Climate and Meteorological Impact on Tropospheric Ozone

Climate change and meteorological processes impact tropospheric ozone abundance through a variety of ways as detailed in **Figure 1-2**. NO_x is produced through natural emissions from soil, lightning, biosphere, wildfires and wetlands. Soil NO_x, which accounts for about 15% of global NO_x emissions is expected to increase significantly with warming temperatures that may worsen of tropospheric ozone pollution (Huber et al., 2024; Lu et al., 2021). Lightning NO_x also accounts for 10-15% of global NO_x emissions although its impact on tropospheric ozone production is harder to estimate since it is released in the

upper troposphere (Lu et al., 2019; Nault et al., 2017). Lightning NO_x emissions are expected to increase with warming temperatures due to frequent and more intense convection, however, the subsequent impact on surface ozone concentration is still unclear (Schumann and Huntrieser, 2007). Wildfires produce large amounts of tropospheric ozone through the emission of NO_x , VOCs and CO. With changing climate, wildfires are probably going to increase in frequency, intensity, and spatial distribution leading to increase in tropospheric ozone production (IPCC, 2023; Lu et al., 2016).

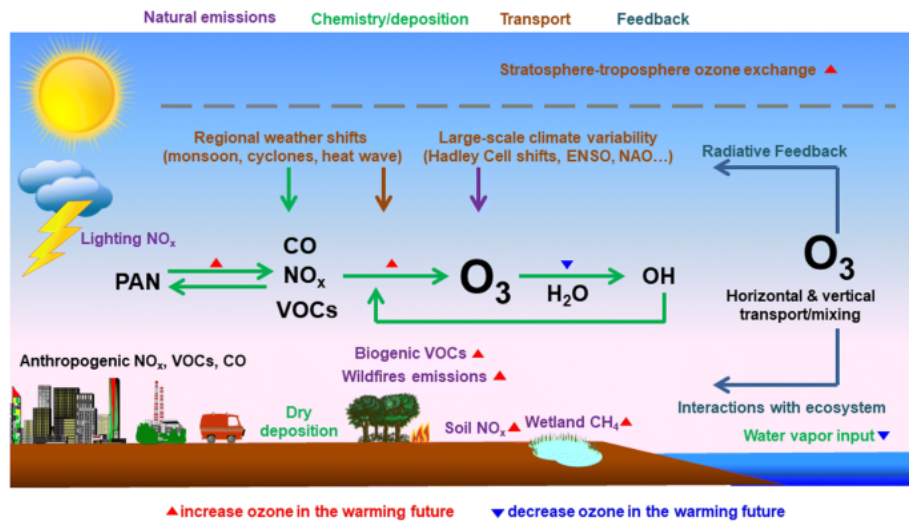


Figure 1-2: Pathways of interaction between meteorology/climate changes and tropospheric ozone. The red (blue) triangles represent that at global scale future climate will increase (decrease) tropospheric ozone through the specific pathway based on current understanding. Figure 1 from (Lu et al., 2019)

VOCs are produced in large amounts through natural sources from vegetation and plants. Climate change causes land use and land cover to vary, which impacts the production of VOCs. Temperature is one of the biggest factors in these changes as rising temperatures increases photosynthesis rates causing increase in biogenic VOCs emissions especially isoprene and monoterpenes (Janyasuthiwong et al., 2022; Zhang et al., 2023a).

This expected increase in VOC emissions will lead to increases in tropospheric ozone concentrations. However, the impact of climate change on tropospheric ozone through biogenic VOCs is complicated due to extreme temperatures, drought conditions, isoprene chemistry, and increasing CO₂ emissions that can lead to potential suppression of the emissions (Gu et al., 2021; Ito et al., 2009; Lam et al., 2011; Marvin et al., 2017; Yáñez-Serrano et al., 2020).

Meteorological processes like boundary layer dynamics, synoptic-scale circulations, temperature, humidity, solar radiation, and advection also impact tropospheric ozone. High temperatures have long been linked with increased ozone production in the troposphere. The climate penalty factor quantifies how much tropospheric ozone concentrations will increase with increasing temperatures, even if the emissions of its precursors remain constant (Bloomer et al., 2009; Rasmussen et al., 2013). In areas of high humidity, aerosol optical depth (AOD) increases, leading to higher UV flux and higher photochemical production rates of tropospheric ozone (Bloomer et al., 2009; Dickerson et al., 1997). Mesoscale level sea breezes arise due to temperature differences across the land-water interface, leading to horizontal pressure gradients that can recirculate pollution in the PBL and lead to poor air quality near the coast (Loughner et al., 2014; Mazzuca et al., 2019). Some of the most densely populated cities in the US (and around the world) are located near the coast, leading to an inherent condition of increased ozone pollution due to sea breezes, in addition to that from anthropogenic forcings. Deep convective storms also carry polluted air from the PBL to the upper troposphere, increasing ozone production (Anderson et al., 2016; Dickerson et al., 1987). Mountain breezes due to temperature differences

between the air over the mountain and adjacent air at the same altitude can reduce ozone pollution being carried away from urban hotspots located near the mountain, worsening urban air quality (Reddy and Pfister, 2016). Another factor to note is that regions that are downwind of electrical generating units (EGUs) tend to have high ozone concentrations (OAR US EPA, 2016).

1.4. HCHO and NO_x Overview

Here we provide a brief overview of prior efforts to regulate NO_x emissions in the US. In 1998, the US EPA issued the Nitrogen Oxides State Implementation Program (NO_x SIP Call) in response to increasing anthropogenic emissions of NO_x, resulting in the NO_x Budget Trading Program (NBP), the Ozone Transport Commission (OTC) NO_x Budget Program, as well as various other national regulations (US EPA, 2002). Anthropogenic NO_x emissions in the US have decreased by 70% from 2002 to 2022 (US EPA, 2023a), a reduction captured by satellite observations of the NO₂ tropospheric column over time (Duncan et al., 2016; Georgoulias et al., 2019; Goldberg et al., 2015; H. He et al., 2013; Kim et al., 2006; Lamsal et al., 2015; Roberts et al., 2022; Russell et al., 2012; Schneider et al., 2015; Tong et al., 2015). Consequently, this reduction lowered interstate ozone transport and substantially decreased surface ozone concentrations (Butler et al., 2011; Canty et al., 2015; Duncan et al., 2010; Foley et al., 2015; G  go et al., 2007; Vinciguerra et al., 2017). In recent decades, the reduction of NO_x has been particularly effective in lowering concentrations of surface ozone (Butler et al., 2011; Duncan et al., 2010; Goldberg et al., 2015; H. He et al., 2013; Roberts et al., 2022; Simon et al., 2015).

While formaldehyde (HCHO) has been widely monitored by satellites since 1995 due to its strong and distinct spectral absorption in the near-UV range, satellites cannot monitor most other VOCs due to their low concentrations and spatial variabilities (Boeke et al., 2011; Burrows et al., 1999; Chance et al., 2000). An important exception is glyoxal (CHOCHO), a short-lived decomposition product of VOCs (Kaiser et al., 2015; Miller et al., 2014). Many VOCs, including biogenic VOCs such as isoprene, are oxidized in the atmosphere to HCHO and CHOCHO on the way to carbon dioxide (CO₂) and water vapor (H₂O). Field campaigns such as Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality (DISCOVER-AQ), Intercontinental Chemical Transport Experiment (INTEX-A), Long Island Sound Tropospheric Ozone Study (LISTOS), SASS (Subsonics Assessment) Ozone and NO_x Experiment (SONEX), Studies of Emissions and Atmospheric Composition, Clouds and Climate Coupling by Regional Surveys (SEAC⁴RS) have provided detailed VOC measurements, but our interpretations are constrained by their limited spatial and temporal range (Crawford et al., 2014; INTEX-A Science Team, 2006; NESCAUM, 2018; Singh et al., 1999; Toon et al., 2013). Emission inventories, based on “bottom-up” estimates of emissions from individual source sectors, show that anthropogenic VOC emissions in the US decreased by 22% from 1997 to 2016 (US EPA, 2017). This decrease is attributed to reduced vehicular emission of VOCs from tailpipes due to widespread use of catalytic converters and to declines in the industrial emissions of VOCs (Simon et al., 2015; Warneke et al., 2012).

With warming temperatures, biomass burning emissions have increased in the southeast and western US leading to increased production of HCHO (Jin et al., 2023; Palmer et al., 2003; Rice et al., 2023; Zhu et al., 2017b). Emissions of VOCs from volatile chemical products (VCPs) such as various personal care items, solvents, and adhesives are now a significant contributor to the production of urban HCHO following the above-mentioned decline in the emission of VOCs from automotive tailpipes (Coggon et al., 2021; McDonald et al., 2018). VCPs now account for ~50% of all petrochemical VOCs in the national budget (McDonald et al., 2018). Anthropogenic VCP emissions can contribute significantly to ozone production and are difficult to regulate due to the wide variety of their sources and their lack of ground monitoring, leading to limited inclusion in regulatory air quality model emissions inventories (McDonald et al., 2018; Yang et al., 2016; Zhao et al., 2014).

1.5. Measurements of Ozone and its Precursors (NO_x and VOCs)

Ground-based observations, such as those within the EPA monitoring networks, also serve to validate regional Air Quality Models (AQMs), which are necessary for policy and regulation. Measuring both HCHO and NO_2 at the surface is necessary because the ratio of formaldehyde to NO_2 (FNR) is a useful method for identifying ozone production regimes and satellite data are often not sensitive to surface conditions (Duncan et al., 2010; Schroeder et al., 2017; Singh et al., 2025a). However, the existing AQS coverage is sparse due to the high operational costs associated with these ground-based monitoring sites (Dobkin and Kerr, 2024; Grainger and Schreiber, 2019; Kelp et al., 2023; Pedde and Adar, 2024; Roque et al., 2025; Wang et al., 2024). As a result, there has been an increase in the

deployment of low-cost sensor networks, such as PurpleAir and mobile vehicle-based monitoring, which help fill observational gaps in areas lacking an AQS (PurpleAir, 2026). Despite helping to meet an important need, the monitoring by low-cost sensors is sparse, and further research is needed to determine calibration standards and measurement accuracy (Apte and Manchanda, 2024; Barkjohn et al., 2021; Considine et al., 2023; deSouza and Kinney, 2021; Dickerson et al., 2024; Kramer et al., 2023; Lu et al., 2022). These ground-based non-AQS networks are also not considered for attainment decisions of NAAQS for 8-hour average ozone (US EPA, 2015a). However, data from these instruments have an impact on mitigation and siting decisions (Northcross et al., 2020).

Although ground-based and aircraft measurements help validate AQ models, the constraints they provide are limited by their spatial and temporal coverages. Many studies have compared FNRs from satellite retrievals and aircraft observations to the output from air quality models to identify inconsistencies between the modeled and measured representation of ozone precursors (Canty et al., 2015; Choi et al., 2012; Duncan et al., 2010; Jin et al., 2020; Johnson et al., 2023; Jung et al., 2022; Martin et al., 2004; Mazzuca et al., 2016; Schroeder et al., 2017; Souri et al., 2023). These inconsistencies exist because instruments on satellites retrieve column-integrated measurements with varying sensitivity as a function of altitude, often with low sensitivity to column values of ozone precursors in the planetary boundary layer (PBL). Another reason for these inconsistencies is the uncertainty in satellite retrievals from systematic and random biases (Souri et al., 2023). Although instruments on low-Earth orbit satellites only provide constraints on ozone photochemistry once or twice per day, instruments on geostationary satellites such as

Tropospheric Emissions: Monitoring Pollution (TEMPO) over North America, the Sentinel-4 over Europe and Geostationary Environmental Monitoring Spectrometer (GEMS) over East Asia are beginning to provide observations of column NO₂ and HCHO every 40-60 minutes, enabling an examination of the diurnal variation of FNR (Chance et al., 2019; J. Kim et al., 2020; Stark et al., 2019; Zoogman et al., 2017).

1.6. Health Impacts of Ozone, NO_x and VOCs

Long-term exposure to ozone at high concentrations can harm human health, materials and ecosystems (Bell et al., 2006; Haagen-Smit, 2002; Lefohn et al., 2018; Nowroz et al., 2024; West et al., 2009). Since the passing of the Clean Air Act Amendments (CAAA) in 1990, the United States (US) Environmental Protection Agency (EPA) has prioritized the regulation of tropospheric ozone (US EPA, 1990). For this reason, US states are required to attain the National Ambient Air Quality Standard (NAAQS) of 70 ppbv for 8-hour average ozone (US EPA, 2015).

Exposure to ozone can impact human health, ranging from respiratory and cardiovascular problems to systemic problems (Bell et al., 2006; Nuvolone et al., 2018). Health impacts can range from acute symptoms to chronic and life-altering symptoms. Ozone exposure also disproportionately impacts the vulnerable populations, such as the elderly, children and immunocompromised people. The number of people globally who have died from exposure to ozone is estimated to have increased by 46% between 2000 and 2019 (Malashock et al., 2022). This increasing trend is more visible in densely populated urban areas. Hospital admissions due to exposure to ozone have also increased,

primarily due to respiratory and cardiovascular causes (Zheng et al., 2021). The cardiovascular impacts due to ozone exposure include heart attacks, strokes, and other cardiovascular diseases, leading to premature morbidity and mortality (Goodman et al., 2015; Hua et al., 2025; Wang et al., 2019). The respiratory impacts from ozone exposure include sore throat and irritation, lung inflammation, asthma attacks and the increased risk of hospitalizations (Kim et al., 2020). Other systemic impacts due to ozone exposure include damage to the immune system, impact on cognitive functions, Alzheimer's, Parkinson's, multiple sclerosis (MS), attention deficit/hyperactive disorder (ADHD), sleep quality and impacts on reproductive health (González-Guevara et al., 2014; Martínez-Lazcano et al., 2013; Nuvolone et al., 2018; Zhang et al., 2023b; P. Zhou et al., 2023).

Figure 1-3 shows a schematic with the different types of health effects due to exposure to ozone and a qualitative representation of the number of people affected due to them.

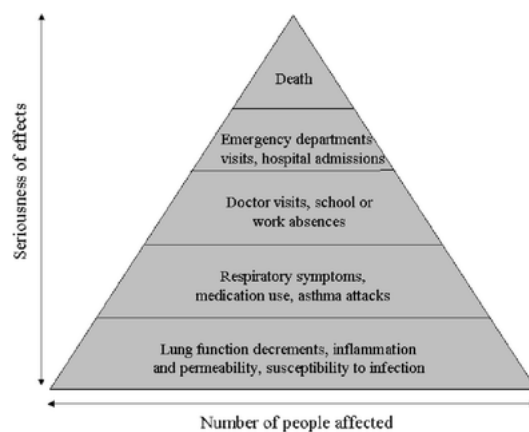


Figure 1-3: Pyramid of health effects caused by ozone. Figure 1 from (Nuvolone et al., 2018)

Exposure to elevated concentrations of NO_2 has been associated with increased mortality, worsening of chronic conditions such as asthma, and increased risk of adverse

infant outcomes, including neonatal intensive care unit admission (Phiri et al., 2025; Wang et al., 2021; Zheng et al., 2021). Children and elderly individuals face disproportionately higher risks due to their developing or compromised immune systems, making them more susceptible to the inflammatory effects of exposure to elevated concentrations of NO₂.

Exposure to VOCs causes respiratory, neurological and carcinogenic impact on human health (Liu et al., 2022; Ren et al., 2017; Zhou et al., 2023). A schematic of some of the health impacts due to VOCs are shown in **Figure 1-4**. HCHO, which is the VOC of focus in this dissertation, is a high-impact carcinogen that is severely under-monitored across the US (Reingruber and Pontel, 2018; Zhu et al., 2017a).

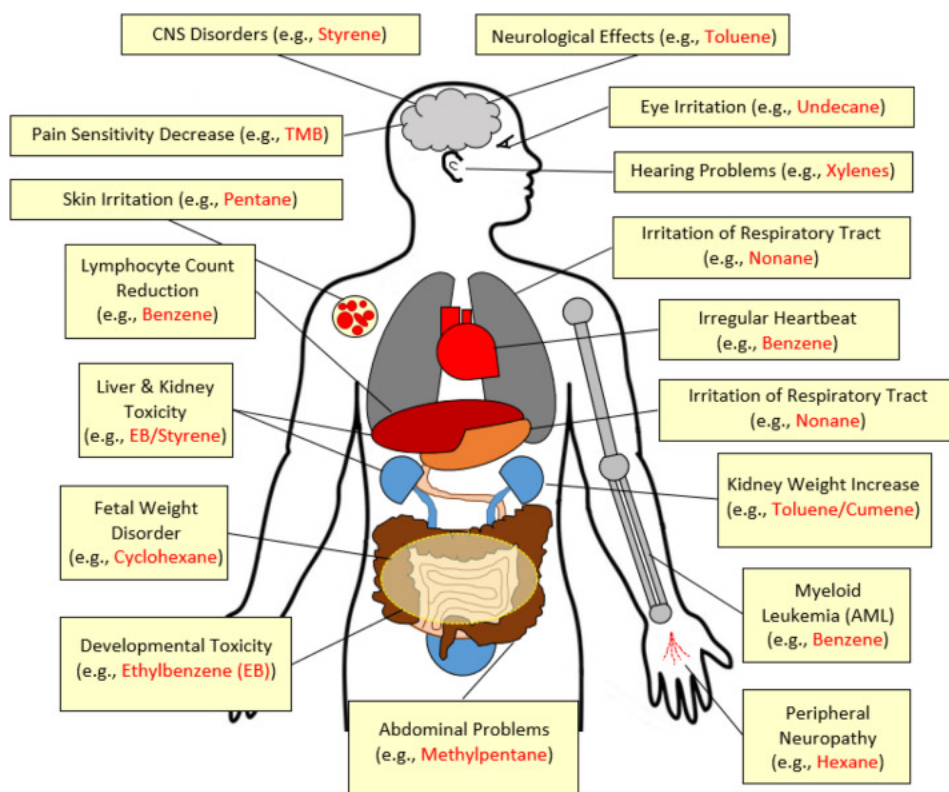


Figure 1-4: Major impacts of VOCs on human health. Figure 1 from (Rajabi et al., 2020)

1.7. Unequal Distribution of Tropospheric Ozone

A common motto for air quality research is that “we do not all breathe the same air”. This motto reflects the growing recognition that exposure to air pollution and associated health risks are not evenly distributed. Despite the traditional understanding that air quality and its adverse health effects are shared amongst all demographic groups, more recent perspectives acknowledge that there exists unequal exposure and risk across demographics (Bravo et al., 2016; Miranda et al., 2011; Tessum et al., 2019). This uneven distribution of air quality burdens has been extensively documented in recently published papers (Camilleri et al., 2023; Clark et al., 2014; Geldsetzer et al., 2024; Hajat et al., 2015; Jbaily et al., 2022; Kerr et al., 2024, 2023, 2021; Li et al., 2024; Liu et al., 2021; Rosofsky et al., 2018; Wang et al., 2024; Zwickl et al., 2014). Despite research showing disparities in both exposure to and health effects of ozone, gaps in the siting and capabilities of the EPA monitoring network’s Air Quality System (AQS) sites limit the ability to fully account for these inequalities. People living in cities and close to pollution sources tend to be from underserved communities and therefore suffer the bulk of the consequences (Dressel et al., 2022; Landrigan et al., 2018; Miranda et al., 2011; Sayyed et al., 2024).

The US Environmental Protection Agency (EPA) defines environmental justice (EJ) as “the fair treatment and meaningful involvement of all people regardless of race, color, national origin, or income, with respect to the development, implementation, and enforcement of environmental laws, regulations, and policies.” Fair and inclusive participation in decisions that impact public and environmental health is essential to ensure that all communities are adequately protected. This approach emphasizes that individuals,

regardless of their backgrounds, should have the opportunity to be involved in and considered for environmental decision making and receive equitable protection from environmental and health risks. To support informed policy and planning, tools such as the US EPA's Environmental Justice Screening and Mapping Tool (EJScreen) have been developed to help identify areas with heightened vulnerability to environmental and health impacts ("EJScreen TSD," 2024; US EPA, 2025, 2014a).

In the US, research has consistently shown that communities with predominantly minority and lower-income populations face disproportionately high levels of air pollution. These pollution burdens coincide with other social challenges, creating compounded stress that makes communities more vulnerable to health impacts. While the Clean Air Act has successfully lowered national pollution levels over recent decades, it has less effectively addressed relative disparities between communities. The same neighborhoods that bore the heaviest pollution burdens years ago continue to experience the worst air quality today, particularly communities of color. This persistence suggests that despite improvements in average air quality, the fundamental inequities in how pollution affects different populations persist (Chambliss et al., 2021; Currie et al., 2023; Tessum et al., 2019).

Figure 1-5 shows the three primary mechanisms that drive disproportionate pollution exposure in communities of color: market dynamics (facility siting and demographic shifts), sociopolitical factors (limited political power to resist undesirable land uses), and racist planning practices (historical segregation and discriminatory zoning). These causes lead to health, economic, and social consequences that create a feedback loop, reinforcing

the original mechanisms and perpetuating environmental injustice (Ash and Boyce, 2018; Bullard, 1990; Lane et al., 2022; Morello-Frosch, 2002; Pastor et al., 2001; Pulido, 2017; Whittemore, 2017).

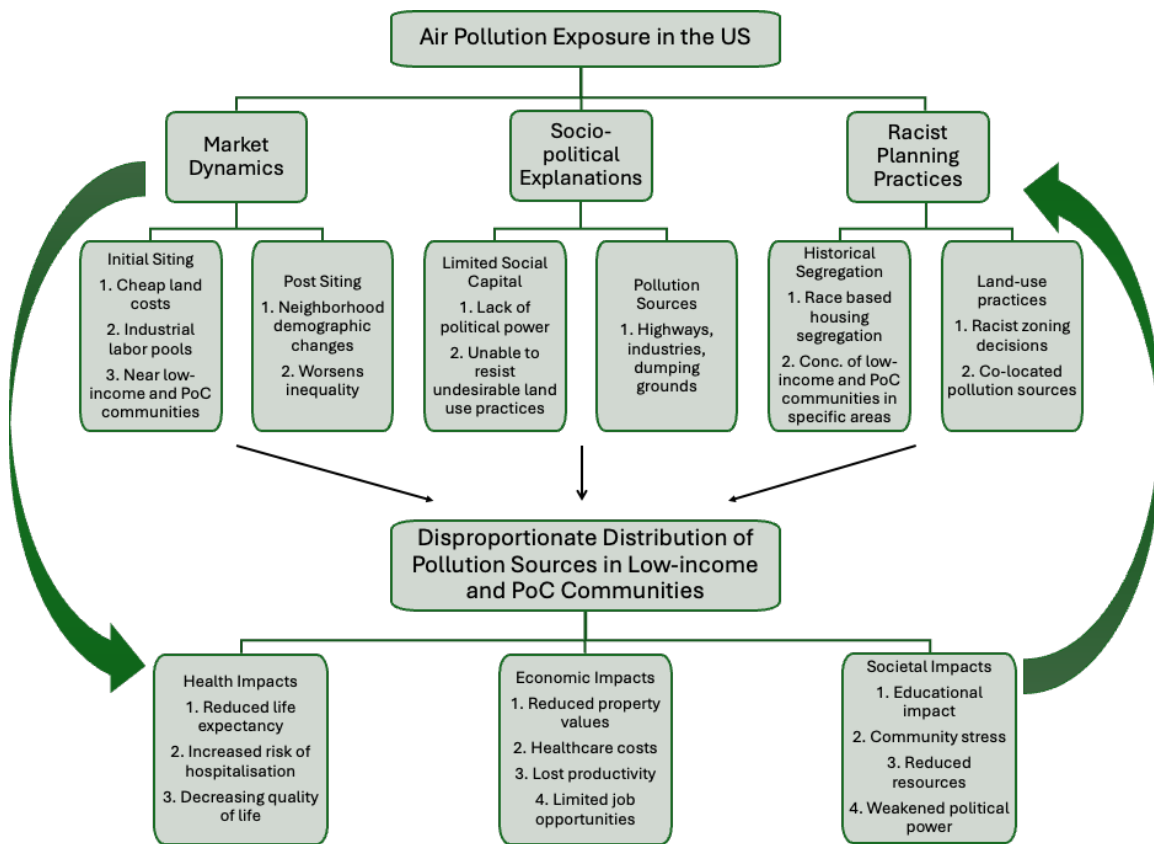


Figure 1-5: Conceptual framework of air pollution inequalities in the United States.

Understanding tropospheric ozone formation requires knowledge of its precursors, primarily HCHO and NO₂. The OPR determines whether ozone formation is limited by VOCs or NO_x, which is essential for designing mitigation strategies. However, characterizing OPR and ozone precursor distributions presents significant challenges. Ground-based monitoring networks provide limited spatial coverage, particularly for HCHO and NO₂, while satellite observations offer broad spatial extent but lack the

temporal and vertical resolution needed to capture surface-level chemistry. This thesis aims to address these limitations by integrating satellite retrievals, regional air quality models, and ground-based observations to better understand ozone photochemistry across the continental United States.

This thesis is organized into the following chapters. Chapter 2 examines OPRs across CONUS during summer 2016 by combining OMI satellite retrievals with CAMx model output, developing a new metric to quantify where satellite column observations reliably represent surface chemistry. Chapter 3 addresses spatial gaps in ground-based monitoring by developing a flexible framework for placement of HCHO and NO₂ monitors that combines pollution patterns, population density, and socioeconomic vulnerability. Chapters 4 and 5 evaluate CMAQ model performance in predicting MDA8 ozone against AQS observations from 2003 to 2019, examining temporal trends, spatial patterns, and potential sources of model-observation discrepancies including evaluation methodology, wildfire smoke representation, and land-water interface processes.

2. Inferring Near-Surface Ozone Production Regimes Using Satellite Remote Sensing and CAMx Modeling (published as (Singh et al., 2025a))

2.1. *Abstract*

Surface ozone regulation policies rely heavily on air quality models, such as CAMx, for guidance. Comparison with observations is crucial to evaluating a model's ability to represent ozone production chemistry. Identifying factors influencing surface ozone formation is complicated because ozone photochemical production rates are non-linearly dependent on concentrations of precursors such as nitrogen oxides (NO_x) and volatile organic compounds (VOCs). We compare ozone production regimes (OPRs) identified from satellite observations and model simulations, as defined by the ratio of column formaldehyde to nitrogen dioxide (FNR, HCHO/NO_2). We performed CAMx simulations for summer 2016 over the Contiguous United States (CONUS) and compared output against two OMI NO_2 and HCHO retrievals. Our analysis spans diurnal and altitudinal variations of OPRs, offering important insights for effective policy formulation. At the time of the OMI overpass ($\sim 1:30$ p.m. LT), OPR is NO_x -limited over most of the CONUS, as determined from OMI column ratios. Analysis of CAMx column ratios shows similar results. In contrast, more regions are VOC-limited when we constrain our ratio to within the Planetary Boundary Layer (PBL). In the morning (~ 9 a.m. LT), the CAMx PBL column ratios shift towards VOC-limited regime compared to the afternoon. We highlight areas of the CONUS where satellite measurements of FNR may not be an accurate indicator of near-surface OPRs. Air quality regulations based on satellite observations should

consider the diurnal variations of surface OPRs and assess how well their ratios represent near-surface OPR. Our results have implications for interpretation of TEMPO data for policy relevant applications.

2.2. *Introduction*

In this chapter we use the Comprehensive Air Quality Model with extensions (CAMx) to investigate the relationship between satellite retrievals of FNR to the distribution of ozone precursors throughout the troposphere over the Contiguous US (CONUS) during the summer months of 2016. CAMx is a regulatory air quality model approved by the US EPA to support policy and regulatory decisions. Several papers have addressed the validity of such regulatory air quality models by comparing the model output with aircraft data and surface air quality monitoring sites (Anderson et al., 2014; Canty et al., 2015; Drosoglou et al., 2017; Goldberg et al., 2022; Hembeck et al., 2019; Kemball-Cook et al., 2015; Nawaz et al., 2023; Zhang et al., 2017; Zyrichidou et al., 2015, 2009). Additional research is necessary to improve agreements between observations and CAMx. Nonetheless, state agencies are required to use the regulatory air quality models (CMAQ and CAMx) to develop pollution attainment strategies. We described science-based improvements we have made to the model for better match with observations in Section 2.2.2.

We quantify insights into the vertical distribution of ozone photochemistry provided by air quality models, as compared to satellite observations by comparing the OPR near the surface to OPRs evaluated using the tropospheric column abundance of HCHO and NO₂.

We highlight regional, diurnal, and altitudinal variations of the OPRs throughout the CONUS. Our research aims to develop a metric that describes where satellite derived FNRs can be used for air quality policy decisions that affect surface ozone, and where it may provide misleading information. Finally, we highlight where additional in situ observations (aircraft and ground-based networks) would be most useful for complementing satellite observations, to assess and improve air quality models.

Several prior papers have examined the seasonal and diurnal variation of OPR (Choi et al., 2012; Jin et al., 2017). Jin et al. (2017) used GEOS CHEM to compare with OMI-derived column FNR in the summertime and wintertime afternoons. They did not specifically examine the diurnal variation of FNR. However, it is important to note that wintertime afternoon ozone chemistry discussed in Jin et al. (2017) is different from summertime morning chemistry (discussed in this paper). 1:30 PM LT in the afternoon during summer and winter have different SZA (for example, Washington DC at 1:30 PM LT in the winter has an SZA of ~ 0.53 while in the summer it is ~ 0.9). Tropospheric ozone chemistry is not symmetric about noon; coming out of nighttime into the morning, the chemistry is different.

2.3. *Methodology*

2.3.1. CAMx Model Setup

For this analysis we use CAMx version 7.2 (Ramboll, 2021). We conduct CAMx simulations for the CONUS at a $12 \text{ km} \times 12 \text{ km}$ horizontal resolution (12US2 domain) (**Figure 2-1**: These simulations use the 12US2 domain shown with respect to other

commonly used domains over the CONUS (US EPA, 2018)) and a 35-layer vertical resolution for summer (June-July-August) of 2016.

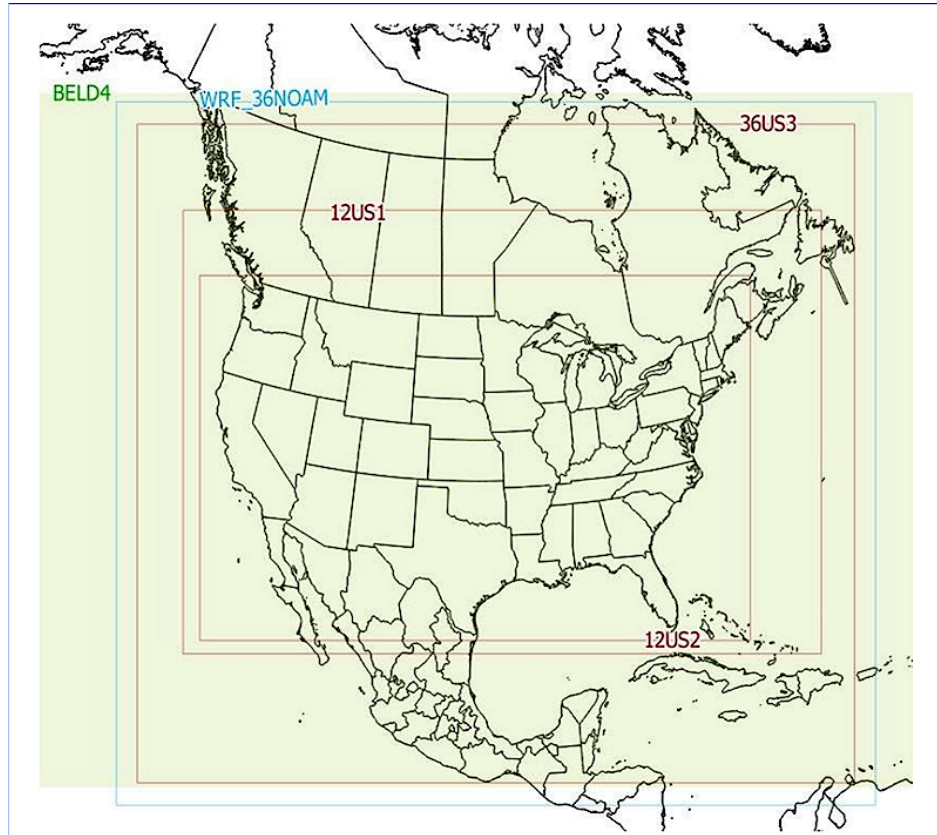


Figure 2-1: These simulations use the 12US2 domain shown with respect to other commonly used domains over the CONUS (US EPA, 2018)

The unequally sized vertical layers extend up to 50 hPa, with the thinnest layers being closest to the surface to better represent dynamics of the PBL. The details of the model configuration are provided in **Table 2-1**.

Table 2-1: CAMx model configuration

Model Codes	CAMx V7.20 – May 2022 release
Horizontal Grid Mesh	12 km, 396 x 246 cells for CONUS

Vertical Grid Mesh	35 vertical layers defined by WRF; no layer collapsing
Grid Interaction	No flexible nesting option used
Initial Conditions	From USEPA 2016 Platform
Boundary Conditions	From USEPA 2016 Platform
Gas Phase Chemistry	CB6r5_CF2_UMD, ISORROPIA (inorganic PM), SOAP2.2 (organic PM)
Horizontal Diffusion	Spatially varying (K-theory)
Vertical Diffusion	Default CAMx vertical diffusion solver (K-theory)
Dry Deposition	Dry deposition scheme for gases and aerosols (Zhang et al., 2003)
Wet Deposition	CAMx-specific formulation, scavenging model for gases and aerosols
Gas Phase Chemistry Solver	Euler Backward Iterative (EBI) Fast Solver
Vertical Advection	Implicit backward-Euler hybrid cantered/upstream (space) solver (Emery et al., 2011)
Horizontal Advection	Piecewise Parabolic Method (Colella and Woodward, 1984)
Photolysis	TUV version 4.8 with OMI total column ozone

We obtain the meteorological inputs for CAMx from the Weather Research and Forecasting (WRF v3.8) model and emissions inventory from the 2016v3 inventory (US EPA, 2021). This inventory, which the EPA supports for the Revised Cross-State Air Pollution Rule (CSAPR) and the Ozone NAAQS standards, relies on the 2014v2 National

Emissions Inventory (NEI) with updated sectoral information (US EPA, 2021a, 2020a, 2020b). Biogenic emissions are derived from the Biogenic Emission Inventory (BEIS) version 3.61 with land use input from the Biogenic Emissions Landuse Dataset (BELD) version 4.1, which includes an updated version of the USDA-USFS Forest Inventory and Analysis (FIA) version 5.1 (Bash et al., 2016; US EPA, 2019a). The Sparse Matrix Operator Kernel Emissions (SMOKE) modelling system (<https://www.cmascenter.org/smoke/>) is used to process emissions of ozone precursors from a wide variety of sectors, as detailed in **Table 2-2**. **Figure 2-2** shows area emissions for HCHO, NO₂ and isoprene from merged and biogenic emissions. **Figure 2-3** shows point source emissions from EGU sector for NO₂ and HCHO. All the emissions are converted to CAMx-ready inputs using the ‘cmaq2camx’ version 2 pre-processor available on the CAMx website (released in 2023). Initial conditions and boundary conditions are also obtained from the US EPA (US EPA, 2019b).

Table 2-2: The emission inventories used for this analysis highlight point sources, area sources, and different sectors¹

Merged Emissions	Not Merged Emissions
onroad_gas ^{or} , onroad_ca_gas ^{or} , onroad_diesel ^{or} , onroad_ca_diesel ^{or}	<i>agfire (agricultural fire)^{fi}</i>
afdust (area source fugitive dust) ^{np}	<i>cmv_c1c2 (commercial marine vehicles)^{nr}</i>
livestock ^{np}	<i>cmv_c3^{nr}</i>
fertilizer ^{np}	<i>egu (electrical generating units)^{pt}</i>
nonpt ^{np}	<i>fire_othna^{fo}</i>
nonroad_gas ^{nr} , nonroad_diesel ^{nr}	<i>fire_rx (prescribed fire)^{fi}</i>
np_oilgas ^{np}	<i>fire_wild^{fi}</i>
othafdust ^{fo} , othptdust ^{fo}	beis (biogenic emissions)
othar (non point and non road outside US) ^{fo}	<i>nonipm^{pt}</i>
airports ^{pt}	<i>oilgas^{pt}</i>
rail ^{nr}	<i>othpt^{fo}</i>

¹We use emissions inventory from the US EPA 2016v3. Point sources are represented in italics and are under the Not Merged Emissions column, while area sources are not italicized and are under the Merged Emissions column. Point sources have a height component at a specific location. While area sources are averaged over a spatial grid and have no height component. EPA provides pre-merged emissions for most area emissions in a single data input file. The only area sources excluded from this merged file are biogenic and residential wood combustion sources, allowing the user to decide whether to include them in their analysis. The point sources are provided as individual files. Here, superscripts stand for different types of emissions such as (nr) non-road mobile sources, (np) non-point sources, (pt) point sources, (fi) fires, (fo) sources outside the US and (or) on-road mobile sources.

solvents ^{np}	rwc (residential wood combustion) ^{np}
canada_ag ^{f0} , canada_og2D ^{f0} , onroad_can ^{f0} , onroad_mex ^{f0}	

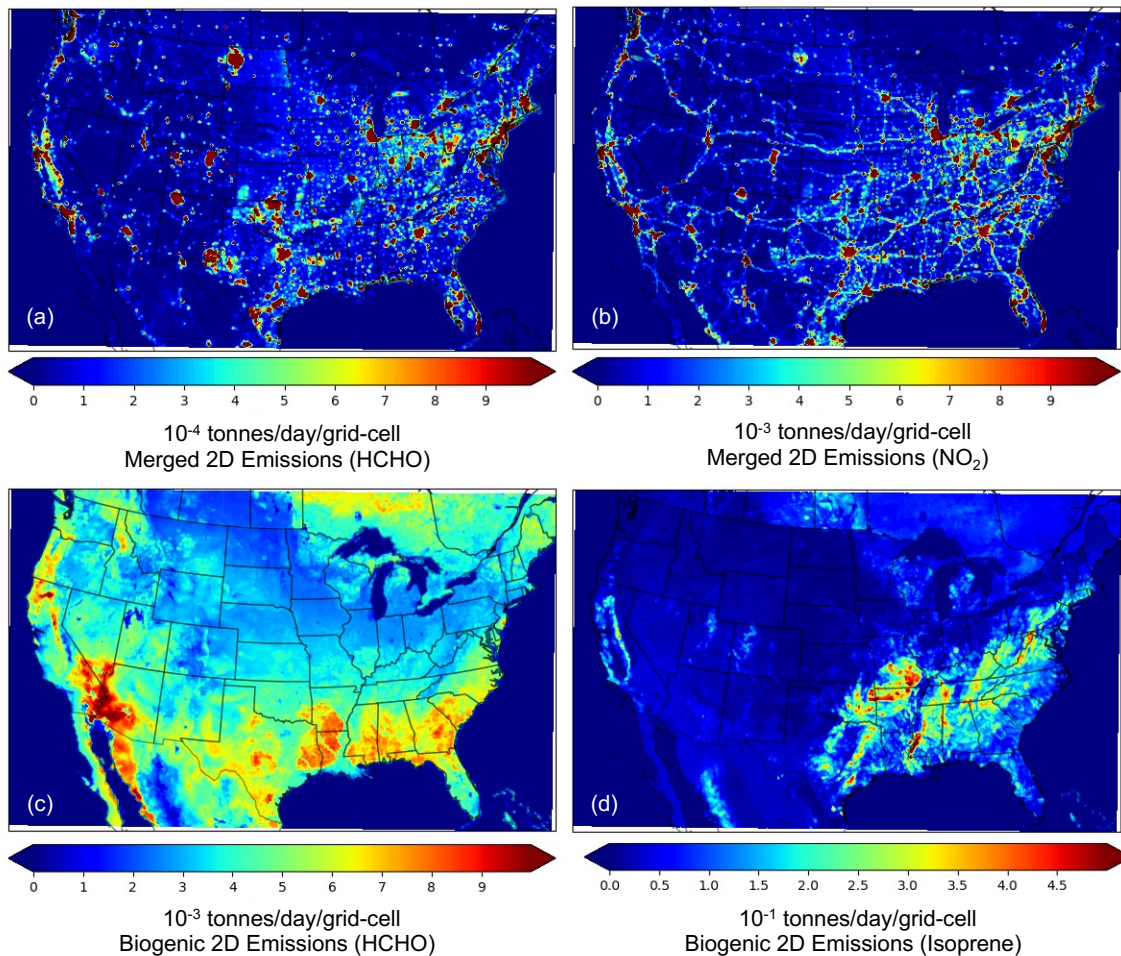


Figure 2-2: Area emission distributions across the CONUS for JJA 2016. (a) merged HCHO emissions, (b) merged NO₂ emissions, (c) biogenic HCHO emissions, and (d) biogenic isoprene emissions. All emissions are shown in tonnes per day.

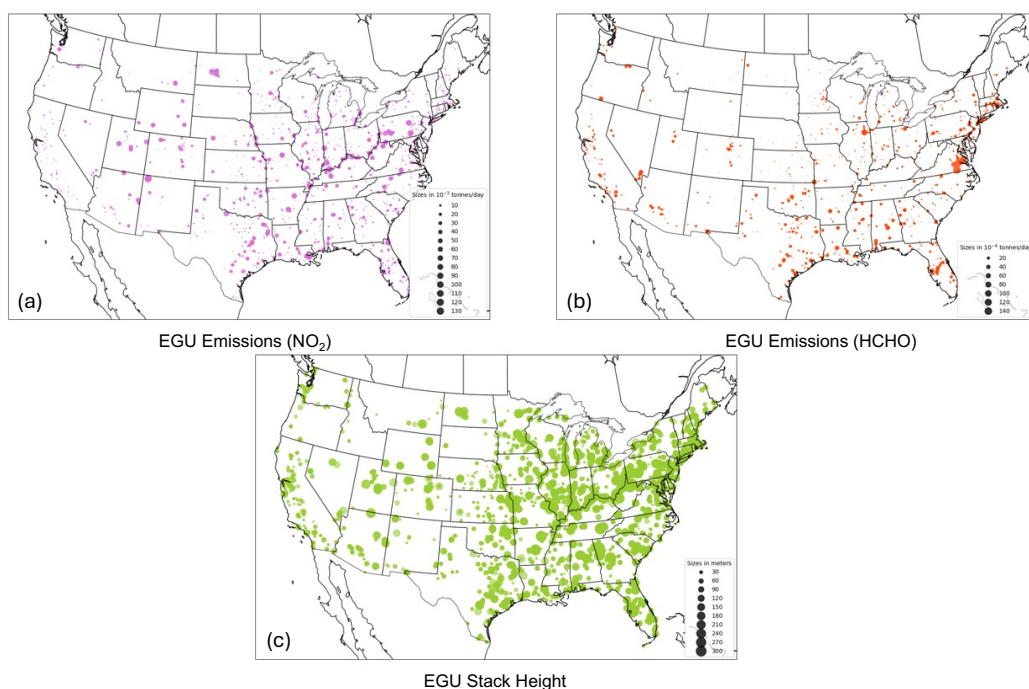


Figure 2-3: Point source EGU emission distributions across the CONUS for JJA 2016. (a) NO₂ emissions in tonnes per day, (b) HCHO emissions in tonnes per day, and (c) stack height in meters

The PBL scheme used for the CAMx model run is the Asymmetric Convective Model version 2 (ACM2) PBL scheme. This scheme has been developed and recommended by the US EPA. It is a well-supported and validated hybrid scheme that uses both a local and non-local approach to simulate mixing within the PBL (Hu et al., 2010; Pleim, 2007a, 2007b; Xie et al., 2012).

We conducted computational sensitivity tests to determine the optimal HPC configuration for CAMx, with the objective of minimizing execution time while maximizing resource efficiency. **Figure 2-4** demonstrates that the optimal configuration occurs at 24 computational units (24 tasks per node $\times$ 1 CPU core per task), where both parallel efficiency and speedup ratio remain consistently high while execution time is

minimized. At lower core counts, the model is underutilized, and execution time is unnecessarily long. Conversely, configurations exceeding 24 cores show reduced performance because the computational tasks become limited by the time required to coordinate between processors, the system's ability to access memory efficiently, and uneven distribution of computational work across the processing units. The intersection of these performance metrics clearly identifies the computational sweet spot that maximizes throughput while avoiding resource waste. This optimized configuration was subsequently adopted for all CAMx simulations throughout this study to ensure both computational efficiency and cost-effectiveness of the modeling framework.

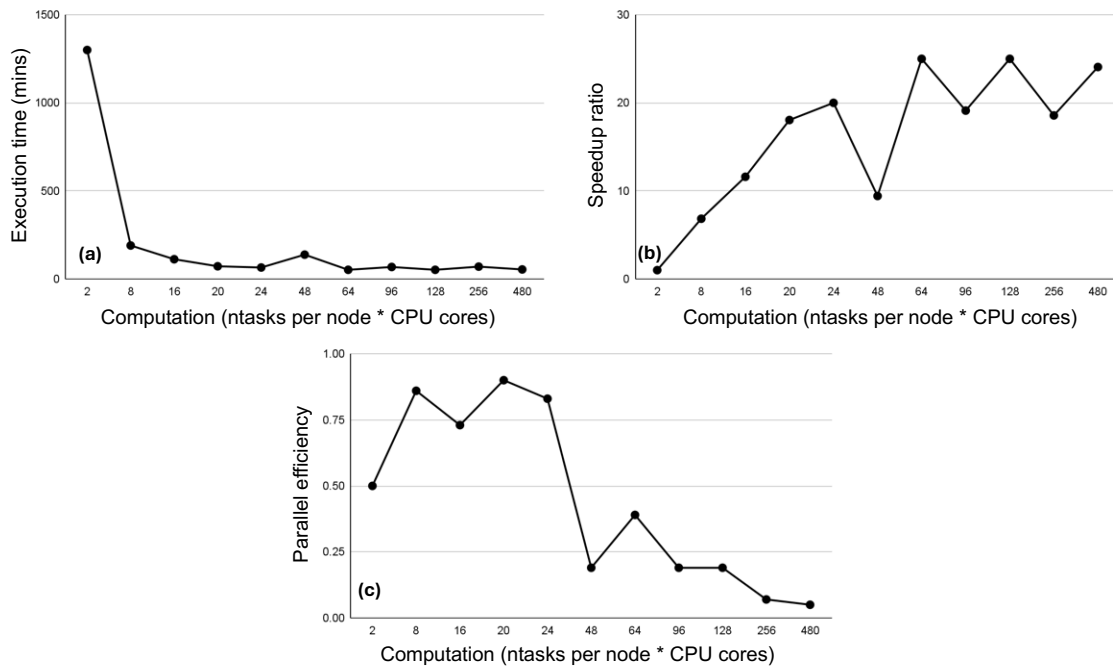


Figure 2-4: Computational sensitivity analysis for optimal CAMx HPC configuration. Sensitivity tests varying computational resources (tasks per node $\times$ CPU cores) to determine optimal CAMx performance. (a) Execution time versus computational configuration. (b) Speedup ratio showing near-linear scaling at low core counts with

deviation from ideal scaling at higher configurations. (c) Parallel efficiency demonstrating optimal performance range before degradation due to communication overhead.²

2.3.2. CAMx Model Chemistry

For complex atmospheric models such as CAMx, a chemical mechanism that balances accuracy and computational efficiency is required. This analysis uses the latest available carbon bond mechanism which is Carbon Bond 6 revision 5 (CB6r5) (Beardsley, 2020; Yarwood et al., 2010). To better represent atmospheric photochemistry, we have modified the CB6r5 chemical mechanism to account for the latest chemistry updates based on published papers identifying critical adjustments to certain chemical mechanism equations. We address the low bias in HCHO production in the second and late generations of isoprene degradation (Marvin et al., 2017), and corrected peroxyacyl nitrates (PAN) equilibrium rate constants (Hembeck et al., 2019). The changes made to the kinetic parameters and reaction mechanisms are provided in **Table 2-3**.

² Speedup Ratio = T_1/T_p where T_1 is execution time using one processor and T_p is execution time using p processors
Parallel Efficiency = Speedup Ratio/Number of Processors

Table 2-3: Changes made to kinetic parameters and reaction mechanism to resolve discrepancies between modeled and measured quantities³

Suggested Changes	Off the Shelf Version (CB6r5)	UMD Science Platform (CB6r5-UMD)
C ₂ O ₃ + NO ₂ = PAN (update PAN equil. rate constants; IUPAC14)	$k(0) = 2.70 \times 10^{-28} (T/300)^{-7.1}$ $k(\text{inf}) = 1.20 \times 10^{-11} (T/300)^{-0.9}$	$k(0) = 3.28 \times 10^{-28} (T/300)^{-6.87}$ $k(\text{inf}) = 1.125 \times 10^{-11} (T/300)^{-1.105}$
PAN = NO ₂ + C ₂ O ₃ (update PAN equil. rate constants; IUPAC14)	$k(0) = 4.90 \times 10^{-3} \exp(-12100/T)$ $k(\text{inf}) = 5.40 \times 10^{16} \exp(-13830/T)$	$k(0) = 1.10 \times 10^{-5} \exp(-10100/T)$ $k(\text{inf}) = 1.9 \times 10^{17} \exp(-14100/T)$
Add HCHO as a product of GLYD + OH	GLYD + OH = 0.2 GLY + 0.2 HO ₂ + 0.8 C ₂ O ₃	GLYD + OH = 0.2 GLY + 0.2 HO ₂ + 0.8 FORM
Add HCHO as a product of MVK + OH and MACR + OH instead of PAR	ISPD + OH = 0.022 XO ₂ N + 0.521 XO ₂ + 0.115 MGLY + 0.115 MEO ₂ + 0.269 GLYD + 0.269 C ₂ O ₃ + 0.457 OPO ₃ + 0.117 PAR	ISPD + OH = 0.022 XO ₂ N + 0.521 XO ₂ + 0.115 MGLY + 0.115 MEO ₂ + 0.269 GLYD + 0.269 C ₂ O ₃ + 0.457 OPO ₃ + 0.117 FORM + 0.137 ACET +

³ Necessary modifications can be found in (Marvin et al., 2017) and (Hembeck et al., 2019). The UMD Science Platform reflects the changes that was made to the chemistry from the Off the Shelf Version. The suggested changes describe what was changed between the two. The species names and description are available in the appendix of https://www.camx.com/Files/CAMxUsersGuide_v7.20.pdf.

	+ 0.137 ACET + 0.137 CO + 0.137 HO ₂ + 0.658 RO ₂	0.137 CO + 0.137 HO ₂ + 0.658 RO ₂
Add HCHO as a product of HPALD + hv	HPLD + hv = OH + ISPD	HPLD + hv = OH + ISPD + FORM
Change product fraction of HCHO and PAR in EPX ₂ + HO ₂	EPX ₂ + HO ₂ = 0.275 GLYD + 0.275 GLY + 0.275 MGLY + 1.125 OH + 0.825 HO ₂ + 0.375 FORM + 0.074 FACD + 0.251 CO + 2.175 PAR	EPX ₂ + HO ₂ = 0.275 GLYD + 0.275 GLY + 0.275 MGLY + 1.125 OH + 0.825 HO ₂ + 0.815 FORM + 0.074 FACD + 0.251 CO + 1.735 PAR
Change product fraction of HCHO and PAR in EPX ₂ + HO ₂	EPX ₂ + NO = 0.275 GLYD + 0.275 GLY + 0.275 MGLY + 0.125 OH + 0.825 HO ₂ + 0.375 FORM + NO ₂ + 0.251 CO + 2.175 PAR	EPX ₂ + NO = 0.275 GLYD + 0.275 GLY + 0.275 MGLY + 0.125 OH + 0.825 HO ₂ + 0.848 FORM + NO ₂ + 0.251 CO + 1.702 PAR
PANX + OH = ALD2 + NO ₂ (update rate constant)	k = 3.0E-10	k = 3.0E-11

2.3.3. Satellite Data Description

Satellite retrievals of NO₂ and HCHO are obtained from the Ozone Monitoring Instrument (OMI) aboard NASA's EOS Aura satellite, a sun-synchronous satellite with a

daily daytime overpass at $\sim 13:40$ local time (Levelt et al., 2018, 2006). The spatial resolution of OMI ranges from $13 \text{ km} \times 24 \text{ km}$ at nadir to $28 \text{ km} \times 160 \text{ km}$ at swath edges. Although Aura was deployed in 2004, a partial external blockage of the radiance port in 2008 caused a row anomaly that has impacted around 50% of OMI observations (Schenkeveld et al., 2017).

This analysis uses two operational retrievals of tropospheric column NO_2 and two operational retrievals of total column HCHO. For NO_2 , we use the Quality Assurance for Essential Climate Variables (QA4ECV) version 1.1, level 2 product provided by the Royal Netherlands Meteorological Institute (KNMI) (Boersma et al., 2018; Zara et al., 2018) as well as the NASA Goddard Space Flight Center (GSFC) OMNO2 version 3, level 2 (Krotkov et al., 2019; Lamsal et al., 2021) product. For HCHO, we use the QA4ECV HCHO version 1.2, level 2 product provided by KNMI (De Smedt et al., 2017; Zara et al., 2018) as well as the SAO OMHCHO version 3, level 2 product (Chance, 2007; González Abad et al., 2015).

All four satellite products are gridded to the CAMx domain ($12 \text{ km} \times 12 \text{ km}$) using a nearest neighbor resampling method. Here, the satellite data are time-averaged over three months: June-July-August for the year 2016. Although it is recommended by the OMI read me files that NO_2 tropospheric column data have a stricter cloud fraction cut-off of 20%, we use a cloud fraction cut-off of 40% for all four satellite products to be consistent with the recommendations for using OMI retrievals of column HCHO (Boersma et al., 2017b; De Smedt et al., 2017). We perform data filtering to account for row anomalies and only

grid points that have at least 3 data points over the 3-month period. Lastly, data from the five outermost pixels along the swath are ignored due to their large footprints compared to nadir pixels. The satellite data used in this study along with the applied filters are shown in **Table 2-4**.

Table 2-4: Satellite retrievals used in this study with the specific filters applied⁴

	File Name	Author	Long Name	Version	Filters
NO₂	OMI- Aura_L2- OMNO2	Goddard Space Flight Center (GSFC)	OMI/Aura Nitrogen Dioxide (NO ₂) Total and Tropospheric Column 1-orbit L2 Swath 13x24 km	V003	CF < 0.4 VCD QF = 0 XTRACK QF = 0
HCHO	OMI- Aura_L2- OMHCHO	Smithsonian Astrophysic al Observatory (SAO)	OMI/Aura Formaldehyde (HCHO) Total Column 1-Orbit L2 Swath 13x24km	V003	CF < 0.4 XTRACK QF = 0 Main Data QF = 0
NO₂	QA4ECV_L 2_NO2_OMI	BIRA-IASB & IUPB & KNMI &	QA4ECV nitrogen dioxide (NO ₂)	DOMIN O v3	CF < 0.4 Error Flag = 0

⁴ Here CF stands for cloud fraction, QF stands for quality flags, VCD stands for vertical column density and XTRACK stands for row anomaly flagging.

		MPIC & WUR	tropospheric column data	TM5- MP	Column Uncertainty $y > 0$
HCHO	QA4ECV_L 2_HCHO_O MI	BIRA-IASB & IUPB & KNMI & MPIC & WUR	QA4ECV formaldehyde (HCHO) column data	v1.2	Error Flag = 0 CF < 0.4

2.3.4. Model Column Values Calculation

Profiles of CAMx hourly output are used to calculate column values of NO₂ and HCHO. We use the box integration method, wherein we calculate the partial column values for each grid cell using height and atmospheric density information. We then sum up the column content of all “boxes” over each grid point to determine the tropospheric column abundances. We also compute column values up to the top of the PBL in a similar manner, using the PBL heights found in the WRF meteorological input files.

We use the model output time closest to the satellite overpass time (average of 1 PM LT and 2 PM LT) to compare model and satellite data. Output from CAMx is interpolated to the pressure grid used in the satellite retrieval, to ensure a consistent approach for sampling in the vertical. We consider four distinct time zones over the CONUS to get the correct local times (**Figure 2-5**). To calculate tropospheric columns of

NO₂ and HCHO using model output that replicate the satellite sensitivity to different layers in the atmosphere, we utilize scattering weights (SW) from NASA, averaging kernels (AK) from QA4ECV, as well as air mass factors (AMFs) associated with the respective retrievals (Boersma et al., 2017b; De Smedt et al., 2017; González Abad et al., 2015; Harkey et al., 2020; Krotkov et al., 2019).

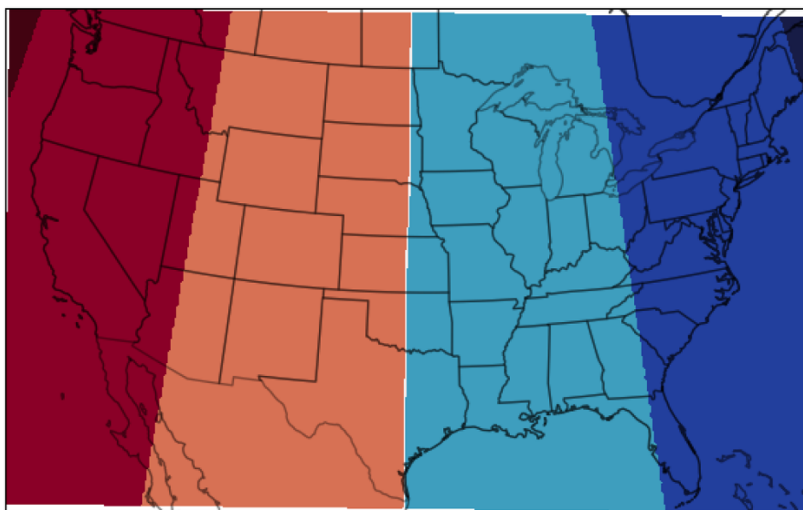


Figure 2-5: The four time zones considered for all the analysis to ensure that the local time in each area matched the OMI overpass time of ~1:30 PM and our morning time of 9:30 AM.

2.4. Results and Discussions

2.4.1. Model Surface Analysis

Figure 2-6 shows CAMx model surface concentrations for NO₂ and HCHO during afternoon and morning for summer 2016. Since ozone formation is a photochemical process, ozone concentrations peak in the afternoon, while precursor species concentrations are greater in the morning (Finlayson-Pitts and Pitts, 1993; Jin et al., 2020). The left panels of Figure 2-6 (a and d) show that NO₂ concentrations tend to be highest in

cities and urban areas. We also see the presence of enhanced NO_2 at several locations, including where coal combustion occurs, such as the Powder River basin in eastern Wyoming and the northern and central Appalachian basins in West Virginia and Kentucky. Oil and gas operations, which lead to emissions of NO_x are also visible in the Bakken Basin in North Dakota. Similarly, large emissions of NO_x from power plants can also be easily seen in the 4-corners power plant (between Arizona, New Mexico, Colorado, and Utah), Montana and Nevada.

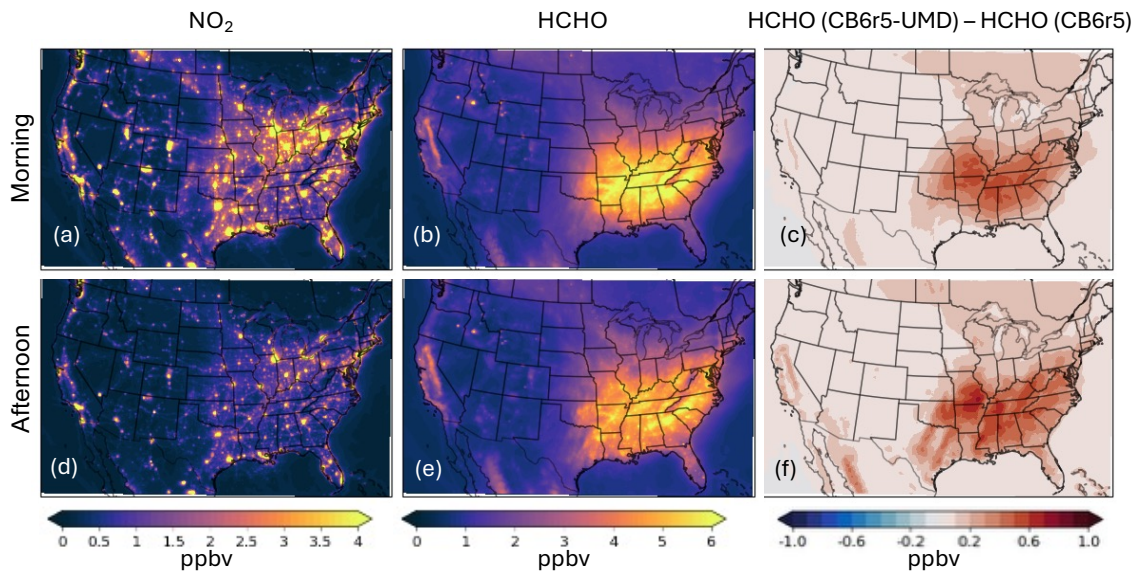


Figure 2-6: Surface concentrations averaged over summer 2016 from CAMx model platform. Morning refers to 9:30 AM local time and afternoon refers to 1:30 PM local. (a) Morning NO_2 , (d) Afternoon NO_2 , (b) Morning HCHO, (e) Afternoon HCHO. Panels (c) and (f) indicate the difference in HCHO between the updated “UMD Science Platform” and the off the shelf version of the CAMx model

The center panels of Figure 2-6 (b and e) show that the concentration of HCHO peaks in the southeast US due to biogenic isoprene sources from broadleaf trees such as oaks. The Missouri Ozarks, along with much of the southeast US have a high density of oak trees that are efficient isoprene emitters due to the warm temperatures and high

moisture levels, leading to the formation of an “isoprene volcano” (Kaiser et al., 2018; Palmer et al., 2006, 2003; Wiedinmyer et al., 2005). Atmospheric degradation of VOCs generally leads to HCHO, therefore the influx of isoprene in this region causes elevated HCHO. The right panels (c and f) highlight the morning and afternoon impact of the improvements to the chemical mechanism on HCHO. These changes have resulted in about a 5% increase in HCHO over the southeast US.

We compared surface CAMx output to ground-based air quality monitoring sites for NO₂ and HCHO. Air Quality Stations (AQS) monitor NO₂ hourly every day, while HCHO is measured over a collection time (3, 8, 12, or 24 hours) mostly every sixth day. CAMx data is compared over equivalent ranges in each case and then time averaged over summer. **Figure 2-7 and Figure 2-8** provide these scatter plots and comparisons. These comparisons of AQS measurements of ground based NO₂ with surface CAMx model output shows good agreement with correlations of $r \sim 0.7$ for different parts of the US.

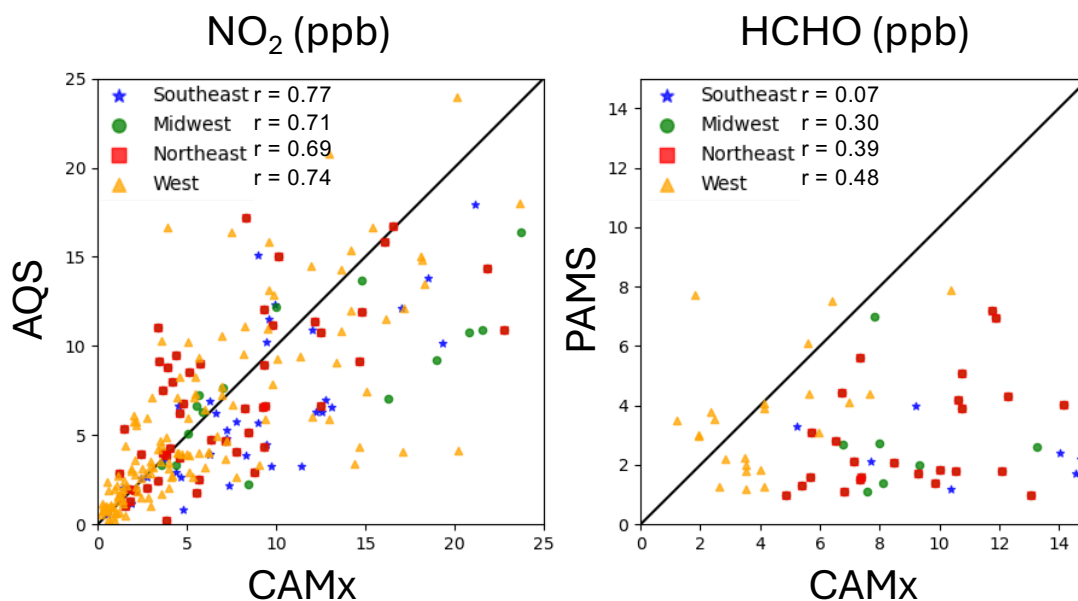


Figure 2-7: Scatter plots between NO₂ and HCHO from AQS and PAMS ground based observations and CAMx surface outputs.

We find small to moderate correlation between ground-based observations of HCHO from Photochemical Assessment Monitoring Stations (PAMS) and CAMx model output with the highest $r = 0.48$ in western US and going as low as $r = 0.07$ in the southeast US with the model being biased high. HCHO is measured using 2,4-dinitrophenylhydrazine (DNPH) cartridges that have a known negative bias of as much as -25% . This low bias and the high uncertainty in the measurement of HCHO have been reported in numerous papers (Achatz et al., 1999; Arnts and Tejada, 1989; Dunne et al., 2018; Hak et al., 2005; Harkey et al., 2020; Mouat et al., 2024; Oommen et al., 2020; Wang et al., 2022). Comparisons of modeled and measured HCHO are also difficult because the CAMx spatial footprint is much larger than a point AQS/PAMS site measurement, which is particularly problematic for a compound such as HCHO with large geographical

heterogeneity. A more thorough examination of these biases is outside the scope of this thesis.

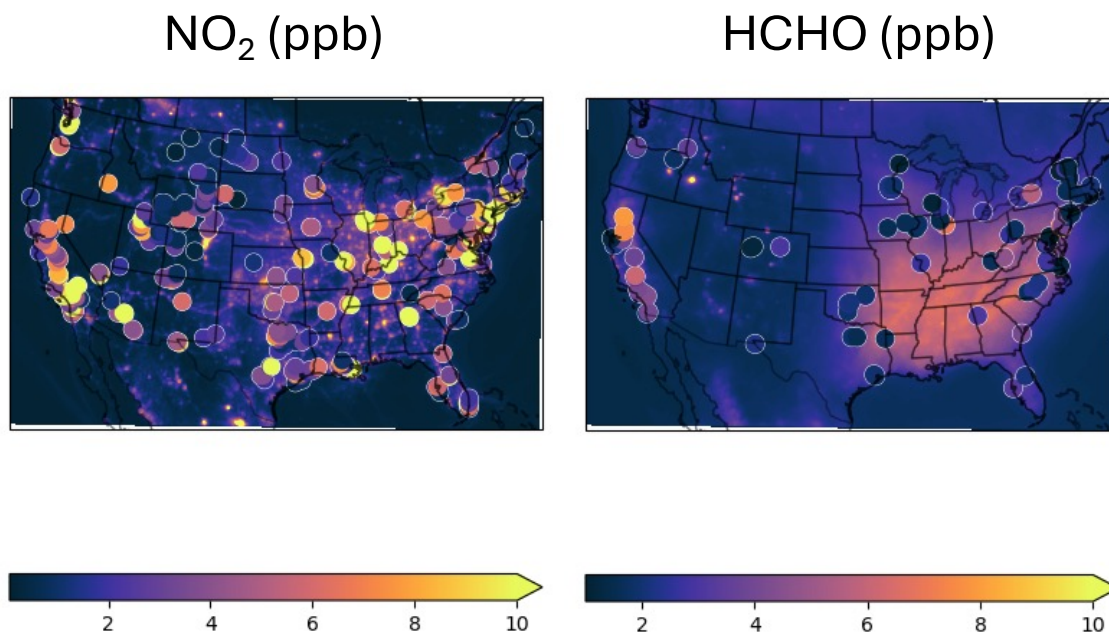


Figure 2-8: NO₂ and HCHO from AQS and PAMS ground based observations plotted on CAMx surface outputs.

2.4.2. Model and Satellite Column Comparisons

Figure 2-9 shows satellite retrievals of tropospheric column NO₂ from QA4ECV, NASA, and CAMx for summer 2016. The CAMx columns are biased low with respect to the satellite products but agree reasonably well when multiple metrics are considered (see **Table 2-11**).

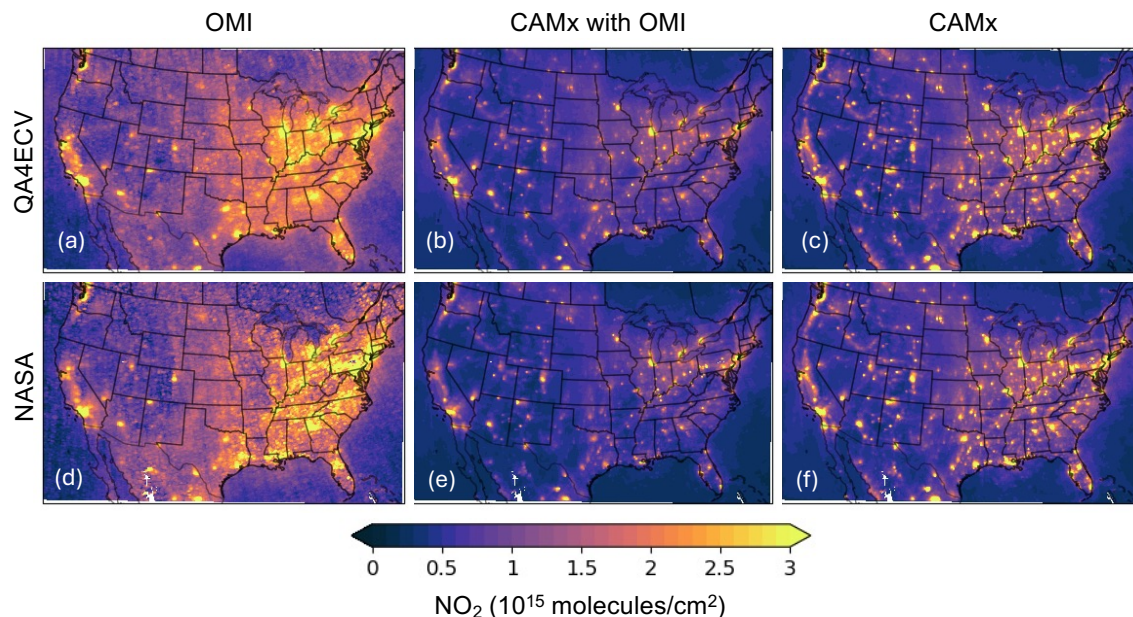


Figure 2-9: Average column NO_2 for summer 2016 from (a) QA4ECV retrieval, (b) CAMx model output with AK and AMF from the QA4ECV retrieval, (c) CAMx model output with grid boxes corresponding to pixels from the QA4ECV retrieval, (d) NASA retrieval, (e) CAMx model output with SW and AMF from the NASA retrieval and, (f) CAMx model output with grid boxes corresponding to pixels from the NASA retrieval. Level 2 data for both the retrievals were screened and regridded onto the CAMx model domain. Only grid points with cloud fraction less than 40% and at least 3 days of data for both the NO_2 and HCHO retrievals are used.

The recalculation ensures that we perform an "apples to apples" comparison of satellite retrieval and model output. Most importantly, this recalculation accounts for the differences in the vertical pressure coordinates and the sensitivity to the surface between the model and satellite. A detailed description of our application of SWs/AKs to modeled NO_2 is provided in **Table 2-5** and **Table 2-6**.

Table 2-5: Recalculation of CAMx NO₂ based on the QA4ECV OMI NO₂ retrieval⁵

Variables used from QA4ECV OMI NO₂ retrieval:		
Variables	Description	Units
latitude	pixel center latitude	degrees north
longitude	pixel center longitude	degrees east
tropospheric_no2_vertical_column	tropospheric vertical column of nitrogen dioxide	molecules cm-2
amf_total	total air mass factor	1
amf_trop	tropospheric air mass factor	1
averaging_kernel	averaging kernel	1
tm5_surface_pressure	Surface pressure of the ground pixel, adjusted based on the TM5 surface pressure	hPa
tm5_tropopause_layer_index	TM5 layer index of the highest layer in the tropopause	1
tm5_pressure_level_a	TM5 hybrid A coefficient at upper and lower interface levels	Pa

⁵ We convert CAMx NO₂ concentration from ppmv to molecules/cm³ using air density. We then calculate the satellite AMF ratio (amf_total/amf_trop) and multiply this factor with the averaging kernel. We then calculate the TM5 pressure profile for the satellite retrieval ((tm5_pressure_level_a*0.01)+ tm5_surface_pressure* tm5_pressure_level_b). We then interpolate CAMx NO₂ concentrations and altitude onto the TM5 pressure profile. We calculate the NO₂ partial column until the tropopause and sum up all the partial columns to get the tropospheric column NO₂ value (Boersma et al., 2017b).

tm5_pressure_level_b	TM5 hybrid B coefficient at upper and lower interface levels	1
processing_error_flag	Flag indicating whether the processing was successful (0) or failed (1)	1
tropospheric_no2_vertical_column_uncertainty	uncertainty of the tropospheric vertical column of nitrogen dioxide	molecules cm-2
cloud_fraction	effective cloud fraction from the cloud product	1
Variables used from METCRO3D files:		
PRES	air pressure	Pa
DENS	density of air	Kg/m^3
ZF	full-layer height above ground	m
Variables used from CAMx output files		
NO ₂		ppmv

Table 2-6: Recalculation of CAMx NO₂ based on the NASA OMI NO₂ retrieval⁶

Variables used from NASA OMI NO₂ retrieval:		
Variables	Description	Units
Latitude	Latitude of the centre of the ground pixel	degrees north

⁶ We convert CAMx NO₂ concentration from ppmv to molecules/cm³ using air density. We then interpolate CAMx NO₂ concentrations and altitude onto the NASA OMI pressure profile. We calculate the NO₂ partial column and sum up all the partial columns to get the total column HCHO value (Krotkov et al., 2019).

Longitude	Longitude of the centre of the ground pixel	degrees east
ColumnAmountNO2Trop	ColumnAmountNO2Trop	molecules cm-2
ScatteringWeight	Scattering weight profile	1
TropopausePressure	Pressure of the tropopause	hPa
ScatteringWtPressure	Pressures for scattering weight profile	hPa
AmfTrop		1
CloudRadianceFraction	Radiative cloud fraction at 440 nm	1
XTrackQualityFlags	The cross-track quality flags indicate specific likely problems with the radiance measurements, due to the row anomaly	1
VcdQualityFlags	This variable contains quality assurance information for the tropospheric vertical column	1
Variables used from METCRO3D files:		
PRES	air pressure	Pa
DENS	density of air	Kg/m ³
ZF	full-layer height above ground	m
Variables used from CAMx output files		
NO ₂		ppmv

Applying the satellite averaging kernel (AK) and scattering weights (SW) reduces the sensitivity of the CAMx columns to NO₂ and HCHO near the surface, because the

satellite observational sensitivity (as represented by both AK and SW) is largest at the top of the troposphere and decreases towards the surface (**Figure 2-10**).

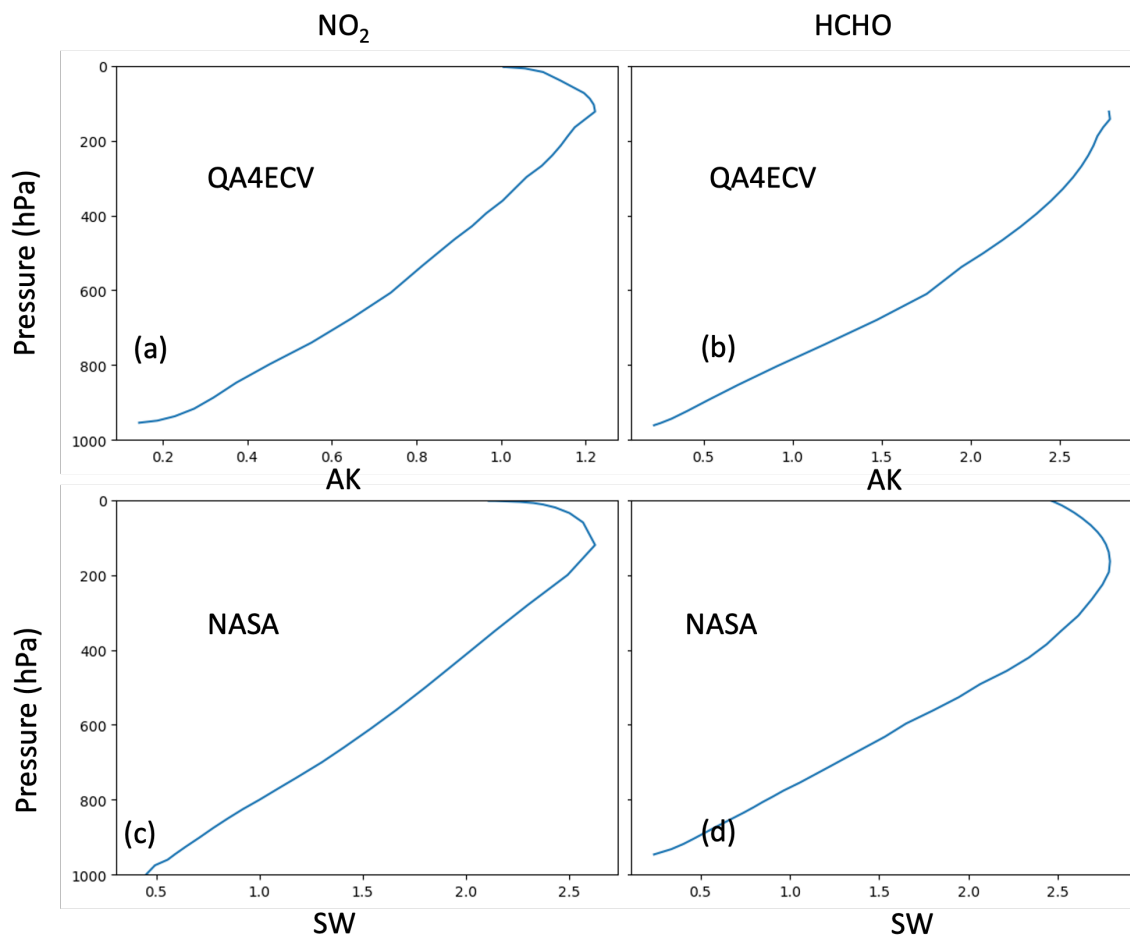


Figure 2-10: This figure illustrates satellite sensitivity to the surface. The profiles represent the (a) NO₂ averaging kernel from QA4ECV retrieval, (b) HCHO averaging kernel from QA4ECV retrieval, (c) NO₂ scattering weights from NASA retrieval and (d) HCHO scattering weights from NASA retrieval.

The tendency of modeled column NO₂ to fall below the measured column could be due to multiple factors, including biases in the retrievals. The NASA OMI NO₂ product has uncertainty ranging from 20% to 60% based on pollution levels (Bucsela et al., 2013). The QA4ECV OMI NO₂ product has a low bias in polluted regions but performs well in cleaner

regions (Compernelle et al., 2020). OMI retrievals of NO₂ have a high bias in less polluted regions due to underestimation of free tropospheric NO₂ in the *a priori* profile used in the retrieval algorithm leading to low values of AMF (Boersma et al., 2004; Johnson et al., 2023; Lamsal et al., 2014; Silvern et al., 2019). Another reason for this model/measurement difference can be slow or inadequate vertical advection of anthropogenic emissions in the model framework, causing more of the NO₂ emissions to build up in the PBL than occurs in the actual atmosphere. A portion of the low bias in the model is due to missing emissions in the model, such as lightning-NO_x and aircraft-NO_x (Silvern et al., 2019). Another possible reason for the model deficit in column NO₂ could be the neglect of downwelling NO_x from the stratosphere by CAMx.

In **Table 2-11**, we provide error metrics associated with Figure 2-9. The two satellite products have similar mean column abundances (1.10×10^{15} molec. cm⁻² for NASA OMI and 1.21×10^{15} molec. cm⁻² for QA4ECV OMI). The two recalculated model columns also have similar means (0.54×10^{15} molec. cm⁻² when NASA SWs are used versus 0.65×10^{15} molec. cm⁻² when QA4ECV AKs are used). RMSEs for both the retrievals are relatively low but there are systemic biases in both the NASA and QA4ECV OMI recalculation products as indicated by the normalized mean biases.

We further evaluate the uncertainty associated with tropospheric vertical column density of OMI NO₂ in **Figure 2-11** and **Figure 2-12**.

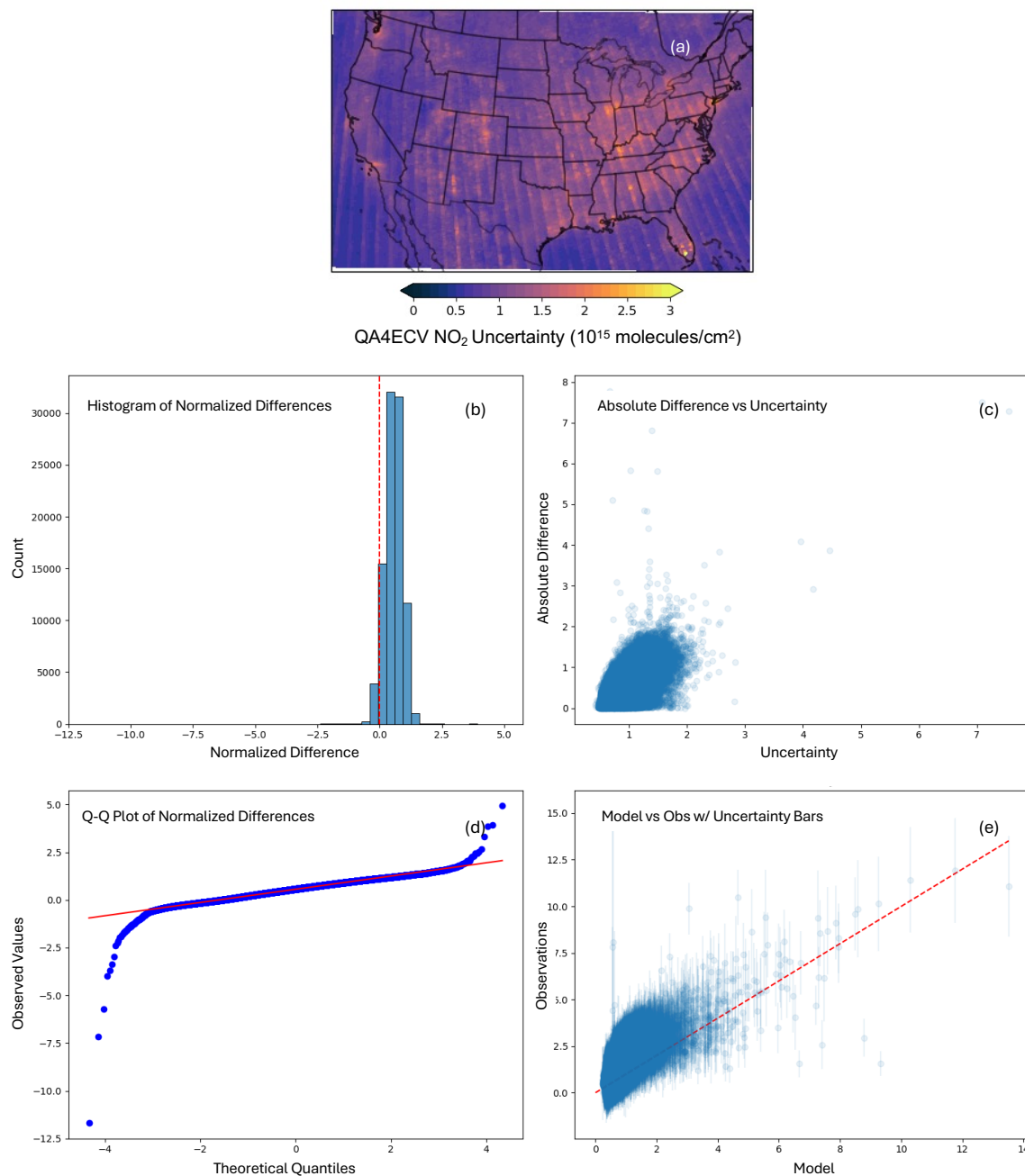


Figure 2-11: Uncertainty analysis of QA4ECV OMI NO₂ tropospheric column values. Here panel (a) shows the uncertainty on tropospheric vertical column, (b) shows the histogram of normalized differences between OMI observations and CAMx model values normalized by OMI uncertainty, (c) shows a plot of absolute difference between OMI observations and CAMx model values vs satellite uncertainty, (d) shows a Q-Q plot of normalized differences and (e) shows CAMx model vs OMI observations with satellite uncertainty error bars. We use the individual pixel uncertainty estimate which is the best guess of the total retrieval uncertainty and contains both random and systematic components. The striping seen in (a) is a known error for this retrieval and a de-striping correction is applied to the retrieved tropospheric column NO₂ values (van Geffen et al., 2020).

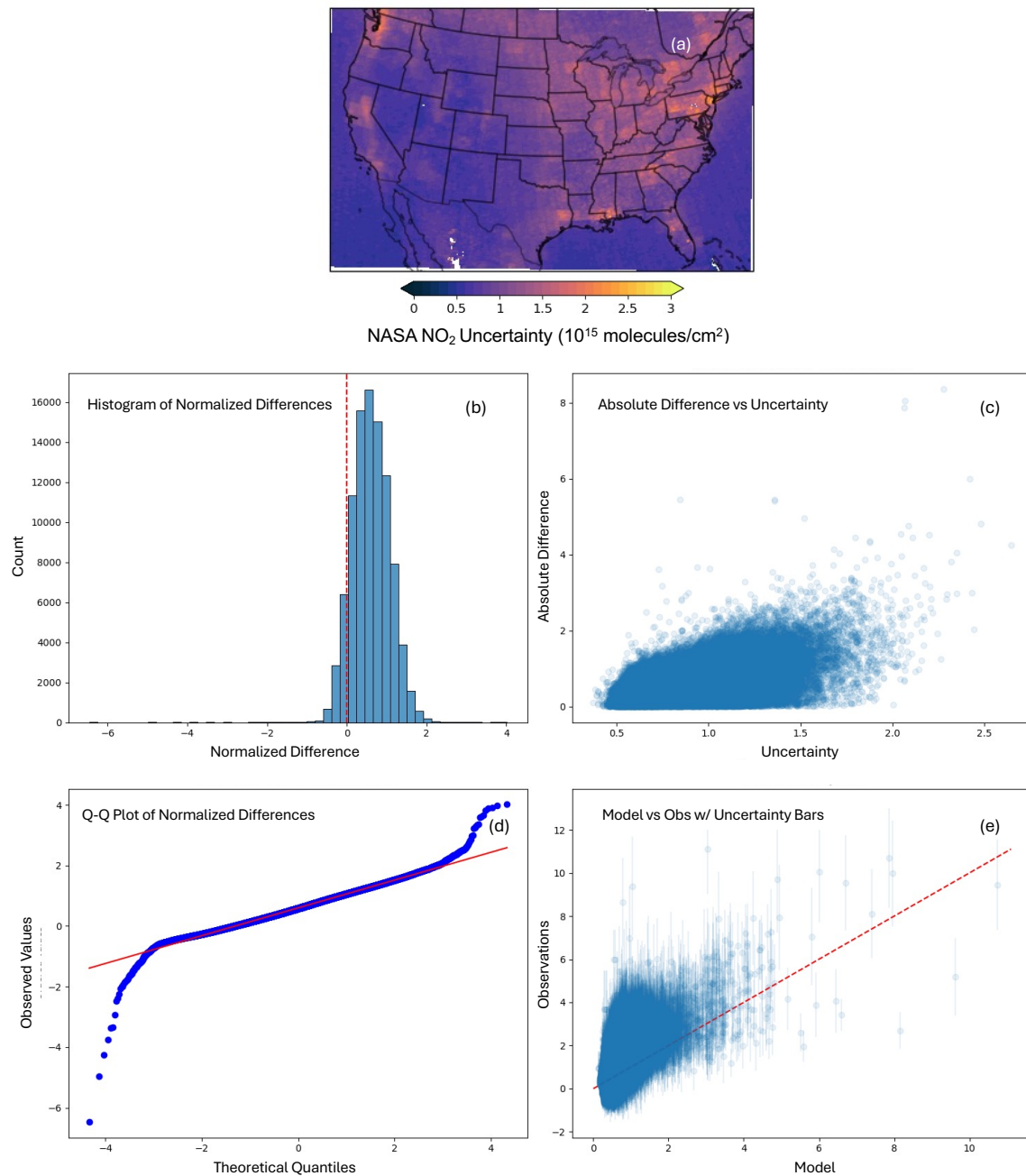


Figure 2-12: Uncertainty analysis of NASA OMI NO₂ tropospheric column values. Here panel (a) shows the uncertainty on tropospheric vertical column, (b) shows the histogram of normalized differences between OMI observations and CAMx model values normalized by OMI uncertainty, (c) shows a plot of absolute difference between OMI observations and CAMx model values vs satellite uncertainty, (d) shows a Q-Q plot of normalized differences and (e) shows CAMx model vs OMI observations with satellite uncertainty error bars. We use tropospheric vertical column uncertainty estimate.

We calculate reduced chi-squared (χ^2) to define the goodness of fit between modeled and observed quantities. We define χ^2 using **Equation 2-1** where $\langle \Delta S_{sat,j} \rangle$, $\langle \Delta S_{CAMx,j} \rangle$, and $\sigma_{sat,j}$ represent the summer 2016 averaged satellite observed NO₂ or HCHO, the summer 2016 averaged CAMx modeled NO₂ or HCHO and the summer 2016 averaged uncertainty of the satellite observed NO₂ or HCHO, respectively. N_{obs} represents the total number of grid points in the CONUS domain.

$$\chi^2 = \frac{1}{N_{obs}-1} \times \sum_{j=1}^{j=N} \frac{1}{\sigma_{sat,j}^2} (\langle \Delta S_{sat,j} \rangle - \langle \Delta S_{CAMx,j} \rangle)^2 \quad \text{Equation 2-1}$$

The reduced chi-squared values of 0.44 and 0.57 for QA4ECV and NASA OMI products (see **Table 2-7**) indicate that our model results are well within the range of satellite uncertainty for tropospheric column NO₂.

Table 2-7: Reduced chi-squared (χ^2) values of CAMx modeled NO₂ and HCHO in comparison with satellite observations

	NASA	QA4ECV
NO₂	0.57	0.44
HCHO	0.11	0.5

Figure 2-13 compares satellite retrievals of tropospheric column HCHO from QA4ECV, NASA, and CAMx for summer 2016. The CAMx columns of HCHO are biased slightly low with respect to the satellite products but agree reasonably well when multiple metrics are considered (see **Table 2-11**).

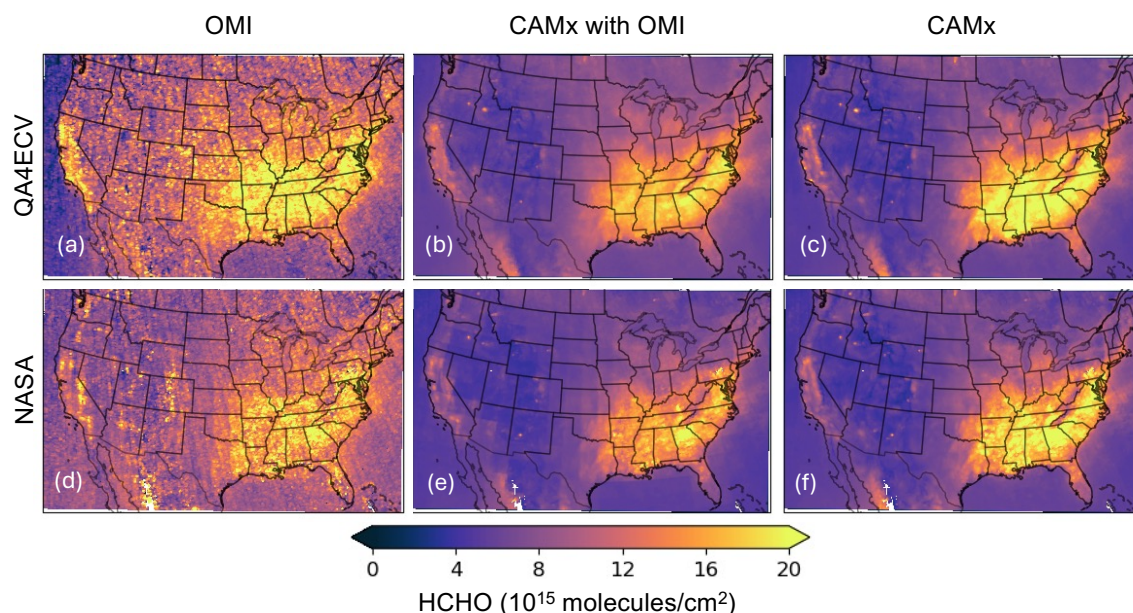


Figure 2-13: Average column HCHO for summer 2016 from (a) QA4ECV retrieval, (b) CAMx model output with AK and AMF from the QA4ECV retrieval, (c) CAMx model output with grid boxes corresponding to pixels from the QA4ECV retrieval, (d) NASA retrieval, (e) CAMx model output with SW and AMF from the NASA retrieval and, (f) CAMx model output with grid boxes corresponding to pixels from the NASA retrieval. Level 2 data for both the retrievals were screened and regridded onto the CAMx model domain. Only grid points with cloud fraction less than 40% and at least 3 days of data for both the NO₂ and HCHO retrievals are used.

As with NO₂, model HCHO columns are substantially lower than the retrieved columns. Panels (b) and (e) of Figure 2-13 show the model output after application of AK and AMF values from the QA4ECV retrieval and SW and AMF values from the NASA retrieval, respectively. Results in panels (b) and (e) show an underprediction in HCHO compared to satellite observations (left panels Figure 2-13 (a and d)) especially where HCHO column values are low. Similar to NO₂, the satellite AKs and SWs have high sensitivity to the presence of HCHO in the middle to upper troposphere, and lower sensitivity to HCHO close to the surface.

The QA4ECV and NASA retrievals of column HCHO agree reasonably well. The retrievals of HCHO tend to be noisier than the retrievals of NO₂ due to remote sensing challenges, with the dominant source of error coming from uncertainty in the estimation of the AMF (Palmer et al., 2001). HCHO retrievals are also challenging due to more Rayleigh scattering at the shorter wavelengths (327.5-356.5 nm) compared to the wavelengths used for the retrieval of NO₂ (405-465 nm). The remote sensing challenge for HCHO arises because the absorption of light by this molecule peaks at the wavelength range with high ozone optical depth, leading to a weak signal for HCHO. The NASA OMI HCHO product has uncertainty ranging from 45% to 105% due to AMF calculations (González Abad et al., 2016, 2015; Zhu et al., 2020). The QA4ECV OMI HCHO product is biased low in polluted regions and biased high in cleaner regions (De Smedt et al., 2021). A detailed description of our application of SWs/AKs to modeled HCHO is provided in **Table 2-8** and **Table 2-9**.

Table 2-8: Recalculation of CAMx HCHO based on the QA4ECV OMI HCHO retrieval⁷

Variables used from QA4ECV OMI HCHO retrieval:		
Variables	Description	Units
latitude	pixel centre latitude	degrees north

⁷ We convert CAMx HCHO concentration from ppmv to molecules/cm³ using air density. We then calculate the TM5 pressure profile for the satellite retrieval ((tm5_pressure_level_a*0.01)+tm5_surface_pressure*tm5_pressure_level_b). We then interpolate CAMx HCHO concentrations and altitude onto the TM5 pressure profile. We calculate the HCHO partial column and sum up all the partial columns to get the total column HCHO value (De Smedt et al., 2017; Harkey et al., 2020).

longitude	pixel centre longitude	degrees east
tropospheric_hcho_vertical_column	tropospheric vertical column of nitrogen dioxide	molecules cm-2
amf_trop	tropospheric air mass factor	1
averaging_kernel	averaging kernel	1
tm5_surface_pressure	Surface pressure of the ground pixel, adjusted based on the TM5 surface pressure	hPa
tm5_tropopause_layer_index	TM5 layer index of the highest layer in the tropopause	1
tm5_pressure_level_a	TM5 hybrid A coefficient at upper and lower interface levels	Pa
tm5_pressure_level_b	TM5 hybrid B coefficient at upper and lower interface levels	1
processing_error_flag	Flag indicating whether the processing was successful (0) or failed (1)	1
cloud_fraction	effective cloud fraction from the cloud product	1
Variables used from METCRO3D files:		
PRES	air pressure	Pa
DENS	density of air	Kg/m^3

ZF	full-layer height above ground	m
Variables used from CAMx output files		
HCHO		ppmv

Table 2-9: Recalculation of CAMx HCHO based on the NASA OMI HCHO retrieval⁸

Variables used from NASA OMI HCHO retrieval:		
Variables	Description	Units
Latitude	Latitude of the centre of the ground pixel	degrees north
Longitude	Longitude of the centre of the ground pixel	degrees east
ReferenceSectorCorrected VerticalColumn	Total column amount for each ground pixel obtained after correcting the retrieved VCD with the reference sector	molecules cm-2
ScatteringWeights	Scattering weights used in the AMFs calculation	1
ClimatologyLevels	Pressure Levels	hPa
AirMassFactor	Molecule specific air mass factor for each ground pixel, including scattering weights, clouds, and vertical distribution of HCHO	1

⁸ We convert CAMx HCHO concentration from ppmv to molecules/cm³ using air density. We then interpolate CAMx HCHO concentrations and altitude onto the NASA OMI pressure profile. We calculate the HCHO partial column and sum up all the partial columns to get the total column HCHO value (González Abad et al., 2015; Harkey et al., 2020).

AMFCloudFraction	Adjusted Cloud Fraction for AMF Computation	1
MainDataQualityFlag	Main flag to indicate data quality	1
XtrackQualityFlags	The cross-track quality flags indicate specific likely problems with the radiance measurements, due to the row anomaly	1
Variables used from METCRO3D files:		
PRES	air pressure	Pa
DENS	density of air	Kg/m ³
ZF	full-layer height above ground	m
Variables used from CAMx output files		
NO ₂		ppmv

Table 2-11 provides error metrics associated with **Figure 2-13**. The mean value of column HCHO over the CONUS for summer 2016 of the QA4ECV satellite product (10.06×10^{15} molec. cm⁻²) for HCHO is slightly higher than that of the NASA product (9.53×10^{15} molec. cm⁻²). We further evaluate the uncertainty associated with the tropospheric vertical column density of OMI HCHO in **Figure 2-14** and **Figure 2-15**. The small reduced chi-squared values of 0.50 and 0.11 for QA4ECV and NASA OMI products (see Table S7) indicate that our model results are well within the range of satellite uncertainty for tropospheric column HCHO.

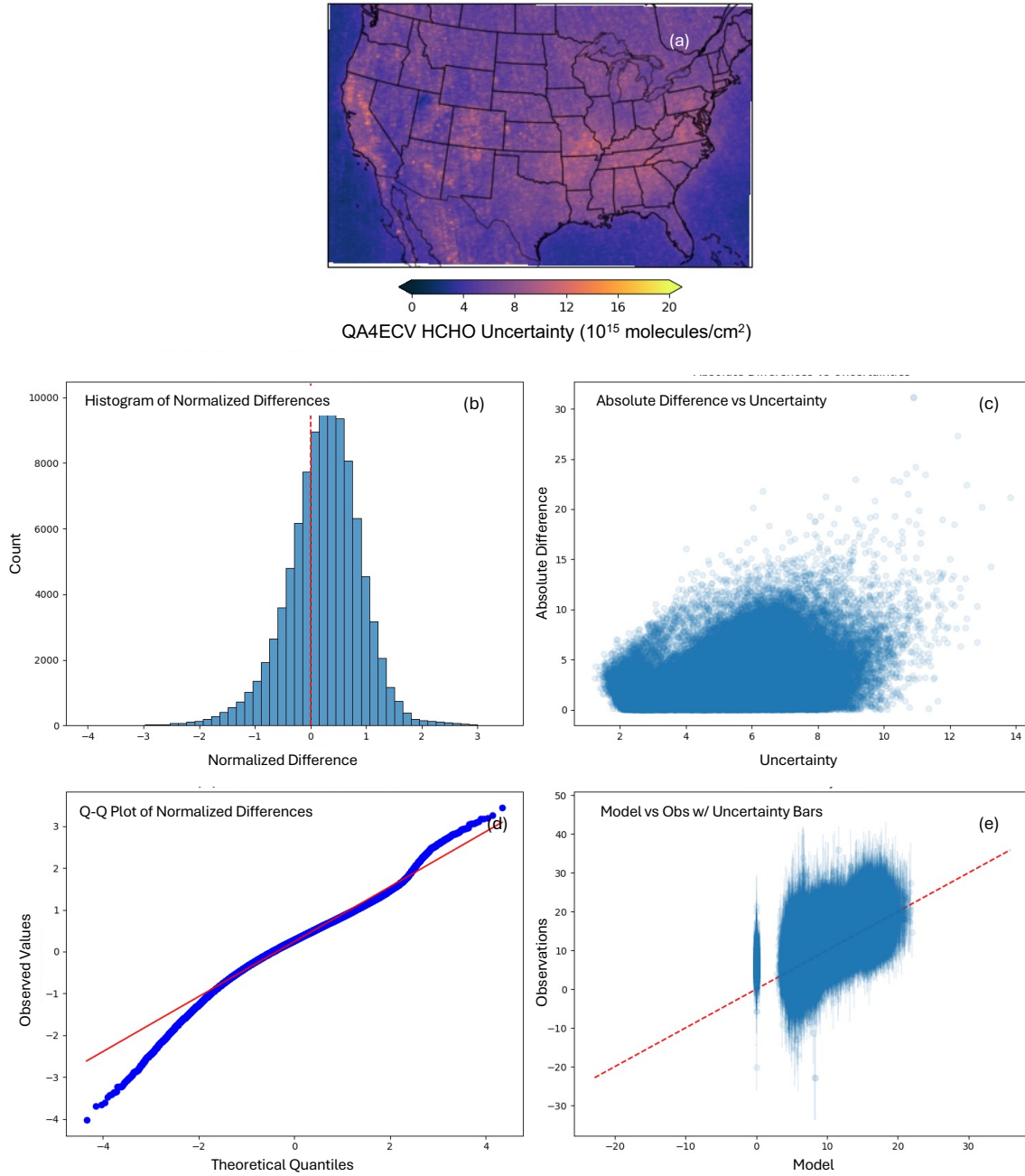


Figure 2-14: Uncertainty analysis of QA4ECV OMI HCHO column values. Here panel (a) shows the uncertainty of the vertical column, (b) shows the histogram of normalized differences between OMI observations and CAMx model values normalized by OMI uncertainty, (c) shows a plot of absolute difference between OMI observations and CAMx model values vs satellite uncertainty, (d) shows a Q-Q plot of normalized differences and (e) shows CAMx model vs OMI observations with satellite uncertainty error bars. We use random and systematic uncertainties and combined them using Equation 2-2 where σ_{sys}^2 is the systematic error, σ_{rand}^2 is the random error and σ_T^2 is the combined error.

$$\sigma_T^2 = \frac{\sigma_{rand}^2}{N} + \sigma_{syst}^2 \quad \text{Equation 2-2}$$

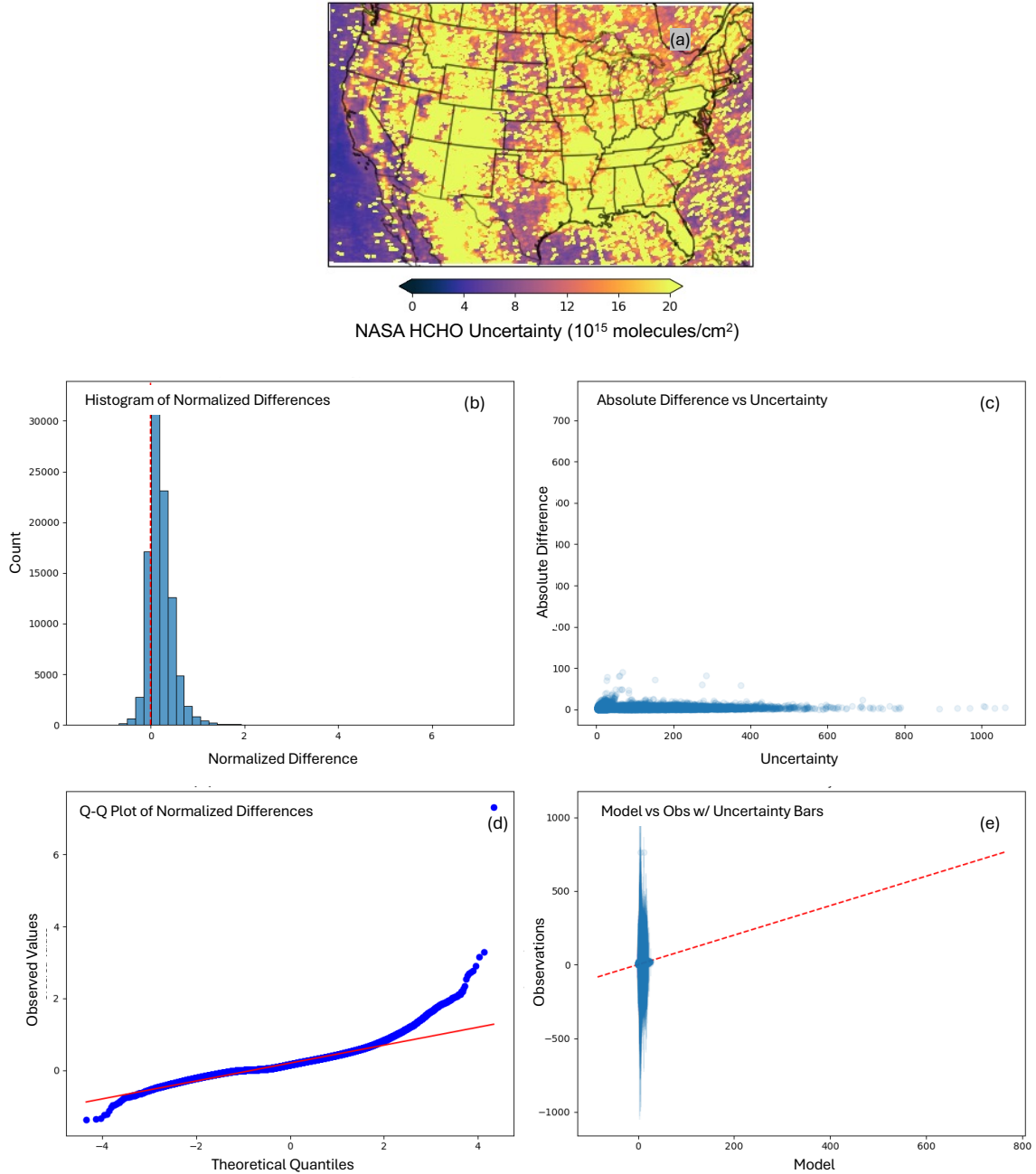


Figure 2-15: Uncertainty analysis of NASA OMI HCHO column values. Here panel (a) shows the uncertainty of the vertical column, (b) shows the histogram of normalized differences between OMI observations and CAMx model values normalized by OMI uncertainty, (c) shows a plot of absolute difference between OMI observations and CAMx model values vs satellite uncertainty, (d) shows a Q-Q plot of normalized differences and

(e) shows CAMx model vs OMI observations with satellite uncertainty error bars. We use total column amount uncertainty of each individual pixel.

2.4.3. Column Ozone Production Regimes

In this section we will discuss FNR calculations using both satellite observations and model output. Using the satellite data, we will compute tropospheric column FNR in the afternoon; while using the model, we will calculate FNR for both tropospheric and PBL column during afternoon and morning times. We compute two FNRs (see **Equation 2-3**) for the CONUS region using the CAMx model output to probe the importance of the vertical distribution of NO₂ and HCHO on the interpretation of satellite data. The first calculation utilizes the partial column values of both NO₂ and HCHO up to top of the PBL (from WRF meteorological input file), for both morning (9:30 AM LT) and afternoon (1:30 LT), which is referred to as FNR_{PBL}. More discussion of the implications of this ratio will be given in the next section. The second set of FNRs relies on tropospheric column values of NO₂ and HCHO from CAMx (total column CAMx because it is a tropospheric model), this will be referred to as FNR_{TC}.

For satellite observations, we determine the FNR_{TC} value by calculating the ratio of total column HCHO to tropospheric column NO₂. The HCHO retrievals of satellite observations do not separate stratospheric and tropospheric contributions because HCHO column values in the stratosphere are negligible (Millet et al., 2006). The FNR values for satellite observations are only available in the afternoon at the OMI overpass time.

$$FNR = \frac{HCHO \text{ Partial Column (molecules cm}^{-2}\text{)}}{NO_2 \text{ Partial Column (molecules cm}^{-2}\text{)}} \quad \text{Equation 2-3}$$

FNR values are representative of the ozone production regime, a critical metric for implementing effective ozone mitigation policy. **Table 2-10** provides the FNR thresholds (Duncan et al., 2010) used in this analysis, and describes their implications. Since the Duncan et al. (2010) paper was published, other studies have continued to advance the community’s understanding of the spatial variabilities of FNR (Choi et al., 2012; Jin et al., 2020; Jung et al., 2022; Schroeder et al., 2017; Sourì et al., 2023). For this analysis of the CONUS domain, we continue to use the FNR classification values as per Duncan et al. (2010) to provide context with earlier studies.

Table 2-10: HCHO to NO₂ Ratio (FNR) values and their Implication on the Ozone Production Regimes (OPRs)

FNR Value	Classification (Duncan et al., 2010)
< 1	Region is VOC-limited
1-2	Region is in transition between VOC and NO _x -limited
>2	Region is NO _x -limited

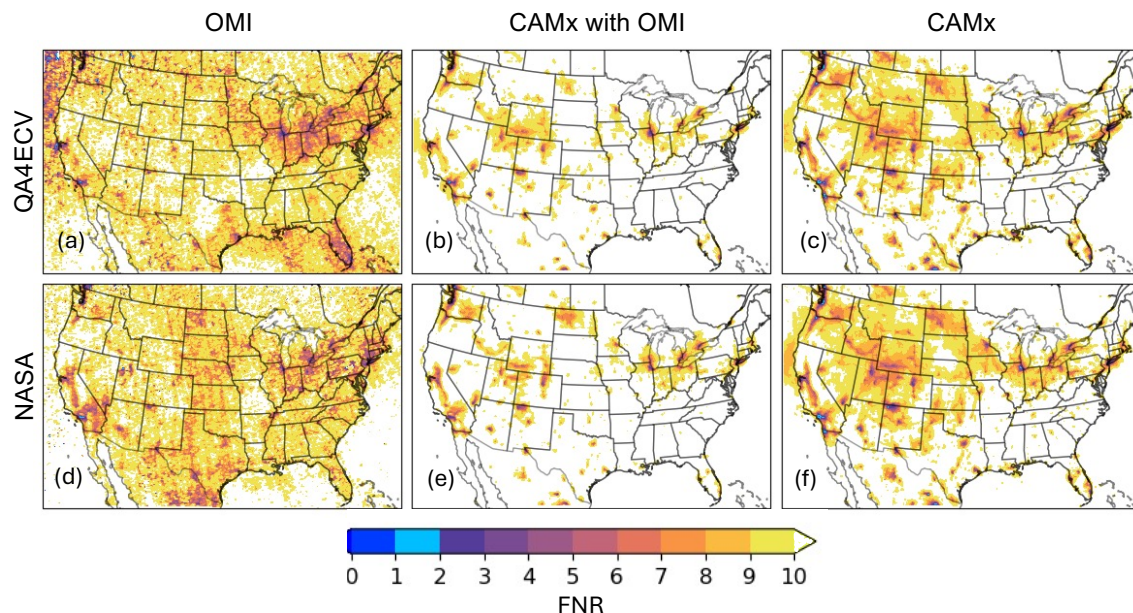


Figure 2-16: Average FNR_{TC} for summer 2016 from (a) QA4ECV retrieval, (b) CAMx model output with AK and AMF from the QA4ECV retrieval, (c) CAMx model output with corresponding pixels from the QA4ECV retrieval, (d) NASA retrieval, (e) CAMx model output with SW and AMF from the NASA retrieval and, (f) CAMx model output with corresponding pixels from the NASA retrieval. Level 2 data for both the retrievals were screened and regridded onto the CAMx model domain. Only grid points with cloud fraction less than 40% and at least 3 days of data for both the NO₂ and HCHO retrievals are used. White color represents regions with FNR > 10 (highly NO_x-limited).

The left panels of **Figure 2-16** (a and d) indicate that according to the satellite data, some scattered rural regions and some metropolitan regions are VOC-limited, whereas the overwhelming majority of CONUS is NO_x-limited. The ratios from the re-calculated model fields (panels b and e) indicate that the majority of CONUS is NO_x-limited (>99% of the pixels). There is strong agreement between all the panels of Figure 2-16 that the CONUS is primarily in the NO_x-limited regime for the production of tropospheric ozone. In **Table 2-11**, we see error metrics associated with Figure 2-16.

Table 2-11: NO₂, HCHO, and FNR (HCHO to NO₂ Ratio) from CAMx Model Output and their Associated Error Metrics Compared to the NASA and QA4ECV OMI Retrievals⁹

	Sat. Col.	Model Col.	Bias	NMB	RMSE	Ratio
	10 ¹⁵ mol/ cm ²	10 ¹⁵ mol/ cm ²	10 ¹⁵ mol/ cm ²	%	10 ¹⁵ mol/ cm ²	unitless
NO₂						
NASA OMI	1.10±0.63	0.54±0.34	-0.56±0.46	-50.73	0.73	0.56±0.28
QA4ECV OMI	1.21±0.60	0.65±0.37	-0.56±0.39	-45.92	0.68	0.58±0.24
HCHO						
NASA OMI	9.53±4.84	7.16±3.15	-2.37±4.42	-24.90	5.02	0.79±0.34
QA4ECV OMI	10.06±4.44	8.36±3.43	-1.70±3.23	-16.88	3.65	0.95±0.52
FNR (no units)						
NASA HCHO/ NASA NO ₂	11.18±7.52	15.10±5.86	3.96±8.12	35.45	9.04	1.70±1.08

⁹ These numbers are for summer averages over 2016. CAMx model output has been convolved with AK/SW information from the respective satellite retrievals. For NO₂ metrics, we have not counted values less than 0.2 x 10¹⁵ molecules/cm² as the model output did not go below this value. Similarly, for HCHO, we have not counted values less than 2 x 10¹⁵ molecules/cm². Both these criteria were considered for the FNR calculations.

QA4ECV HCHO/ QA4ECV NO ₂	9.16±4.20	13.88±4.53	4.72±5.55	51.46	7.29	1.78±1.02
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2.4.4. Diurnal Variation in OPR

CAMx broadly reproduced satellite observations of NO₂ and HCHO and, subsequently, the FNR_{TC} to a reasonable extent. By comparing model output with satellite and ground-based observations, we show that CAMx can represent the chemistry of the troposphere. Thus, we can use CAMx to provide insight into the diurnal variation of ozone precursor species and ozone production regimes, important to policy makers, while polar-orbiting satellites provide data for a single daylight overpass time. Additionally, CAMx provides details of near-surface chemistry, which is challenging to ascertain from satellites due to reduced sensitivity to conditions near the surface. Understanding ozone chemistry within the PBL is important because pollution control strategies generally focus on limiting the abundance of ozone near the surface, since surface ozone is most important for human health concerns (Bell et al., 2007, 2006; Berman et al., 2012; Fleming et al., 2018; Lefohn et al., 2018; Nuvolone et al., 2018; Stowell et al., 2017).

Figure 2-17 shows the morning (9:30 AM LT) to afternoon (1:30 PM LT) variation of FNR_{TC} and FNR_{PB}. These times were chosen to demonstrate the diurnal variation of ozone precursor species. Again, we are following the FNR designations of Duncan et al. (2010) shown in Table 1. We indicate FNR > 10 (highly NO_x-limited) as white in Figure 2-17 to highlight the differences. Clearly, the PBL columns (bottom panels) have lower

ratios that the tropospheric columns (top panels) and therefore are more likely to be VOC-limited or at least in the transitional regime than the tropospheric columns.

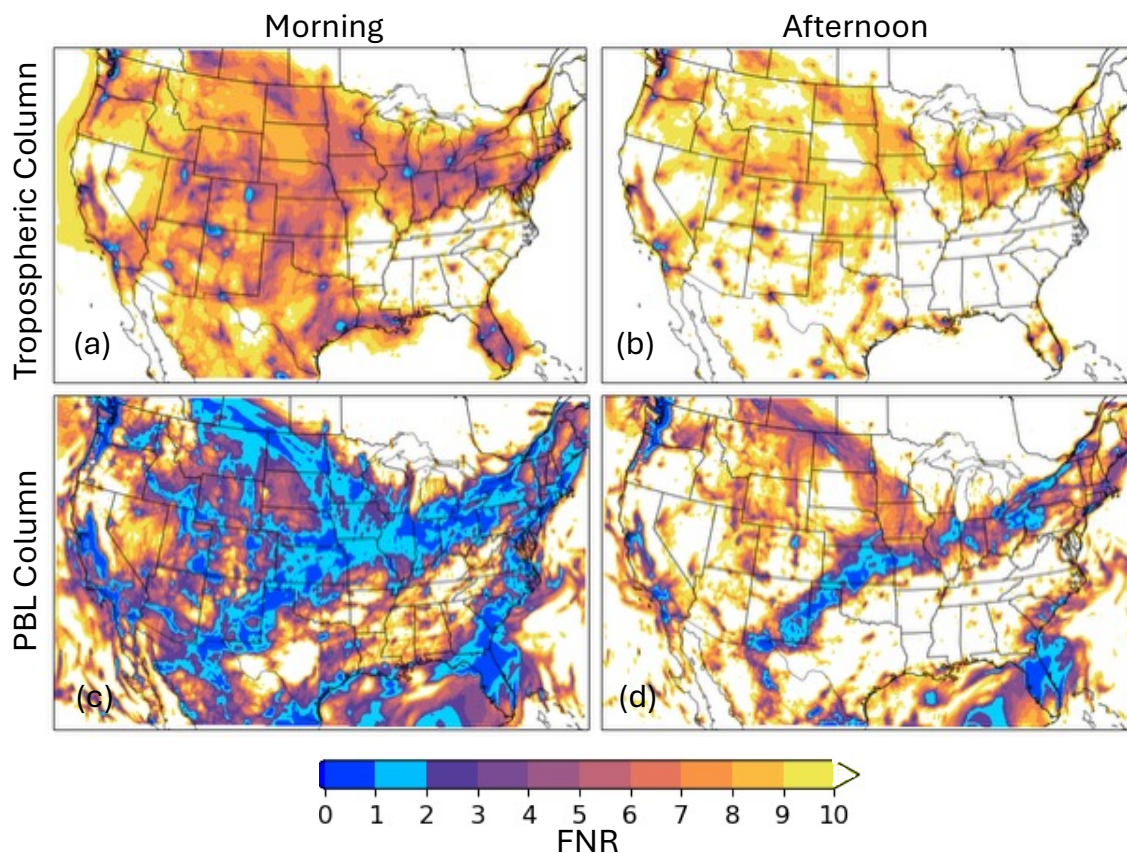


Figure 2-17: Panels (a), (b), (c) and (d) show the column ratios of HCHO to NO₂ averaged over summer 2016 from the CAMx model platform. Morning refers to 9:30 AM local time while afternoon refers to 1:30 PM local time. Panels (a) and (b) give tropospheric column ratios (FNR_{TC}) while panels (c) and (d) give PBL column ratios (FNR_{PBL}). White color represents regions with $FNR > 10$ (highly NO_x-limited regime). The AK and SW of the retrievals are not applied to the model output, because this information is unavailable for the morning.

The FNR_{PBL} plots (panels (c) and (d)) of Figure 2-17 show that OPR is in the VOC-limited regime for large swaths of the US, especially in urban areas and cities. The importance of VOC chemistry in the PBL is not revealed by the FNR_{TC} shown in Figure 2-17 panels (a) and (b). OPRs within the PBL are often quite different from those

represented by the tropospheric column. Analysis of PBL ozone production regime shows some near-surface areas are more VOC-limited than are indicated by the NO_x -limited column FNRs. These areas include significant roadways like Interstate-40 (I-40) and I-95, a horseshoe bend in Idaho where many fracking activities occur, and a strong signature of the Four Corners power plant between New Mexico, Arizona, Utah, and Colorado.

The OPR for the PBL (that is, FNR_{PBL}) is more likely to be VOC-limited than the OPR for the tropospheric column because the fraction of NO_y existing as NO_x ($\text{NO} + \text{NO}_2$) is larger in the PBL than in the free troposphere (Dang et al., 2023; Luke et al., 1992; Yang et al., 2023). As altitude increases, the NO_x to NO_y ratio falls off due to the stability of PAN and the conversion to organic nitrates, nitric acid, and nitrate aerosols (Jacob, 1999). NO_x also has a shorter lifetime than NO_y , and many of the NO_y species are reservoirs that can later contribute to making ozone upon reentering the PBL. The lifetime of NO_x and NO_y are longer at higher altitudes. In the free troposphere, anthropogenic NO_x is commonly converted to these species, resulting in the OPR averaged over the troposphere (FNR_{TC}) being more NO_x -limited than in the PBL.

CAMx output in Figure 2-17 (panels a and c) show that the morning is usually more VOC-limited than the afternoon, for both FNR_{TC} and FNR_{PBL} with the FNR_{PBL} being more VOC-limited than FNR_{TC} . This knowledge, not captured by polar orbiting satellites, is important for developing effective pollution reduction strategies for surface ozone. With the April 2023 launch of TEMPO, a geostationary satellite centered over North America, we now have 40-60 minute measurements of column NO_2 , HCHO, and ozone (Chance et

al., 2019; Zoogman et al., 2017). With TEMPO, the diurnal variation of FNR_{TC} can be measured and compared to models. However, information regarding FNR_{PBL} will not be provided by TEMPO.

2.4.5. Sensitivity of the Satellites to the Surface: Understanding the Ratio of FNR_{PBL} to FNR_{TC} (β)

In the previous section, we calculated FNR_{TC} using satellite observations and model output and found that they both showed mainly NO_x -limited conditions over CONUS. To better understand OPR as a function of height, we leverage our model output to determine locations where the FNR_{TC} is representative of near-surface ozone chemistry and regions where it is not. We consider the ratio of CAMx-derived FNR_{PBL} to FNR_{TC} as Beta (β), defined below in **Equation 2-4**.

$$\beta = \frac{\text{FNR}_{\text{PBL}}}{\text{FNR}_{\text{TC}}} \quad \text{Equation 2-4}$$

A value of 1 for β means the same message about photochemical control of ozone applies throughout the tropospheric column as in the PBL. The further β deviates from 1, the less representative the satellite-retrieved FNR_{TC} is of photochemical conditions within the PBL that directly affect surface ozone. **Table 2-12** provides further details regarding the implications of particular values of β . We believe that inferring β is a unique way of looking into these variations and can provide a regional picture of the height dependence of OPR.

Table 2-12: β Values and their Implication on the Ozone Production Regimes (OPRs)

β Value	Classification
<1	PBL column is more VOC-limited than tropospheric column
1	PBL Column and tropospheric column are in general agreement
>1	PBL column is more NO _x -limited than tropospheric column

In **Figure 2-18**, panels (a) and (b) show β for morning and afternoon, respectively. We then plot only the regions from panels (a) and (b) that switch OPR when comparing FNR_{TC} and FNR_{PBL} and show them in Figure 2-18, panels (c) through (h). These focus regions (panels (c) through (h)) represent areas in which FNR_{TC} indicates that the region is NO_x-limited, but FNR_{PBL} indicates the production of ozone is VOC-limited. There is never a situation where FNR_{PBL} is NO_x-limited while FNR_{TC} is VOC-limited. Hence, we only see values less than 0.8 highlighted in panels (c) through (h). In the morning, there are more regions where tropospheric column derived ozone chemistry does not represent the near-surface ozone chemistry. These regions of low β are often over urban regions, or regions with significant NO_x sources during the morning and afternoon.

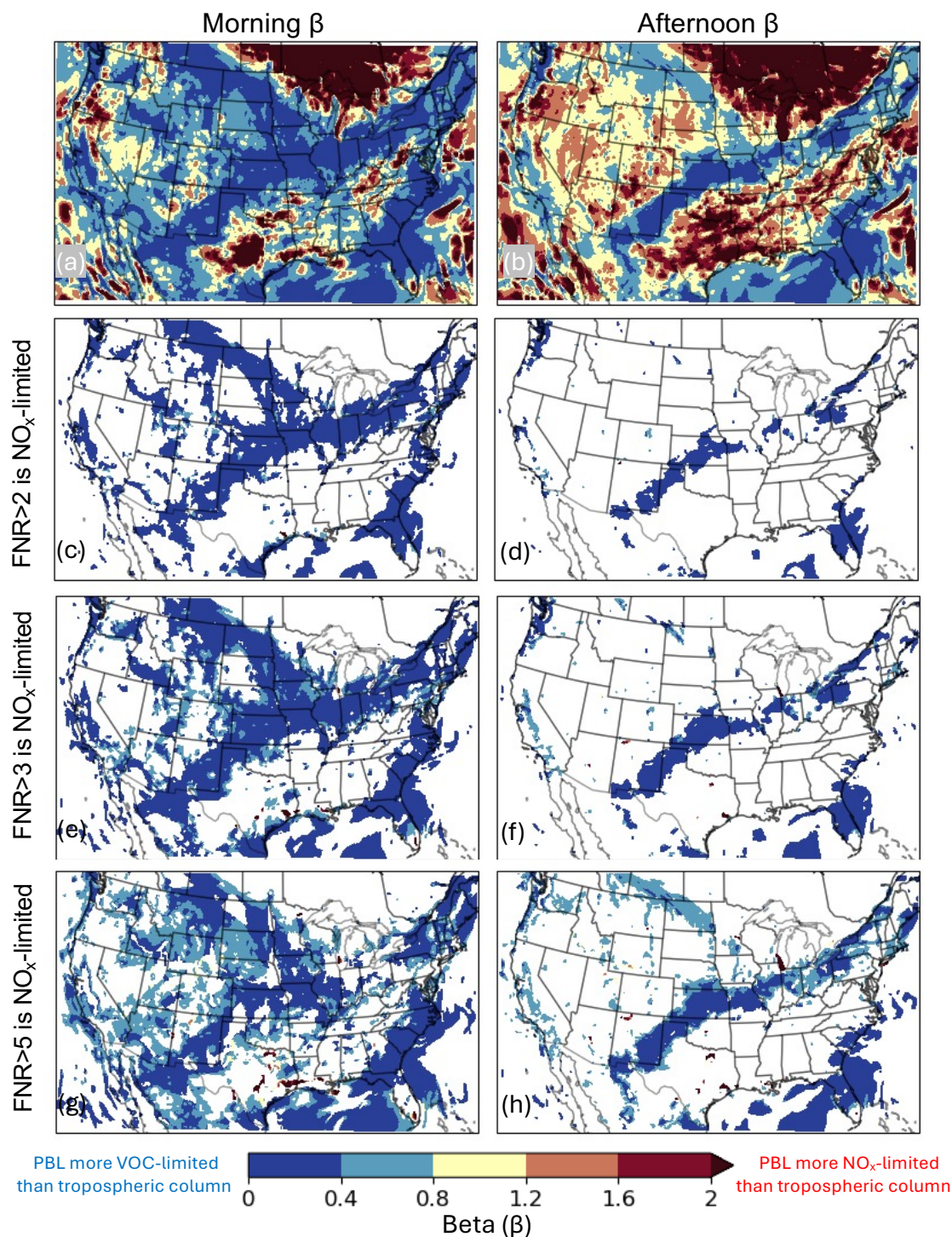


Figure 2-18: This figure represents the metric Beta (β) which we developed to understand tropospheric column FNR applicability to the surface. Panels (a) and (b) show β (the ratio of FNR_{PBL} to FNR_{TC}) for morning and afternoon, respectively. Panels (c) (morning) and (d) (afternoon) highlight the regions where FNR_{TC} is NO_x-limited, but FNR_{PBL} is transition/VOC-limited if FNR > 2 represents NO_x-limited regime. Panels (e) and (f) are

similar to panels (c) and (d), but for $\text{FNR} > 3$ representing a NO_x -limited regime, while panels (g) and (h) use $\text{FNR} > 5$ to represent a NO_x -limited regime.

Figure 2-18 shows that for large regions of CONUS, OPRs indicated by FNR_{TC} and measurable from space are different from OPRs indicated by FNR_{PBL} that can only be obtained from models. Thus, models can be used to gain additional insight into the OPR. Our analysis shows that tropospheric column-based estimates underestimate the importance of VOC chemistry in the U.S. This figure illustrates the need for increased surface observations (especially increasing Photochemical Assessment Monitoring Stations (PAMS) coverage for measuring VOCs), bottom-up column observations and in-situ flight observations, to provide a better understanding of the near-surface tropospheric ozone chemistry. Souri et al. (2023) investigated several types of uncertainty in using tropospheric column satellite retrieval to inform PBL chemistry, including retrieval errors, errors due to the ability of FNR to describe the $\text{HO}_x\text{-RO}_x$ cycle, errors due to spatial heterogeneity and errors due to translation of column FNRs to PBL FNRs. They found that retrieval errors are the most significant source of error in satellite-derived FNR in the summertime. This finding adds to our message about being cautious when using satellite retrievals to inform policy.

The Duncan et al. (2010) classification for identifying the transition regime for OPR that is central to our analysis focused on southern California in 2007 (Figure 2-18 panels (c) and (d)). We illustrate how the FNR threshold as found in Schroeder et al., 2017 impacts β (Figure 2-18 panels (e) through (h)). They found that over Colorado, the transition regime using column densities for FNR are in the range of 1.1-3 (Figure 2-18 panels (e) and (f)).

They also found that over Houston, the range is 1.3-5 (Figure 2-18 panels (g) and (h)). It is evident from these panels that the regions where there are disagreements between FNR_{PBL} and FNR_{TC} tend to become broader as the transition point to NO_x -limited regime increases. With increasing threshold, we observe additional regions fall under this disagreement, namely across EPA-designated regions 8, 9, and 10 (US EPA, 2020c). However, regions, such as parts of Ohio, Indiana, and Michigan during the morning agree better as the threshold increases.

A map of the regions of the CONUS that are in non-attainment of the current US EPA 8-hour surface ozone standard as of 2023 is shown in **Figure 2-19**. Several of the non-attainment regions are geographically consistent with the blue regions shown in Figure 2-18. This geographical consistency implies that many regions where FNR_{PBL} are VOC-limited, especially in the morning, coincide with regions of non-attainment of the 8-hour ozone standard, leading to significant implications for surface ozone reduction policies. In theory, β could also be used to scale tropospheric column FNRs to PBL column FNRs (Jin et al., 2017; Souri et al., 2023). However, for this paper, we use β to highlight areas where there could be disagreements between the satellite retrieval derived column FNR and model derived PBL FNR. This metric is specifically crafted for policy purposes.

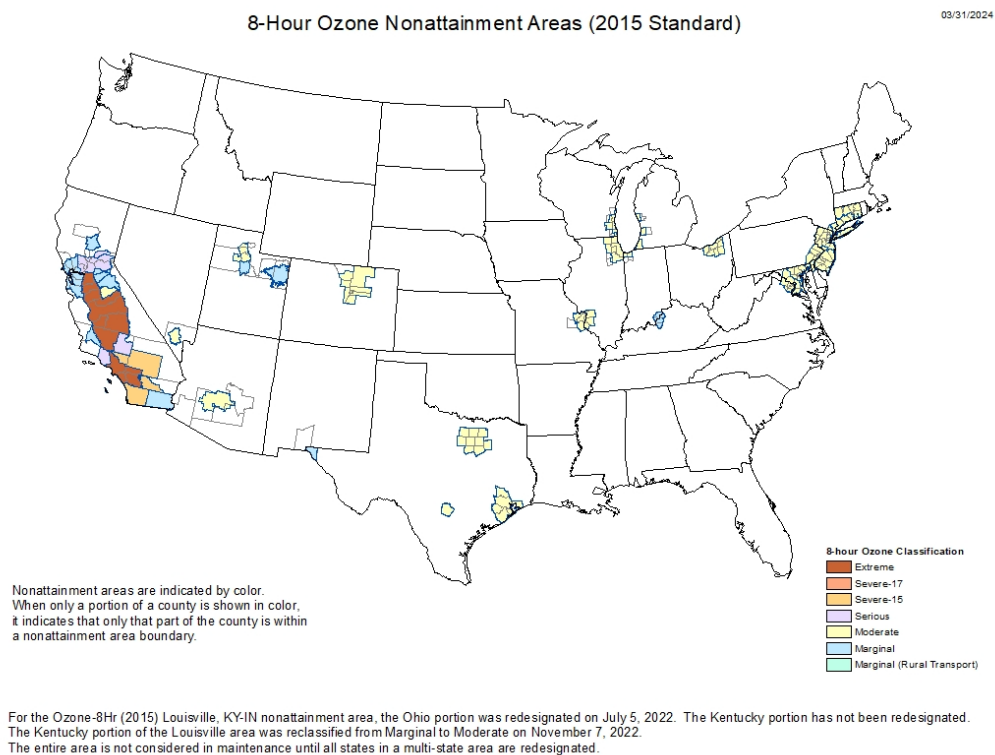


Figure 2-19: Figure represents a 2024 map of the CONUS highlighting regions that are in non-attainment of the 8 hour ozone standard set by the US EPA (US EPA, 2024).

2.4.6. Vertical Distribution of HCHO, NO₂ and FNR

AQMs like CAMx provide detailed information about the vertical distribution of atmospheric species that complements both surface observations and satellite retrievals. The vertical profiles presented in **Figure 2-20** and **Figure 2-21** illustrate the contrasting behavior of HCHO/NO₂ ratios between urban and rural regions across the CONUS. Urban areas are defined as the 30 most populous cities over CONUS, while rural regions encompass the remaining areas. The cumulative ratio represents the summation of partial column formaldehyde to partial column nitrogen dioxide from the surface to the nth model layer (Figure 2-20) and from top of the model to the nth layer (Figure 2-21).

Consistent with previous analysis, urban regions exhibit VOC-limited to transitional ozone chemistry near the surface, as indicated by lower HCHO/NO₂ ratios. However, this relationship changes with altitude and becomes more NO_x-limited in the upper atmospheric layers. In contrast, rural areas remain consistently NO_x-limited throughout the vertical profile due to higher biogenic VOC emissions and lower anthropogenic NO_x emissions in these regions.

Comparison with satellite retrievals reveals notable differences in model-observation agreement between urban and rural areas. NASA OMI and QA4ECV OMI show better agreement with modeled distributions in rural regions compared to urban areas. This enhanced agreement in rural areas is due to a more homogeneous chemical environment compared to the complex, heterogeneous conditions of urban environments. The satellite retrieval challenges in urban areas may stem from sub-grid scale variability and boundary layer mixing complexities.

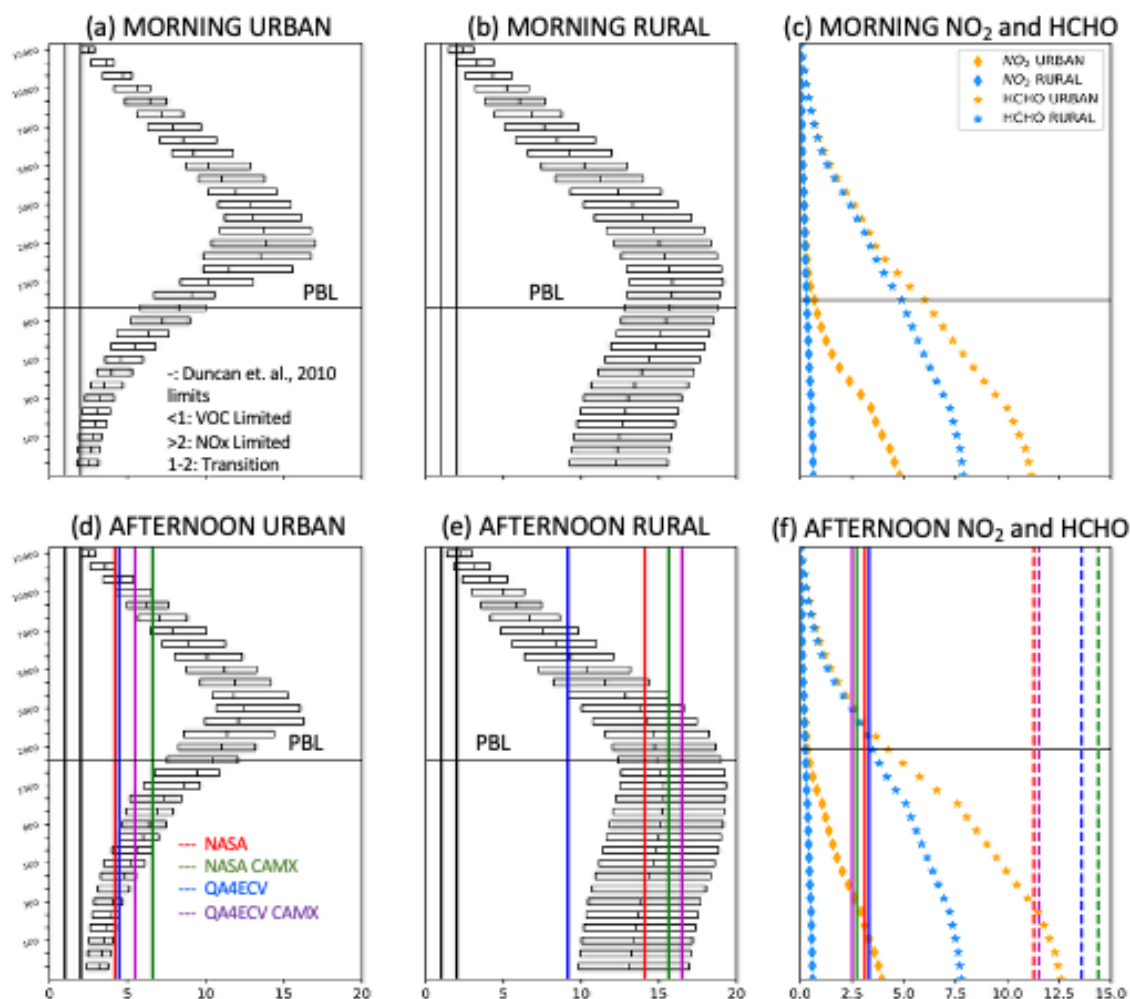


Figure 2-20: Vertical distributions averaged for JJA 2016 from the CAMx model platform. Panels (a) and (d) show the distribution of the top-down cumulative ratios of HCHO to NO₂ over urban areas of the CONUS for morning and afternoon, respectively. Panels (b) and (e) show the distribution of the top-down cumulative ratios of HCHO to NO₂ over rural areas of the CONUS for morning and afternoon, respectively. Panels (c) and (f) show the distribution of the top down cumulative NO₂ and HCHO over both urban and rural areas of the CONUS for morning and afternoon, respectively. Here, afternoon refers to 1:30 PM local time while morning refers to 10:30 AM local time. The vertical lines in red, blue, green and magenta represent the averaged values of the NASA and QA4ECV OMI satellite retrieval and their recalculated counterparts for urban and rural areas, respectively.

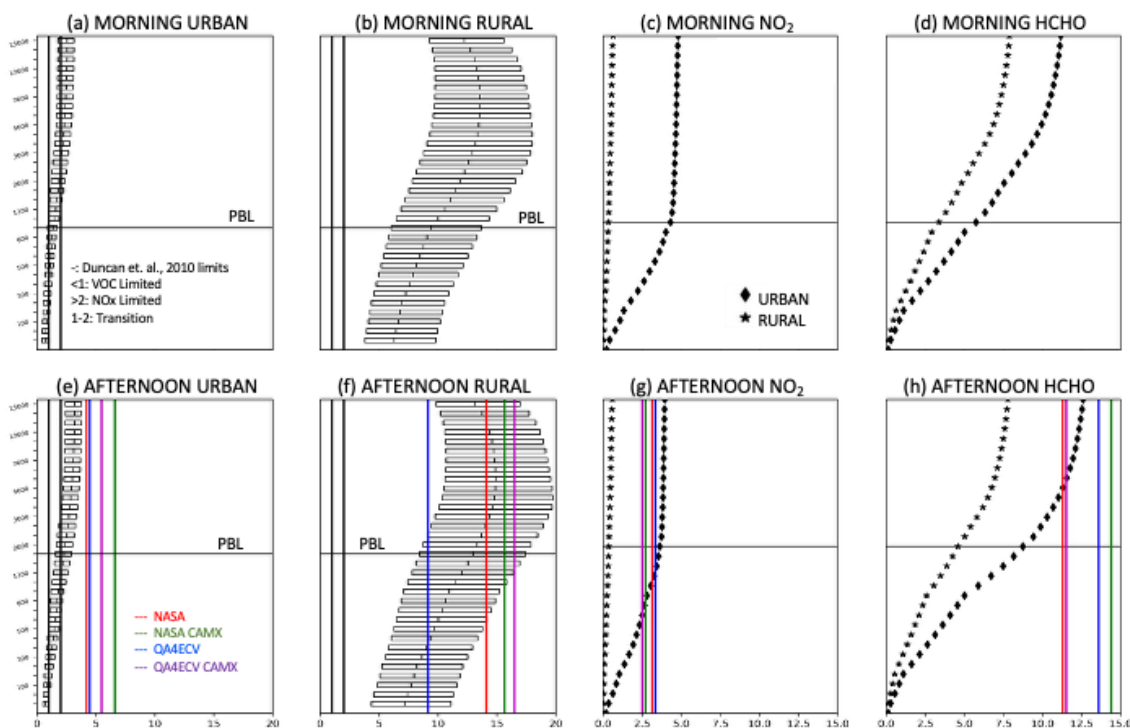


Figure 2-21: Vertical distributions averaged for JJA 2016 from the CAMx model platform. Panels (a) and (e) show the distribution of the bottom-up cumulative ratios of HCHO to NO₂ over urban areas of the CONUS for morning and afternoon, respectively. Panels (b) and (f) show the distribution of the bottom-up cumulative ratios of HCHO to NO₂ over rural areas of the CONUS for morning and afternoon, respectively. Panels (c) and (g) show the distribution of the bottom up cumulative NO₂ over both urban and rural areas of the CONUS for morning and afternoon, respectively. Panels (d) and (h) show the distribution of the bottom-up cumulative HCHO over both urban and rural areas of the CONUS for morning and afternoon, respectively. Here, afternoon refers to 1:30 PM local time while morning refers to 10:30 AM local time. The vertical lines in red, blue, green and magenta represent the averaged values of the NASA and QA4ECV OMI satellite retrieval and their recalculated counterparts for urban and rural areas, respectively.

2.4.7. Impact on Policy

We have shown that the photochemical production of ozone in the PBL over the CONUS during the summer of 2016 tended to be more VOC-limited in the morning, with a transition to being more NO_x-limited in the afternoon. The transition between the two regimes marks the time of peak photochemical production of ozone. We utilize CAMx

output to determine the time when a region transitions from the VOC-limited to the NO_x-limited regime: results are shown in **Figure 2-22**.

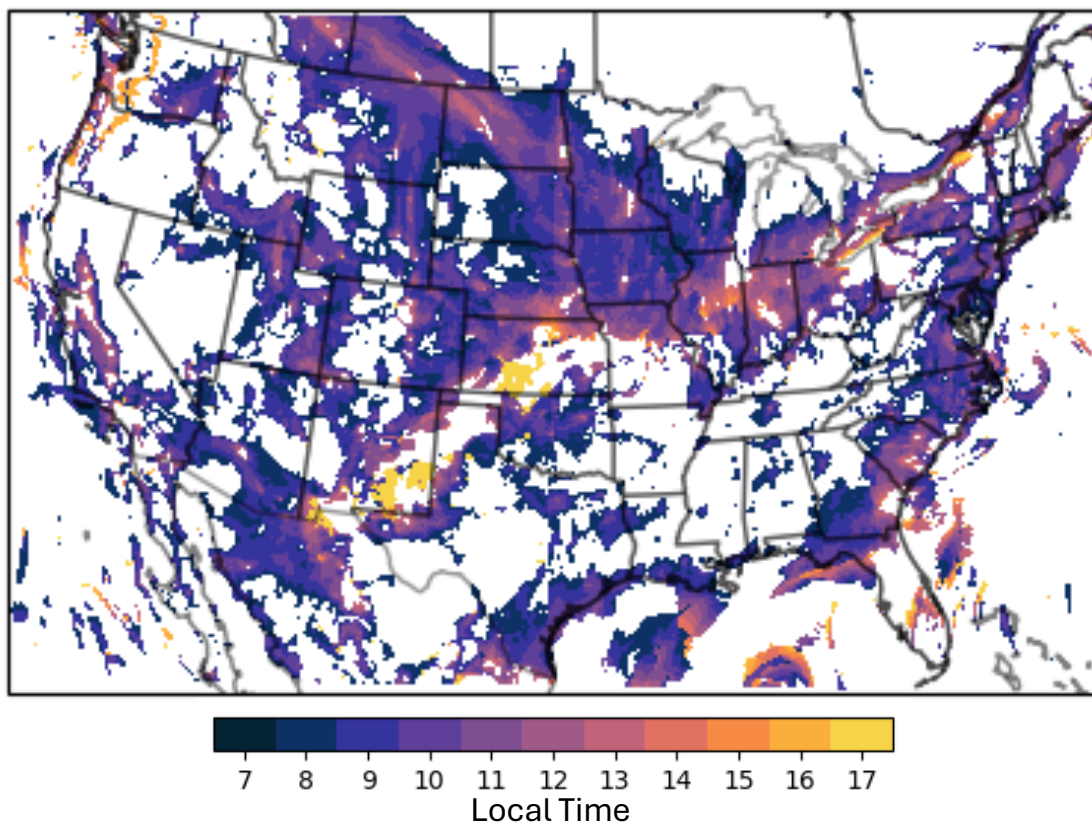


Figure 2-22: Spatial distribution of transition times from VOC-limited to NO_x-limited photochemical ozone production regimes over CONUS during summer 2016, derived from CAMx model output. The color scale indicates the local time when each grid cell transitions between chemical regimes. White areas indicate regions that remain consistently NO_x-limited throughout the day.

Figure 2-22 shows that for most of the CONUS during the summer of 2016, the transition from VOC to NO_x-limited regimes occurs between 10 AM and 12 noon. This transition time is generally when peak ozone production takes place. Policy makers can use this information to enact regulations in areas that exhibit a transition during the day. Ideally, for these regions, it would be best to focus policy on reducing VOC emissions in the morning and reducing NO_x emissions in the afternoon. Alas, such a time-sensitive focus

is likely not practical. Consequently, policy measures could be implemented to reduce both VOC and NO_x emissions in such a manner that as the local photochemical production of ozone moves more fully into the NO_x-limited regime, the peak formation rate of ozone also declines. The simultaneous reduction of emissions of VOCs and NO_x for the Baltimore-Washington region was essential for causing local levels of ozone to steadily improve, as this transition occurred (Roberts et al., 2022).

Figure 2-23a shows the difference in the OPR between urban and rural regions of the CONUS within the PBL. We define urban as the 36 km² grid around the top 30 densely populated metropolitan statistical areas and rural as the rest of the grid cells within the model domain. Rural areas generally remain NO_x-limited throughout the day, while urban areas tend to remain largely VOC-limited. This difference between ozone production regime for urban and rural regions suggests customized strategies could be considered for the mitigation of surface ozone for various parts of the CONUS. Surface ozone levels in rural regions will continue to benefit from a NO_x reduction strategy, while urban areas would benefit most from an effort to reduce anthropogenic emissions of both VOCs and NO_x.

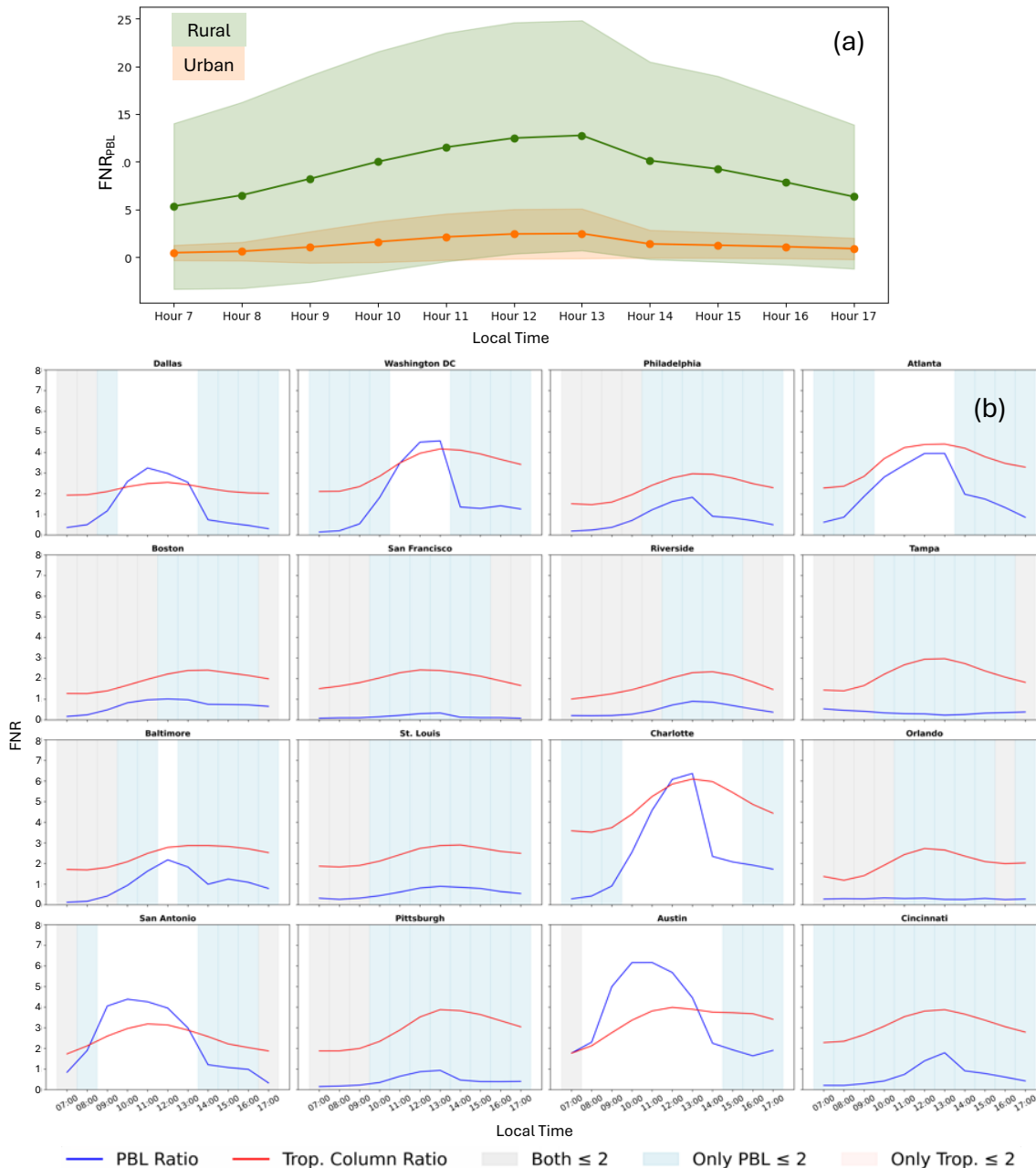


Figure 2-23: (a) Time series of FNR_{PBL} for CONUS urban and rural areas averaged over summer 2016. We define urban as the 36 km² grid around 30 metropolitan statistical areas and rural as the rest of the grid cells. The shaded regions represent one standard deviation for urban (orange) and rural (green). (b) Time series of FNR_{PBL} (blue line) and FNR_{TC} (red line) at a few urban locations in the CONUS averaged over summer 2016. The rest of the urban locations considered in this study are shown in Figure S11. The gray-shaded regions are where both FNR_{PBL} and FNR_{TC} are in the VOC-limited or transition regime (<2), the blue-shaded regions are where only FNR_{PBL} is in the VOC-limited or transition regime (<2), the pink shaded regions (not seen in this figure) are where only FNR_{TC} is in the VOC-limited or transition regime (<2), and the unshaded regions are where both FNR_{PBL} and FNR_{TC} are in the NO_x -limited regime.

Figure 2-23(b) highlights the OPR inferences across select urban centers in the CONUS, where tropospheric and PBL columns yield contrasting results. In the panels, the red line represents FNR_{TC} , and the blue line represents FNR_{PBL} . When the two FNRs agree about the OPRs being less than 2, the hour is highlighted with gray; when only FNR_{PBL} is less than 2, the hour is highlighted with blue. Both FNRs are solidly in the NO_x -limited regime in the unshaded or white regions. Out of the 30 urban centers we analyzed in this paper, we show 16 of them in Figure 2-23(b); the rest of the urban centers are shown in **Figure 2-24**.

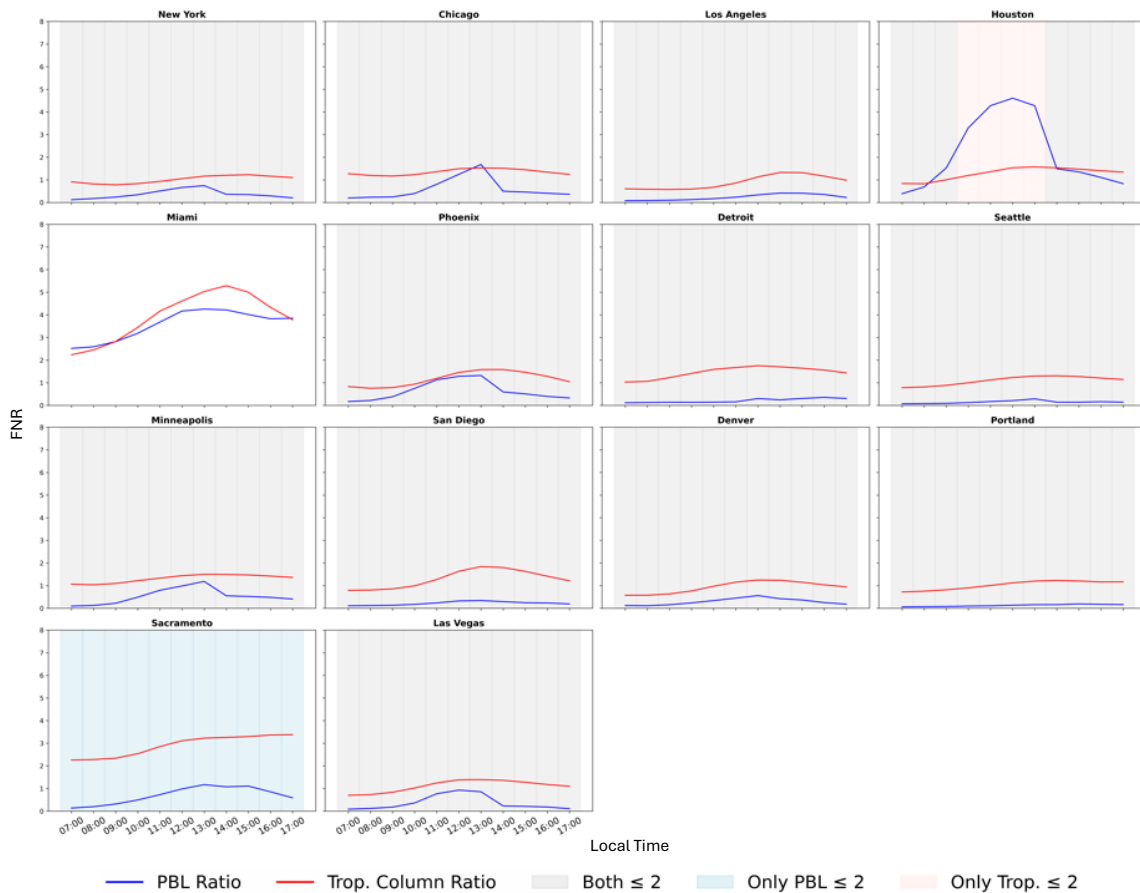


Figure 2-24: Time series of FNR_{PBL} (blue line) and FNR_{TC} (red line) at a few urban locations in the CONUS averaged over summer 2016. The gray-shaded regions are where

both FNR_{PBL} and FNR_{TC} are in the VOC-limited or transition regime (<2), the blue-shaded regions are where only FNR_{PBL} is in the VOC-limited or transition regime (<2), the pink shaded regions are where only FNR_{TC} is in the VOC-limited or transition regime (<2), and the unshaded regions are where both FNR_{PBL} and FNR_{TC} are in the NO_x -limited regime.

We see large discrepancies between FNR_{TC} , and FNR_{PBL} for some urban areas, indicating that FNR_{TC} may not always be accurate enough to understand the photochemical production of ozone within the PBL. For instance, Cincinnati (lower right panel in Figure 2-23b) is consistently in the VOC-limited regime within the PBL throughout the day; however, if we tried to understand ozone production only by looking at the tropospheric column, we would assess the situation as being NO_x -limited. This mismatch could lead to wrong policy decisions, and worsening conditions for surface ozone, at least initially. Other cities, such as New York City (shown in Figure 2-24), show excellent agreement between column and PBL FNRs and lie solidly in the VOC-limited regime throughout the day.

In general, FNR_{TC} varies less with time of day than FNR_{PBL} . Changes in PBL height affect the photochemical production of ozone and, subsequently, the OPRs. This information about the variation in PBL height is washed out when we look at the tropospheric column FNR, leading to inaccuracies when using satellites to determine surface FNR. With these results, we aim to provide time-of-day instances when VOC emissions controls would be the most effective in controlling ozone production.

The difference between FNR_{TC} , and FNR_{PBL} in relation to OPRs for much of the country (see Figure 2-18 panels c-h) demonstrates how using satellite-derived FNR alone (FNR_{TC}) could lead to conclusions regarding the regime of surface ozone production that

could lead to ineffective emissions reductions policies. It is crucial for policymakers to understand that due to the nonlinear nature of the photochemical production of tropospheric ozone, reducing anthropogenic emissions of NO_x alone could lead to an increase in tropospheric ozone production in a VOC-limited regime while a decrease in VOC emissions alone could lead to an increase in tropospheric ozone production in a NO_x -limited regime. To develop effective surface ozone production policy, information about surface pollution levels is essential. Therefore, in addition to satellite data, surface observations are critically important to provide surface observations of ozone and its precursors, emphasizing the importance of expanding ground-level monitoring networks in addition to using satellite observations.

2.5. Conclusions and Future Perspectives

Policymakers must use air quality model simulations, despite their limitations, to test mitigation strategies and because their high temporal and spatial resolution can be used to fill in the gaps between surface, satellite, and aircraft observations. Photochemical models such as CAMx capture diurnal variations of NO_2 and HCHO essential to understanding the variation in Ozone Production Regimes (OPRs) throughout the day over the CONUS. This diurnal variation cannot be captured by polar sun-synchronous satellite observation systems such as OMI and TROPospheric Monitoring Instrument (TROPOMI) because they have one daytime observation period at approximately 1:30 PM local time. Understanding the diurnal variation of OPRs is crucial because peak ozone production commonly occurs as OPRs transition from morning (VOC-limited) to afternoon (NO_x -limited) (Chen and Brune, 2012; Mao et al., 2010; Ring et al., 2023).

Our analysis shows that in the morning within the PBL for many regions of the CONUS, ozone production is in a VOC-limited regime and the photochemistry shifts to a NO_x-limited regime in the afternoon, with peak production of ozone likely occurring during midday when the chemistry is in the transition regime. Satellite measurements of tropospheric column NO₂ and HCHO, more heavily weighted to the tropospheric column than the PBL, often fail to capture the true photochemical environment of ozone within the PBL. Our analysis suggests that successful regulation of surface ozone in many areas of the CONUS should prioritize future reductions in the emissions of both VOCs and NO_x.

This study defines the tropospheric column Formaldehyde to NO₂ Ratio (FNR_{TC}) divided by the FNR ratio from the PBL (FNR_{PBL}) as Beta (β) to identify regions where satellite observations can be a sufficient analogue for surface ozone chemistry and where they might not be appropriate. In particular, the β metric can be used to determine where satellite-derived tropospheric column estimates of ozone production regimes mischaracterize surface ozone chemistry. Specifically, tropospheric column-based estimates underestimate the importance of VOC-chemistry. These limitations must be understood as satellite observations are increasingly being used to examine surface ozone chemistry and production regime. Our study emphasizes that although most of the U.S. is in a NO_x-limited regime, VOC emission reductions are still beneficial, especially in areas of the CONUS as highlighted by β (Figure 2-18). These areas include many densely populated urban regions with important implications for human health. Furthermore, this

kind of analysis may benefit state and local regulators, as ozone standards are slated to become more strict (US EPA, 2023b).

TEMPO, a geostationary satellite launched in 2023, is measuring NO₂ and HCHO hourly over the CONUS, thus resolving the temporal disadvantage of sun-synchronous satellites described above. As with all satellite observational systems, TEMPO observations are less sensitive to near surface chemistry than to free troposphere chemistry. For understanding near surface ozone chemistry, photochemical air quality models like CAMx are useful, as they provide concentrations of these species at each layer of the troposphere. In this study, we find that OPRs estimated using PBL columns are more VOC-limited than those estimated using total tropospheric columns.

We plan to extend this analysis to TEMPO data to investigate the ability of FNR_{TC} to properly assess the production regime of surface ozone, by comparing OPR regimes derived from the satellite fields to those inferred from ground-based measurements (Roberts et al., 2022). Future studies can also investigate decadal trends of β to determine how emission changes affect its spatial distribution. In particular, future studies could use higher resolution models for input into health impact assessment studies to develop targeted pollution reduction methods for communities most adversely affected by high concentrations of NO₂ and exceedances of the current US EPA standard for 8-hour ozone, which tend to be low income communities often with overrepresentation from racial and ethnic minorities (Kerr et al., 2024).

3. Monitoring Exposure to Tropospheric Ozone Precursors: AQS Site Evaluation and Recommendation (published as (Singh et al., 2025b)

3.1. *Abstract*

Current air quality monitoring through the EPA’s Air Quality System (AQS) network faces significant coverage gaps particularly in vulnerable communities that experience disproportionate exposure to air pollutants. While satellite instruments provide extensive geographic coverage for monitoring tropospheric ozone (O_3) precursors, such as nitrogen dioxide (NO_2) and formaldehyde (HCHO), these space-based measurements cannot replace ground-based observations for an accurate assessment of air quality conditions near the surface. Attainment of the National Ambient Air Quality Standards for tropospheric O_3 is determined using surface measurements rather than satellite-derived column values. Using the Environmental Justice Screening and Mapping demographic and health variables, we identify underserved counties, those that lack adequate ambient air quality monitoring. We present a comprehensive method for optimizing AQS site placement by integrating satellite data from NASA’s Tropospheric Emissions: Monitoring Pollution instrument, demographic indicators, and population density. We introduce the Integrated AQS Placement Index (I_{IAP}), which combines normalized demographic overlap, satellite-measured HCHO or NO_2 column values, and population density to prioritize future monitoring locations. Our analysis reveals significant monitoring gaps in the Eastern and Southeastern United States, notably in the ‘isoprene volcano’ region, as well as clusters along the I-95 corridor in the Northeast. These areas are characterized by high population,

high concentrations of HCHO, which is an under-monitored carcinogen, and vulnerable demographic profiles. We identify existing AQS sites that could benefit from expanded species monitoring as an economical approach to comprehensive coverage. This research underscores the critical need for proactive policies in air quality monitoring to address disparities and ensure that resources are allocated to protect the most vulnerable populations.

3.2. *Introduction*

AQS ground-based sites are typically selected to represent regional air quality and have historically been located in areas distant from major point sources, such as power plants. Siting is based on population size, traffic volume, and ozone design values. We assess whether siting should also consider demographic indicators to help monitor and address conditions across neighborhoods that are most impacted by poor air quality. We use EJScreen demographic and health variables to identify vulnerable counties that lack ambient air quality monitoring sites. We also use data from the newly launched NASA TEMPO instrument, in a geostationary orbit centered over North America that provides column measurements of NO₂ and HCHO throughout the day (Chance et al., 2019; Zoogman et al., 2017). Using these data, we present a new index for siting that considers both satellite observations and demographic factors. We suggest this new index could be used to assist future siting decisions to improve equitable access to air quality data.

3.3. *Methodology*

3.3.1. Demographic Data Description

We use EJScreen demographic indicators for the contiguous United States (CONUS) for 2024 (“EJScreen TSD,” 2024). EJScreen data provides information on the total population of each census tract, which ranges from 1200 to 8000 people, along with the proportion of the population within each tract that falls into various demographic categories. **Table 3-1** describes the ten demographic indicators we use to determine if AQS sites used to monitor ozone precursors are equitably distributed.

To analyze this dataset at the county level, we first calculate the population of each county by summing census tract data. For each county, we then determine the percentage of the population in each demographic category. Next, we rank the counties from lowest to highest percentage of each demographic indicator. This analysis gives the percentile (PCTL) ranking, where a higher PCTL indicates a higher proportion of the population in that demographic category compared to other counties. **Table 3-2** presents values for the 50th, 75th, and 90th PCTLs for the ten indicators used in the analysis. **Figure 3-1** shows county level PCTLs for each of the ten indicators over the CONUS.

Table 3-1: Demographic and health indicators from the US EPA EJScreen used in this analysis¹⁰

Indicator Name	Description
People of Color	Race other than white alone and/or ethnicity as Hispanic/Latino
Low Income Population	Household income is below twice the federal poverty level
Unemployed Population	Did not have a job and made effort to find one
People with Disabilities	Self-reported hearing, vision, cognitive, ambulatory, self-care, and independent living disability
People with Less than High School Education	People aged 25 or older who did not obtain a high school diploma
Limited English-Speaking Households	A household where members aged 14 and above have difficulty communicating in English
People Under Age 5	Population aged less than 5 years old
People Over Age 64	Population aged greater than 64 years old

¹⁰ EJScreen indicators for 2024 use demographic data obtained from the American Community Survey (ACS) from the US Census for 2018-2022 and the geographic framework is based on the 2022 Census TIGER/Line data (US Census, 2022). Low life expectancy data are from the Centers for Disease Control and Prevention (CDC) and the National Center for Health Statistics (NCHS) (NVSS, 2024). Traffic proximity and volume data in EJScreen are from the 2020 Highway Performance Monitoring System (HPMS) dataset of the Department of Transportation (DOT) National Transportation Atlas Database (NTAD) (HPMS, 2020). Traffic closer to a household is given more weight than traffic further from the household, using inverse distance weighting. Traffic proximity and volume are linked with increased exposure to toxic gases and pollutants and increased risk of adverse health outcomes such as asthma, cardiovascular diseases, coronary heart diseases and overall mortality (Health Effects Institute, 2010).

Traffic Proximity and Volume	Average annual daily traffic count at major roads within 10 km, divided by distance in km
Low Life Expectancy	$1 - (\text{Life Expectancy} / \text{Max Life Expectancy})$

Table 3-2: Demographic indicators from the US EPA EJScreen used in this analysis

Field Name	Percentile at County Level		
	50 th	75 th	90 th
Percent People of Color	18%	38%	60%
Percent Low Income Population	33%	40%	48%
Percent Unemployed Population	4%	6%	8%
Percent People with Disabilities	15%	19%	22%
Percent People with Less than High School Education	10%	15%	19%
Percent Limited English-Speaking Households	1%	2%	5%
Percent People Under Age 5	5%	6%	6%
Percent People Over Age 64	19%	22%	25%
Traffic Proximity and Volume	-	-	-
Percent Low Life Expectancy	20%	22%	23%

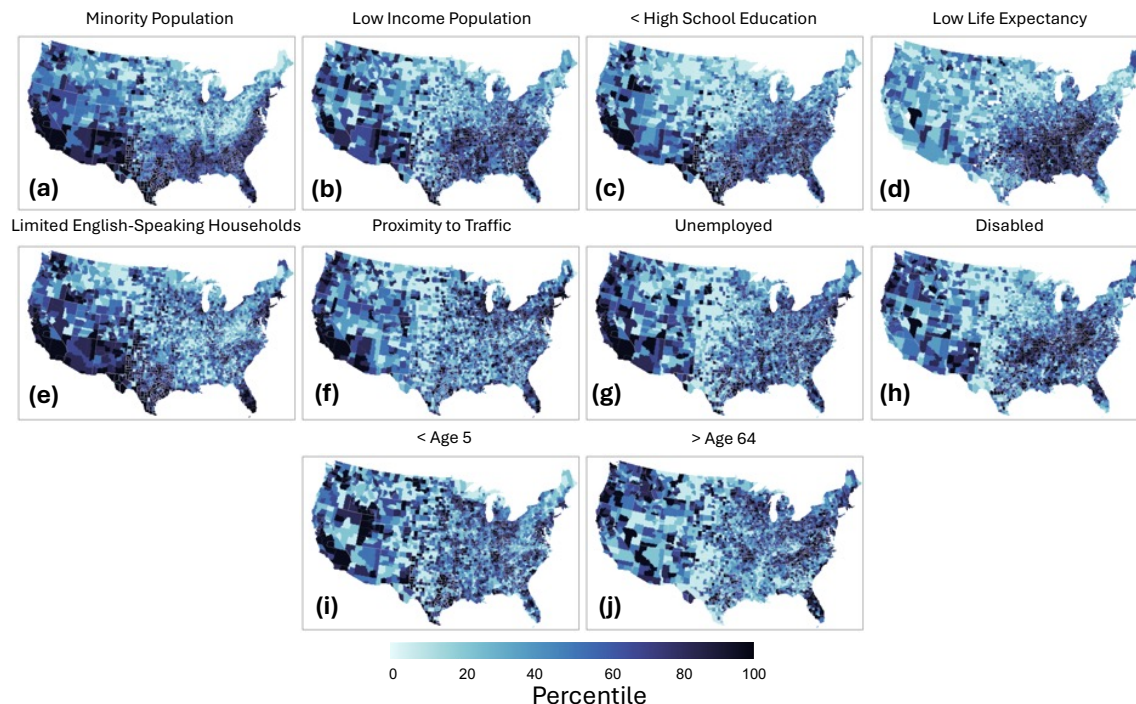


Figure 3-1: County level PCTLs computed across the CONUS for the ten demographic indicators used in this study as defined in Table 1. We show the PCTL distribution of (a) people of color, (b) low income, (c) less than high school education (d) low life expectancy (e) limited English-speaking, (f) proximity to traffic, (g) unemployment rate, (h) disability, (i) age less than 5 and (j) age greater than 64 populations over the CONUS

3.3.2. Ground-based Air Quality Monitoring Sites

Several ground-based measurement networks monitor ozone, NO_2 , and HCHO in the US. As of 2024, NO_2 and ozone stations overlap the most, with 308 stations measuring both quantities (**Figure 3-2**). Station monitoring of HCHO has the least overlap with both ozone (40 stations in common) and NO_2 (35 stations in common). Only 34 sites in the US measure all three species.

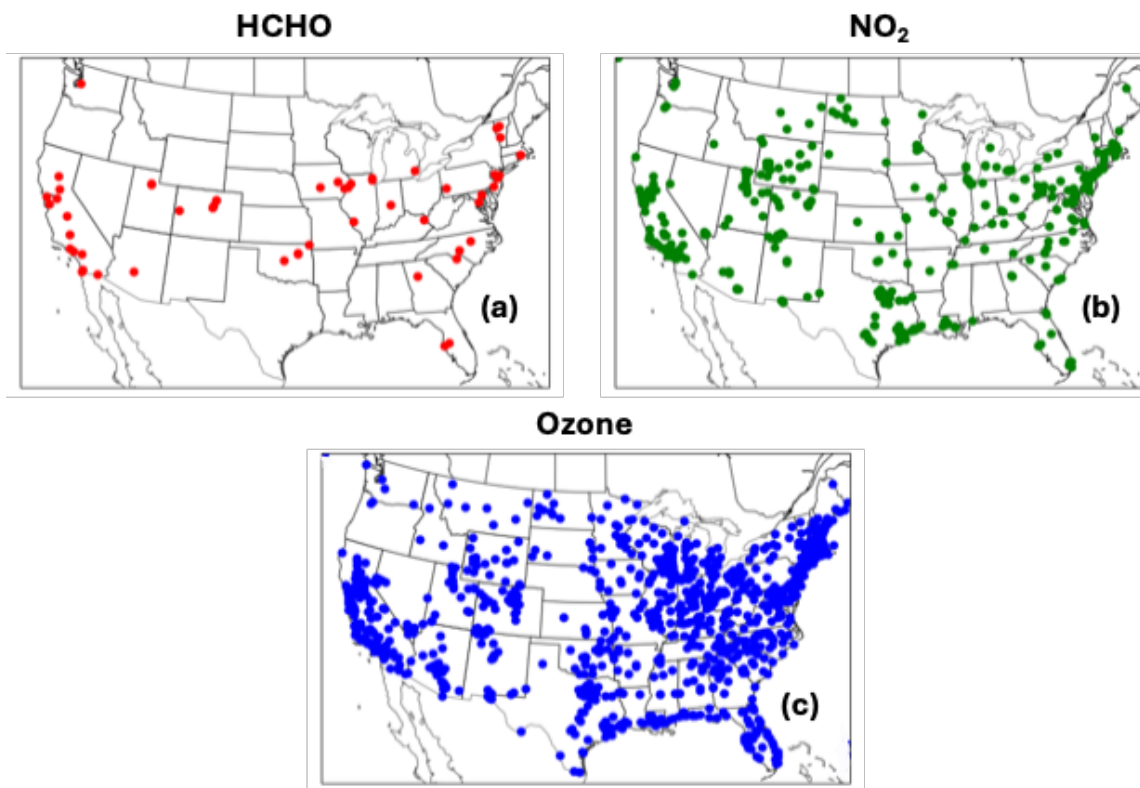


Figure 3-2: Ground-based (AQS) air quality monitoring site locations for (a) HCHO (55 sites), (b) NO₂ (414 sites) and (c) ozone (1095 sites) in 2024.

Monitoring of NO₂ and ozone is conducted using State and Local Air Monitoring Stations (SLAMS), which are distributed according to population and ozone design values, and are therefore primarily located in urban areas (US EPA, 2016, 2014b, 2013). Within SLAMS, monitoring is accomplished using either a National Core (Ncore) station or a Photochemical Assessment Monitoring Stations (PAMS) sampler (US EPA, 2021b, 2019c). Each state is required to have at least one Ncore Station, with ozone monitoring needed throughout the year (LII, 2025). Additionally, if the population of the Ncore Core Based Statistical Area (CBSA) exceeds 1 million people, the site is required to have a PAMS sampler (LII, 2025). PAMS samplers, which usually measure HCHO, are needed to monitor ozone for a minimum of June, July and August (LII, 2025). The concentration of

NO₂ must also be measured at near-road sites if the Metropolitan Statistical Area (MSA) has a population greater than 1 million (US EPA, 2020d). Additional near-road sites are required as the population increases or road traffic volume increases. The concentration of surface ozone is also measured at Clean Air Status and Trends Network (CASTNET) locations, which cover rural areas and provide broader geographic coverage (US EPA, 2015b). In addition to PAMS, HCHO is also measured through the Interagency Monitoring of Protected Visual Environments (IMPROVE) and National Air Toxics Trends Stations (NATTS) (IMPROVE, 2025; US EPA, 2020e).

3.3.3. TEMPO Satellite Data Description

Satellite retrievals of NO₂ and HCHO are obtained from the Tropospheric Emissions: Monitoring Pollution (TEMPO) instrument aboard the Intelsat satellite, a geostationary satellite over North America launched in April 2023 (<https://tempo.si.edu>). During daylight hours, TEMPO samples a given location every 40 to 60 minutes at a spatial resolution of 2.0 km N/S × 4.75 km E/W. Our study uses hourly tropospheric column NO₂ and total column HCHO data obtained during July 2024. We use the version VO3Beta NASA/SAO L2 product for both species. The NO₂ retrieval is in the 405-465 nm spectral window, while HCHO retrieval is in the 328.5-356.5 nm fitting window (TEMPO User Guide). Using a nearest neighbor resampling method, the satellite products are gridded and averaged to the US county domain. The satellite data used in this study, along with the applied filters, are presented in

Table 3-3. Mild striping affects the NO₂ retrieval in the N-S direction, which has yet to be addressed in the data version used for this analysis (TEMPO User Guide).

Table 3-3: TEMPO satellite data description¹¹

	File Name	Author	Long Name	Version	Filters
TEMPO NO ₂	TEMPO_ NO2_L2	SAO	Nitrogen dioxide tropospheric and stratospheric vertical columns	V03	Main Data Quality Flag = 0 CF < 0.4
TEMPO HCHO	TEMPO_ HCHO_L2	SAO	Formaldehyde vertical columns	V03	Main Data Quality Flag = 0 CF < 0.4

3.4. Results and Discussions

3.4.1. Current Measurement Distribution

Here we examine the distribution of AQS stations within the CONUS for counties exceeding the 90th PCTL for each of the 10 demographic and health indicators. **Figure 3-3** shows the status of AQS site coverage (e.g. no AQS site, only ozone measured, etc.) for each respective demographic indicator category in 2024. Overall, AQS monitoring was not conducted in many counties with high values of demographic or health indicators. Surface ozone is the most extensively measured quantity, followed by NO₂. AQS sites are most

¹¹ SAO: Smithsonian Astrophysical Observatory

common in counties with high traffic. This distribution is likely due to vehicular exhaust pollution being one of the leading sources of NO_x and VOCs. The surface measurement coverage for HCHO is lacking in every demographic and health category, including those in high-traffic proximity. Most importantly, HCHO is severely under monitored in counties exceeding the 90th PCTL of the “most low-income” and “disabled population” indicators.

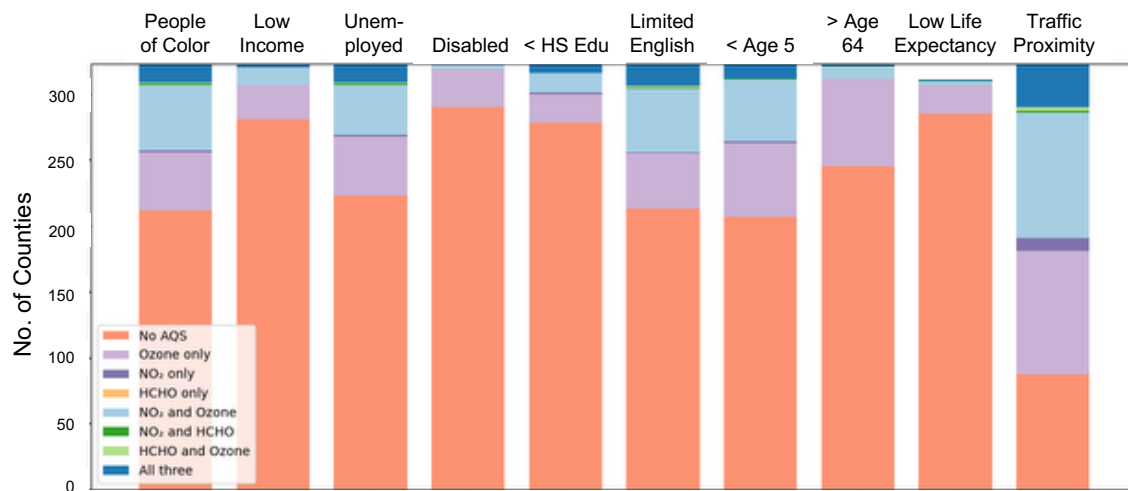


Figure 3-3: Counties within the CONUS (out of 3226 counties) exceeding the 90th PCTL for each of the ten indicators considered in this study, stratified by AQS monitoring extent as indicated in the legend. Note: The number of counties in the low life expectancy category is smaller than in other categories due to incomplete data coverage for this indicator in certain counties.

Figure 3-4 illustrates the percentage of counties missing AQS sites as a function of PCTL thresholds for the ten indicators presented in Figure 3-1. Figure 3-4 shows the contrast in access to AQS measurements, based on the demographic and health indicators. For example, in Figure 3-4(a), the percentage of counties with missing AQS data increases for counties with higher percentages of residents who have low incomes, low life expectancies, high disability rates, and are without high school education. Near-surface air quality is underreported in counties with populations characterized by individuals who

have lower life expectancies, lower incomes, lower education levels, and higher disability rates. An exception to this tendency is observed for people who live in areas of high traffic proximity. As seen in Figure 3-4(c), AQS site location selection has historically been dependent upon regions with a high volume of traffic, that is, near-road monitors.

Figure 3-4(b) illustrates the absence of AQS measurements for the remaining indicators considered in this study: people of color, unemployed, limited English speaking, and age extremes (notes the small range of scale in Figure 3-4b). Communities with higher percentages of these four indicators tend to overlap with those of the traffic proximity indicator, as these indicators tend to be high for populations residing in urban centers with high traffic volumes. Due to this geographic factor, the populations associated with the indicators shown in Figure 3-4(b) tend to have more equitable access to AQS sites than populations with high values of the indicators featured in Figure 3-4(a).

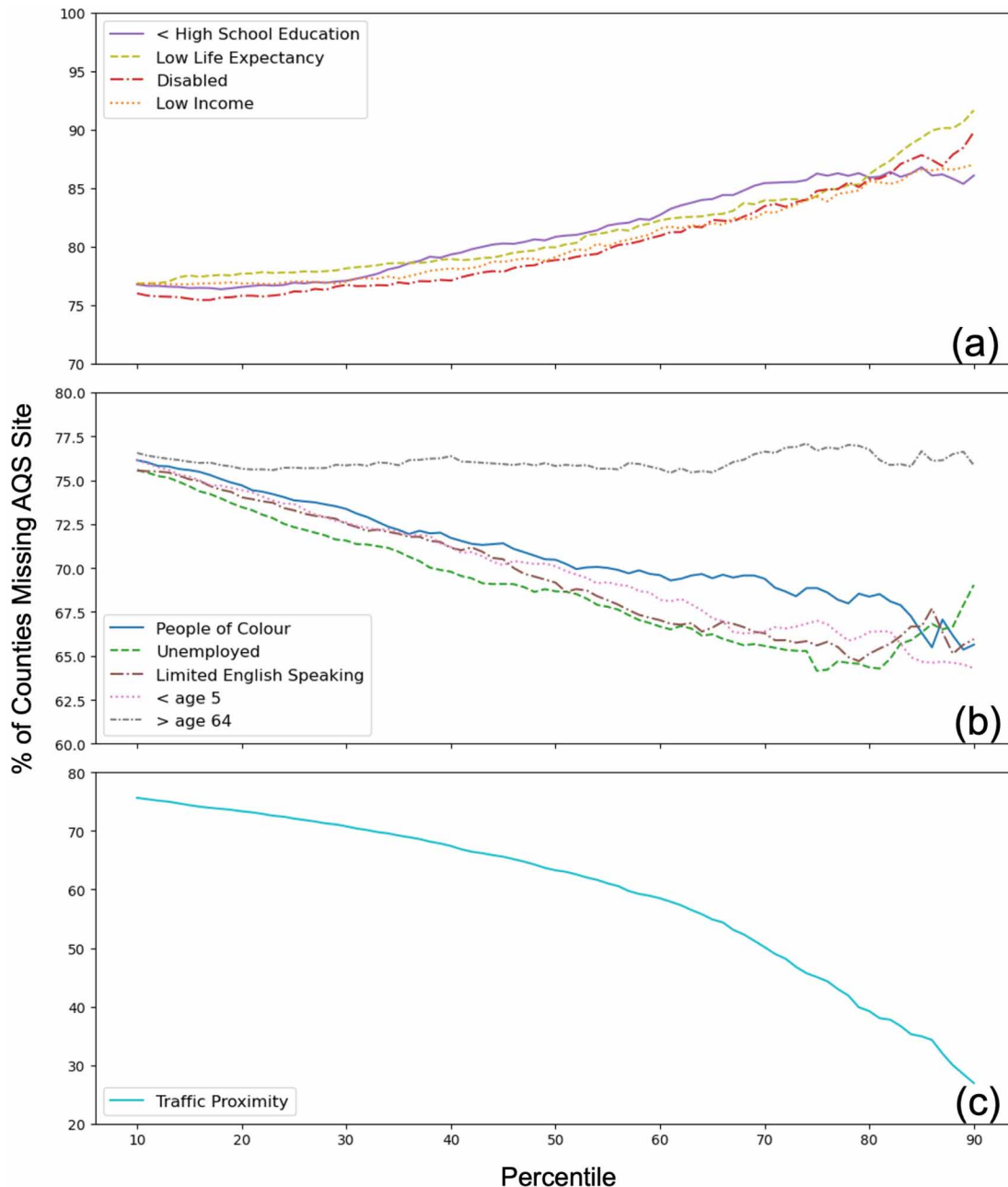


Figure 3-4: Percentage of counties within the CONUS in 2024 that lacked access to AQS sites, evaluated across the ten demographic and health indicators used in this study. The figure presents results from the 10th to 90th PCTLs for each category. The categories are indicated in each panel's respective legend, stratified into panels based on percentages of counties missing AQS for interpretability. Panel (a) shows indicators where access to AQS sites decreases as counties become more disadvantaged. Panel (b) includes indicators where access either slightly increases or remains relatively unchanged across PCTLs. Panel (c) highlights traffic proximity, where access to AQS sites tends to increase as traffic proximity rises.

3.4.2. Introduction of the Integrated AQS Placement Index (I_{IAP})

We develop an index for prioritizing future AQS sensor placement based on air pollution patterns, demographic indicators, and population density. We define the Integrated AQS Placement Index as:

$$I_{IAP} = DM_N \times HCHO_N \text{ or } NO2_N \times POP_N \quad \textbf{Equation 3-1}$$

where DM_N is the ‘normalized demographic overlap’, $HCHO_N$ or $NO2_N$ is the normalized column value distribution of HCHO or NO_2 measured by TEMPO, and POP_N is the normalized population density. Equal weighting was chosen to provide a balanced approach that stakeholders can modify based on their specific priorities. The variables are normalized using min-max scaling, defined as:

$$X_N = \frac{X - X_{min}}{X_{max} - X_{min}} \quad \textbf{Equation 3-2}$$

Where X is the variable (demographic overlap, species distribution or population density). Min-max scaling is applied to ensure the three variables have a similar numerical range and weighting. In this section, we first describe these three variables and then use this index to identify the counties that could most benefit from future air quality monitoring.

3.4.2.1. First Variable: Demographic Overlap (DM_N)

Using the EJScreen indicators from Table 3-1, we first identify counties that are at or above the 75th PCTL for each indicator. We then aggregate the number of indicators that

exceed this threshold per county and plot these county-level values on a CONUS map (Figure 3-5). The variable shown in Figure 3-5 allows us to identify counties with greater cumulative air-quality inequalities. Depending on the available resources, counties with higher overlap should be prioritized for AQS monitoring due to enhanced intersections of vulnerability. For example, a county colored dark green corresponding to the number 4 indicates that 4 out of 10 variables are exceeding the 75th PCTL in that county.

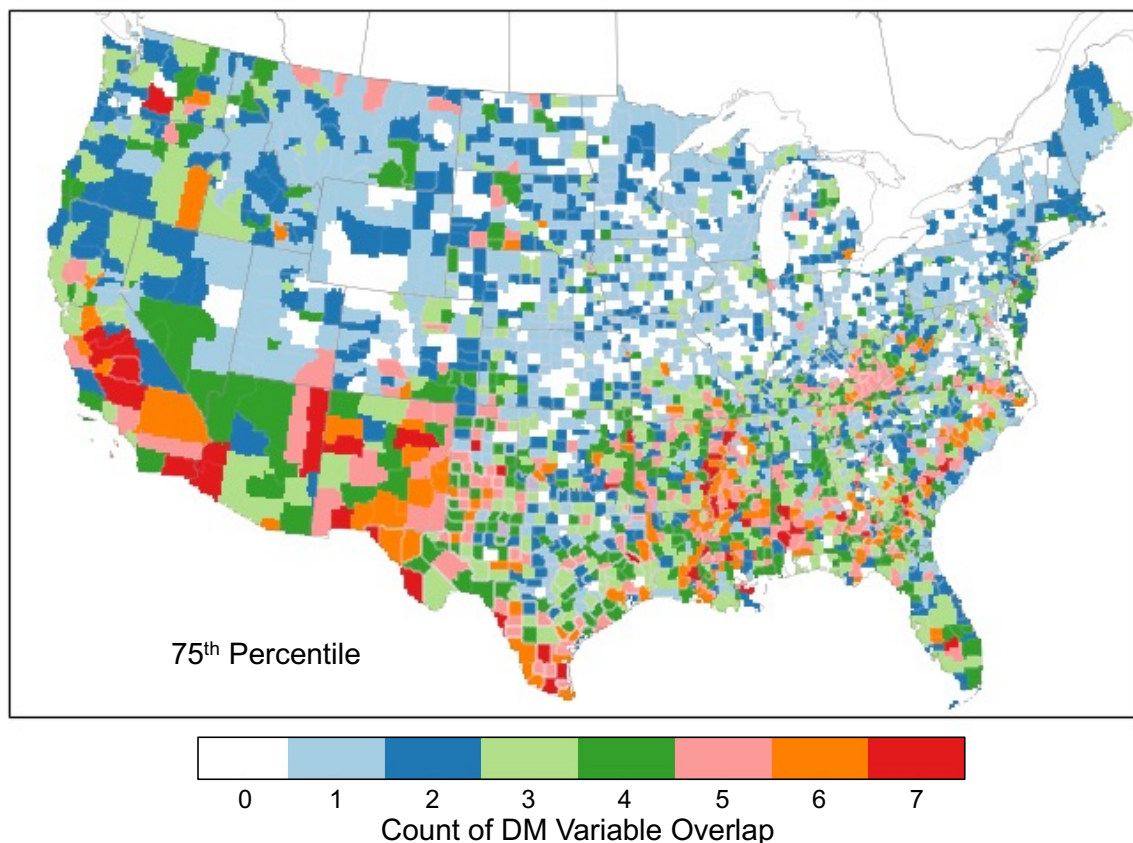


Figure 3-5: Demographic overlap per county for 2024 as indicated by the color bar. Higher magnitude values indicate greater cumulative vulnerability. For example, a county with a value of 4 exceeds the 75th PCTL in 4 of 10 indicators.

Several distinct geographic clusters emerge from this analysis, including hotspots along the Mississippi River corridor (encompassing portions of Louisiana’s “Cancer Alley”),

California’s Central Valley, Appalachian counties extending across multiple states, counties throughout the southeastern United States (particularly in Georgia, South Carolina, and North Carolina), Apache County in Arizona where the Navajo Nation is located, and border counties in Texas and New Mexico adjacent to Mexico.

The overlap of demographic indicators depends on the chosen PCTL threshold. We selected the 75th PCTL based on the sensitivity analysis shown in **Figure 3-6** and **Table 3-4**. The 75th PCTL represents a sufficiently high threshold that limits the number of counties that are omitted, ensuring the resulting DM_N metric spans a wide portion vulnerable counties in the US. We use the min-max normalized values (Equation 3-2) of the data shown in Figure 4 in our I_{IAP} calculation.

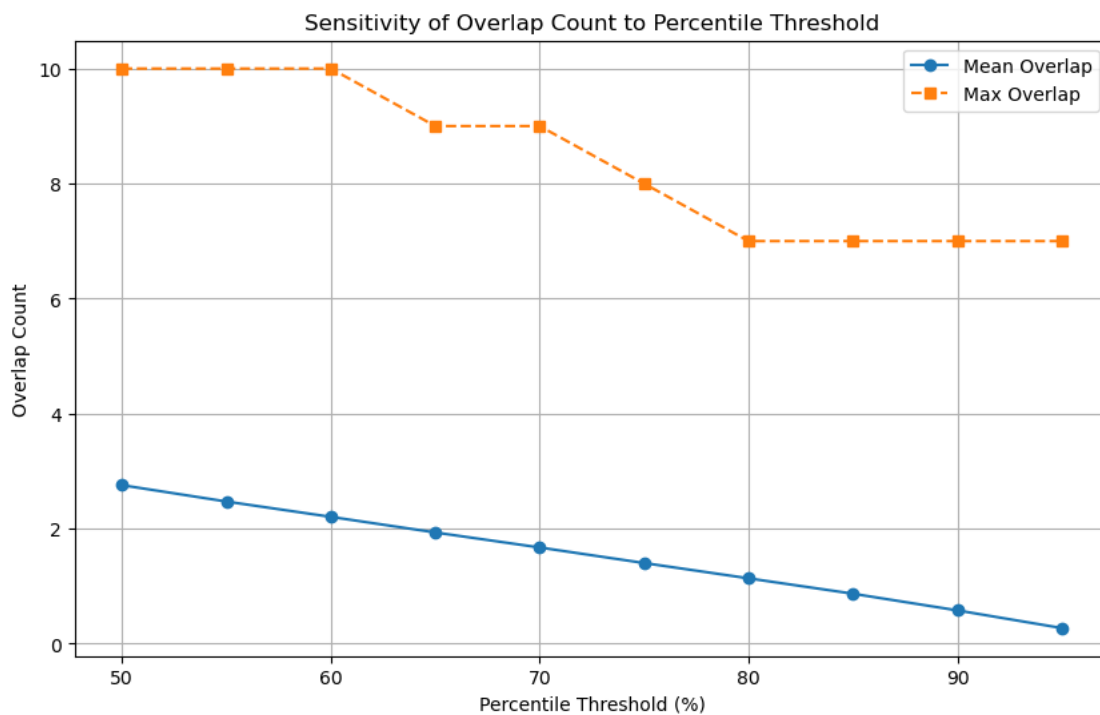


Figure 3-6: Variation of demographic overlap count by PCTL threshold

Table 3-4: Statistics of the variation of overlap count by PCTL threshold.

Percentile	Mean Overlap	Max Overlap	Min Overlap	Std Dev
50	2.75	10	0	2.95
55	2.47	10	0	2.73
60	2.20	10	0	2.52
65	1.93	9	0	2.3
70	1.67	9	0	2.09
75	1.40	8	0	1.88
80	1.13	7	0	1.65
85	0.86	7	0	1.42
90	0.57	7	0	1.14
95	0.27	7	0	0.72

3.4.2.2. Second Variable: Distribution of HCHO and NO₂ (HCHO_N or NO_{2N})

Column values of NO₂ and HCHO exhibit seasonal variations. However, since many AQS sites are mandated to measure ozone only during the so-called ozone season (April to September) and the ozone design values for attainment of the ozone standard are also calculated during these months, we take data collected in July 2024 as an indicator of the entire ozone season. **Figure 3-7(a)** shows TEMPO NO₂, averaged for July 2024. These NO₂ columns tend to be highest in cities and urban areas – enhanced NO₂ occurs near high temperature combustion processes. Figure 3-7(b) shows TEMPO satellite observations of tropospheric column HCHO, again for July 2024. Column HCHO peaks in the southeast US due to biogenic isoprene sources from broadleaf trees, such as oaks. The Missouri Ozarks, along with much of the southeast US, have a high density of deciduous trees (due

to the warm temperatures and high moisture levels) that are efficient emitters of isoprene, leading to the formation of the so-called “isoprene volcano” (Kaiser et al., 2018; Palmer et al., 2006, 2003; Wiedinmyer et al., 2005). Since atmospheric oxidation of VOCs leads to the formation of RO_2 , HO_2 , and HCHO , the influx of isoprene causes elevated HCHO in this region. Elevated HCHO is also present in the agriculturally active region of California, due to biogenic emission of VOCs (Wang et al., 2022). **Table 3-5** shows statistics on the difference in NO_2 and HCHO between the urban and rural areas.

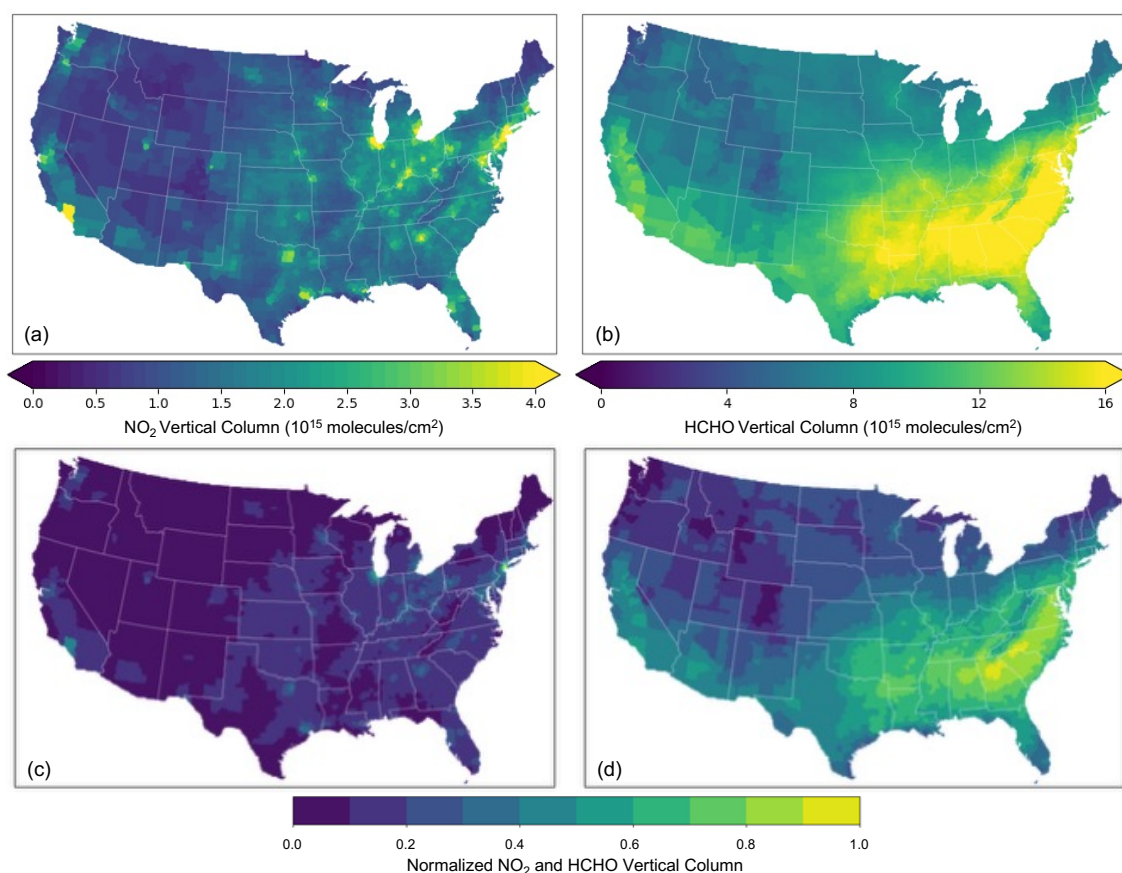


Figure 3-7: July 2024 average values from TEMPO Level 2 data, filtered and regridded to the county level for (a) tropospheric column NO_2 and (b) total column HCHO . Panels (c) and (d) show the corresponding normalized vertical column values using Equation 3-2 for NO_2 and HCHO , respectively (HCHO_N or NO_2N).

To represent NO₂ and HCHO on a uniform scale, we normalize them using min-max normalization, depicted in Figure 3-7(e) and Figure 3-7(d). We use the normalized distributions of NO₂ and HCHO, so that potential new AQS sites identified using our proposed index would be located in regions with high concentrations of these species, which are indicative of potentially harmful health impacts.

Table 3-5: NO₂ and HCHO from TEMPO observations over urban and rural areas of the CONUS¹²

Variable	Urban Mean	Urban Median	Urban Std. Dev.	Rural Mean	Rural Median	Rural Std. Dev
HCHO (molecules/cm ²)	12.59	12.25	4.80	8.49	7.65	3.83
NO₂ (molecules/cm ²)	3.93	3.42	2.62	1.08	0.92	0.74

3.4.2.3. Third Variable: Population Density (POP_N)

Figure 3-8(a) shows the population density for each county in the CONUS. **Figure 3-8(b)** is the normalized population density calculated using Equation 3-2. The distribution of population density is shown on a logarithmic scale, as there is substantial variation across the US. The eastern US tends to have small geographically sized counties with large populations, while the Midwest has larger counties with smaller populations. For the

¹² We define urban as the 36 km² grid around the top 30 densely populated metropolitan statistical areas and rural as the rest of the grid cells in CONUS

placement of AQS sites, we consider population density to ensure that new sites benefit as many people as possible. **Figure 3-9** shows the population and area of each county over the CONUS.

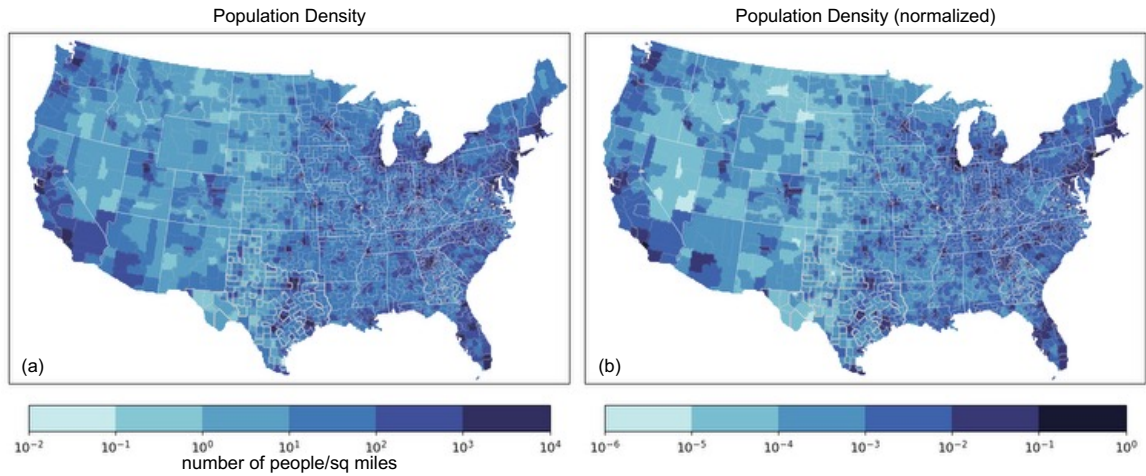


Figure 3-8: (a) Population density and (b) normalized population density distribution (POP_N) using Equation 3-2 across counties in the CONUS. Population density is calculated as the total population of each county divided by its area (square miles). The data is presented on a logarithmic scale to account for the wide variation in density.

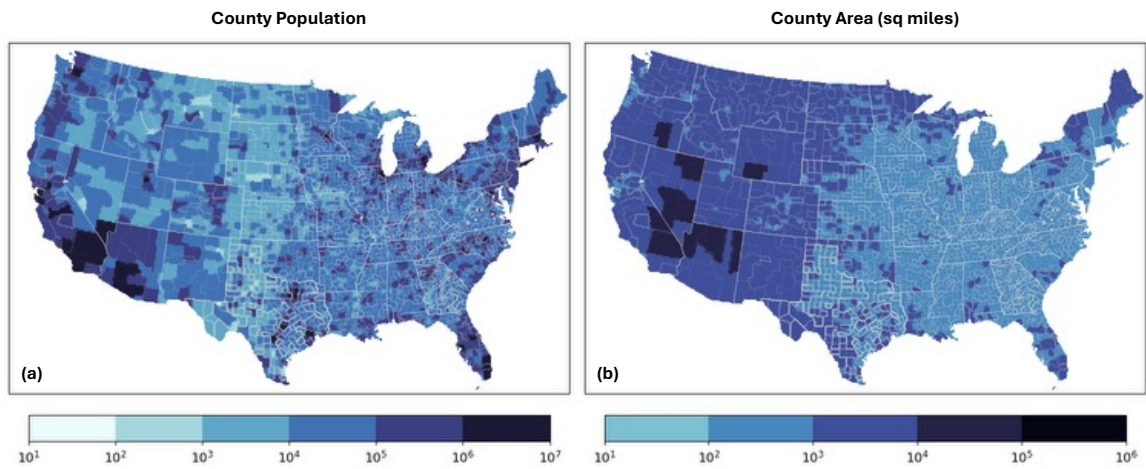


Figure 3-9: (a) County population and (b) county area (in square miles) distribution across the CONUS. The data is presented on a logarithmic scale

3.4.2.4. Integrated AQS Placement Index (I_{IAP})

We now demonstrate how the Integrated AQS Placement Index (I_{IAP}) is used to identify high-priority placements for new AQS sites. **Figure 3-10(a)** and **(b)** show I_{IAP} for NO_2 and HCHO, respectively, excluding counties that already have AQS sites. The southeast, northeast I-95 corridor (e.g., Washington, D.C., to Boston, MA) and western US have higher I_{IAP} compared to the rest of the CONUS. Therefore, these areas may require additional AQS site measurements for both HCHO and NO_2 . Based on the I_{IAP} values, we identified the 30 counties that would most benefit from additional AQS sites for public health concerns (**Figure 3-10(c)** and **Figure 3-10(d)**). In **Figure 3-10(e)** and **Figure 3-10(f)**, we show the county with the highest I_{IAP} within each state.

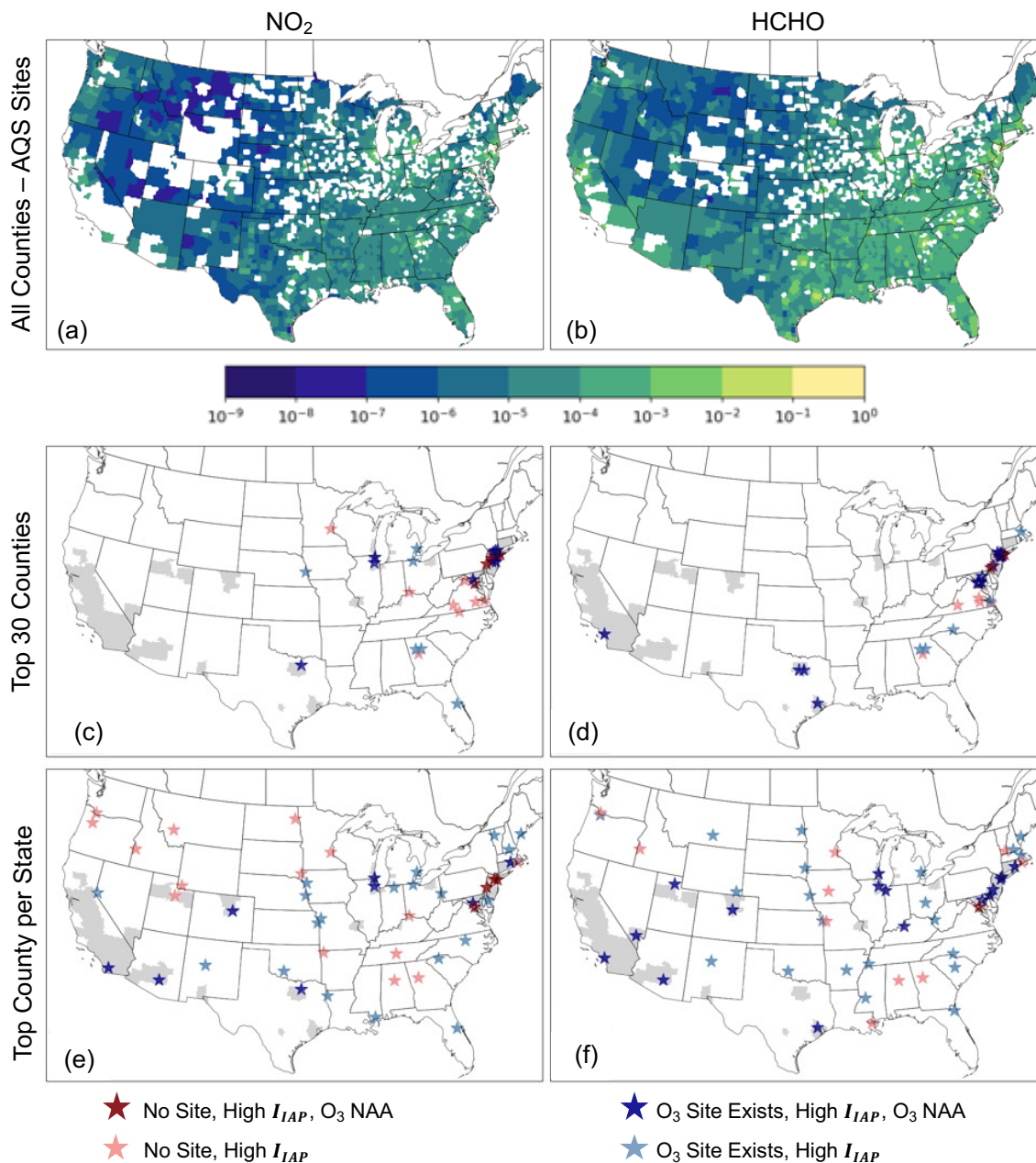


Figure 3-10: Panels (a) and (b) illustrate the I_{IAP} for NO_2 and HCHO , respectively, excluding counties that already host AQS sites. Panels (c) and (d) identify the top 30 counties from (a) and (b) that should be prioritized for new AQS site placement for NO_2 and HCHO , respectively, based on I_{IAP} . Panels (e) and (f) identify the top county per state from (a) and (b) that should be prioritized for new AQS site placement for NO_2 and HCHO , respectively, based on I_{IAP} . Star markers indicate proposed site categories, differentiated by color. Dark red stars represent counties that are not in attainment of the NAAQS for ozone (O_3), have a high I_{IAP} , and lack existing AQS infrastructure. Pink stars mark counties that are in attainment of O_3 standards, also have a high I_{IAP} , and similarly lack AQS infrastructure. Dark blue stars represent counties that are not in attainment, have a high I_{IAP} , and already have existing AQS infrastructure. Light blue stars indicate counties that

are in attainment, have a high I_{IAP} , and possess existing AQS infrastructure. Grey shaded regions represent areas in non-attainment of the 8-hour ozone standard.

The identified sites for new measurements, marked by stars in Figure 3-10(c), Figure 3-10(d), Figure 3-10(e), and Figure 3-10(f), can be grouped into four distinct categories based on their ozone attainment status and the presence of existing monitoring infrastructure. Category one includes the dark red stars, which represent counties currently designated as ozone non-attainment areas with high I_{IAP} values and are presently lacking AQS monitoring of ozone. These counties also lack monitoring of NO_2 and HCHO, indicating that these counties should be prioritized for the establishment of new monitoring sites. Category two consists of pink stars, which indicate counties with high I_{IAP} values and no existing AQS infrastructure of any kind. The dark blue stars represent counties that are in ozone non-attainment, have high I_{IAP} values, and already monitor ozone. We suggest these counties would benefit from the addition of NO_2 or HCHO monitoring, since the necessary infrastructure for obtaining pollution measurements is already in place. These sites present an opportunity for relatively low-effort expansion, with the potential for a high impact on understanding pollution sources and advancing progress toward attainment. The light blue stars represent the final category, which identifies counties with high I_{IAP} values that currently monitor ozone and could be further enhanced by adding measurements for the other two pollutants. The equal weighting scheme shows good agreement with existing non-attainment areas, validating this methodological approach (**Figure 3-11**).

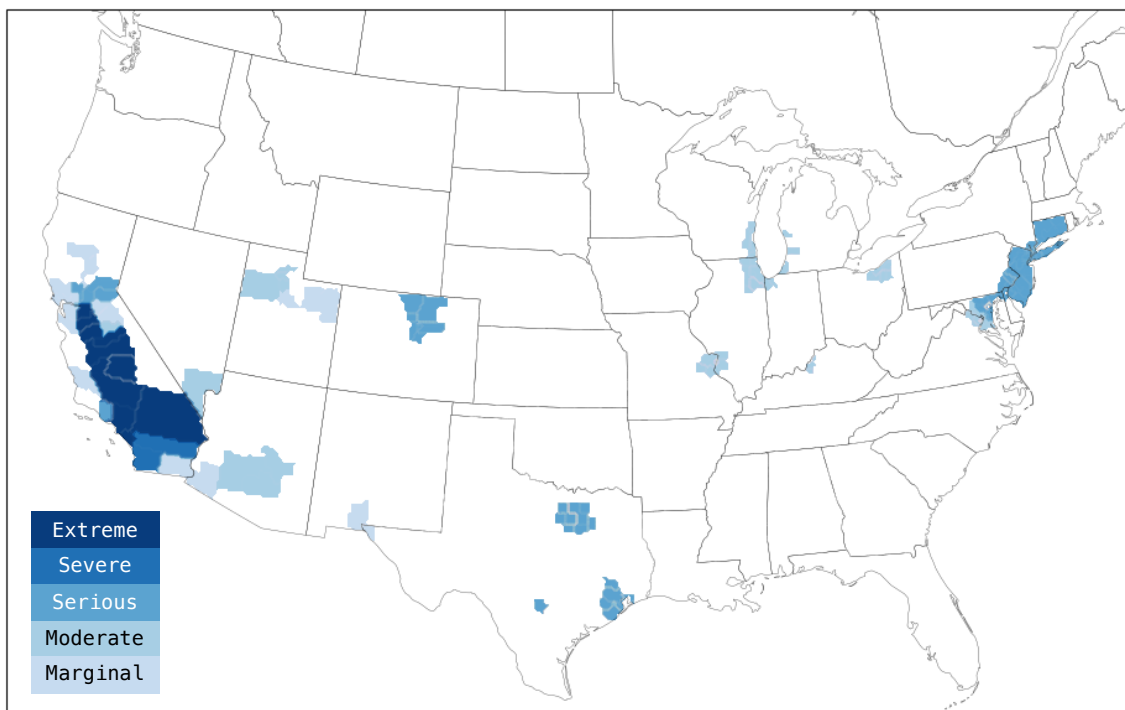


Figure 3-11: 8-hour ozone non-attainment areas in 2024 according to the 2015 ozone standard (US EPA, 2024b)

We conducted a sensitivity analysis of I_{IAP} to TEMPO satellite retrieval uncertainties of NO_2 and HCHO column values. The analysis shows strong ranking stability due to min-max normalization with detailed results in **Figure 3-12**, **Figure 3-13**, **Figure 3-14** and **Table 3-6**.

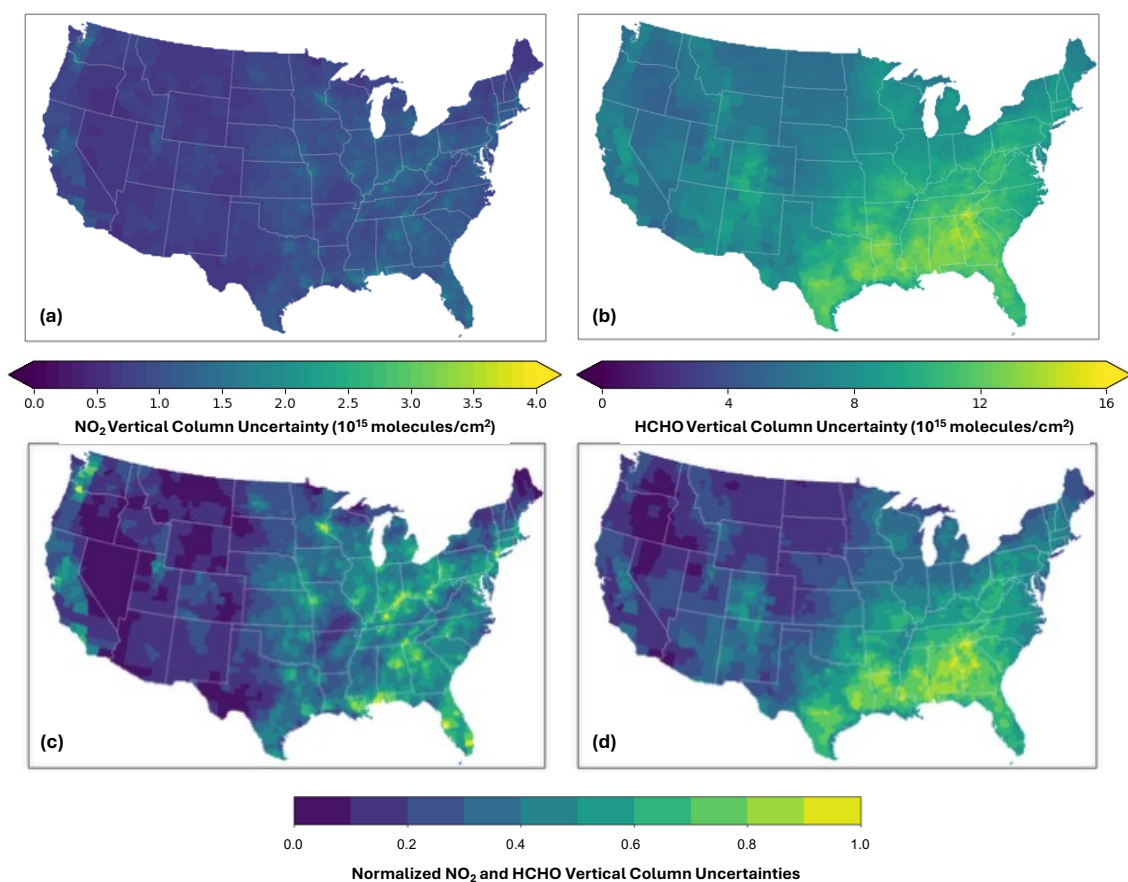


Figure 3-12: July 2024 average values from TEMPO Level 2 data, filtered and regridded to the county level for (a) tropospheric column NO₂ uncertainty and (b) total column HCHO uncertainty. Panels (c) and (d) show the corresponding normalized vertical column uncertainty values using Equation 3-2 for NO₂ and HCHO, respectively.

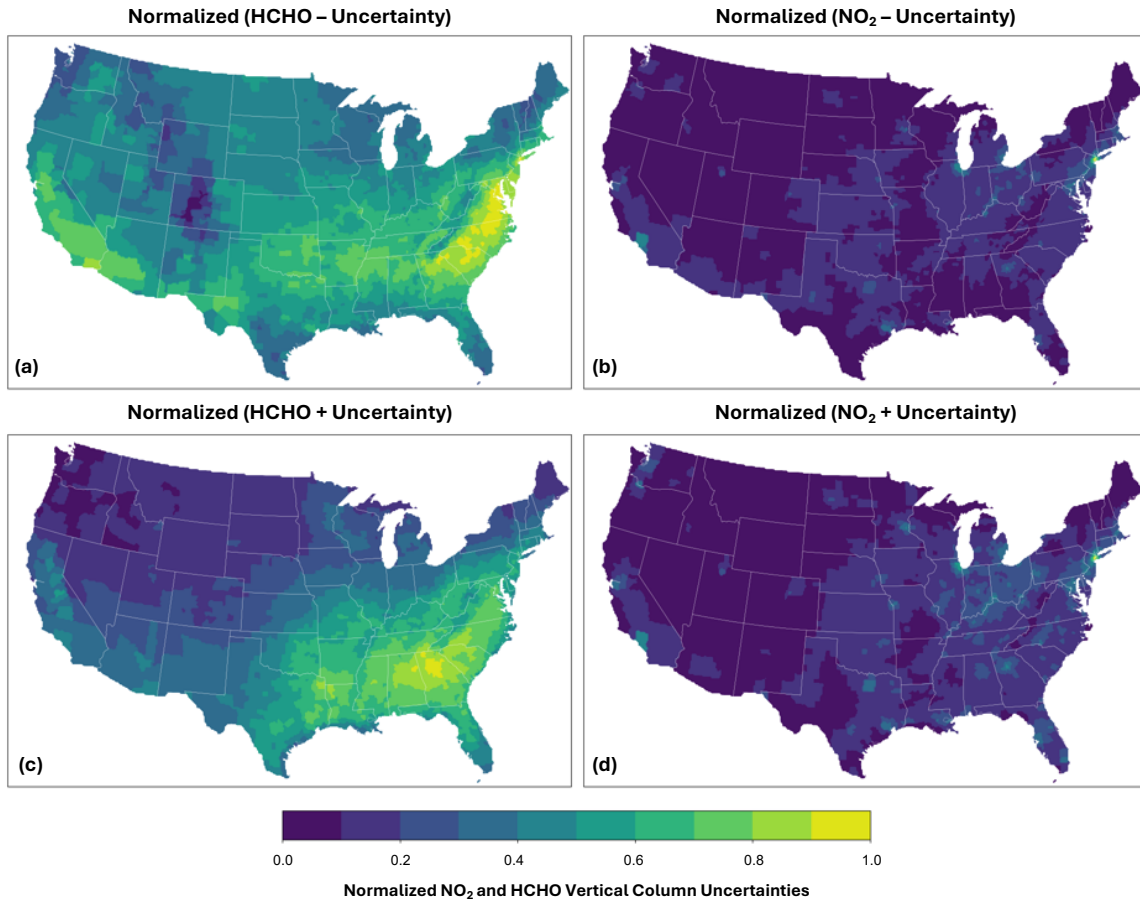


Figure 3-13: July 2024 average values from TEMPO Level 2 data, filtered and regridded to the county level for (a) HCHO column values minus uncertainties (HCHO-UC), (b) NO₂ column values minus uncertainties (NO₂-UC), (c) HCHO column values plus uncertainties (HCHO+UC), and (d) NO₂ column values plus uncertainties (NO₂+UC). Panels show the normalized column values using Equation 3-2.

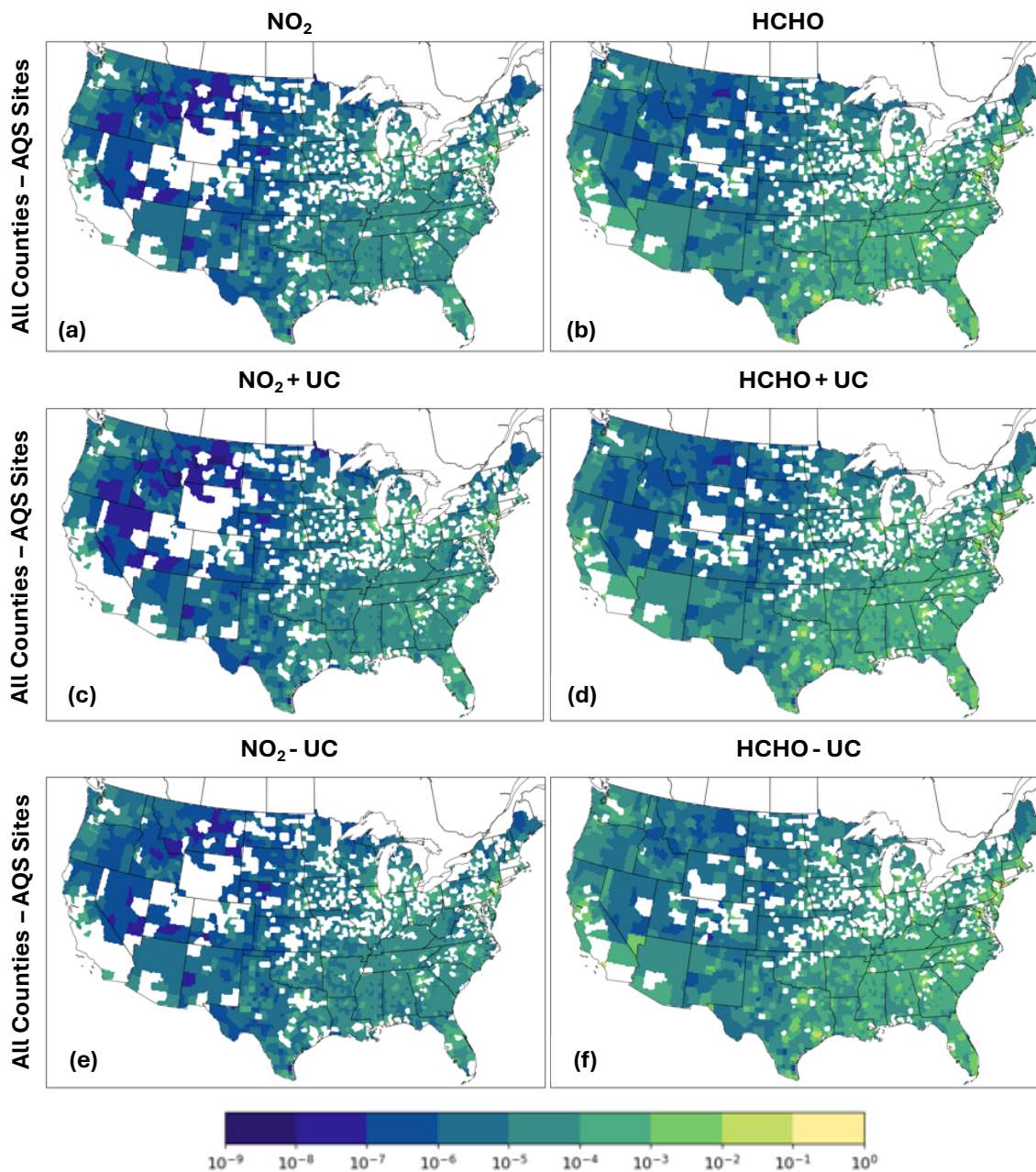


Figure 3-14: Panels (a) and (b) illustrate the I_{AP} for NO_2 and HCHO , respectively, excluding counties that already host AQS sites. Panels (c) and (d) show I_{AP} calculated using column values plus uncertainties ($\text{NO}_2 + \text{UC}$ and $\text{HCHO} + \text{UC}$), and panels (e) and (f) show I_{AP} calculated using column values minus uncertainties ($\text{NO}_2 - \text{UC}$ and $\text{HCHO} - \text{UC}$), all excluding counties with existing AQS sites.

Table 3-6: Sensitivity analysis of I_{IAP} rankings to TEMPO retrieval uncertainties. Values indicate the number of counties that retained their original ranking when I_{IAP} was recalculated using uncertainty perturbed column values¹³

Category	NO ₂ +UC	NO ₂ -UC	HCHO+UC	HCHO-UC
Top 30 Counties	29/30	30/30	29/30	28/30
Top County per State	46/48	46/48	45/48	43/48

3.5. *Conclusions and Future Perspectives*

AQS data are vital for assessing the impacts of pollutants on health and for evaluating satellite-based observations and air quality models. We suggest that current coverage of surface air quality monitors could be expanded and distributed more effectively and equitably. We rank communities based on the need for AQS monitors, using demographic indicators, satellite observations and population. While the US EPA has established the NAAQS for six criteria pollutants, including ozone, surface sites often lack measurements of ozone precursors HCHO and NO₂ (US EPA, 2014a, 2015b, 2020a). We identify

¹³ Top 30 replacements due to uncertainty

NO₂+UC: State 13, County 59 replaced State 34, County 25

HCHO+UC: State 13, County 121 replaced State 42, County 45

HCHO-UC: State 27, County 123 replaced State 13, County 67

State 51, County 700 replaced State 48, County 439

Top county per state replacements due to uncertainty

NO₂+UC: State 9: County 13 replaced County 15

State 47: County 125 replaced County 149

NO₂-UC: State 9: County 5 replaced County 15

State 28: County 33 replaced County 47

HCHO+UC: State 4: County 19 replaced County 21

State 9: County 9 replaced County 11

State 30: County 93 replaced County 111

HCHO-UC: State 9: County 7 replaced County 11

State 30: County 93 replaced County 111

State 36: County 47 replaced County 5

State 39: County 35 replaced County 49

State 54: County 69 replaced County 11

underserved counties (counties that lack AQS monitoring), many of which are in the southeastern and southern U.S. (notably in the “isoprene volcano” region) and we also see a cluster of sites along the I-95 corridor in the northeastern US. In these regions, data from AQS sites can support health studies and enhance data coverage.

While TEMPO satellite observations provide extensive spatial coverage and hourly temporal resolution, it should be supplemented with aircraft and ground-based observations for critical policy decisions, such as identifying ozone production regimes to guide mitigation strategies. Significant discrepancies have been observed between ozone production regimes inferred from tropospheric column content measured with remote sensing and those within the planetary boundary layer in urban areas (Singh et al., 2025a; Souri et al., 2023). Relying solely on satellite derived ozone production regimes can lead to incorrect policy decisions and exacerbate surface ozone levels. Therefore, despite the advantages of satellite data in terms of coverage, ground-based AQS sites remain a critical source of near-surface ozone measurements.

We identify underserved counties based on three essential criteria: (1) population density, (2) demographics and (3) satellite-observed HCHO and NO₂ tropospheric column values. This method ensures that the recommended AQS locations will serve a large population of underserved communities that live in high-pollution areas, so that there is an efficient use of limited financial resources on air pollution monitoring. We highlight counties that have existing AQS infrastructure, are in non-attainment areas, and would

benefit from the monitoring of additional species as a cost-effective method for expanding AQS coverage.

It is possible that the current ozone standards will eventually be lowered from the current level of 70 ppb to 55-60 ppb as has been recommended by the US EPA's Clean Air Scientific Advisory Committee (CASAC) based on scientific evidence about the adverse effects of ozone exposure to human health (US EPA, 2023c). If so, it will be imperative for states to have comprehensive monitoring of ozone precursors to understand how best to attain this future ozone standard. With increasing temperatures, ozone concentrations may rise even if emissions are held constant, a phenomenon known as the 'climate penalty' (Lu et al., 2019). Identifying how surface ozone as well as ozone precursors fluctuate throughout the day using data from additional monitoring sites will be crucial for guiding effective air quality attainment policy decisions. Our current methodology focuses on photochemical production of ozone in the summer. In the future, we plan to extend our work to incorporate winter satellite observations to address seasonality in ozone chemistry.

One of the major advantages of the I_{IAP} methodology is its flexibility and ease of implementation. Additional variables can be incorporated or removed as appropriate, and the analysis can be conducted at finer spatial resolutions, such as the census tract level within individual states. For example, if a state wishes to prioritize AQS site placement based on neighborhood-level childhood asthma rates, such criteria can be readily integrated into this framework. While demonstrated here using TEMPO data over North America, the I_{IAP} methodology can be applied globally using other geostationary satellites such as

GEMS over East Asia and Sentinel-4 over Europe and northern Africa, which provide similar high-resolution NO₂ and HCHO observations, with locally available demographic indicators and population datasets substituted as appropriate

Comparing Figure 3-2, Figure 3-5 and Figure 3-10, we can use our index to identify areas that are in non-attainment of the ozone standard and are currently not monitored. Many new recommended sites are concentrated around the I-95 corridor, which is heavily driven by high populations in small counties (see Figure 3-10). In contrast, there are many large counties in California that have a monitor within the county but would benefit from a higher density of monitors as the region still suffers from non-attainment. For these regions, we suggest this analysis be performed at a sub-county level. If we look at the top 30 counties nationwide (Figure 3-10(c) and Figure 3-10(d)), the I_{IAP} methodology for choosing new sites does not identify the need for additional monitors in several states currently in non-attainment of the ozone standard, namely Connecticut, Arizona, Utah, and Indiana, due to their (1) low population density and (2) low demographic overlap at a county-level. These states would still benefit from additional ground-based observations from a purely air quality standpoint, especially with the potential of a stricter ozone standard being implemented in the future. If we apply our methodology on a state-by-state basis, as shown in Figure 3-10(e) and Figure 3-10(f), then we find that many of these counties, that were not selected for monitoring previously, are now identified. This change in recommended site locations highlights the utility of our methodology, which enables site selection at the county (sub-county), state, or national scale. In future work, we plan to

prioritize site selection based on proximity to existing sites rather than limiting it by county boundaries.

Proactive policy is critical for addressing underlying disparities and preventing disproportionate impacts on communities that are more susceptible to environmental and health risks. Such policies ensure that resources, such as AQS monitoring, are equitably distributed to protect those who are most at risk. By prioritizing preventative measures, policymakers can promote health equity, empower affected populations, and foster resilience against environmental challenges, helping to close gaps in environmental burdens and benefits while making the most effective use of limited resources.

4. Long-term Trends in Surface Ozone: A Comparison of Air Quality Model Simulations and Surface Observations from 2003 to 2019 over the Contiguous US (Singh et al., *in prep*)

4.1. Introduction

Tropospheric ozone remains a challenge for policymakers and scientists across the United States, despite decades of emission control efforts. The EPA's NAAQS ozone standard, based on the Maximum Daily 8-Hour Average (MDA8) concentration of 70 ppb, requires accurate measurements and predictions to protect the public from adverse health effects. Effective ozone control strategies must focus on reducing the atmospheric emission of its precursor species (NO_x and HCHO). Substantial progress has been made in this regard, leading to improvements in air quality attributed to ozone reduction across the US (Bloomer et al., 2009; Butler et al., 2011; Cooper et al., 2014; G  go et al., 2007; Goldberg et al., 2015; Hao He et al., 2013; He et al., 2020a; Marufu et al., 2004; Oltmans et al., 2006; Roberts et al., 2022). Despite these gains, ozone concentrations in rural areas have remained steady or increased slightly in recent decades (Canty et al., 2015; Cooper et al., 2014, 2012; Goldberg et al., 2014; Sicard, 2021).

Regulatory air quality models like Community Multiscale Air Quality (CMAQ) have become essential for regulatory agencies for demonstrating attainment with EPA standards (US EPA, 2016). CMAQ has been used by states to develop implementation plans for nonattainment areas (SIP) (US EPA, 2023). Model performance is fundamentally limited by the quality of emissions inventories. We use the EPA's EQUATES (EPA's Air

QUALity Time Series) modeling platform for this analysis. However, CMAQ shows a wide range in its ozone prediction capabilities across regions and seasons. These challenges have been well-documented in literature and mainly focus on its difficulty in simulating summer photochemistry and nighttime ozone processes (Appel et al., 2012, 2007; Canty et al., 2015; Foley et al., 2015; Harkey et al., 2015; Ring et al., 2018). While numerous studies have evaluated CMAQ's ability to reproduce observed concentrations, fewer have systematically examined how well the model predicts exceedances of regulatory thresholds over extended periods (Astitha et al., 2017; He et al., 2020b).

We evaluated CMAQ's MDA8 ozone predictions across the CONUS from 2003 to 2019, focusing on the model's performance at identifying exceedance events above the NAAQS threshold. Using a quadrant-based framework, we assessed model performance in distinguishing exceedance from non-exceedance conditions and examined how this capability varies by region, season, and time. We also identified potential exceedance events in unmonitored areas to highlight gaps in current surveillance coverage that may compromise effective air quality management.

4.2. *Methodology*

4.2.1. EQUATES Data Product

The emissions data utilized in this study are derived from the EQUATES (EPA's Air QUALity Time Series) project that provides meteorology and emissions inventories from 2003 through 2019 (<https://www.epa.gov/cmaq/equates>). The datasets cover the CONUS at a 12km horizontal grid spacing using the WRF model version 4.1.1 for simulating

weather conditions and EPA's Community Multiscale Air Quality (CMAQ) model version 5.3.2 for air quality modeling. CMAQ v5.3.2 includes extensive science updates compared to previous CMAQ timeseries (Appel et al., 2021). Previous decadal CMAQ simulations used emissions datasets from different NEIs or employed base year NEI data with scaling factors based on activity data and emission control information. In contrast, the EQUATES emissions data were developed using consistent input data and methods across all years to avoid artificial step-changes in emissions and air quality estimates due to methodological changes.

The EQUATES base year emissions are derived from the 2017 NEI, with emissions for the entire 2003-2019 time period estimated using four distinct approaches applied to each sector: (1) development of new methods for creating consistent emissions for all years, (2) use of 2017 model platform emissions with scaling factors based on activity data and emission control information, (3) utilization of existing modeling platform data, or (4) maintaining emissions flat at 2017 NEI levels (Foley et al., 2023; US EPA, 2021c).

Important emissions updates in EQUATES include the use of EPA's MOtor Vehicle Emissions Simulator version 3 (MOVES3) for onroad emissions modeling, consistent fire emissions inventories, consistent oil and gas emissions using EPA's Oil and Gas Emission Estimation Tool, new fertilizer emissions based on the Environmental Policy Integrated Climate (EPIC) model to support CMAQ v5.3.2, and new volatile chemical product (VCP) emissions following updated methodological frameworks (Foley et al., 2023; Seltzer et al., 2021; O. US EPA, 2021, 2015).

4.2.2. Long-term EPA AQS Network Data

Surface ozone observations utilized in this study are obtained from EPA's AQS, which serves as the agency's repository of ambient air quality data from ozone monitoring stations operated by EPA, state, local, and tribal air pollution control agencies across the United States (US EPA, 2014b). The AQS database contains hourly ozone concentration measurements along with descriptive information about each monitoring station including geographic location. Under Clean Air Act (CAA) requirements, ozone monitoring must employ measurement methods designated by EPA as either Federal Reference Methods (FRMs) or Federal Equivalent Methods (FEMs) so that standard measurement data quality is maintained across the network (O. US EPA, 2020). The EPA reference method for ozone measurement is based on continuous automated measurement of the intensity of characteristic chemiluminescence released by the gas phase reaction of ozone in sampled air with either ethylene (C_2H_4) or nitric oxide (NO) gas (CFR, 2025a). The calibration procedure is based on ultraviolet (UV) photometry, utilizing the photometric assay of ozone concentrations in a dynamic flow system where ozone concentration in an absorption cell is determined from measurement of the amount of 254 nm light absorbed by the sample (CFR, 2025a).

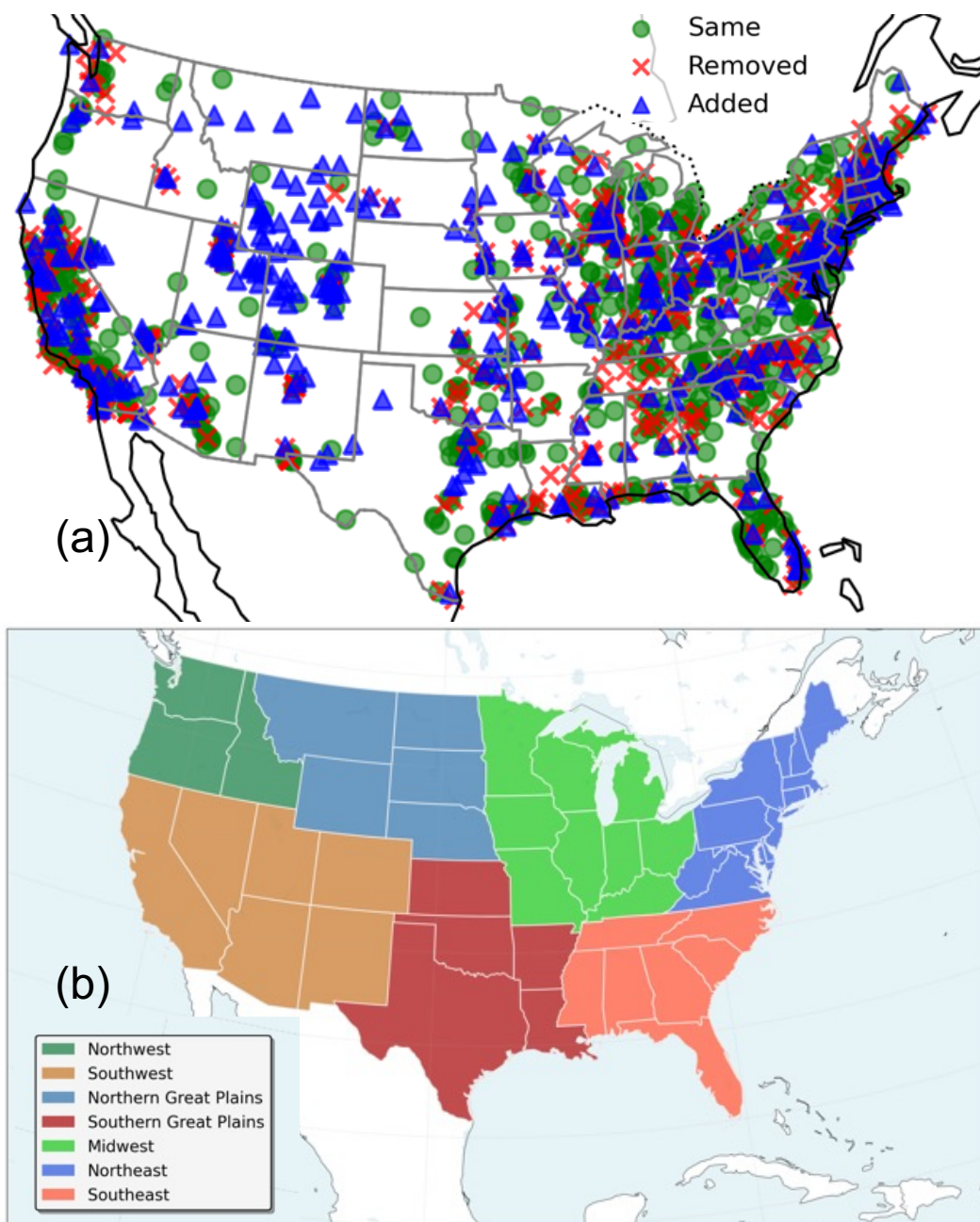


Figure 4-1: (a) Changes in AQS ozone monitoring station locations across the contiguous United States, Alaska, Puerto Rico, and Hawaii from 2003 to 2019. Station status is indicated by symbol type and colour: added stations (404, blue triangles), persistent stations (838, green circles), and removed stations (430, red crosses). (b) Regional divisions of the contiguous United States used in ozone analysis. Different colours represent the seven regions: Northwest, Southwest, Northern Great Plains, Southern Great Plains, Midwest, Northeast, and Southeast.

Figure 4-1(a) shows the distribution of the AQS ozone monitoring network during the study period (2003 to 2019). The network experienced substantial changes with monitoring stations being added, removed, or maintained throughout the contiguous United States, Alaska, Puerto Rico, and Hawaii. The figure marks stations that operated continuously throughout the study period, stations that were discontinued during this timeframe, and new stations that were added to improve spatial coverage or address emerging air quality concerns.

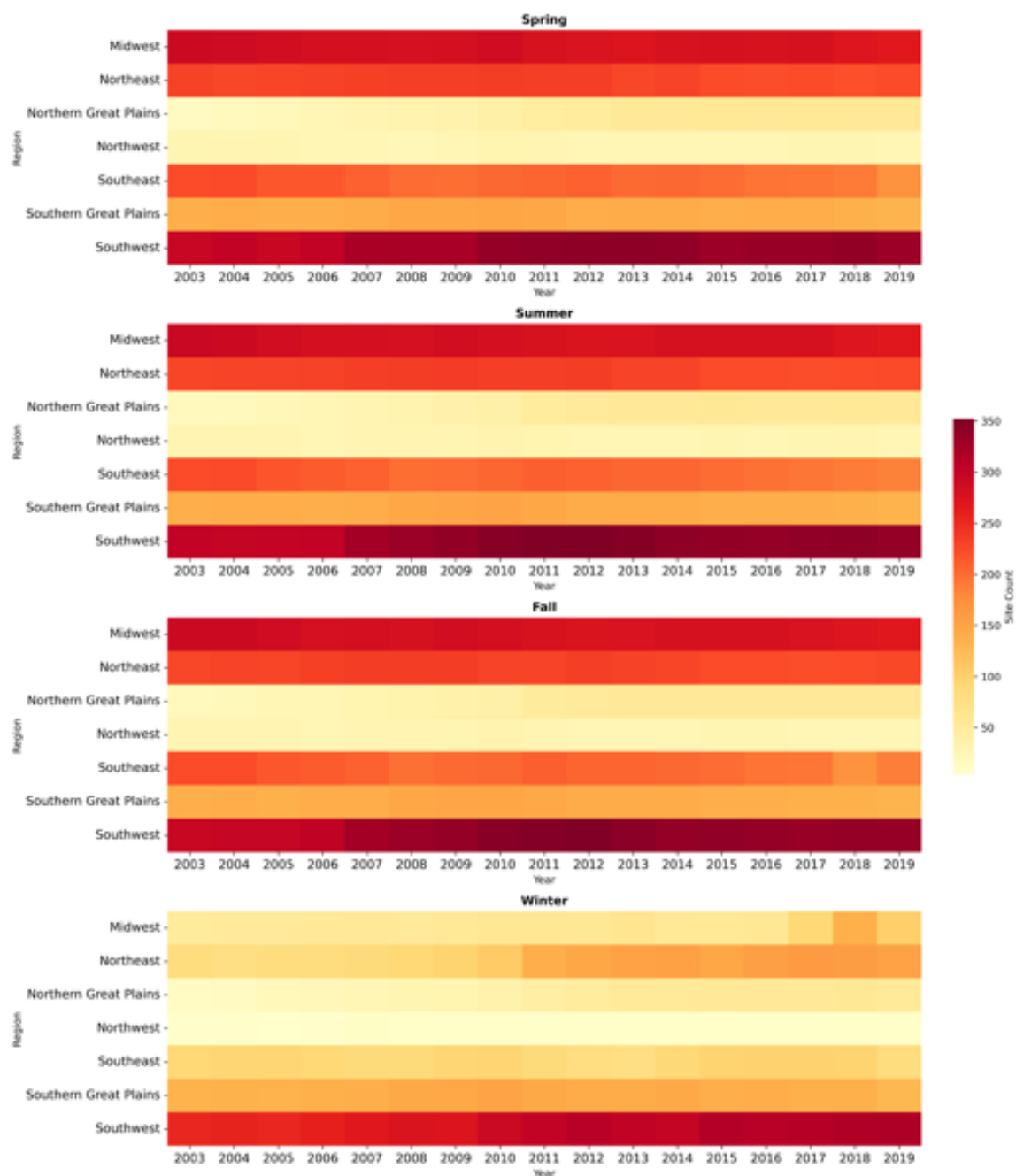


Figure 4-2: Heat map of AQS ozone monitoring site coverage by region and season from 2003-2019. Each panel represents a season (Spring, Summer, Fall, Winter) with rows corresponding to the seven geographic regions (Midwest, Northeast, Northern Great Plains, Northwest, Southeast, Southern Great Plains, Southwest) and columns representing years 2003-2019. Color intensity indicates the number of functioning ozone monitoring sites, with dark red representing higher monitoring coverage and light yellow indicating lower coverage.

The heatmap in **Figure 4-2** shows the temporal and spatial patterns in AQS density for different seasons and regions of the CONUS (**Figure 4-1a**). The Northern Great Plains and Northwest show the lowest overall site densities, though the Northern Great Plains maintains consistent year-round monitoring while the Northwest demonstrates reduced winter coverage. The Southeast and Southwest show the highest monitoring densities, with the Southeast reducing winter operations while the Southwest maintains consistent operations across seasons. The Midwest and Northeast also scale back winter monitoring activities. The Southern Great Plains demonstrates consistent monitoring throughout all seasons. There is not much change in the total number of operational monitoring sites in this study period except for an increase in sites remaining operational during winter. This increase is likely due to a growing recognition of the importance of year-round ozone monitoring.

4.2.3. MDA8 Calculation

The Maximum Daily 8-hour Average (MDA8) ozone concentration is the primary metric assessing compliance with the US NAAQS (US EPA, 2023d). MDA8 is calculated as the highest of consecutive 8-hour averages of surface ozone concentrations per day (CFR, 2025b). The regulatory design value is calculated as the annual fourth-highest daily maximum 8-hour ozone concentration averaged over three consecutive years, with NAAQS compliance achieved when this 3-year average is ≤ 70 ppb (CFR, 2025b). Quality assurance protocols must exclude data affected by exceptional events (CFR, 2025b). The 8-hour averaging period better captures cumulative health exposure patterns compared to shorter periods. This metric determines nonattainment designations, triggering mandatory

emission controls, transportation planning requirements, and industrial permitting restrictions.

For AQS observations, MDA8 values were derived directly from the 8-hour average concentrations provided by the AQS database, with the daily maximum selected for each location. For CMAQ model output, we first computed 8-hour running averages, from which daily maximum values were extracted for each grid cell. Model-observation comparisons were facilitated by identifying the nearest CMAQ grid cell to each AQS monitoring site and selecting the maximum MDA8 value from a 3×3 grid centred on the closest grid point to account for spatial representativeness and potential misalignment between point observations and grid-averaged model predictions.

4.3. *Results and Discussions*

4.3.1. Time Series Analysis

In **Figure 4-3** we show the temporal evolution of MDA8 ozone, from AQS observations and CMAQ model output for MDA8 ozone from 2003 to 2019 across CONUS. The data reveal a marked decrease in AQS-observed MDA8 ozone concentrations throughout this period, consistent with steadily improving ozone air quality in the US. Notably, the lower-percentile MDA8 values observed by AQS shows a slight increase with time. This slight increase in lower percentile MDA8 values has been observed in previous studies (Goldberg et al., 2015). Several factors may explain this pattern such as surface ozone abatement strategies may have primarily targeted high-pollution sources while leaving background concentrations in non-exceedance areas

relatively unchanged, or surface ozone may be increasing in previously clean regions despite better control of peak concentrations.

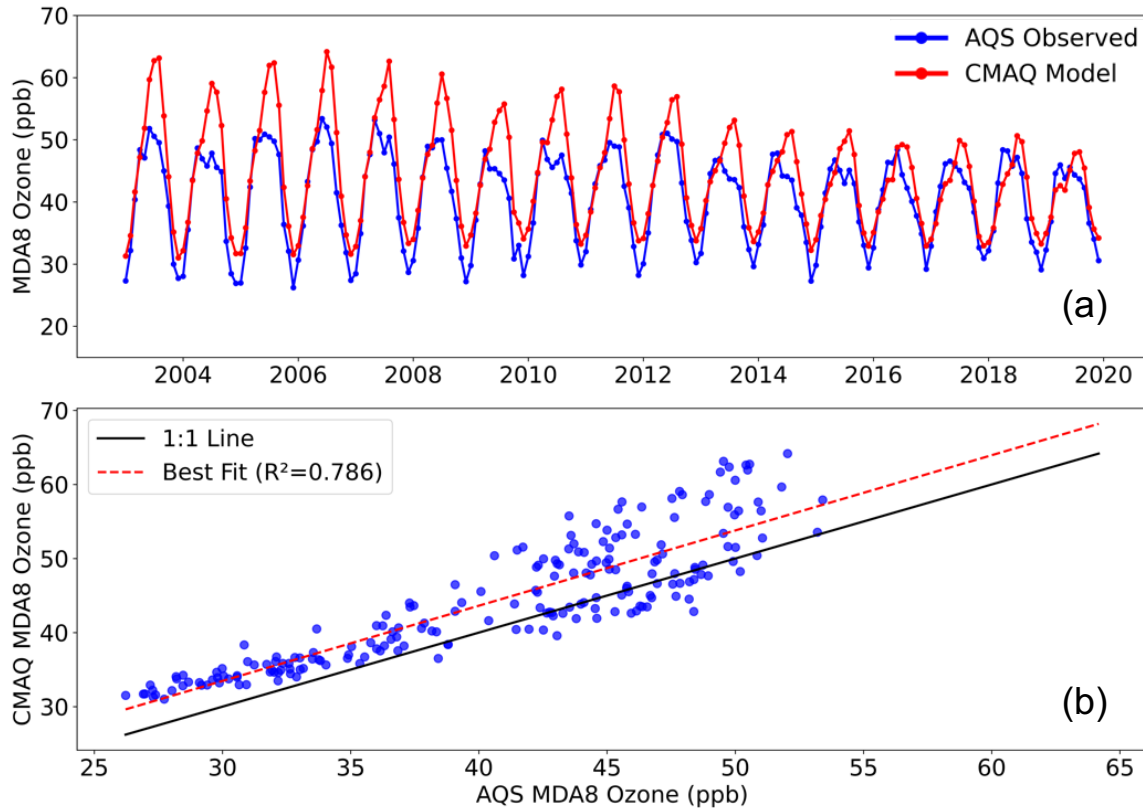


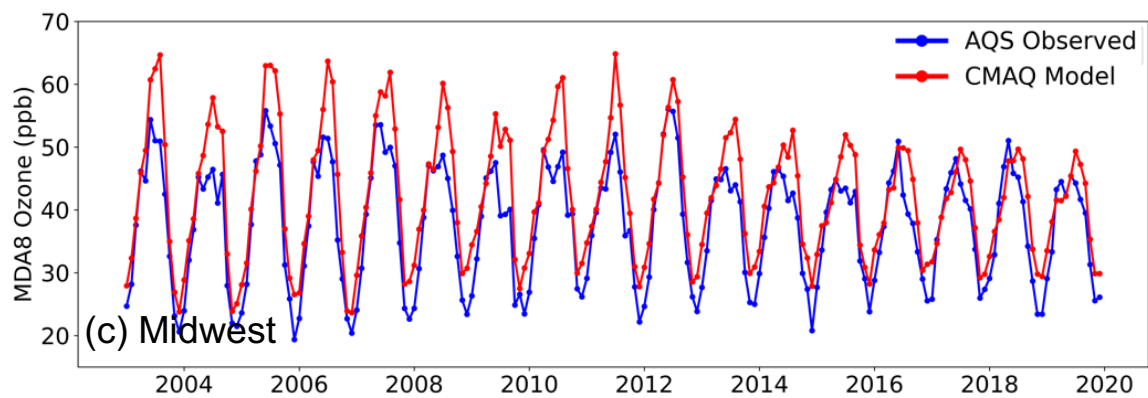
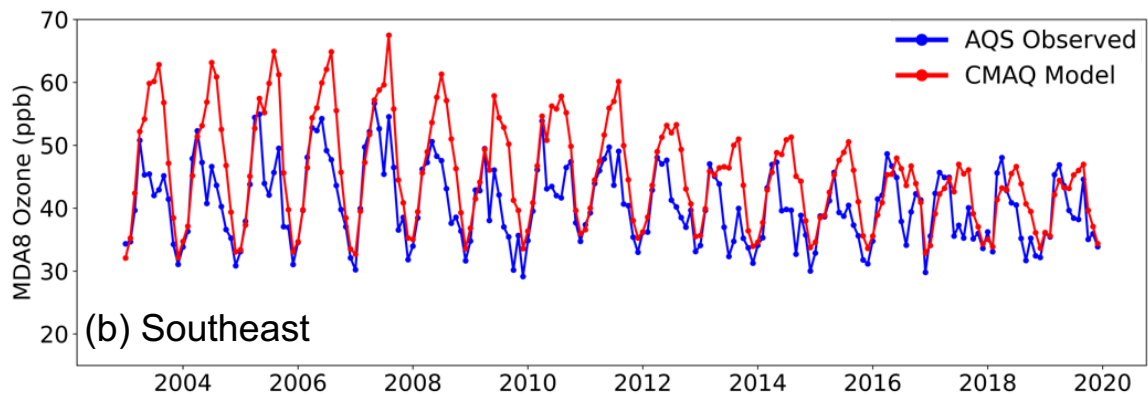
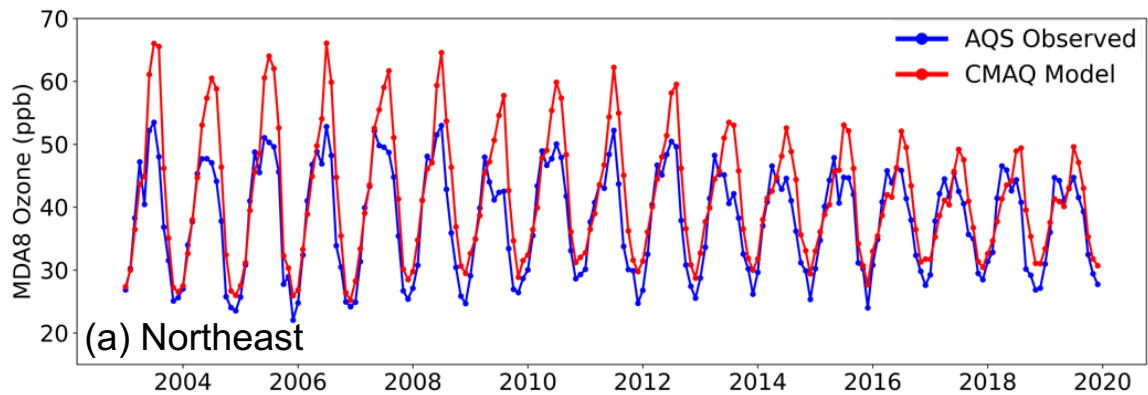
Figure 4-3: Comparison of observed and modeled MDA8 ozone concentrations from 2003 to 2019 for CONUS. (a) Average monthly MDA8 from AQS monitoring sites (blue) and CMAQ model output (red) (b) Scatter plot of monthly averages of AQS observations (x-axis) and CMAQ model output (y-axis) with the best fit line (red dashed) and one-one line (black)

CMAQ model output of MDA8 shows considerable improvement over time, achieving better correlation with AQS observations after 2014. Prior to 2014, the model consistently overestimated concentrations of MDA8 ozone by a significant margin. A continued limitation of the model output is its inability to capture the lowest AQS observations. This shortcoming may be due to modeling challenges such as inadequate representation of nighttime ozone chemistry, poor simulation of nighttime stratification, or difficulties in

parameterizing of the PBL height and dynamics. The overall R^2 of 0.786 for observed vs modeled MDA8 across CONUS represents strong model performance.

4.3.1.1. Regional Time Series

In **Figure 4-4** we examine the temporal evolution of monthly averaged MDA8 ozone from AQS observations and CMAQ model output across seven geographic subdivisions of CONUS, as shown in Figure 4-1(b). The strongest correlations between model and observations occur in the Midwest ($R^2 = 0.862$) and Southern Great Plains ($R^2 = 0.777$). The Northeastern and Southwestern US exhibit patterns similar to the overall CONUS time series, with improved agreement after 2014. In the Southeastern US, the model adequately reproduces ozone magnitudes but struggles to capture seasonal patterns post-2014, resulting in significantly degraded correlation ($R^2 = 0.556$). The Northern Great Plains present a different challenge: while the model captures the magnitude of MDA8 highs and lows even before 2014, it fails to reproduce seasonal variability patterns. The Northwestern US also demonstrates poor model performance ($R^2 = 0.619$). Here, the model consistently underperforms in simulating low MDA8 values and exhibits apparent systematic positive bias across all seasons throughout the study period.



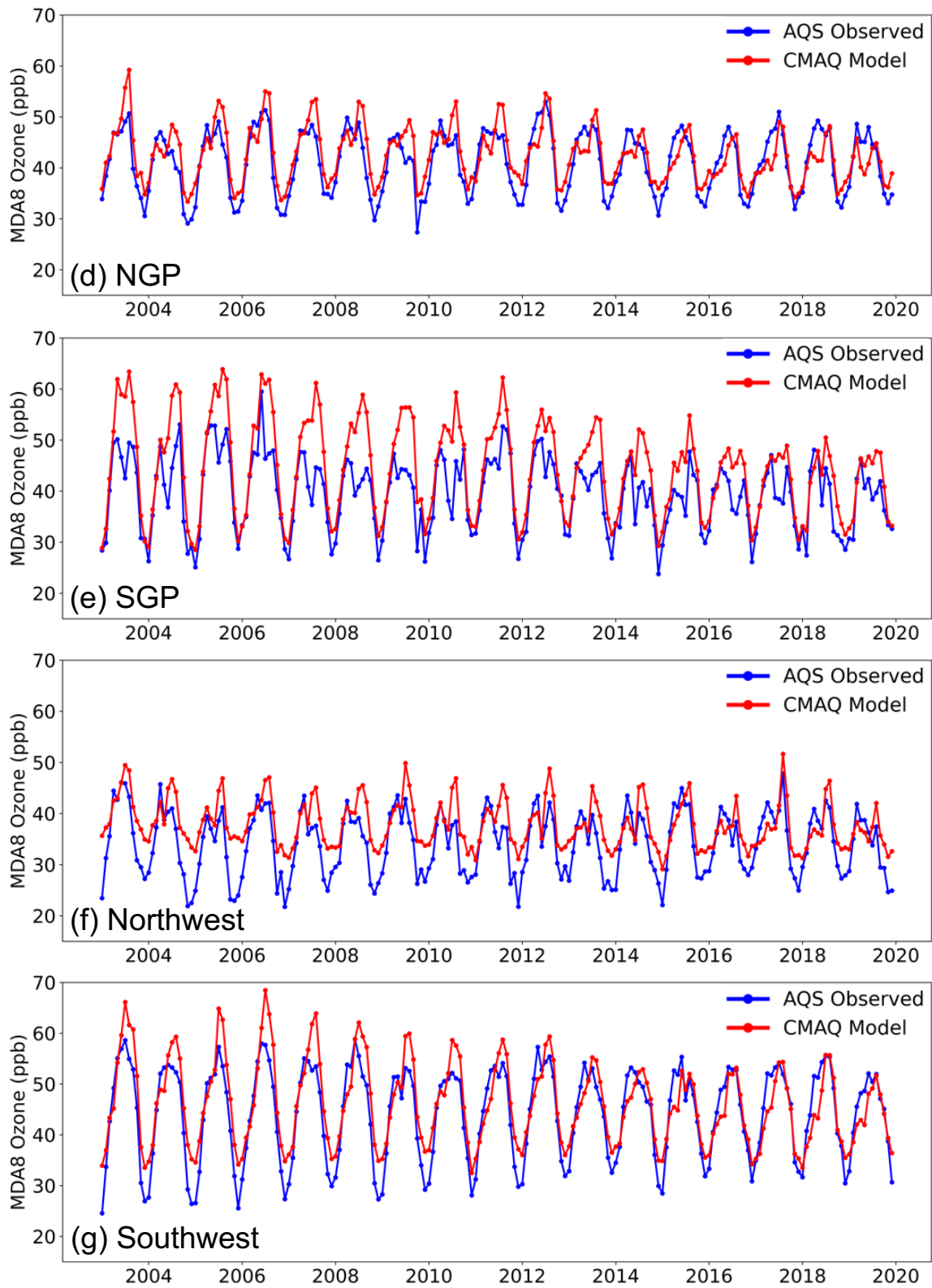


Figure 4-4: Comparison of observed and modeled MDA8 ozone concentrations from 2003 to 2019 for different regions of CONUS. We see the monthly averaged MDA8 from AQS monitoring sites (blue) and CMAQ model output (red) for (a) Northeast, (b) Southeast, (c)

Midwest, (d) Northern Great Plains, (e) Southern Great Plains, (f) Northwest and (g) Southwest of the US.

The statistical metrics shown in **Table 4-1** reveal distinct regional patterns in model bias and accuracy. Across CONUS, the model exhibits a consistent positive bias of 3.63 ppb (8.95% NMB), with the Southern Great Plains, Midwest and Southeast showing the largest absolute biases of 5.08 ppb, 4.51 ppb and 4.78 ppb, respectively. Despite these biases, the Southern Great Plains and Midwest maintain strong correlations ($R^2 = 0.777$ and 0.862), suggesting the model captures temporal variability well even while systematically overestimating concentrations of ozone. The Southeast, however, combines high bias with lower correlation ($R^2 = 0.556$) and the highest RMSE (7.31 ppb), reflecting the seasonal pattern issues identified earlier. The Northern Great Plains demonstrates the smallest bias (1.39 ppb, 3.39% NMB) and lowest RMSE (3.69 ppb), indicating good overall accuracy despite the seasonal variability challenges noted earlier. Conversely, the Northwest shows moderate bias (3.63 ppb) coupled with low correlation ($R^2 = 0.619$), confirming the model's struggle with the seasonal variability of ozone in this region.

4.3.1.2. Seasonal Time Series

We next examine seasonal trends in MDA8 ozone and model performance using yearly averages. **Figure 4-5** shows yearly averaged MDA8 ozone from model and AQS observations for Summer (June-July-August), Fall (September-October-November), Spring (March-April-May), and Winter (December-January-February) for CONUS. The data reveal that MDA8 values for summer, spring, and fall have declined over time for both model and observations, while winter values exhibit an upward trend. This trend represents

the first instance in our seasonal or regional analysis where MDA8 ozone concentrations increase across the study period. During summer and fall, the model consistently overestimates observations across all years, though this bias decreases with time. In spring we see an unusual pattern where the model exceeds observations until 2012 but underestimates concentrations post-2012, suggesting a possible shift in model behavior or changes in springtime ozone chemistry that the model struggles to capture accurately.

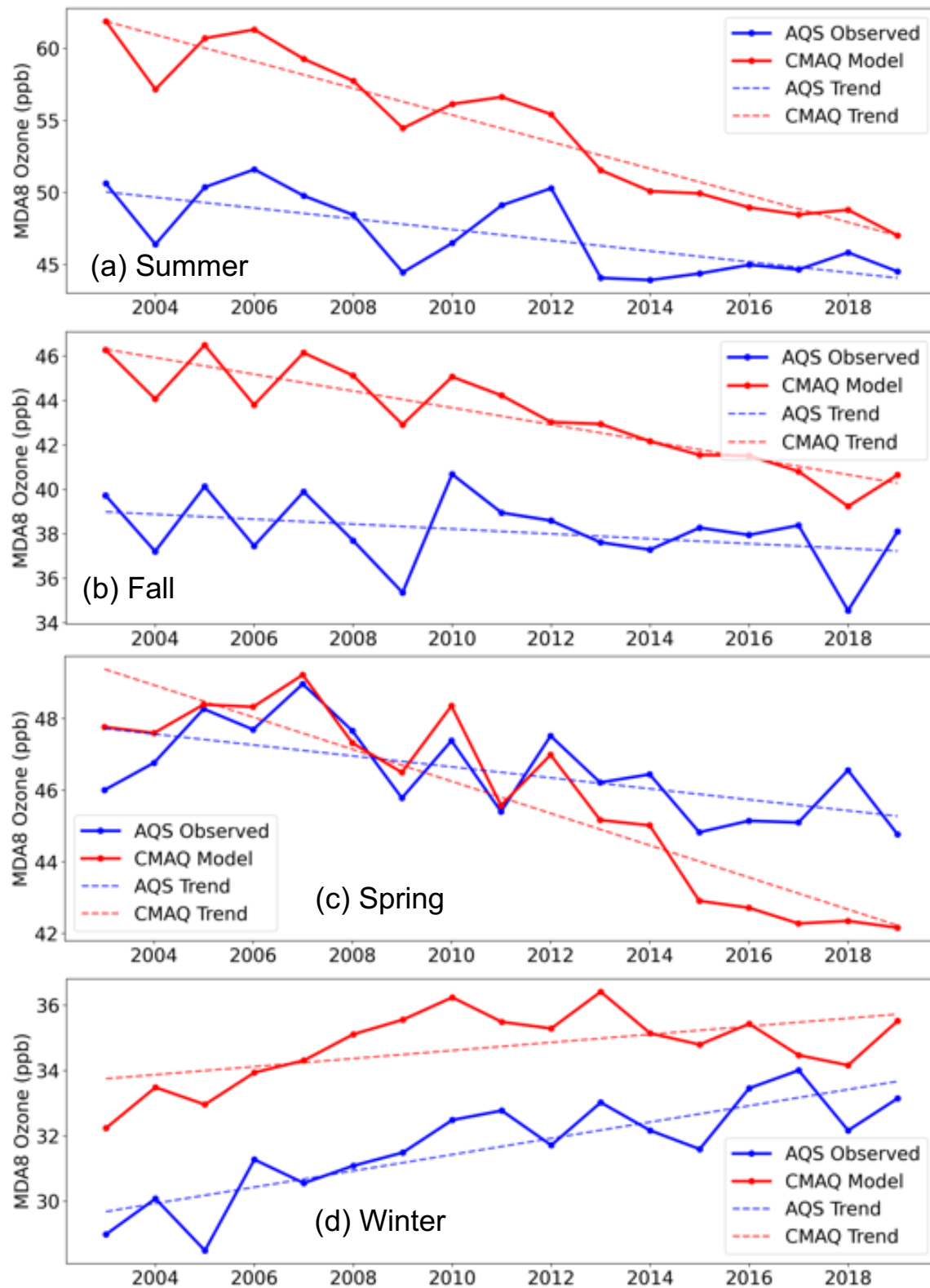


Figure 4-5: Comparison of observed and modeled MDA8 ozone concentrations from 2003 to 2019 for the four seasons across CONUS. We see the yearly averaged MDA8 from AQS

monitoring sites (blue) and CMAQ model output (red) for (a) Summer, (b) Fall, (c) Spring, and (d) Winter. Note the scale is different for each panel to highlight the variabilities.

The increasing winter ozone trend likely stems from multiple factors including expanded oil and gas extraction activities, oil tar sands operations, enhanced snow-sun reflectance increasing photochemical activity, weakened NO_x titration, increased aviation and shipping emissions, transpacific transport from Asian sources, and changes in large-scale atmospheric circulation patterns (Jhun et al., 2015; Li et al., 2023; Lin et al., 2017; Simon et al., 2015). Weakened NO_x titration in colder months allows background sources to become more important. Overall, wintertime ozone formation operates under different chemistry and dynamics than the well-studied summer photochemical regime.

The seasonal performance statistics (shown in Table 4-1) reveal that summer exhibits poor model performance with the largest bias (7.38 ppb, 15.69% NMB), highest RMSE (7.91 ppb), indicating fundamental challenges in capturing summer ozone photochemistry using CMAQ v5.3.2 driven by EQUATES emissions. This finding contrasts sharply with spring, which shows minimal bias (-0.7 ppb, -1.5% NMB) and the lowest RMSE (1.74 ppb). Fall and winter demonstrate moderate positive biases of 5.18 ppb and 3.06 ppb. These patterns suggest the model struggles most during peak photochemical season when ozone formation processes are most active, and performs reasonably well during transitional seasons and winter.

4.3.1.3. Urban-Rural Time Series

We next examine MDA8 ozone time series analysis between urban and rural regions across the CONUS in **Figure 4-6**. Urban areas, defined as the 36 km² grid cells surrounding the 30 most densely populated metropolitan statistical areas, exhibit higher peak concentrations compared to rural regions (the rest of the grid cells). Both rural and urban regions show a declining trend over the study period. The model performance (shown in Table 4-1) demonstrates a strong correlation between model and observations for both urban and rural CONUS ($R^2 = 0.837$ for urban, $R^2 = 0.771$ for rural), though the model exhibits a systematic positive bias. The higher biases observed in urban regions may reflect uncertainties in representing urban scale processes such as local emissions, urban heat island effects, and atmospheric mixing in areas with complex land use practices.

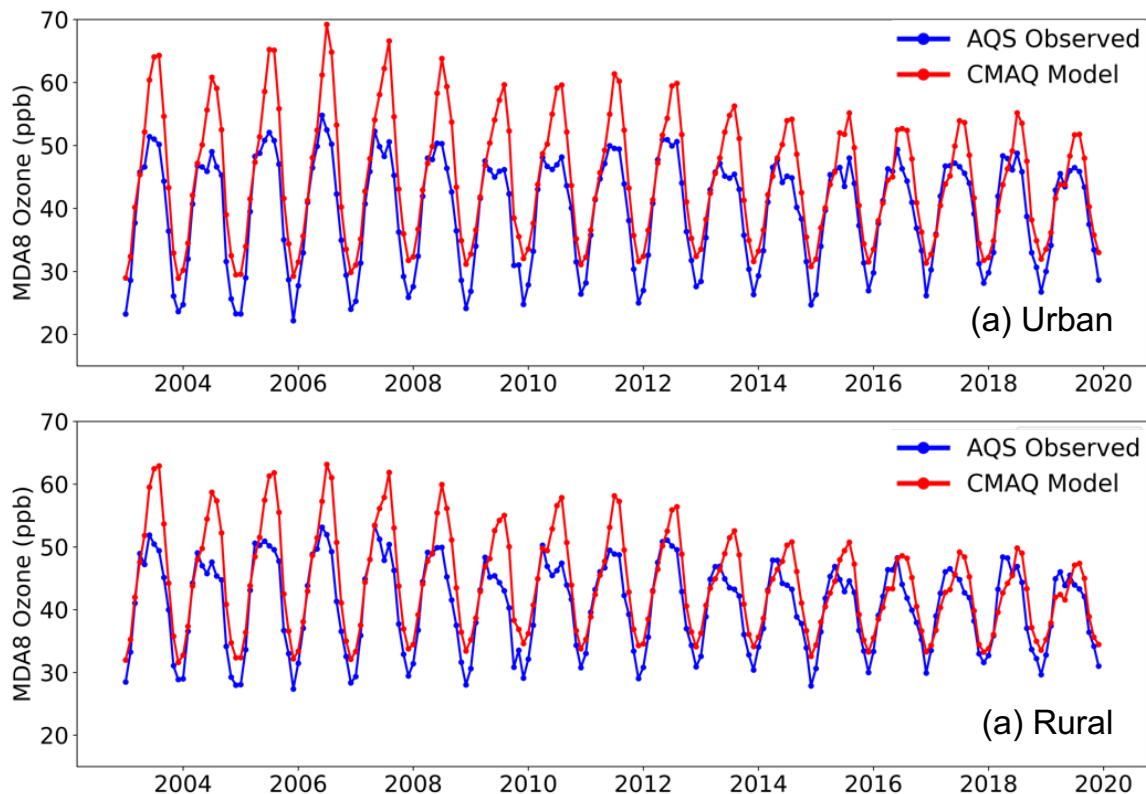


Figure 4-6: Comparison of observed and modeled MDA8 ozone concentrations from 2003 to 2019 for urban and rural CONUS. We see the monthly averaged MDA8 from AQS monitoring sites (blue) and CMAQ model output (red) for (a) Urban and (b) Rural US. We define urban as the 36 km² grid around the top 30 densely populated metropolitan statistical areas and rural as the rest of CONUS.

Table 4-1: Monthly statistical comparison between observed AQS and CMAQ modeled ozone concentrations. Statistics include error metrics (RMSE, mean bias, NMB), and correlation coefficients (R²).

	Obs Mean	Model Mean	Bias	RMSE	NMB	R²
	(ppb)	(ppb)	(ppb)	(ppb)	(%)	
CONUS	40.56	44.2	3.63	5.3	8.95	0.786
Urban	39.59	44.58	4.99	6.41	12.61	0.837
Rural	40.82	44.17	3.34	5.1	8.19	0.771
Regions						
Northwest	34.2	37.83	3.63	5.31	10.62	0.619

Southwest	44.25	46.1	1.84	4.65	4.17	0.78
NGP	41.11	42.5	1.39	3.69	3.39	0.691
SGP	39.47	44.55	5.08	6.76	12.87	0.777
Midwest	37.67	42.18	4.51	5.88	11.97	0.862
Northeast	37.99	41.68	3.69	5.83	9.71	0.802
Southeast	40.53	45.31	4.78	7.31	11.8	0.556
Seasons						
Spring	46.5	45.8	-0.7	1.74	-1.5	0.658
Summer	47.06	54.44	7.38	7.91	15.69	0.744
Fall	38.11	43.29	5.18	5.41	13.6	0.436
Winter	31.68	34.74	3.06	3.2	9.66	0.585

4.3.2. Quadrant Analysis

We next examine scatter plots of MDA8 ozone between model and observations, partitioned into four quadrants based on the 70 ppb exceedance threshold. The lower left quadrant represents cases where both model and observations fall below the NAAQS standard, while the upper right quadrant shows instances where both exceed 70 ppb. The upper left quadrant identifies "false positives" where the model incorrectly predicts an exceedance event. The lower right quadrant captures "false negatives" where the model fails to detect an exceedance event. This analysis provides insight into model performance, as false positives can impose unnecessary financial burdens on states through unneeded control measures, while false negatives may result in undiagnosed ozone violations and

inadequate pollution mitigation efforts. Given CMAQ's widespread use in regulatory compliance assessments, accurate prediction of exceedance events is essential for effective air quality management and policy implementation.

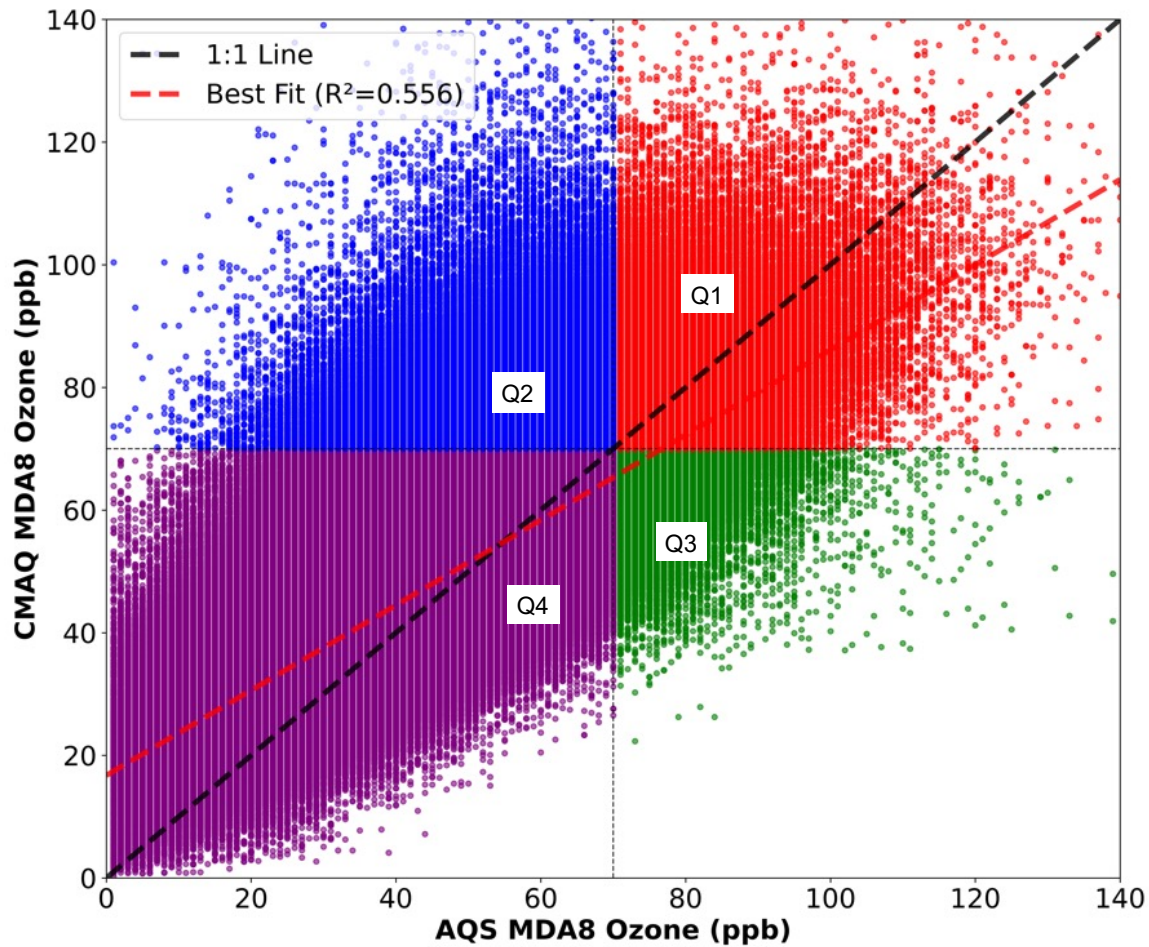


Figure 4-7: Scatter plot of MDA8 ozone concentrations between CMAQ model output and AQS observations for CONUS from 2003-2019. Data points are color-coded by quadrant: Q1 (red) represents both model and observations exceeding 70 ppb, Q2 (blue) shows model-only exceedances, Q3 (green) indicates observation-only exceedances, and Q4 (purple) denotes both below the 70 ppb NAAQS threshold. The black dashed line represents the 1:1 line, while the red dashed line shows the best fit.

In **Figure 4-7** and **Table 4-2** we see the scatter plot analysis of MDA8 ozone across CONUS from 2003-2019 revealing that the vast majority of data points (93.78%) fall

within Q4, where both model and observations remain below the 70 ppb exceedance threshold. However, the model demonstrates a tendency toward false positives, with 3.43% of MDA8 cases in Q2 where the model incorrectly predicts exceedances. Only 1.11% of cases fall in Q3, suggesting the model rarely misses true MDA8 exceedance events across CONUS during this period. Both model and observations exceed the threshold simultaneously in just 1.68% of cases (Q1). The overall correlation of $R^2 = 0.556$ indicates moderate agreement between modeled and observed MDA8 concentrations.

To quantify model performance in predicting MDA8 ozone exceedances, we employ metrics based on the four-quadrant framework as shown in **Equation 4-1, 4-2 and 4-3**. True positives correspond to Q1 cases where both model and observations exceed 70 ppb, false positives represent Q2 cases where only the model predicts exceedance, false negatives are Q3 cases where only observations exceed the threshold, and true negatives correspond to Q4 cases where both remain below 70 ppb. We calculate hit rate, false alarm rate, and overall accuracy to assess the model's capability in correctly identifying exceedance events, which is critical for regulatory applications.

$$\text{hit rate} = \frac{\text{true positives}}{\text{true positives} + \text{false negatives}} \quad \text{Equation 4-1}$$

$$\text{false alarm rate} = \frac{\text{false positives}}{\text{false positives} + \text{true negatives}} \quad \text{Equation 4-2}$$

$$\text{accuracy} = \frac{\text{true positives} + \text{true negatives}}{\text{total points}} \quad \text{Equation 4-3}$$

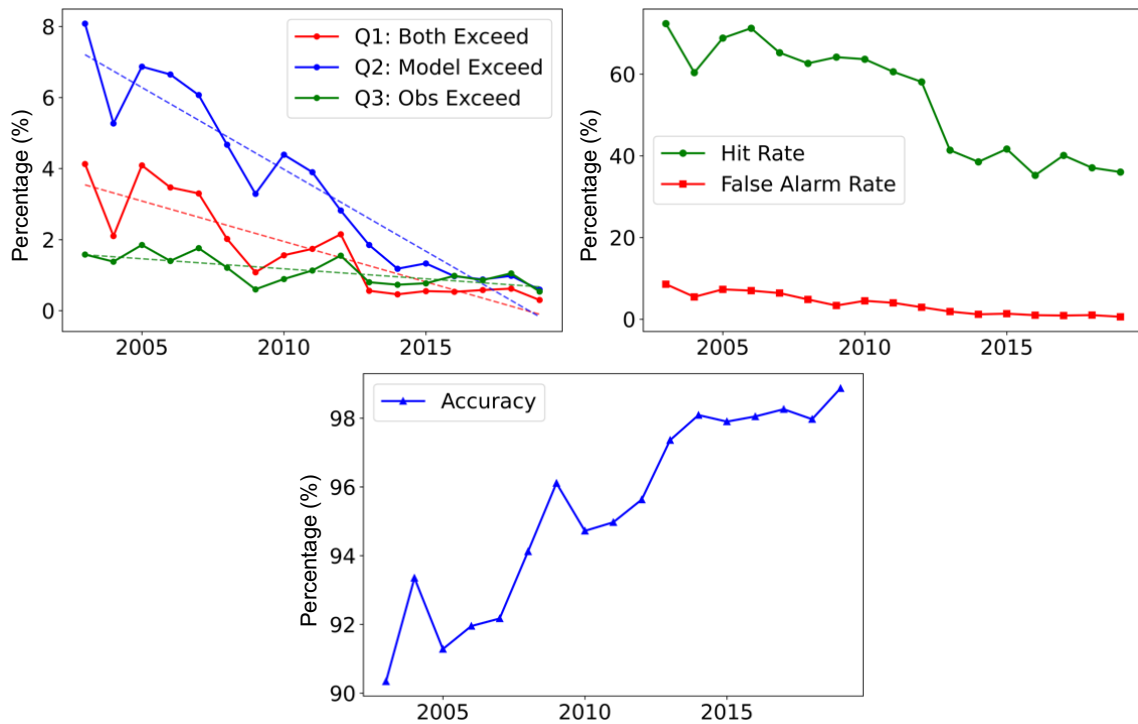


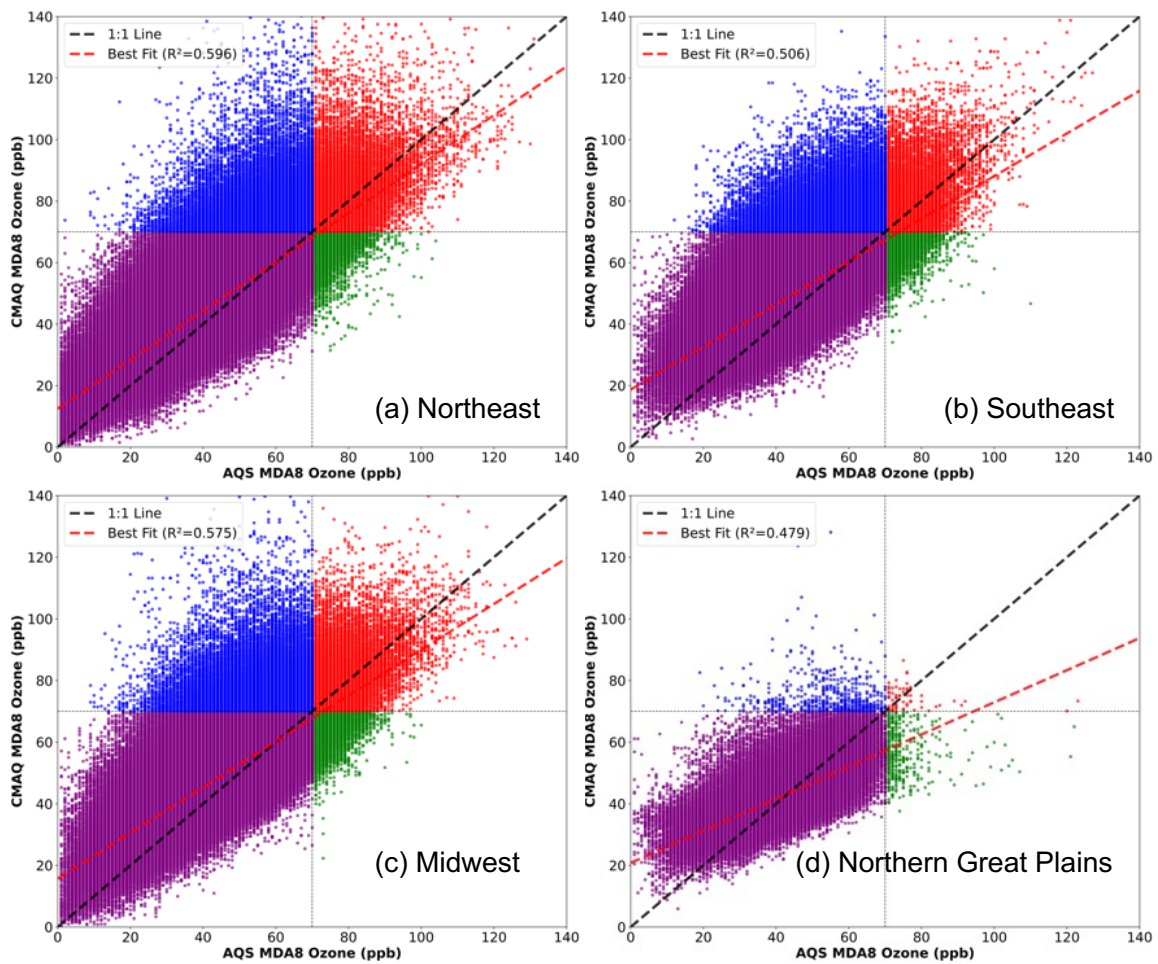
Figure 4-8: Temporal evolution of CMAQ model performance for MDA8 ozone predictions across CONUS from 2003-2019. (a) Annual percentages of exceedance quadrants Q1 (both exceed 70 ppb), Q2 (model-only exceedance), and Q3 (observation-only exceedance), (b) Hit rate (Equation 4-1) and false alarm rate (Equation 4-2) percentages over time, (c) Overall model accuracy (Equation 4-3) over time

Figure 4-8 presents time series of MDA8 ozone quadrant analysis from 2003 to 2019 for CONUS where panel (a) shows the Q1, Q2 and Q3 percentages, panel (b) shows the hit rate and false alarm rate (Equation 4-1 and 4-2) and panel (c) shows the accuracy (Equation 4-3). Figure 4-8 reveals that the percentages of exceedance quadrants Q1 through Q3 have all decreased over time, reflecting the overall improvement in air quality and reduced frequency of MDA8 ozone exceedances across CONUS. While the hit rate has declined over this period, this decrease is primarily due to reduction in exceedance events. The false alarm rate has remained relatively stable with a slight downward trend, indicating consistent model behavior in predicting false positives. Overall model accuracy has

increased with time, suggesting that improvements in emissions inventories and meteorological inputs have improved CMAQ's ability to correctly classify both exceedance and non-exceedance conditions for MDA8 ozone predictions throughout the CONUS.

4.3.2.1. Regional Quadrants

Figure 4-9 shows scatter plots of measured versus modeled MDA8 ozone for the seven regions considered in this chapter: (a) Northeast, (b) Southeast, (c) Midwest, (d) Northern Great Plains, (e) Southern Great Plains, (f) Northwest, and (g) Southwest CONUS. These plots reveal that Northwest exhibits one of the highest proportion of correct predictions with 98.69% in Q4 and minimal false positives (0.69% in Q2), though correlation remains moderate ($R^2 = 0.519$). The Southwest has 92.58% in Q4 and moderate correlation ($R^2 = 0.570$). In contrast, the Midwest demonstrates more complex performance with 93.51% in Q4 and highest false positive rates (4.09% in Q2), while maintaining a moderate correlation ($R^2 = 0.575$). The Southeast and Southern Great Plains show intermediate performance with Q4 percentages around 93-94% and moderate false alarm rates. The Northern Great Plains stands out with lowest true positive rates (0.03 % in Q1) compared to other regions, reflecting infrequent exceedance conditions, though the correlation is weakest ($R^2 = 0.479$). The Northeast shows balanced performance across metrics with 93.74% in Q4 and a strong correlation ($R^2 = 0.596$), indicating reliable model behavior for this region's ozone.



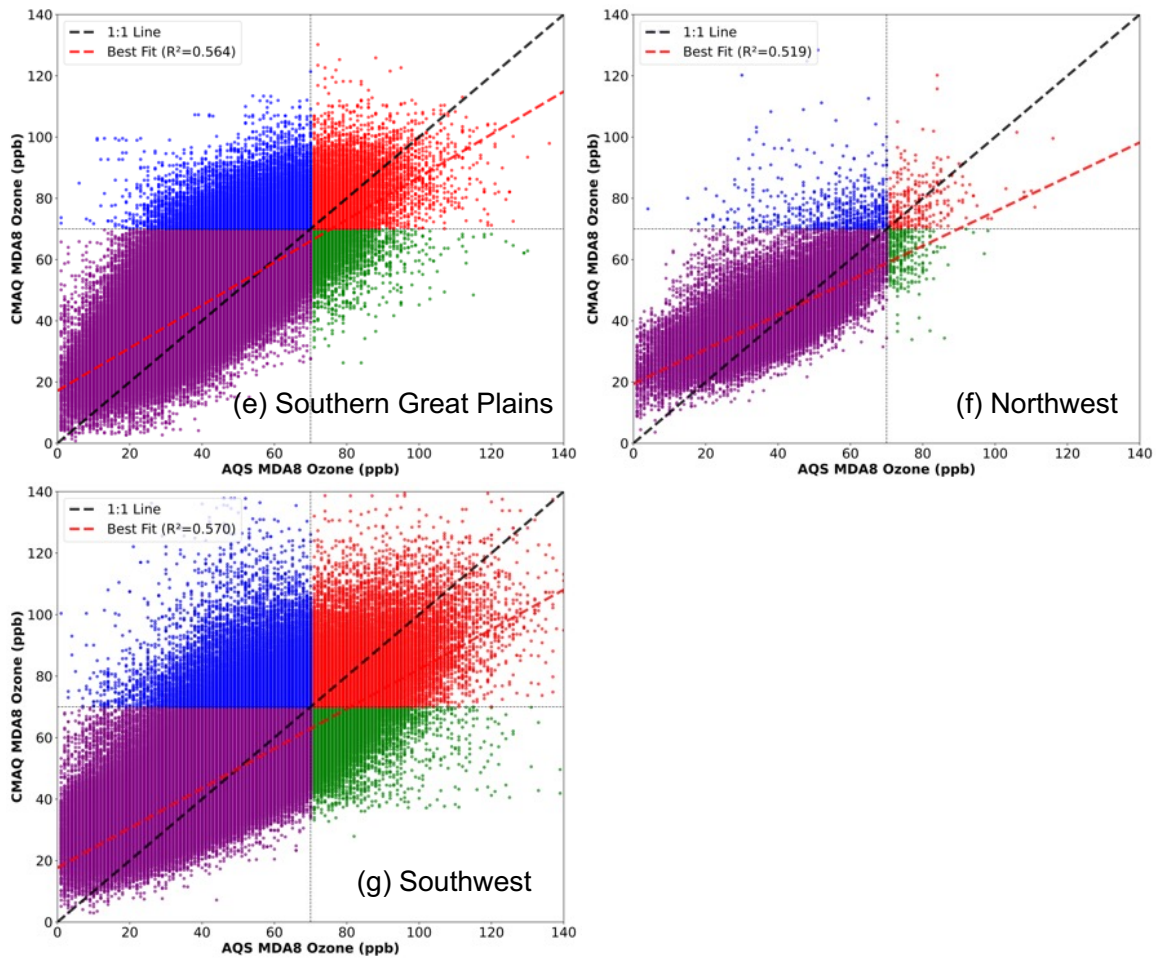


Figure 4-9: Regional scatter plots of MDA8 ozone concentrations between CMAQ model output and AQS observations from 2003-2019 for the seven geographic subdivisions: (a) Northeast, (b) Southeast, (c) Midwest, (d) Northern Great Plains, (e) Southern Great Plains, (f) Northwest, and (g) Southwest. Data points are color-coded by quadrant: Q1 (red) represents both model and observations exceeding 70 ppb, Q2 (blue) shows model-only exceedances, Q3 (green) indicates observation-only exceedances, and Q4 (purple) denotes both below the 70 ppb NAAQS threshold. Black dashed lines represent the 1:1 relationship, while red dashed lines show the best-fit linear regression for each region.

Figure 4-10 presents time series of MDA8 ozone quadrant analysis from 2003 to 2019, where each panel shows one of the seven CONUS regions with corresponding Q1, Q2 and Q3 percentages. Figure 4-10 shows that the Northeast, Midwest, and Southern Great Plains exhibit steady decreases in Q1, Q2, and Q3 percentages over the study period, reflecting consistent improvements in both air quality and model performance. The

Southeast shows a similar pattern with Q2 decreasing steadily and Q1 experiencing a slower decline throughout the period. The Northern Great Plains displays a sharp decrease in Q2 from 2003 to 2004, after which all quadrant percentages remain relatively stable. The Northwest demonstrates an early sharp decline in Q1, Q2, and Q3 percentages followed by steady conditions for the remainder of the period. The Southwest presents the most distinctive pattern among all regions, showing a steady decrease in exceedance quadrants but becoming the only region where Q3 (observation-only exceedances) surpasses both Q1 and Q2 after 2012 by a significant margin, suggesting the model increasingly underestimates MDA8 ozone exceedances in this region during the latter half of the study period.

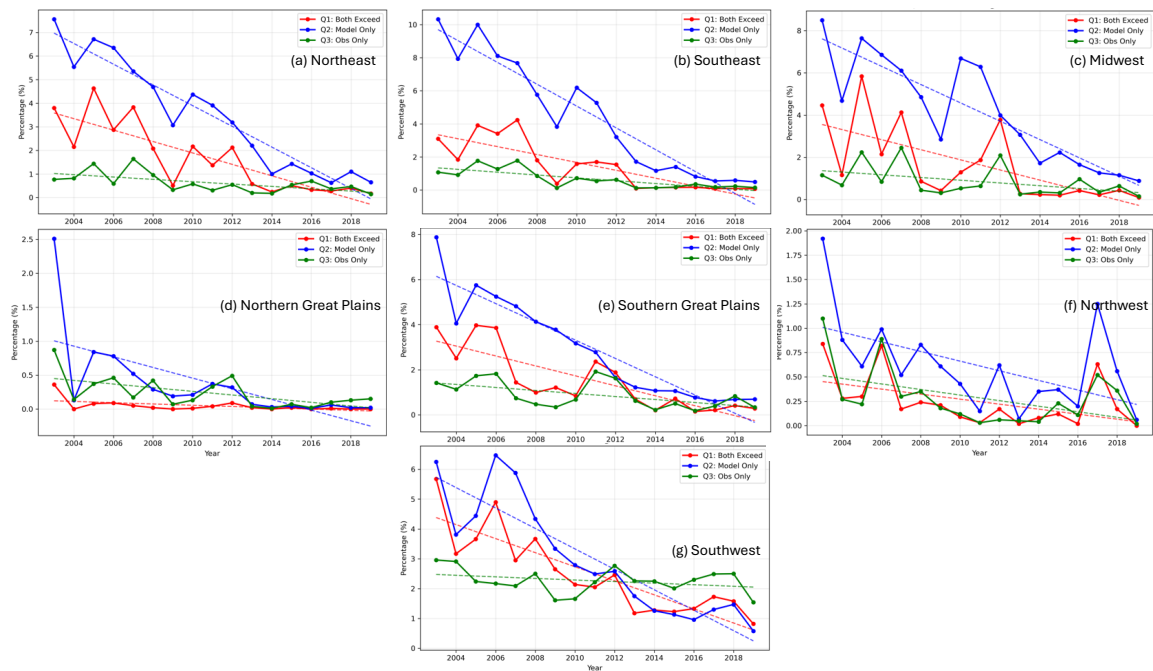


Figure 4-10: Regional time series of MDA8 ozone exceedance quadrant percentages from 2003-2019 for the seven geographic subdivisions: (a) Northeast, (b) Southeast, (c) Midwest, (d) Northern Great Plains, (e) Southern Great Plains, (f) Northwest, and (g) Southwest. Each panel shows the annual percentages of Q1 (red, both model and observations exceed 70 ppb), Q2 (blue, model-only exceedance), and Q3 (green, observation-only exceedance). Note different y-axis limits for each plot.

From Table 4-2, the Northeast demonstrates the highest hit rate at 74.11%, while the Northern Great Plains exhibits the poorest performance at 13.85%, which indicates large regional differences in CMAQ v5.3.2 capabilities. The overall CONUS performance shows a 60.1% hit rate with a 3.53% false alarm rate, reflecting reasonable model skill in distinguishing exceedance from non-exceedance conditions.

4.3.2.2. Seasonal Quadrants

Figure 4-11 shows scatter plots of measured versus modeled MDA8 ozone for the four seasons considered in this chapter: (a) Fall, (b) Spring, (c) Summer, and (d) Winter. Figure 4-11 shows that summer exhibits the highest exceedance activity with 4.19% of cases in Q1 and the largest false positive rate (9.07% in Q2), reflecting the model's tendency to overestimate during peak ozone season, though correlation remains moderate ($R^2 = 0.515$). Spring shows intermediate exceedance frequencies with 0.63% in Q1 and notable false negatives (1.39% in Q3), indicating the model occasionally misses observed exceedances during this transitional season ($R^2 = 0.449$). Fall demonstrates excellent performance with 96.78% of cases correctly classified in Q4 and minimal false alarms, achieving the strongest seasonal correlation ($R^2 = 0.597$). Winter shows very few exceedance events in either model or observations, though the correlation is weakest ($R^2 = 0.423$).

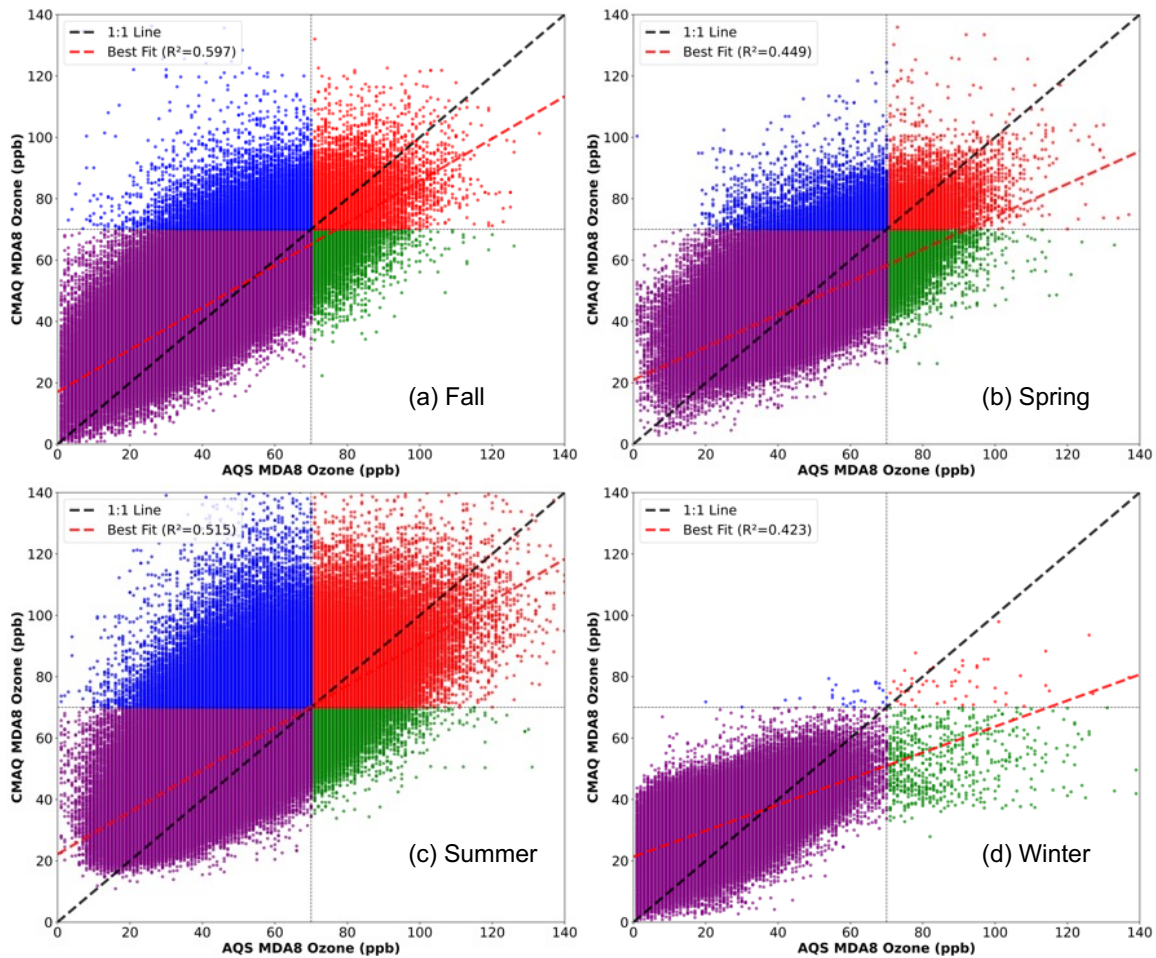


Figure 4-11: Seasonal scatter plots of MDA8 ozone concentrations between CMAQ model output and AQS observations from 2003-2019 for the four seasons: (a) Fall, (b) Spring, (c) Summer, and (d) Winter. Data points are color-coded by quadrant: Q1 (red) represents both model and observations exceeding 70 ppb, Q2 (blue) shows model-only exceedances, Q3 (green) indicates observation-only exceedances, and Q4 (purple) denotes both below the 70 ppb NAAQS threshold. Black dashed lines represent the 1:1 relationship, while red dashed lines show the best-fit linear regression for each region.

Figure 4-12 presents time series of MDA8 ozone quadrant analysis from 2003 to 2019, where each panel shows one of the four seasons with corresponding Q1, Q2 and Q3 percentages. From Figure 4-12, summer and fall exhibit steady decreases in all three exceedance quadrants (Q1, Q2, Q3) over the 2003-2019 period, reflecting consistent improvements in air quality during these seasons. Spring also shows a general declining trend but stands out as the only season where observation-only exceedances (Q3)

consistently exceed both Q1 and Q2 throughout the study period, suggesting the model systematically underestimates springtime ozone formation. Winter presents a contrasting pattern with Q1 and Q2 remaining relatively steady at near-zero levels, while Q3 shows a slight increasing trend over time, indicating the model's growing tendency to miss the infrequent exceedance events that occur during the cold season.

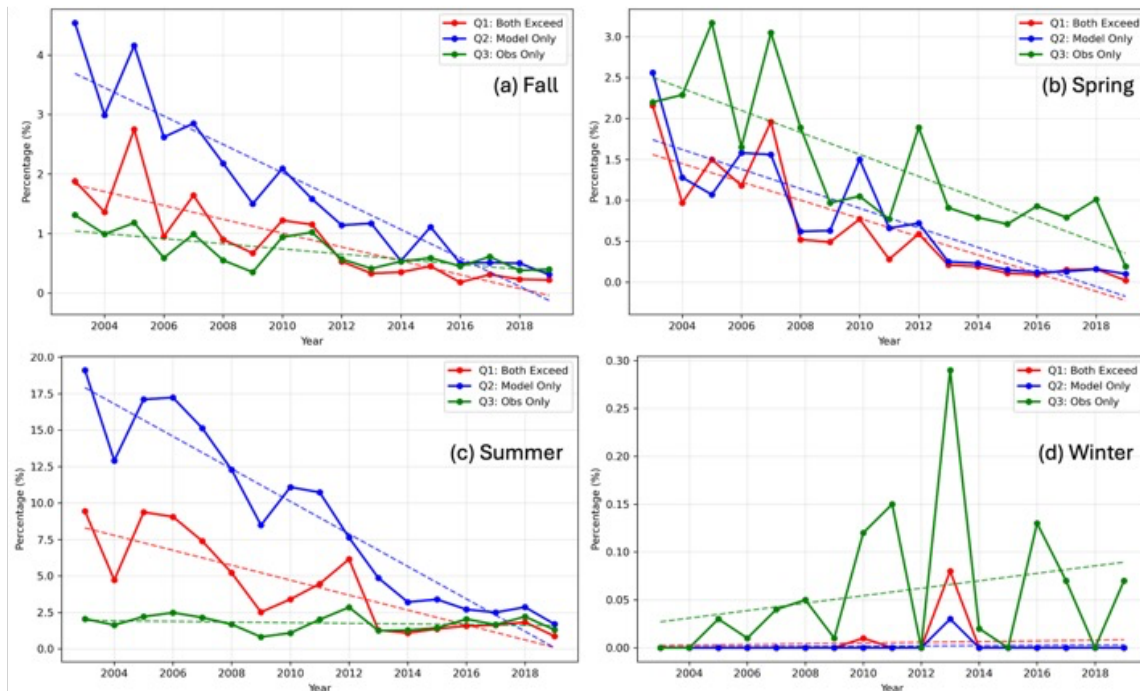


Figure 4-12: Seasonal time series of MDA8 ozone exceedance quadrant percentages from 2003-2019 for the four seasons: (a) Fall, (b) Spring, (c) Summer, and (d) Winter. Each panel shows the annual percentages of Q1 (red, both model and observations exceed 70 ppb), Q2 (blue, model-only exceedance), and Q3 (green, observation-only exceedance). Note different y-axis limits for each plot.

From Table 4-2, summer shows the highest hit rate at 69.97% but also a large false alarm rate at 9.65%, showing that the model tends to overpredict exceedances during ozone season. Spring shows the poorest hit rate at 31.19% with low false alarms (0.76%), indicating that the model frequently misses actual exceedance events during this season.

Winter shows limited activity with only an 8.32% hit rate and zero false alarms, consistent with the rarity of ozone exceedances during cold months.

4.3.2.3. Urban-Rural Quadrants

Figure 4-13 shows scatter plots of measured versus modeled MDA8 ozone for urban and rural CONUS. We define urban as the 36 km² grid around the top 30 densely populated metropolitan statistical areas and rural as the rest of CONUS. We see that urban CONUS exhibits better correlation ($R^2 = 0.607$) than rural CONUS ($R^2 = 0.543$). From Table 4-2, urban areas show a hit rate of 69.05% compared to 57.51% in rural areas, indicating better model performance in capturing ozone exceedances. Urban areas also exhibit a higher false alarm rate (5.19%) relative to rural areas (3.19%), suggesting a tendency for the model to overpredict exceedances. Overall, urban areas have a higher rate of ozone exceedances for both observed and modelled concentrations of ozone.

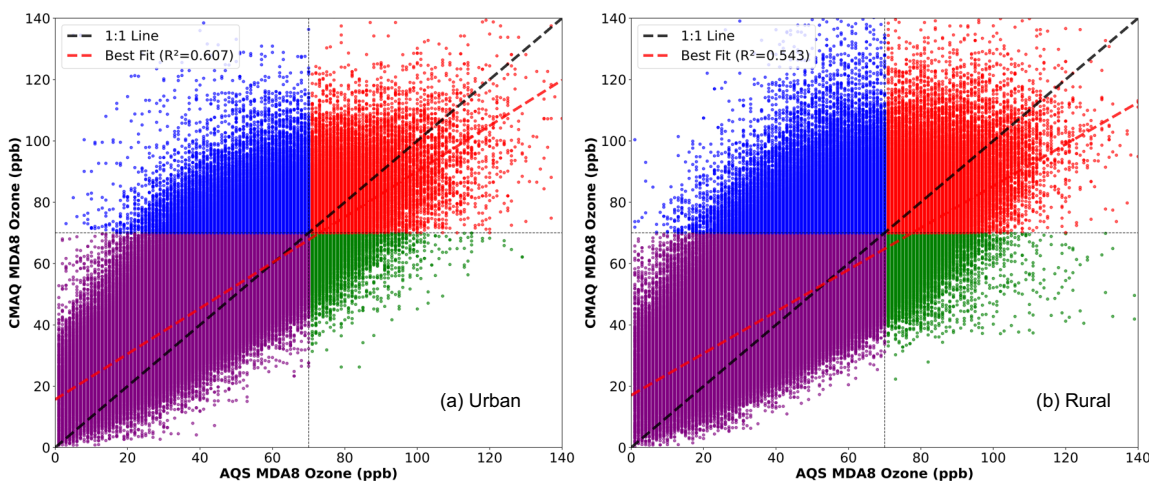


Figure 4-13: Urban and rural scatter plots of MDA8 ozone concentrations between CMAQ model output and AQS observations from 2003-2019. Data points are color-coded by quadrant: Q1 (red) represents both model and observations exceeding 70 ppb, Q2 (blue) shows model-only exceedances, Q3 (green) indicates observation-only exceedances, and Q4 (purple) denotes both below the 70 ppb NAAQS threshold. Black dashed lines represent

the 1:1 relationship, while red dashed lines show the best-fit linear regression for each region. We define urban as the 36 km² grid around the top 30 densely populated metropolitan statistical areas and rural as the rest of CONUS.

Figure 4-14 presents time series of MDA8 ozone quadrant analysis from 2003 to 2019, where each panel shows Q1, Q2 and Q3 percentages for urban and rural classifications. Both urban and rural areas exhibit steady decreases in all three exceedance quadrants (Q1, Q2, Q3) over the 2003-2019 period, reflecting consistent improvements in air quality across CONUS. After 2015, Q3 exceedances remain higher than both Q1 and Q2 exceedances in rural regions, indicating that the model underpredicts rural exceedances. The model has better performance in capturing exceedances in urban regions, with steady improvements over the study period.

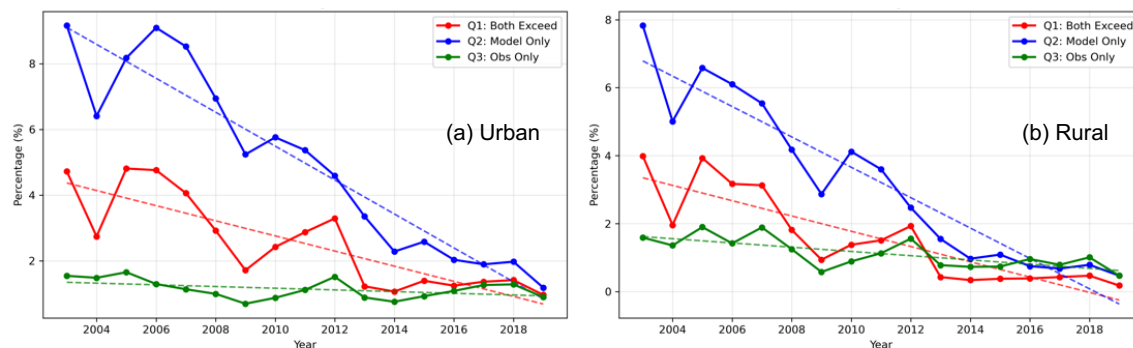


Figure 4-14: Urban-rural time series of MDA8 ozone exceedance quadrant percentages from 2003-2019. Each panel shows the annual percentages of Q1 (red, both model and observations exceed 70 ppb), Q2 (blue, model-only exceedance), and Q3 (green, observation-only exceedance). Note different y-axis limits for each plot.

Table 4-2: Statistics for MDA8 ozone exceedance predictions (>70 ppb) by geographic regions and seasons across CONUS from 2003-2019 using a quadrant analysis framework.

Label	Q1 (%)	Q2 (%)	Q3 (%)	Q4 (%)	Hit (%)	False Alarm (%)	Accuracy (%)	R²	Bias (ppb)	RMSE (ppb)
CONUS	1.68	3.43	1.11	93.78	60.1	3.53	95.46	0.556	3.86	10.4
Urban	2.54	5	1.14	91.33	69.05	5.19	93.86	0.607	5.22	11.48
Rural	1.5	3.11	1.11	94.29	57.51	3.19	95.79	0.543	3.58	10.16
Regions										
NW	0.29	0.69	0.33	98.69	46.42	0.7	98.97	0.519	3.43	9.3
SW	2.32	2.97	2.14	92.58	52.04	3.11	94.89	0.57	1.72	9.89
NGP	0.03	0.23	0.17	99.57	13.85	0.23	99.6	0.479	0.99	7.67
SGP	1.4	3.08	0.84	94.69	62.46	3.15	96.08	0.564	5.16	10.86
MW	1.57	4.09	0.83	93.51	65.33	4.19	95.08	0.575	4.87	10.56
NE	1.76	3.89	0.61	93.74	74.11	3.98	95.5	0.596	4.26	10.36
SE	1.3	4.37	0.63	93.7	67.39	4.46	95	0.506	5.87	11.42
Seasons										
Spring	0.63	0.75	1.39	97.23	31.19	0.76	97.86	0.449	-0.76	8.47
Summer	4.19	9.07	1.8	84.94	69.97	9.65	89.13	0.515	7.39	13.17
Fall	0.84	1.7	0.67	96.78	55.62	1.73	97.62	0.597	5.14	9.84
Winter	0.01	0	0.06	99.93	8.32	0	99.94	0.423	3	8.02

4.3.3. Ozone Exceedance Analysis

Thus far in this chapter, we have compared and validated CMAQ model output against AQS observed MDA8 ozone concentrations. However, large portions of CONUS remain unmonitored by AQS sites. Although ozone is a criteria pollutant with observation stations

in all CONUS states, there are still gaps in the monitoring network, particularly in rural and sparsely populated areas. In this section, we examine CMAQ model derived MDA8 ozone concentrations in these unmonitored areas. We define a monitored area as any CMAQ grid cell containing an AQS site plus the surrounding 3x3 grid cells. All remaining grid cells are classified as unmonitored.

The daily maximum ozone concentrations, in unmonitored areas throughout 2019, exhibit a characteristic bell-shaped curve spanning March through October, with mean maximum values peaking in July and absolute maximum concentrations in April as shown in **Figure 4-15**. Daily exceedance counts are highest during March and April. The monthly mean exceedance counts as shown in **Figure 4-16** show peak values in April and July, indicating sustained periods of elevated ozone concentrations.

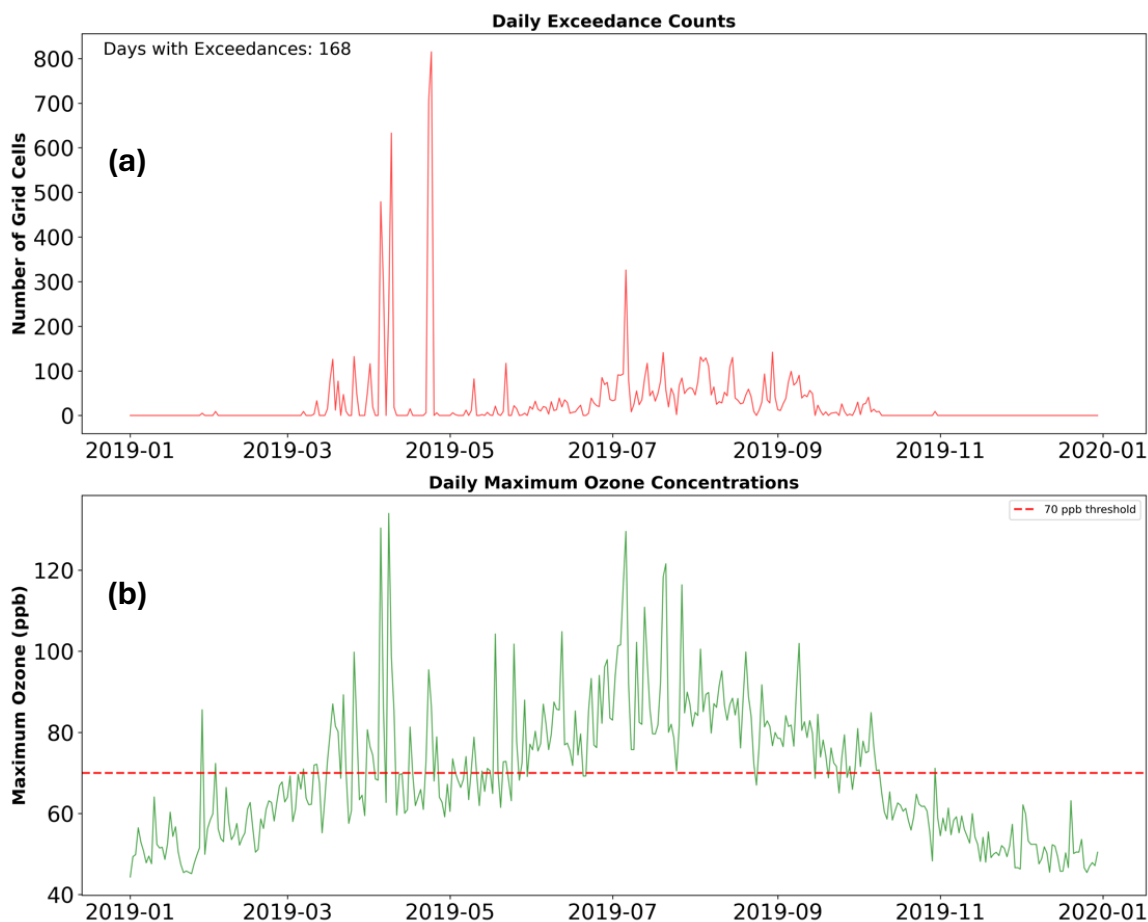


Figure 4-15: Daily potential MDA8 ozone exceedance events (>70 ppb) for 2019 in areas without AQS monitoring sites based on CMAQ model predictions. (a) Daily count of grid cells exceeding the 70 ppb threshold in unmonitored areas. (b) Daily maximum MDA8 ozone concentrations across all unmonitored grid cells. We define a monitored area as any CMAQ grid cell containing an AQS site plus the surrounding 3x3 grid cells. All remaining grid cells are classified as unmonitored.

The data reveal that April is the most problematic month for unmonitored areas, accounting for 3,342 total exceedance events (30% of the annual total) with up to 1.76% of all unmonitored grid cells exceeding the NAAQS threshold simultaneously. July and August also show significant exceedance activity though the spatial extent is more limited. This shows the importance of enhanced monitoring coverage during spring and summer months when photochemical ozone formation is most active in areas currently lacking routine air quality surveillance.

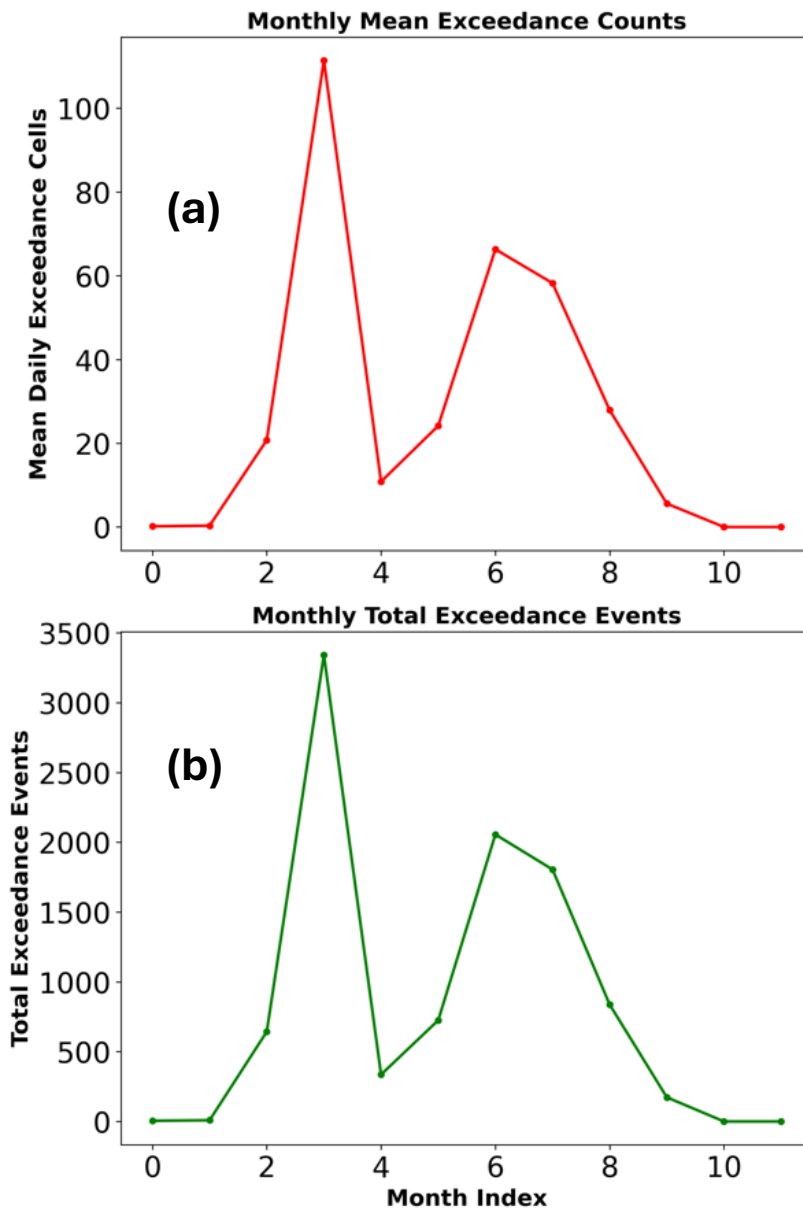


Figure 4-16: Monthly MDA8 ozone exceedance events (>70 ppb) for 2019 in areas without AQS monitoring sites based on CMAQ model predictions. (a) Monthly mean of daily exceedance counts in unmonitored areas. (b) Monthly total exceedance events across all unmonitored grid cells. We define a monitored area as any CMAQ grid cell containing an AQS site plus the surrounding 3x3 grid cells. All remaining grid cells are classified as unmonitored.

The contrast between spring and summer exceedance patterns in unmonitored areas suggests that the current AQS monitoring network may be strategically positioned to

capture summer ozone events but potentially overlooks early spring exceedances. While July shows high mean maximum ozone concentrations, the relatively lower exceedance counts compared to April indicate that existing monitoring stations are likely well positioned in areas prone to summer photochemical ozone formation. The April exceedances suggest that spring ozone formation may occur in geographic areas not adequately represented by the current monitoring network. The current monitoring strategy, designed around well-established summer ozone patterns, may need reevaluation to capture these spring events that could affect air quality management decisions and public health protection in under monitored regions.

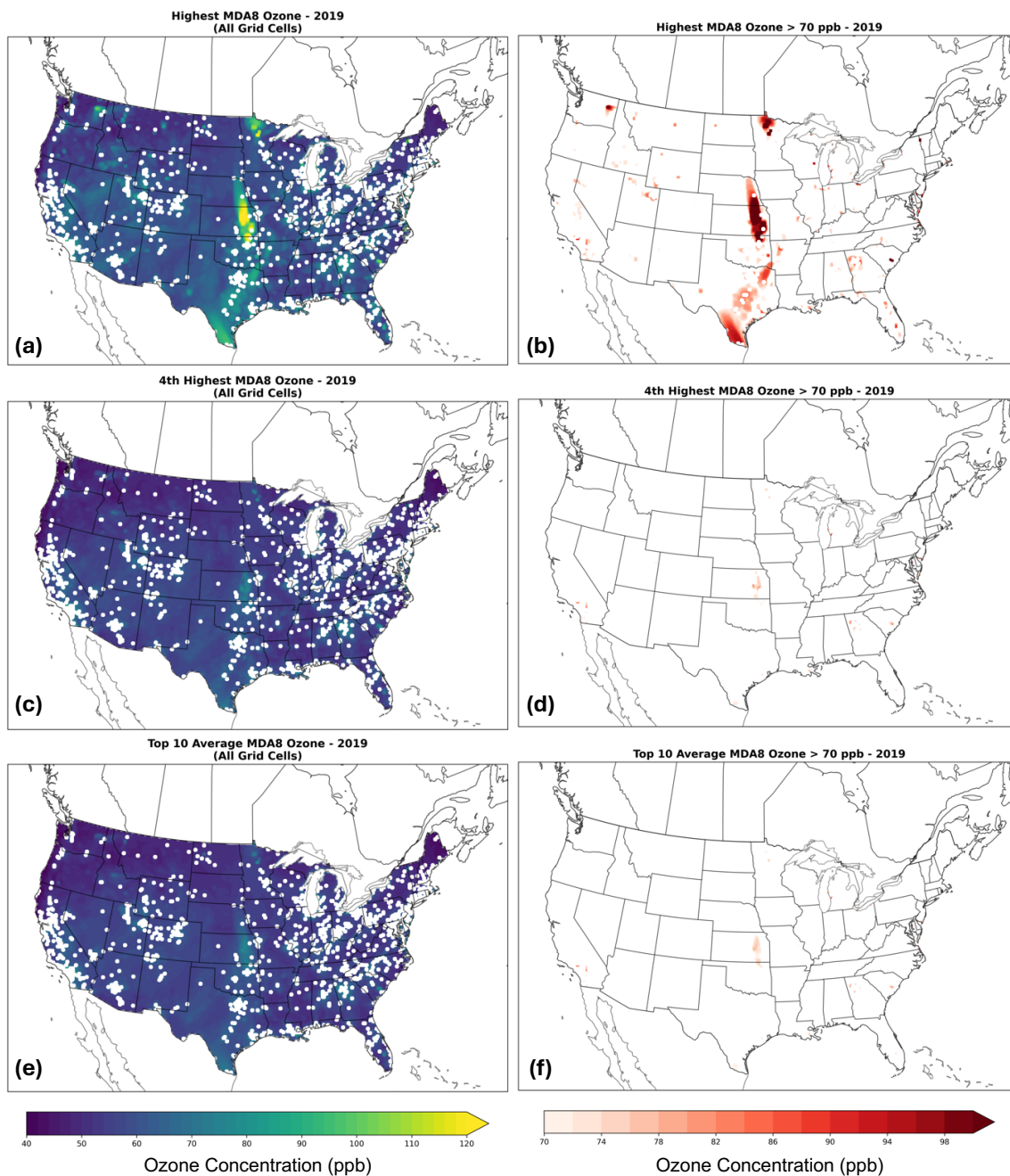


Figure 4-17: Spatial distribution of MDA8 ozone across CONUS for 2019 based on CMAQ model predictions for unmonitored grid cells. (a) Maximum MDA8 ozone values (b) Maximum MDA8 ozone values exceeding 70 ppb (c) Fourth highest MDA8 ozone values (d) Fourth highest MDA8 ozone values exceeding 70 ppb (e) Top 10 average MDA8 ozone values (f) Top 10 average MDA8 ozone values exceeding 70 ppb. All panels show only grid cells excluding AQS monitoring locations. We define a monitored area as any CMAQ grid cell containing an AQS site plus the surrounding 3x3 grid cells. All remaining grid cells are classified as unmonitored.

In **Figure 4-17**, we see large contiguous areas in Texas, Oklahoma, Kansas, Nebraska, and Minnesota show elevated ozone concentrations that are unmonitored by the current AQS station distribution, with substantial overlap with the breadbasket states (the major grain-producing regions of the CONUS) in panels (a) and (b). These areas experience emissions from fertilizer application, livestock operations, crop residue burning, and seasonal prescribed burning practices that can cause localized high ozone concentrations. High ozone areas are also scattered throughout other regions, suggesting that the current monitoring strategy may be primarily focused on urban and industrial centers while potentially overlooking rural and agricultural areas which could impact both agricultural productivity and rural population health. In panels (d) and (f), fewer areas are highlighted but still show regions in the Northeast and California, along with the patch above Texas, indicating that even when considering fourth highest and top 10 average values, significant unmonitored exceedance zones persist.

4.4. Conclusions and Future Perspectives

In this chapter, we performed an evaluation of the CMAQ model performance for MDA8 ozone predictions across CONUS from 2003 to 2019. We first analyze overall model capability, and this analysis reveals that CMAQ demonstrates generally decent performance with an overall $R^2 > 0.7$ of modeled versus observed MDA8 ozone. However, there is a consistent positive bias in the model predictions of MDA8 ozone. We explored the regional and seasonal behavior of MDA8 variability. The Midwest and Southern Great Plains show the strongest correlations of measured versus modeled MDA8 ozone, while the Northwest exhibits the poorest model performance. All regions of the CONUS

experience a systematic overestimation of MDA8 ozone. CMAQ performs best during fall and winter but struggles during summer, showing the largest bias and weakest correlation during this peak photochemical season.

Figure 4-18 presents the time series of CMAQ model accuracy in predicting MDA8 ozone across CONUS, by urban-rural classifications, geographical regions and seasons. The results affirm that urban areas exhibit lower model accuracy than rural areas and, consequently, lower accuracy than the overall CONUS values. Among regions, the Southern Great Plains and Northwest demonstrate the highest overall accuracy across all years. The Southeast begins with the lowest accuracy but shows significant improvement after 2010, while the Southwest currently exhibits the poorest accuracy. Seasonally, winter shows a slight decrease in accuracy over time, although it maintains higher accuracy than other seasons throughout the study period. The most substantial improvement occurs in summer, with model prediction accuracy increasing from less than 80% in 2003 to more than 95% in 2019.

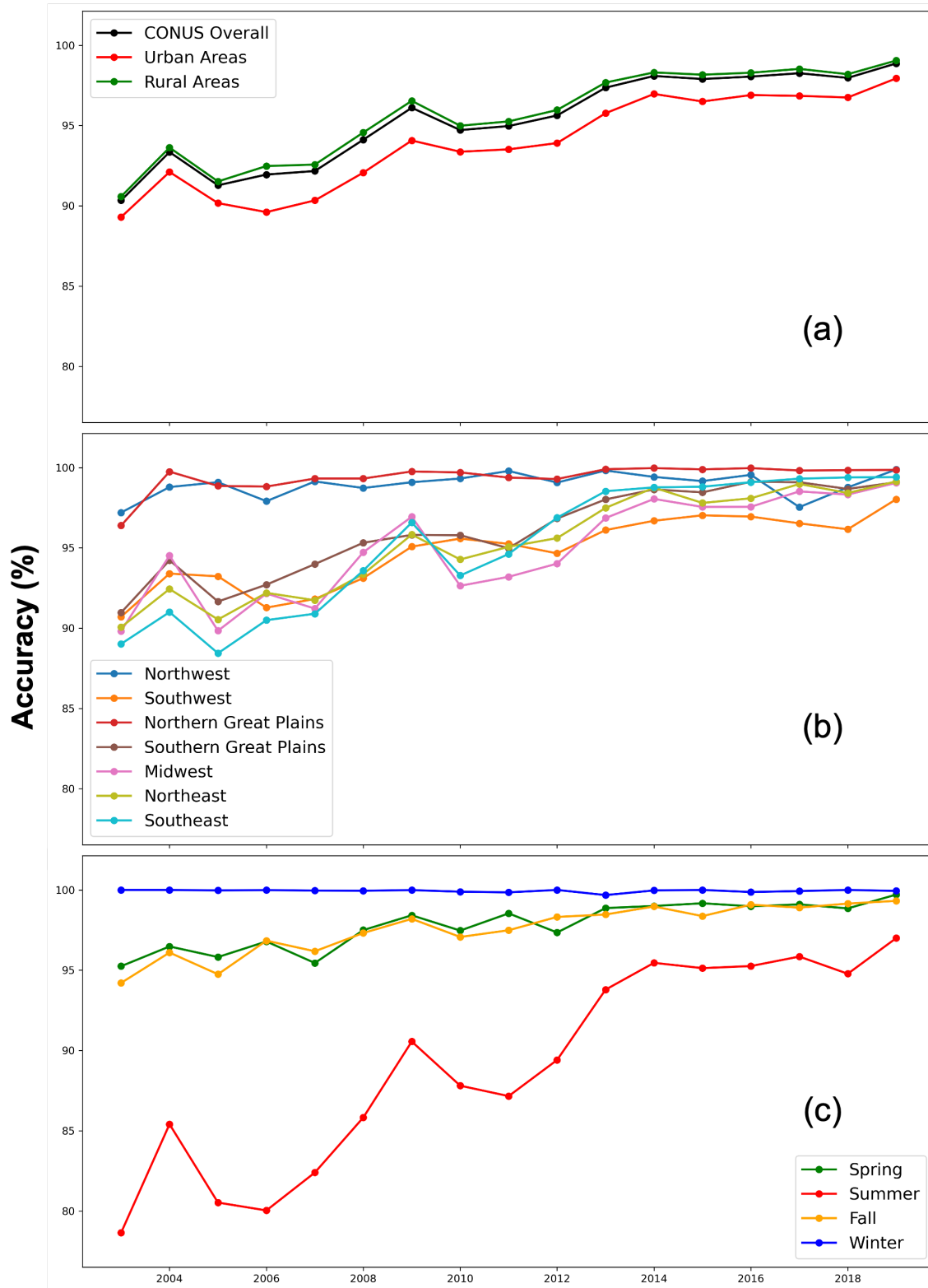


Figure 4-18: Temporal evolution of CMAQ model accuracy (Equation 4-3) in predicting MDA8 ozone across CONUS from 2003 to 2019 by (a) urban-rural classification, (b) geographical regions and, (c) seasons.

Next, we examined model performance in determining ozone exceedances (> 70 ppb NAAQS standard for MDA8 ozone). CMAQ correctly classifies $>90\%$ of non-exceedance conditions. However, CMAQ demonstrates a tendency toward false positives (incorrectly predicting exceedances). The regional disparities in hit rates (accuracy in predicting exceedances) range from very poor performance ($\sim 13\%$) in the Northern Great Plains to decent performance in the Northeast ($>70\%$). Summer exhibits the highest exceedance activity and the largest false positive rate, while spring frequently shows the poorest hit rate, with CMAQ missing the most exceedance events. Summer and fall exceedance quadrants decrease steadily over the years due to improved model performance and ozone conditions in the CONUS.

Spring remains difficult to understand as it is the only season where observational exceedances consistently exceed model predictions. Recent studies show that spring ozone exceedances have different photochemistry than summer events, with the eastern U.S. experiencing a seasonal shift in peak ozone from summer to spring (Chang et al., 2025; Ring et al., 2023). Winter and spring exceedances have also increased in oil and natural gas regions due to temperature inversions and snow albedo effects (Caputi et al., 2025). These changes in seasonal patterns suggest that spring exceedances are not only due to expansion of the traditional ozone season but also due to different meteorological and chemical regimes that current models may not adequately represent. Winter shows a slight increasing trend in missed CMAQ prediction of exceedances, despite having a low number of exceedances.

We then use the CMAQ model output in areas of the CONUS where there are no AQS monitoring sites to understand the current coverage of ozone monitoring. We identify regions with potential MDA8 ozone exceedances, particularly in agricultural breadbasket states such as Texas, Oklahoma, Kansas, Nebraska, and Minnesota. We suggest that current monitoring strategies may overlook significant air quality issues in rural and agricultural regions.

Several key limitations of this analysis point toward future research needs. We evaluate model performance primarily on statistical metrics without examining underlying chemical and meteorological processes driving model errors. We do not answer why the model has a systematic overestimation problem, and why the spring season does not follow the same patterns as the rest of the seasons. We also do not have an explanation of the regional variabilities in the model performance. While revealing concerning exceedance patterns, the unmonitored area analysis lacks ground-truth validation and may reflect model biases rather than actual air quality conditions. This limitation further supports the need for better and wider ground-based measurements from aircraft campaigns and additional monitoring sites.

Future work should incorporate process-level model evaluation, enhanced emissions inventory understanding for agricultural regions, nighttime ozone photochemical representation and field campaigns to validate predicted exceedances in unmonitored areas. The shift toward year-round monitoring from only ozone season monitoring represents

positive progress. Gaps in spatial coverage in the breadbasket states limit understanding and estimating agricultural productivity and the health of rural populations.

5. Concluding Remarks and Future Work Recommendations

5.1. *Chapter Summaries*

In Chapter 1, we study the foundations of ozone chemistry, beginning with the non-linear relationship between ozone and its precursors. We introduced the concept of OPRs and explained why understanding whether ozone formation is VOC-limited or NO_x -limited is essential for designing effective control strategies. Depending on the OPR, reducing one precursor has more impact than the other. This explains the need for OPR specific strategies that ultimately reduce both NO_x and VOCs. We then examined how meteorology and climate change add additional layers of difficulty to understanding surface ozone chemistry, as temperature and atmospheric circulation patterns influence ozone formation and transport, complicating both prediction and mitigation efforts. The chapter provided an overview of ozone precursors, describing their sources, both anthropogenic and biogenic, and the various measurement techniques used to quantify them, from ground-based monitors to satellite retrievals. We discussed the health impacts of ozone and its precursors, establishing why ozone research is a critical public health issue. Finally, we highlight the unequal distribution of tropospheric ozone across the United States. Socioeconomically disadvantaged communities disproportionately experience higher ozone levels due to historical patterns of industrial siting, highway placement, and residential segregation.

In Chapter 2, we looked at OPRs across the CONUS during summer 2016 by comparing HCHO and NO_2 retrievals from OMI with CAMx model output. OMI provides tropospheric column-integrated values once per day in the afternoon, offering valuable

spatial coverage but limited temporal and vertical information. We leveraged CAMx to overcome these limitations, using its hourly output to track the diurnal evolution of OPR and identify when and where OPR transitions occur throughout the day. Additionally, we exploited the model's vertical resolution to calculate OPR within the PBL and for the entire tropospheric column. After validating the model against satellite observations, we used CAMx to reveal limitations in using satellite-derived OPR as a proxy for surface ozone chemistry. To address this gap, we developed a new metric called β that quantifies where satellite information reliably represents surface conditions and where caution is needed. This metric helps identify regions that require additional ground-based and aircraft measurements to properly characterize near-surface ozone production chemistry.

In Chapter 3, we addressed the uneven spatial distribution of ground-based AQS monitoring stations for ozone precursors, specifically HCHO and NO₂. While ozone is measured extensively, its precursors have significant monitoring gaps despite being crucial for understanding ozone formation and its abatement strategies. HCHO measurement is especially necessary because it is also a carcinogen with direct public health implications. We developed a flexible framework for monitor placement that combines socioeconomic variables, population density, and TEMPO-retrieved concentrations of NO₂ and HCHO. This approach identifies where new stations would provide the most balanced coverage by accounting for both pollution patterns and vulnerable populations. We demonstrated this method for summer 2024 across the CONUS at the county level, though the framework is readily adaptable to other time periods, regions, and spatial resolutions. The flexibility of

our approach allows stakeholders to include as many or as few variables as needed depending on their monitoring objectives.

In Chapter 4, we evaluate long-term CMAQ model predictions of ozone from 2003 to 2019 across CONUS, examining model performance across different regions, seasons, and years with particular focus on MDA8 ozone and exceedance detection capability. Using ground-based AQS measurements as truth, we find the model achieves good overall correlation but exhibits consistent positive bias and substantial regional variability, with the strongest performance in the Midwest and poorest in the Northwest. Summer shows the weakest predictive skill despite being the most critical season for regulatory compliance, while the model struggles to capture springtime exceedances. We reveal significant disparities in exceedance detection capability across regions and identify potential annual exceedance events in unmonitored areas, particularly in agricultural breadbasket states. These findings highlight critical gaps in model accuracy and monitoring coverage that impacts regulatory air quality management.

5.2. Future Work Ideas

An important extension of Chapter 2 would be to calculate β during winter months, when ozone concentrations are increasing and models struggle to capture observed trends. Wintertime photochemistry is fundamentally different due to reduced solar radiation, shallower boundary layers, longer NO_x lifetimes, and reduced biogenic VOC emissions. Summer β values likely cannot be reliably used in winter conditions. We would expect winter β to show systematically lower values due to weaker vertical mixing and reduced

photochemical activity, meaning satellite column observations may be even less representative of surface chemistry than in summer.

Chapter 3 analysis can be extended to understand how large an area does each ozone or precursor monitor represent. Future work can address this by mapping coverage areas around existing AQS stations at different distances to identify where measurements remain representative versus where they diverge. We expect urban monitors to represent smaller areas due to steep pollution gradients, while rural monitors likely capture broader regions. Using satellite data, we could determine characteristic distances where correlations break down. This analysis would reveal optimal spacing between monitors.

To enhance the analysis in Chapters 4, it would be valuable to separate and quantify changes in the annual cycle from long-term trends over the entire study period. Given that most improvements in model performance occur during the summer, a straightforward approach would be to analyze JJA averages as a time series. To detect the changes in the annual cycle itself, we could construct a climatological annual mean and plot anomalies relative to this baseline. This approach would help distinguish between systematic bias and random error in the annual cycle versus the mean change, which would strengthen the interpretation of model performance evaluation. Another refinement would be establishing a significance threshold that accounts for combined observational and model uncertainty. AQS monitors have measurement uncertainties, while CMAQ has uncertainties from meteorological inputs, emissions inventories, and chemical parameterizations.

In Chapter 4, we have evaluated CMAQ model performance across various temporal, seasonal and regional scales. We documented instances where the model successfully captures observed ozone patterns as well as cases with substantial discrepancies. These assessments have provided valuable benchmarks for understanding model skill under different conditions and have highlighted both the strengths and limitations of current air quality modeling approaches. However, while identifying where and when the model performs poorly is an important first step, it does not explain why these differences occur. Understanding the underlying causes of model-observation disagreements is essential for improving air quality predictions, refining emissions inventories, and advancing our representation of atmospheric chemical and physical processes.

The work in this section presents preliminary explorations into the factors driving these discrepancies. This work serves as a foundation for future investigations that will more thoroughly examine the reasons for model error. The analyses that follow identify key patterns in where, when, and under what conditions the largest disagreements occur. We establish a roadmap for the deeper diagnostic work needed to advance model development and ultimately improve air quality predictions. The data discussed below has been described in Chapter 4.

Figure 5-1 presents the frequency of absolute differences in the MDA8 ozone concentrations between CMAQ modelling and AQS observations from 2003 to 2019. This figure reveals the extent and magnitude of model-observation discrepancies. The distribution exhibits a smooth, monotonic decrease with increasing difference. This

decrease suggests that while the model captures ozone variability reasonably well for most locations, there are a non-trivial number of instances with substantial bias. The bimodal color scheme differentiates systematic bias direction: red bars indicate instances where CMAQ underestimates MDA8 ozone, while blue bars represent overestimation of MDA8 ozone. The decline in frequency indicates that while extreme model-observation deviations are rare, further investigation is needed to understand the potential sources of these extreme differences.

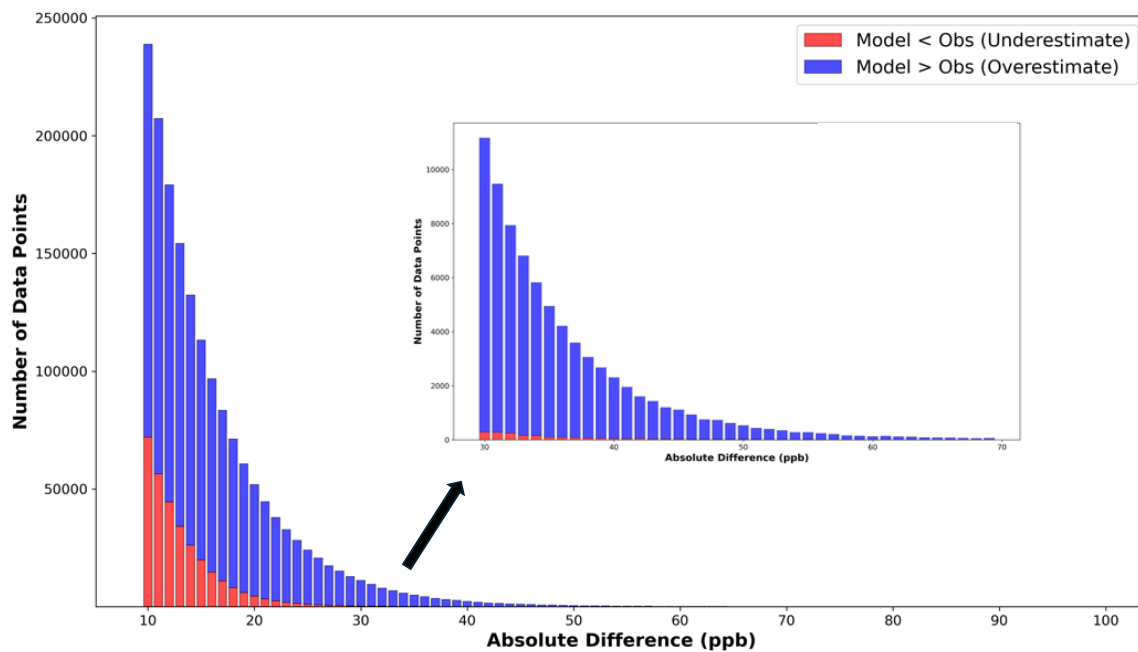


Figure 5-1: Frequency distribution of absolute differences between CMAQ-modeled and AQS-observed MDA8 ozone from 2003 to 2019. Red bars indicate model underestimation (CMAQ < AQS); blue bars indicate overestimation (CMAQ > AQS). Inset shows detail for the 30–70 ppb range.

Looking at the model-observation differences in Figure 5-1, we now want to understand what drives these discrepancies, particularly in cases of extreme differences. We focus on AQS sites where the absolute difference is higher than 70 ppb because these

are instances where model performance is notably poor. As a first step in this analysis, we examine the spatial distribution of these extreme differences across the CONUS to identify whether particular regions or geographic features are associated with larger errors. **Figure 5-2(a)** maps the unique location of all AQS locations with differences of 70 ppb or greater, with color coding to distinguish between inland locations (red) and areas near water bodies (blue). This spatial perspective allows us to assess whether proximity to coastlines, lakes, or other water features plays a role in model bias.

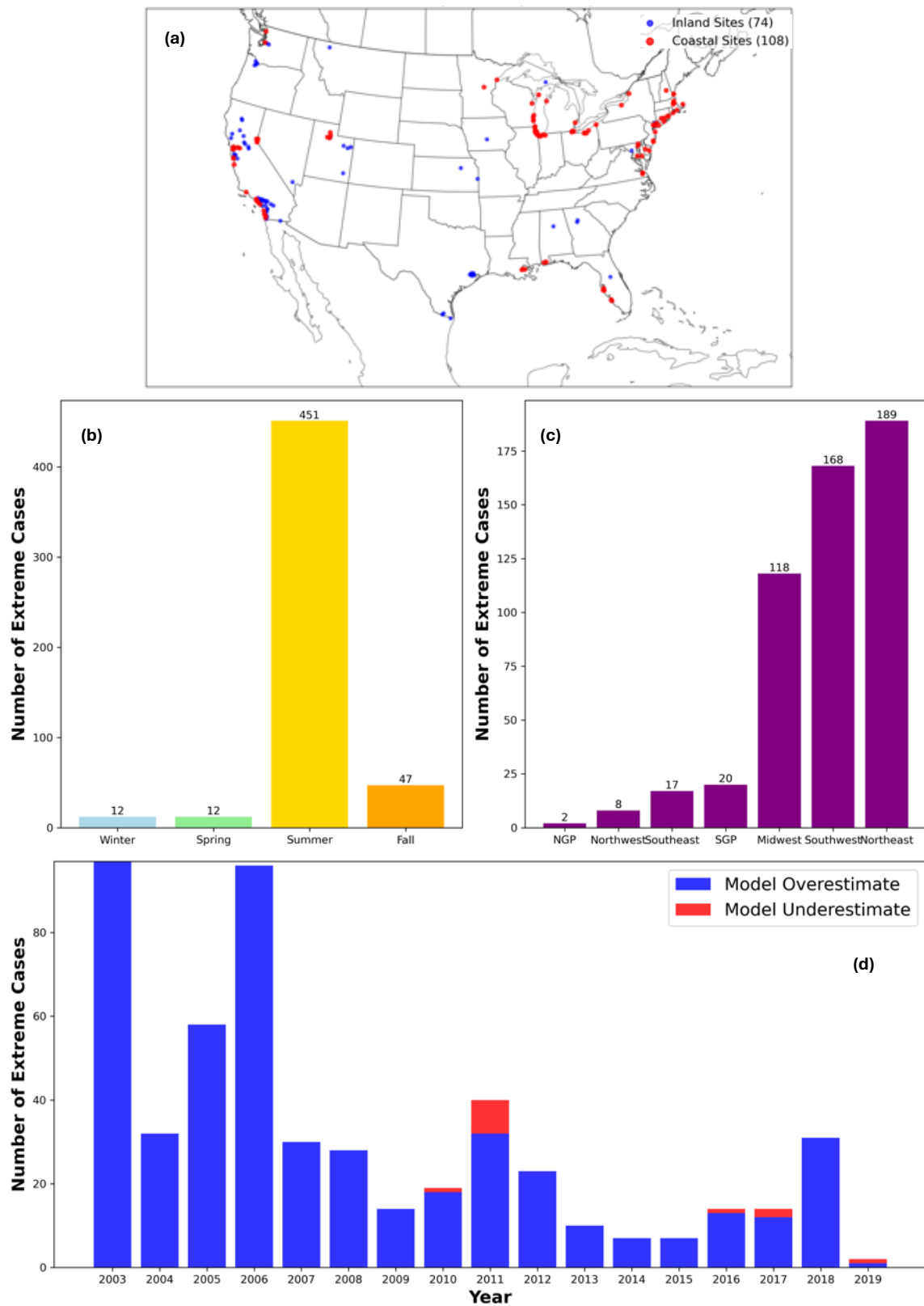


Figure 5-2: AQS locations with absolute differences ≥ 70 ppb between CMAQ-modeled and AQS-observed MDA8 ozone concentrations across CONUS from 2003 to 2019. (a)

spatial distribution where red points indicate inland locations and blue points indicate locations near water bodies, (b) seasonal distribution, (c) regional distribution and (d) timeseries.

Figure 5-2 also details the seasonal and regional patterns of extreme model-observation disagreements, defined as differences exceeding 70 ppb. Panel (b) shows a clear seasonal pattern, with summer recording the highest frequency of extreme differences by a substantial margin, followed by fall. Winter and spring exhibit notably fewer cases. Panel (c) shows the regional distribution across CONUS, revealing that the Northeast, Southwest, and Midwest experience the highest numbers of extreme differences. The remaining regions show considerably lower instances. These extreme differences were most prevalent prior to 2009 and have decreased since as seen in panel (d). However, we still see high frequency of extreme differences in 2011 and 2018.

5.2.1. Possible Sources for Model Discrepancy

5.2.1.1. Reason 1: EPA Gridding Methodology

In Figure 5-1 and Figure 5-2, we followed the standard EPA methodology for comparing AQS observations with model output. This approach identifies the grid cell closest to each AQS monitor location, then takes a 3x3 grid around it and selects the maximum value from those nine cells as the corresponding model value. This methodology was developed under the assumption that each monitor represents the regional chemistry of its surrounding area. However, we suspect that ozone pollution has evolved from a regional problem to a more localized one, making the 3x3 grid approach potentially outdated.

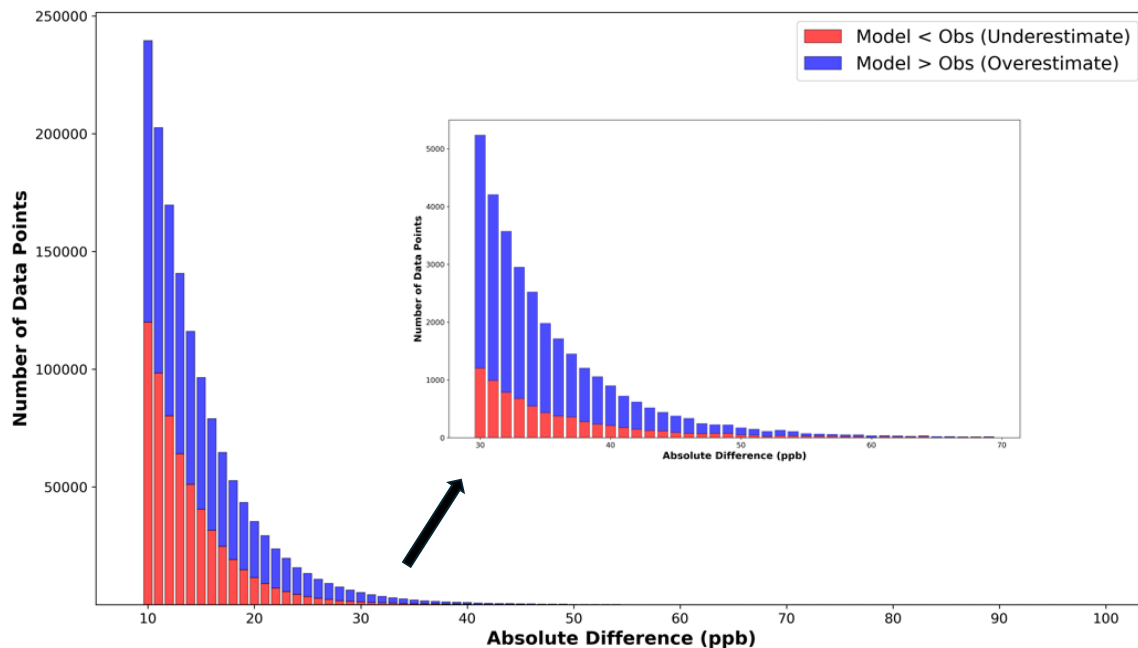


Figure 5-3: Frequency distribution of absolute differences between CMAQ-modeled and AQS-observed MDA8 ozone from 2003 to 2019 using 1x1 grid. Red bars indicate model underestimation (CMAQ < AQS); blue bars indicate overestimation (CMAQ > AQS). Inset shows detail for the 30–70 ppb range.

To test this hypothesis, we recomputed the comparisons using an exact grid match (1x1 grid). We regenerated the analysis as **Figure 5-3** and **Figure 5-4**. We then see notable differences in the model-observation discrepancy patterns. While the frequency distribution still peaks at 10 ppb difference, the decline is steeper and less smooth compared to the 3x3 grid approach. More significantly, the fraction of model underestimations (red portion of the bars) is considerably larger with the 1x1 grid method and remains elevated even when examining the 30-70 ppb range. The number of unique locations showing extreme discrepancies (>70 ppb) drops dramatically from 184 to just 45 sites, indicating that much of the apparent model error was an artifact of the gridding methodology rather than an actual model deficiency. However, we also see an increase in model underestimation with the 1×1 method which suggests that the relationship between

gridding methodology and model performance is more complicated. Further analysis is needed to determine which grid cells within the 3×3 grid contribute to the maximum values. If specific grid cells within the 3×3 grid drive the discrepancies, this would support the gridding methodology hypothesis otherwise it would indicate underlying model issues.

The change in methodology also reveals different seasonal and regional patterns. While summer and fall previously had the highest discrepancies, winter now becomes the second most problematic season, a finding that was missed by the 3×3 grid approach. Regionally, Southwest, Midwest, and Southern Great Plains become the top three regions with the largest discrepancies, while the Northeast drops out of the top three. These findings suggest that gridding methodology substantially influences our interpretation of model performance. However, whether the 3×3 gridding approach conceals genuine model errors requires further investigation.

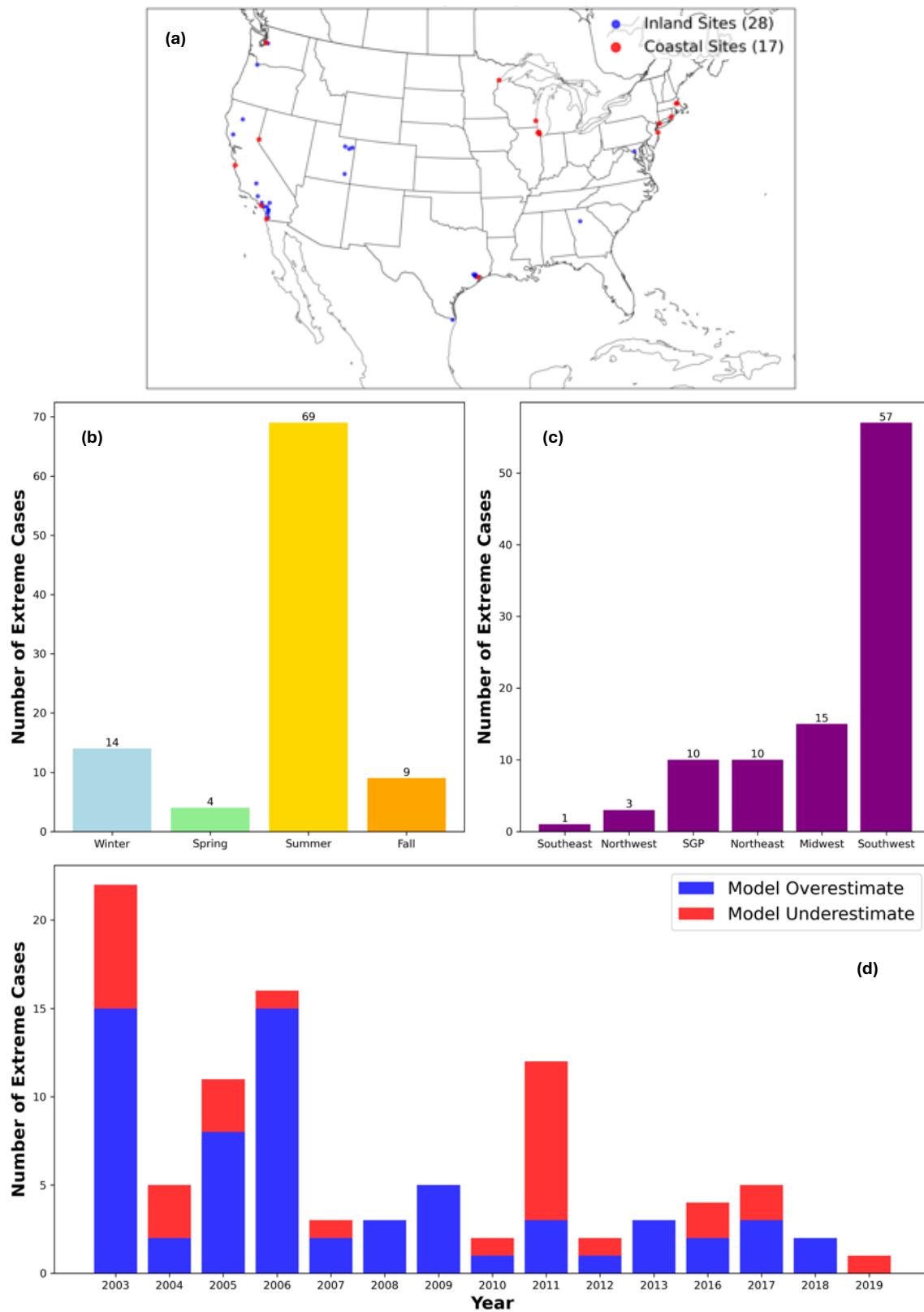


Figure 5-4: AQS locations with absolute differences ≥ 70 ppb between CMAQ-modeled and AQS-observed MDA8 ozone concentrations across CONUS from 2003 to 2019 using

a 1x1 grid. (a) spatial distribution where red points indicate inland locations and blue points indicate locations near water bodies, (b) seasonal distribution and (c) regional distribution and (d) timeseries.

In the future, a comprehensive investigation into gridding methodologies is needed due to the impact of the choice between 3x3 maximum and 1x1 exact matching on our results. Beyond these two approaches, numerous other methods should be analyzed that could lead to different interpretations of model performance. For example, we could use the mean of the nine grid cells, to provide an average representation of the surrounding area. Averaging will potentially smooth out localized highs and lows in the concentration of ozone. We could also take the minimum of the nine cells. This method could better represent background conditions and assess baseline ozone. We could also use the median of the nine cells to reduce the influence of outliers.

We can also explore different weighted gridding methods, such as distance-weighted averaging, where grid cells closer to the site are weighted higher than those further away. A population-weighted approach can be tested that prioritizes grid cells with higher population density. We could also employ an inverse-distance squared weighting scheme that emphasizes nearest neighbors. Angular distance weighting is another approach where weighting grid cells is based on distance and angle from the site. Each of these methodologies represents different assumptions about what the monitor represents and how the model should be evaluated in relation to observations. A systematic comparison across multiple gridding approaches is essential to ensure that our model evaluation is robust and not influenced by methodological choices. Another potential source of model discrepancy may stem from spatial allocation errors in the emissions inventory. Emission sources could

be incorrectly assigned to model grid cells leading to the distribution of emissions across different sectors not accurately representing actual source locations.

5.2.1.2. Reason 2: Wildfire Effects

The second potential source of discrepancy we explore involves wildfire events. One particularly notable case occurred on September 5, 2017, across Washington and Oregon in the Pacific Northwest. During this time, the region experienced intense wildfire activity due to the Eagle Creek Fire that started on September 2 in the Columbia River Gorge and burned over 48,000 acres. The smoke plumes from these fires created severe air quality problems throughout this region. We see that CMAQ overestimated ozone concentrations by more than 70 ppb at multiple monitoring sites on September 5, 2017. This overestimation during an active fire raises questions about how well the model represents wildfire emissions and atmospheric chemistry under smoky conditions. We examine this case in detail to gain a better understanding of what might be driving such significant errors when wildfires are present.

Figure 5-5 shows the differences in modeled and observed concentrations of ozone, PM_{2.5}, NO₂ and HCHO during the wildfire event in the Pacific Northwest on Sept 5, 2017. For PM_{2.5}, AQS observations are substantially higher than CMAQ predictions, indicating that the model significantly underestimates particulate matter concentrations. This underestimation can be from a variety of reasons such as due to errors in wildfire emissions, errors in smoke plume injection heights or limitations in capturing the formation of secondary organic aerosols under high smoke conditions. In contrast, the model

overestimates ozone concentrations relative to observations. This opposing behavior where CMAQ underestimates PM_{2.5} while overestimating ozone suggests possible flaws in how the model handles NO_x titration processes within dense smoke plumes. Under heavy particulate loading, NO_x emitted from fires should react with and consume ozone, suppressing ambient ozone concentrations. These hypotheses warrant further investigation to determine which mechanisms are most responsible for the observed discrepancies.

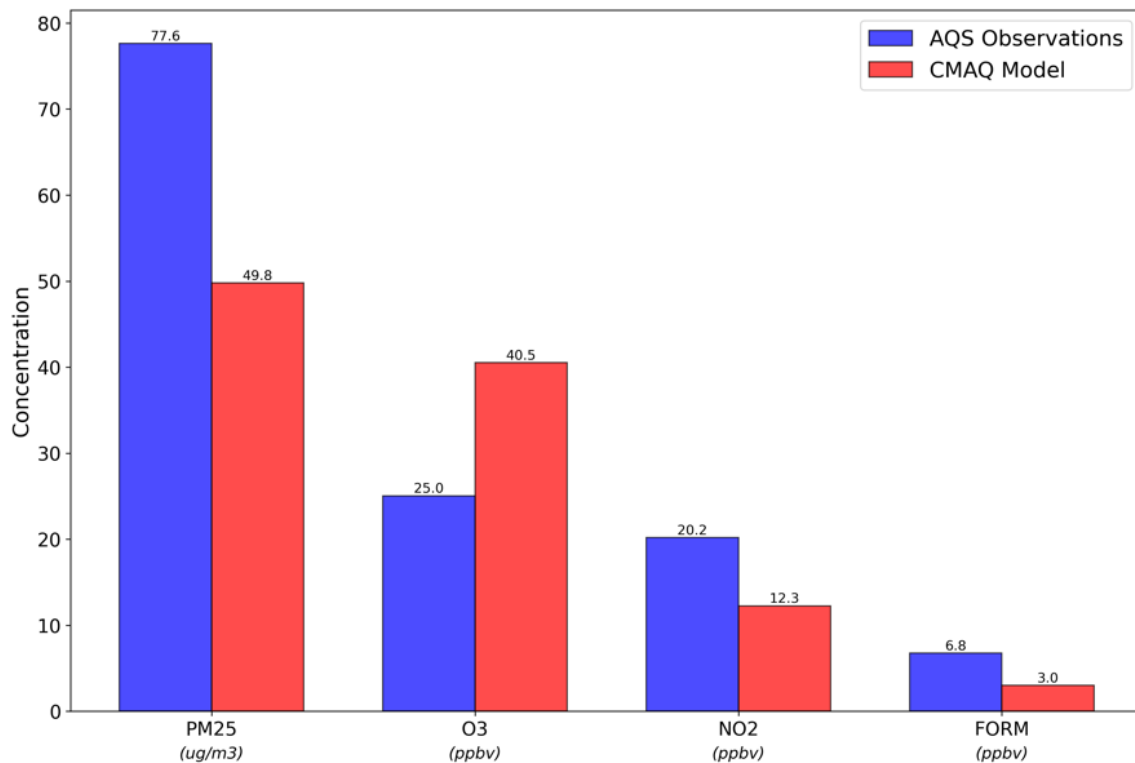


Figure 5-5: Comparison of CMAQ-modeled (red) and AQS-observed (blue) concentrations for PM_{2.5}, ozone, NO₂, and HCHO across the Pacific Northwest on September 5, 2017, during the Eagle Creek Fire event.

Figure 5-6 displays the distribution of CMAQ modeled concentrations across the Pacific Northwest during the wildfire event. HCHO and PM_{2.5} maps show clear fire hotspots with elevated concentrations near the wildfire source regions. NO₂ shows a fainter

spatial signal near the wildfire locations. The ozone map is spatially mixed, lacking any visible wildfire hotspots. The contrasting spatial patterns of these pollutants, with strong wildfire signatures in $\text{PM}_{2.5}$ and HCHO and the lack of a wildfire signature in the distribution of ozone, require further investigation.

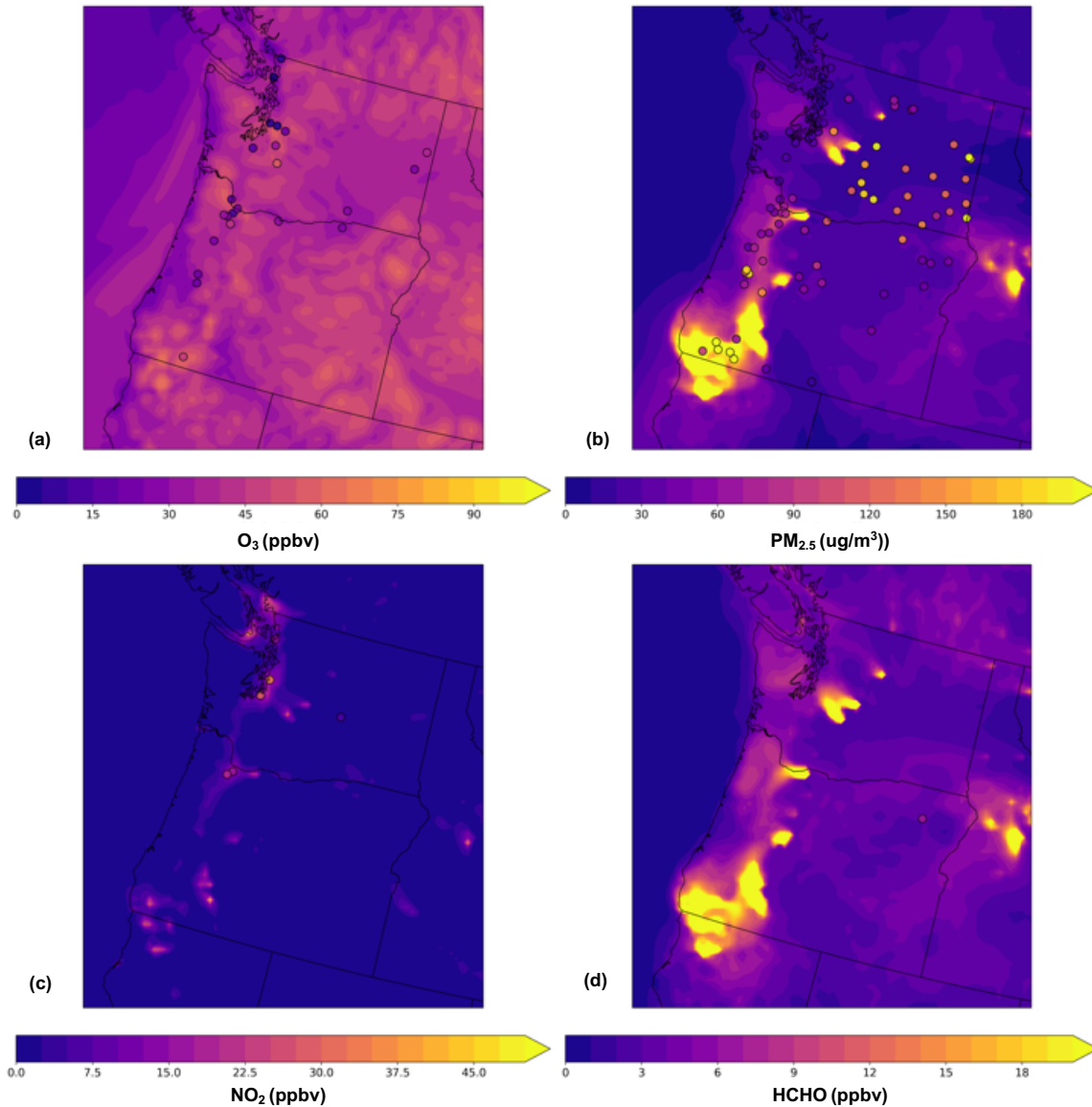


Figure 5-6: Spatial distribution of CMAQ-modeled concentrations on September 5, 2017, during the Eagle Creek Fire event for (a) ozone, (b) $\text{PM}_{2.5}$, (c) NO_2 , and (d) HCHO. Circles indicate AQS monitoring locations with observed values.

Figure 5-7 shows the hourly time series of pollutant concentrations during the wildfire episode. PM_{2.5} observations are elevated throughout the day while CMAQ consistently predicts lower concentrations. For ozone, CMAQ overestimates concentrations during the afternoon while observations drop to their lowest during midday before both curves begin to converge in the evening. NO₂ observations show higher values in the early morning and evening with a distinct midday peak, while the model captures some of this diurnal pattern but misses both the magnitude and timing of the afternoon maximum. These patterns show that the model-observation differences vary throughout the day. The processes driving these differences, whether related to emissions, photochemistry, or plume transport, are sensitive to the diurnal cycles of these pollutants and needs further investigation.

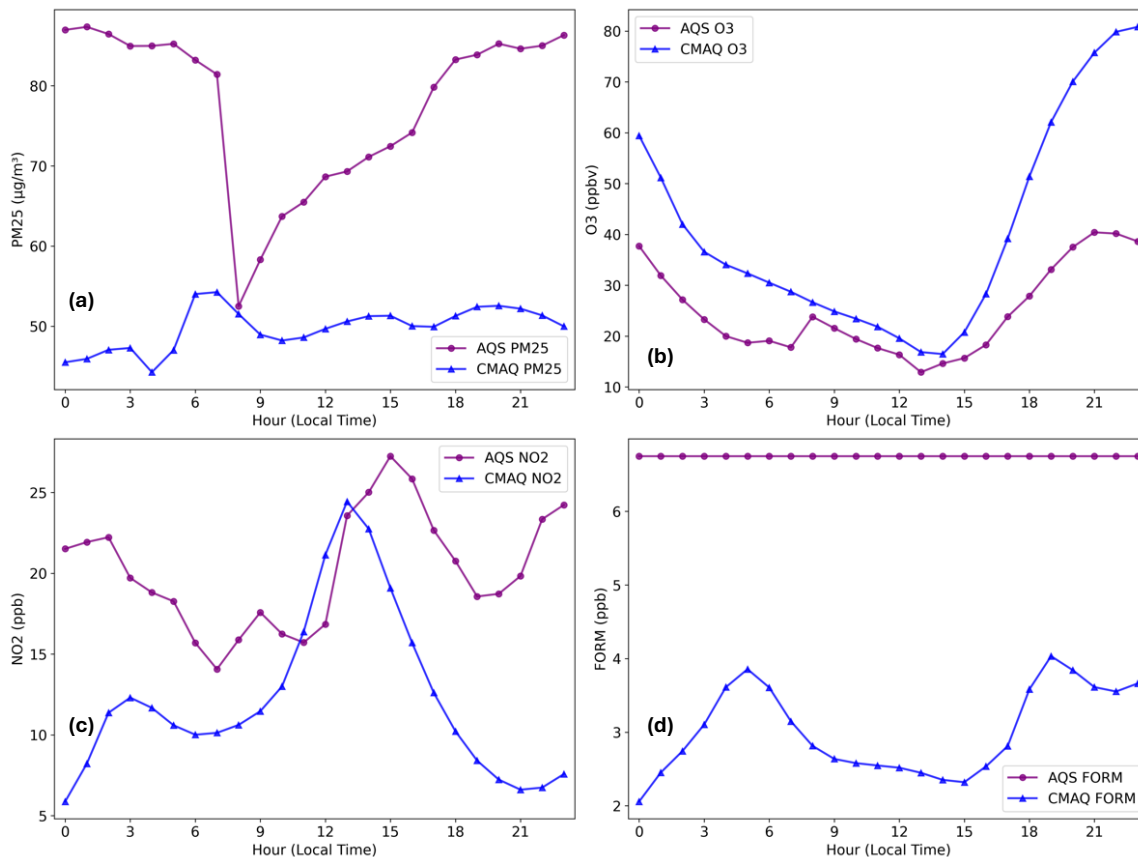


Figure 5-7: Hourly time series on September 5, 2017, comparing CMAQ-modeled (blue) and AQS-observed (purple) concentrations for (a) PM_{2.5}, (b) ozone, (c) NO₂, and (d) HCHO during the Eagle Creek Fire event. Note: we did not have hourly observations of HCHO

5.2.1.3. Reason 3: Land-water Interface

Another potential source of extreme model-observation differences involves the land-water interface. In Figure 5-2(a), we observe that 108 out of 182 locations with extreme differences (>70 ppb) are located near water bodies, representing nearly 60% of all exceedance cases. This disproportionate concentration of large errors at coastal and lakeside locations points to known challenges in how models handle the transition zones between land and water. Air quality models have been known to struggle with accurately representing the meteorological and chemical processes at land-water interfaces (Appel et

al., 2021; Gantt et al., 2017; Torres-Vazquez et al., 2022). These processes include difficulties in representing differential heating, land-sea circulations, boundary layer dynamics, pollutant transport across land-water interface, and pollutant production over water. While this issue has been recognized as a persistent problem in air quality modelling, the magnitude of these discrepancies underscores the need for continued research. Future work should continue to examine the reasons behind these errors. A few reasons could be due to coarse grid model resolution that fails to capture sharp gradients at shorelines (such as abrupt changes in surface roughness and temperature), inadequate representation of marine boundary layer processes (such sea breeze development and nocturnal low-level jets), or limitations in how emissions and deposition are handled in coastal grid cells (such as the treatment of ship emissions or halogen chemistry over ocean surfaces) (Appel et al., 2021; Gantt et al., 2017; Ring et al., 2018; Torres-Vazquez et al., 2022).

5.3. Thesis Conclusions

The first goal of this dissertation was to improve our understanding of the chemistry and characterization of tropospheric ozone. Tropospheric ozone pollution harms both human health and ecosystems as thus it has important policy implications. This dissertation shows that integrating various observational and modeling platforms is necessary for effective tropospheric ozone reduction strategies. Satellites provide broad spatial coverage but lack vertical resolution, ground-based monitors offer high temporal resolution and direct surface measurements but are spatially sparse, and models add vertical and spatiotemporal continuity but exhibit seasonal and spatial biases. By integrating them, we overcome the limitations of individual platforms.

The second goal of this dissertation is to assess ground-based observation network coverage with respect to socioeconomic markers and to identify corresponding gaps in coverage for ozone precursors. We developed a novel approach that considered demographic factors that are not usually considered for monitoring site placement. This work demonstrates that optimal air quality monitoring network design must move beyond purely concentration-based criteria and instead additionally incorporate socioeconomic equity and public health vulnerability.

The final objective of this dissertation is to better understand and characterize long-term ozone trends and assess model capabilities to predict such trends. As tropospheric ozone pollution shifts from a predominantly summer, regional phenomenon to one with an expanded ozone season and an increasingly localized nature, both our monitoring strategies and model parameterizations must adapt accordingly. With changes in meteorological conditions and emissions patterns in winter and spring, models currently tuned for characterizing summer photochemistry require fundamental updates to model physics and chemistry.

Altogether, this dissertation highlights the combined importance of all observation types in characterizing tropospheric ozone and its precursors, and stresses specific individual strategies for their improved usage. In an ever-evolving global atmosphere, this research and its findings are essential to the improved health of our environment and our communities.

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