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Impact of Altering NO/NO_2 Splits in NO_x Emissions of Diesel Sources

REPORT

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1. Introduction

Diesel vehicles dominate the heavy-duty vehicle classifications in the United States, and nitrogen oxides (NO_x) and particle emissions from diesel engines are of concern to the regulatory community. The California State Implementation Plan for ozone calls for significant reductions in NOX emissions from on-road and off-road heavy-duty vehicles. Airborne particulate matter (PM) causes significant health effects and the Air Resource Board has specifically identified particle exhaust from diesel engines as a Toxic Air Contaminant.

For diesel engines, advances in emissions control technology and after-treatment (combined with the use of low/no sulfur diesel fuel) are likely to further reduce the total PM mass emissions mass. However, the overall effect of these controls on diesel emissions is uncertain. In diesel vehicles, while diesel particulate filters do not affect NO_x emissions significantly, they have been found to increase the NO_2 contribution to the total NO_x. Using "late model" transit buses, ARB staff has recently completed the CNG and diesel comparative study, which performed the simultaneous measurement of total NO_x and NO from a trap-equipped diesel during a variety of duty cycles.

Preliminary analyses indicate that not only does total NO_x increase slightly in the trap-equipped diesel engines compared to the baseline engines (equipped with an oxidation catalyst and are tested using low sulfur fuel), approximately 45-50% of the NO_x is in the form of NO_2, versus about 10 percent in baseline engines. The conversion of NO to NO_2 in the trap is an intentional catalytic reaction necessary to enable the regeneration of the trap at temperatures encountered within the typical diesel temperature profiles. More NO_2 is being created than is actually being used in the regeneration process; the excess is being emitted. Findings by ARB and others suggest that NO_2 may account for up to 50% of the total NO_x emitted. The changing of NO to NO_2 ratio appears likely to be an undesirable outcome with potential impact on ozone and PM formation, and it will require careful attention.

The purpose of this research is to conduct an air quality modeling study to investigate how this change in the nature of NO_x emissions may affect the levels of other pollutants in the atmosphere.

2. Materials and Methods

The atmosphere is a complex system where numerous physical and chemical processes occur simultaneously. Ambient measurements provide only an indication of atmospheric conditions at a particular time and cannot be used directly to establish effective air quality control strategies. Moreover, an understanding of the individual processes occurring in the atmosphere does not imply an understanding of the overall system. For this reason, mathematical models have been developed in order to integrate the understanding of individual atmospheric processes, to study their interactions, and to investigate the impacts of various air pollution control strategies.

Summer and fall episodes incorporating aerosol thermodynamics are simulated using the Caltech (CIT) Airshed Model [McRae et al., 1982; McRae and Seinfeld, 1983; Meng et al., 1997] for the South Coast Air Basin of California. The master domain of the model is an 80 by 30 horizontal grid with a resolution of 5 km with a vertical resolution consisting of five layers up to 1100 m above the surface. The computational domain of 994 five-cell columns used for this study encompasses the major ocean, surf, urban and rural regions that influence the air quality of the master domain and contains over 90% of the population of the South Coast Air Basin of California.

The CIT Airshed model employs an extended LCC (Lurmann, Carter and Coyner) gas-phase chemistry mechanism [*Harley et al*., 1993], consisting of 121 chemical reactions, and tracks 47 gas-phase species. Dynamic aerosol computations simulate the fate of 19 aerosol species over 8 size bins, characterized by mass, ranging from 0.039 to 10 micrometers in diameter. Specific inorganic aerosol constituents simulated by the model include ammonium, nitrate, sulfate, sodium, chloride, magnesium, potassium, calcium, carbonates and water. A lumped category for

other inorganic species represents dust and other crustal components. Directly-emitted organic aerosol species are treated in a lumped category as well. Six aerosol species characterize the secondary organic aerosol products from toluene, mono-terpenes and higher aromatics. Elemental carbon completes the array of aerosol constituents simulated by the model.

The thermodynamics module Simulating Composition of Atmospheric Particles at Equilibrium 2 (SCAPE2) is used to describe the gas-aerosol partitioning of inorganic aerosol constituents [*Kim et al.*, 1993; *Meng et al*., 1995]. Aerosol particles are modeled using an internally mixed assumption, i.e. all particles within a size bin are assumed to have the same composition. This assumption provides adequate results, particularly when comparing measurements of 24-hour averaged concentration of aerosol constituents with model predictions [*Meng et al.,* 1988]. Secondary organic aerosol formation is treated using the method of *Odum et al*. [1996, 1997].

Gas-phase emissions were obtained from ARB estimates for the year 2010. Primary particle emissions as described by *Lurmann et al*. [1997] are used in the aerosol model simulations. These values approximate emissions for sulfate, sea-salt, elemental carbon, lumped-organic and lumped-inorganic emissions during the 1987 SCAQS episode. Use of this emission inventory may introduce a certain amount of uncertainty to the absolute value of total particulate matter mass concentrations. However, the main purpose of this study is to investigate the relative effect of altering the NO_x splits from diesel emissions on PM levels due to the changes to the production rate of secondary nitrate aerosol. Thus these emissions are retained for the baseline simulations. For the different evaluation scenarios, elemental carbon particulate emissions were reduced in proportion to the expected reductions from diesel particulate traps.

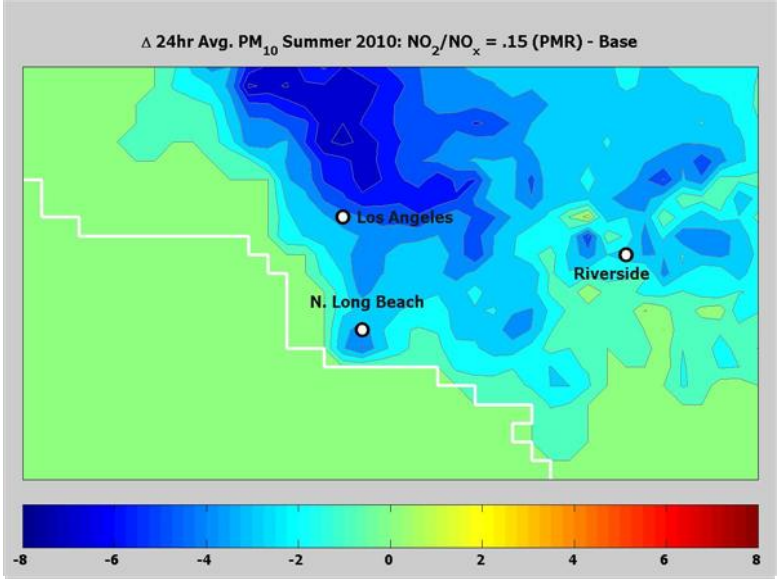
Two meteorological scenarios were chosen for the aerosol simulations. A summer scenario was defined by applying the meteorological data from the late-August 1987 SCAQS episode to the 2010 emissions inventory. Similarly, a fall scenario was defined by applying mid-October 1995 meteorological data [Fred Lurmann, personal communication] to the 2010 emissions

inventory. Whereas the summer episode was characterized by gentle winds and warm temperatures, the fall episode exhibited much stronger currents albeit milder temperatures. The regionally-averaged daily-mean temperature for the summer episode is 23.4 ºC with a mid-afternoon regionally-averaged high of 30.7 ºC compared to values of 19.0 ºC and 23.8 ºC for similar measurements during the fall episode, respectively. Maximum wind speeds reached in excess of 10 m/s for the fall episode in contrast to the gentle, and at times stagnant, conditions of the summer episode. Following is a description of the simulations performed in the analysis:

- Fall/Winter 2010 Base Case: A simulation that serves a reference point for the "experimental" simulations described immediately below.
- Adjusted NO_2/NO_x Fall/Winter 2010 runs: Scenarios where 15, 30 and 50% (molar basis) of NO_x emissions from (area and point) diesel sources are released as NO_2. Any alteration of NO_x emissions must be performed on a molar basis to conserve the discharge of NO_x molecules to the atmosphere.
- Summer 2010 Base Case: A simulation that serves as a reference point for the three "experimental" simulations described immediately below.
- Adjusted NO_2/NO_x 2010 runs: Scenarios where 15, 30 and 50% (molar basis) of NO_x emissions from (area and point) diesel sources are released as NO_2.

3. Graphical Results

On the following pages are graphical results obtained during from the simulations above. Section 4 discusses the results in further detail.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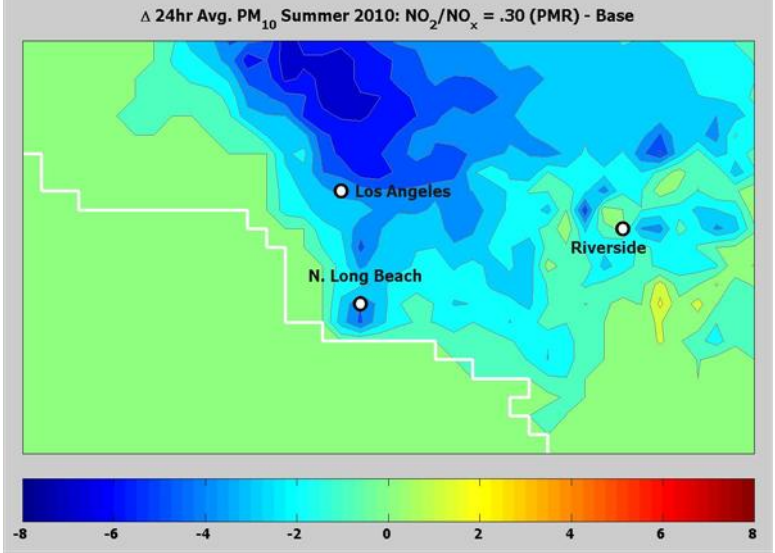
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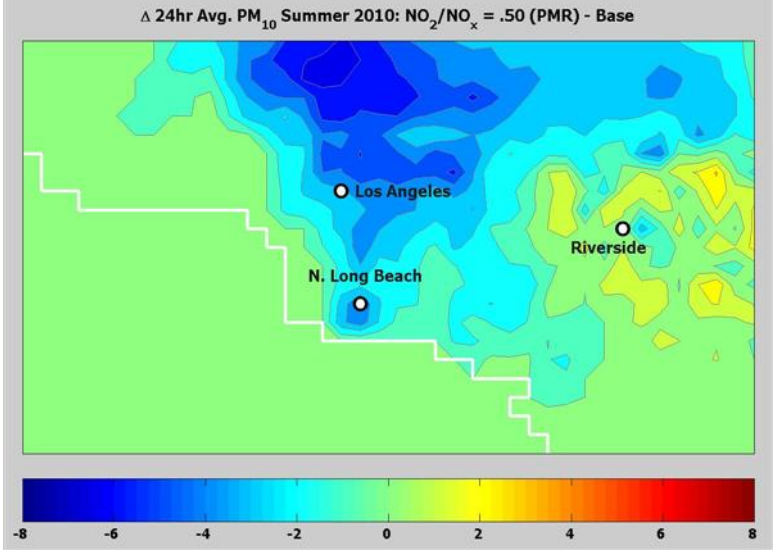
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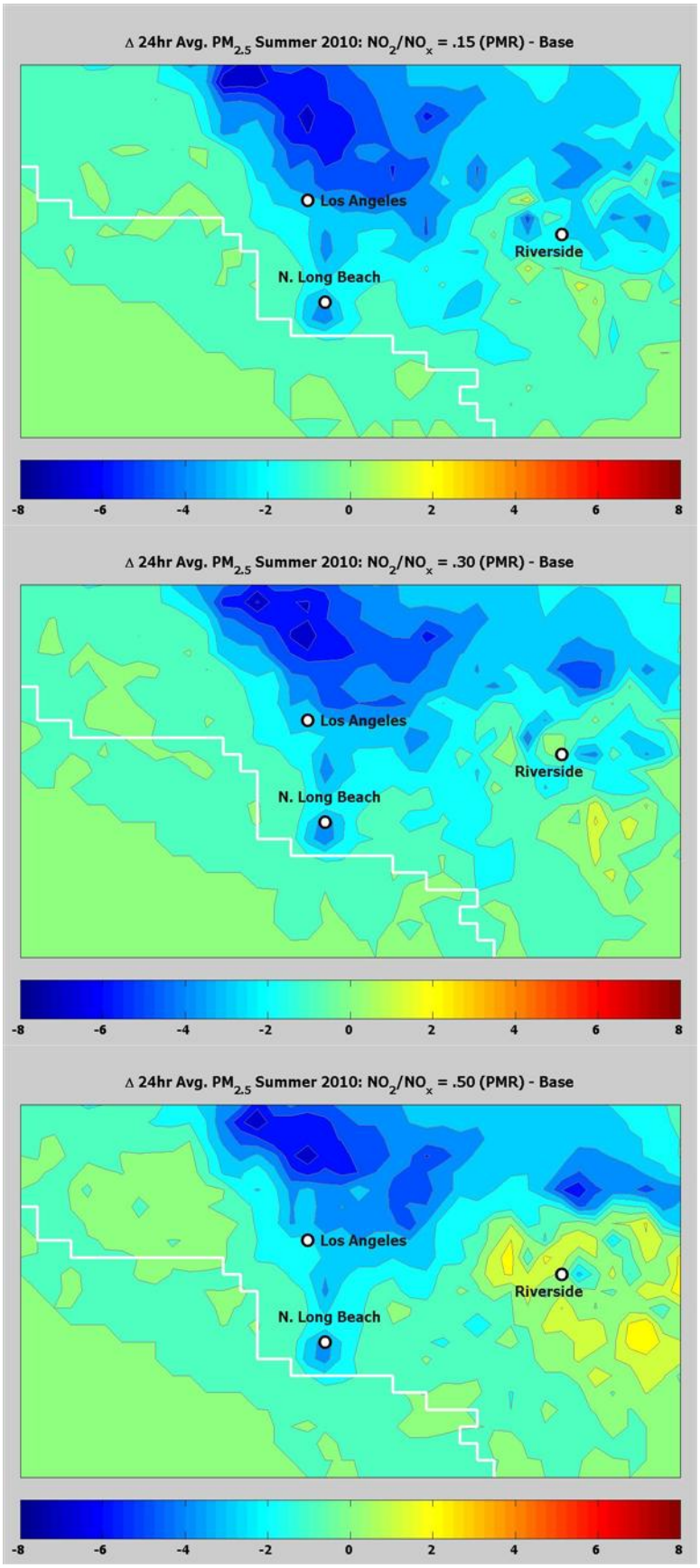
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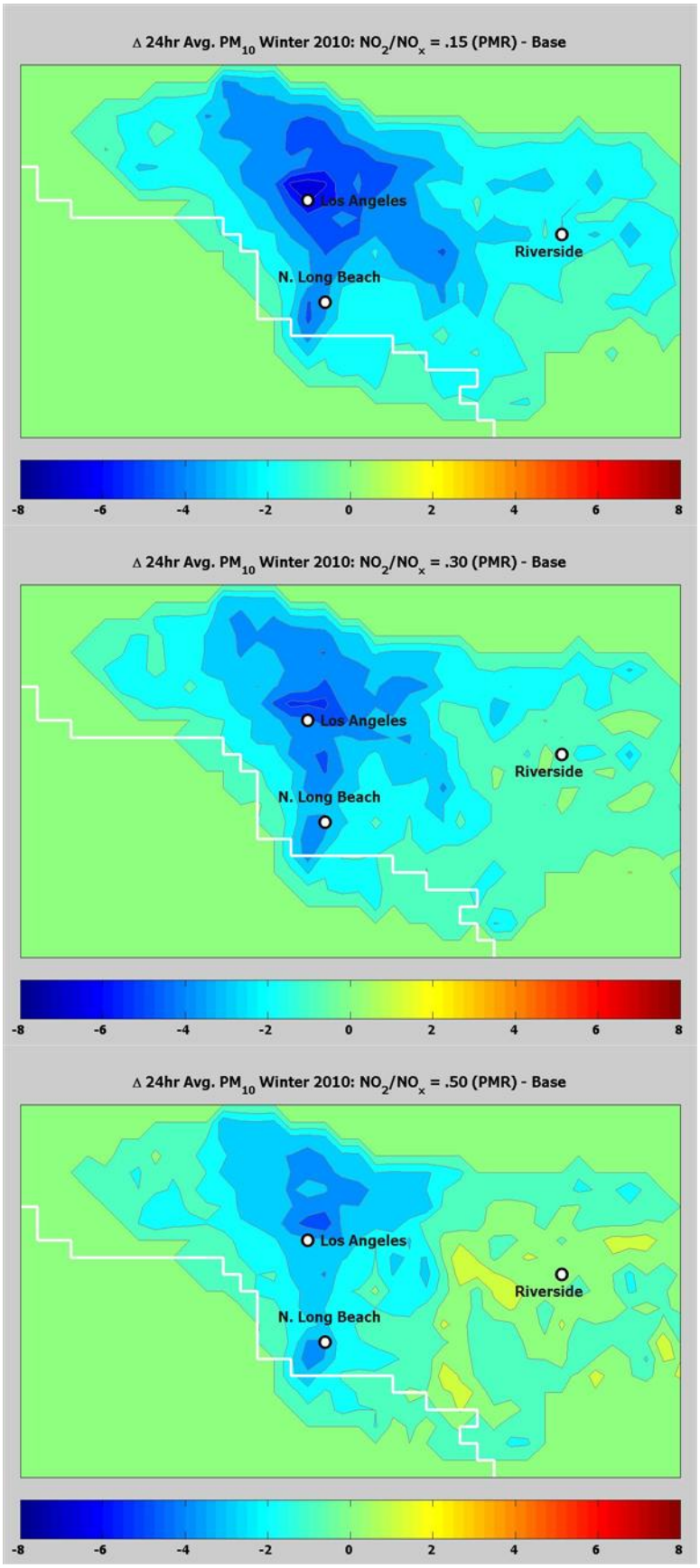
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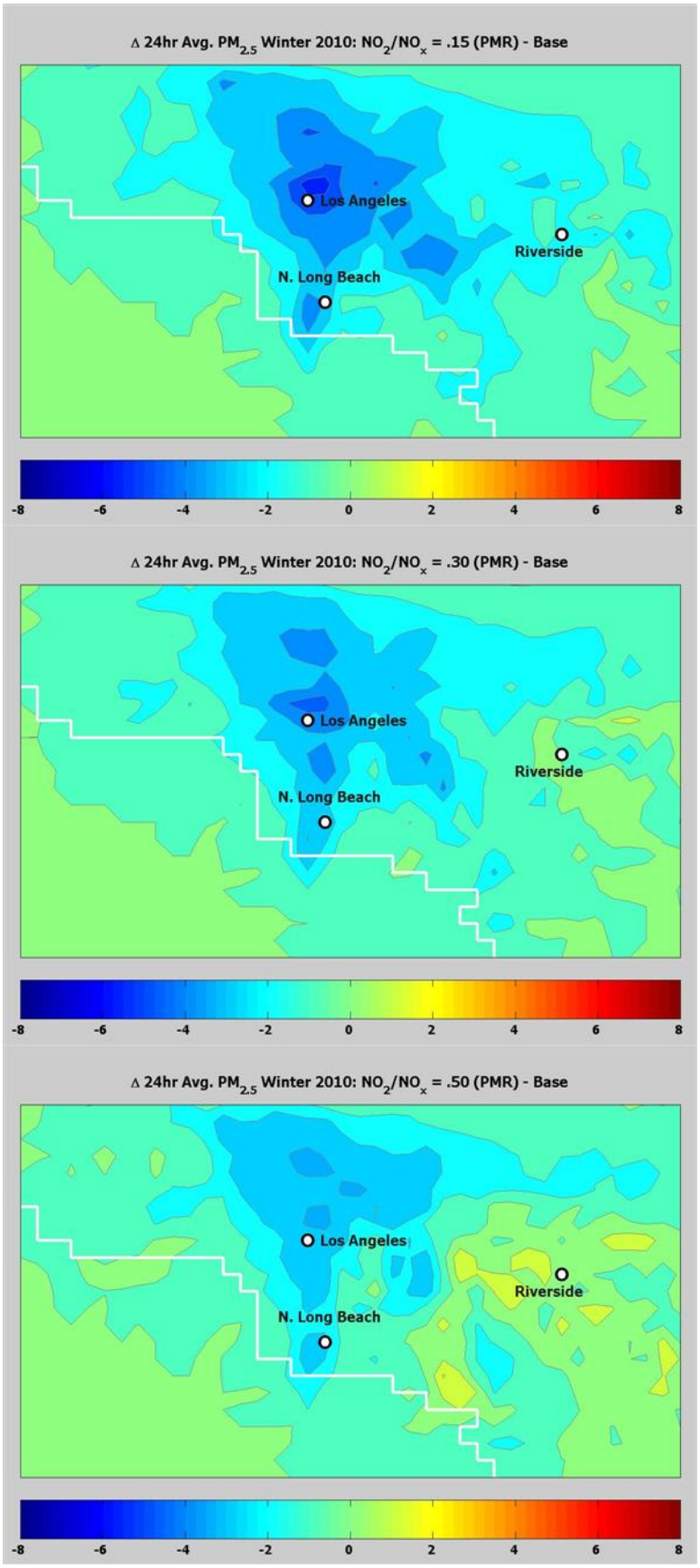
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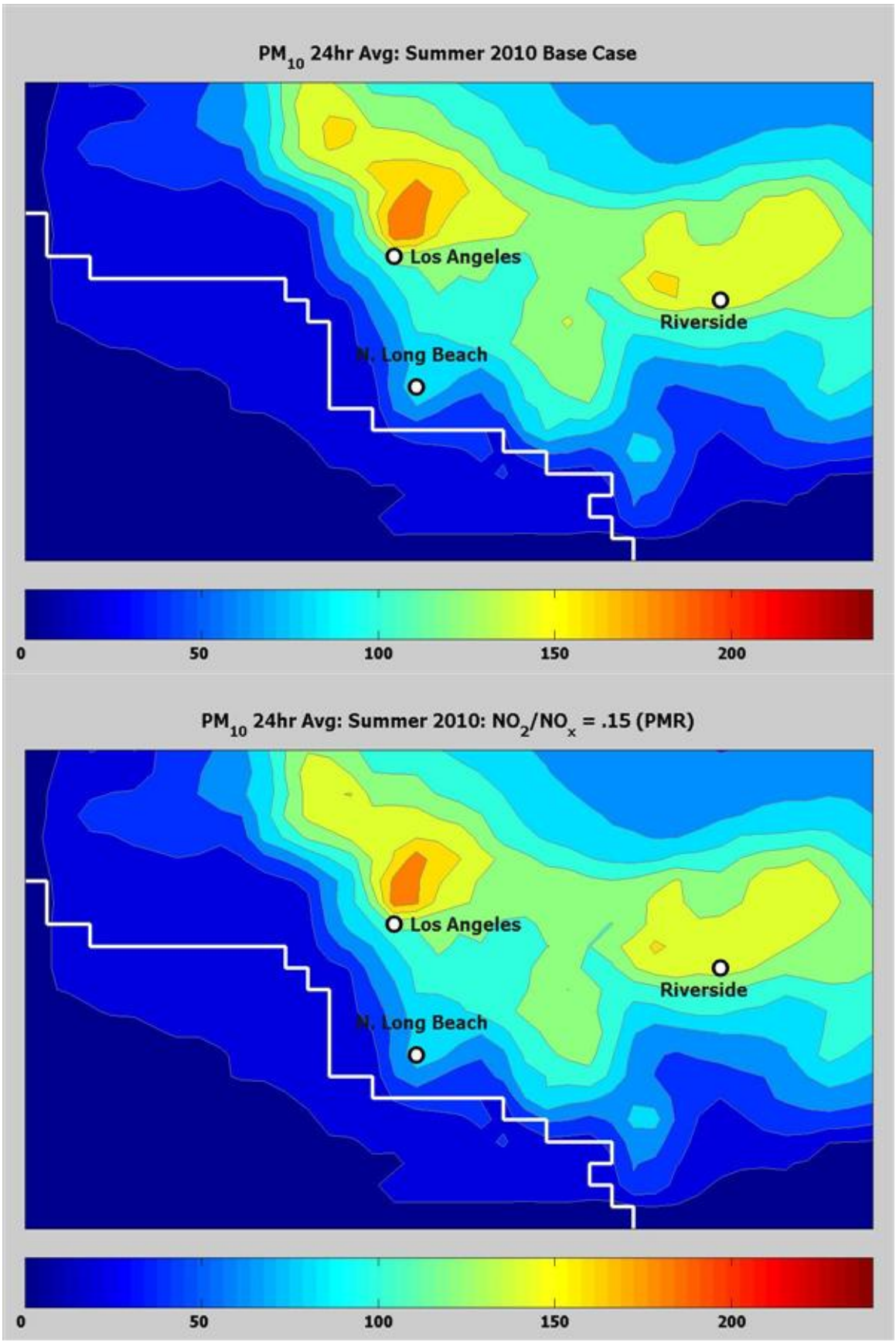
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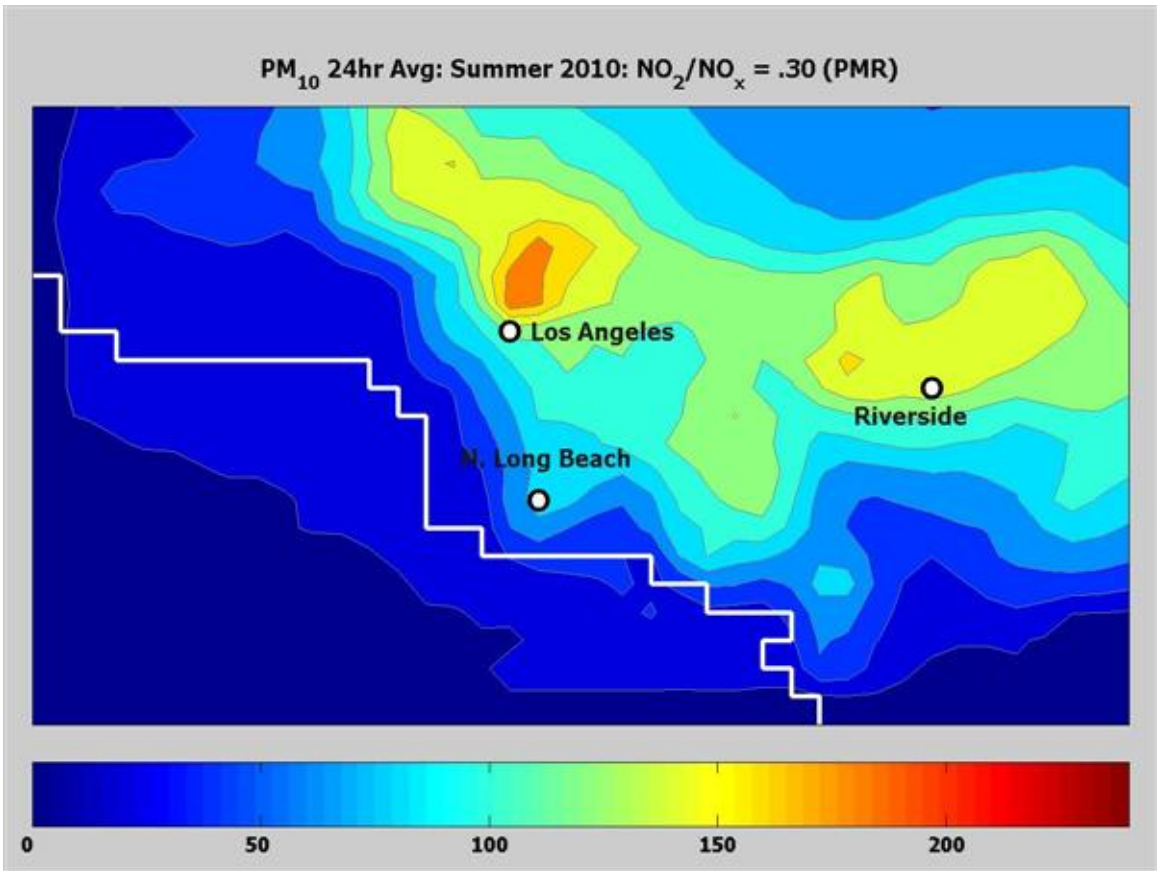
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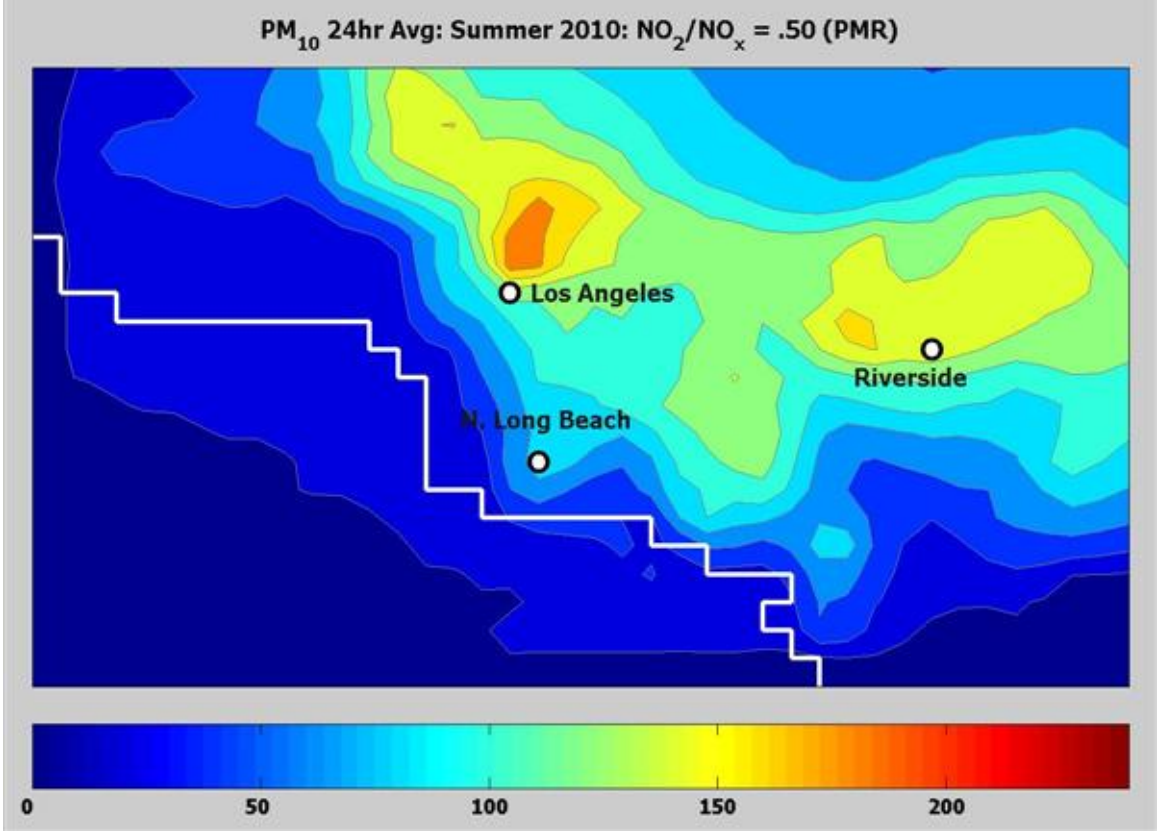
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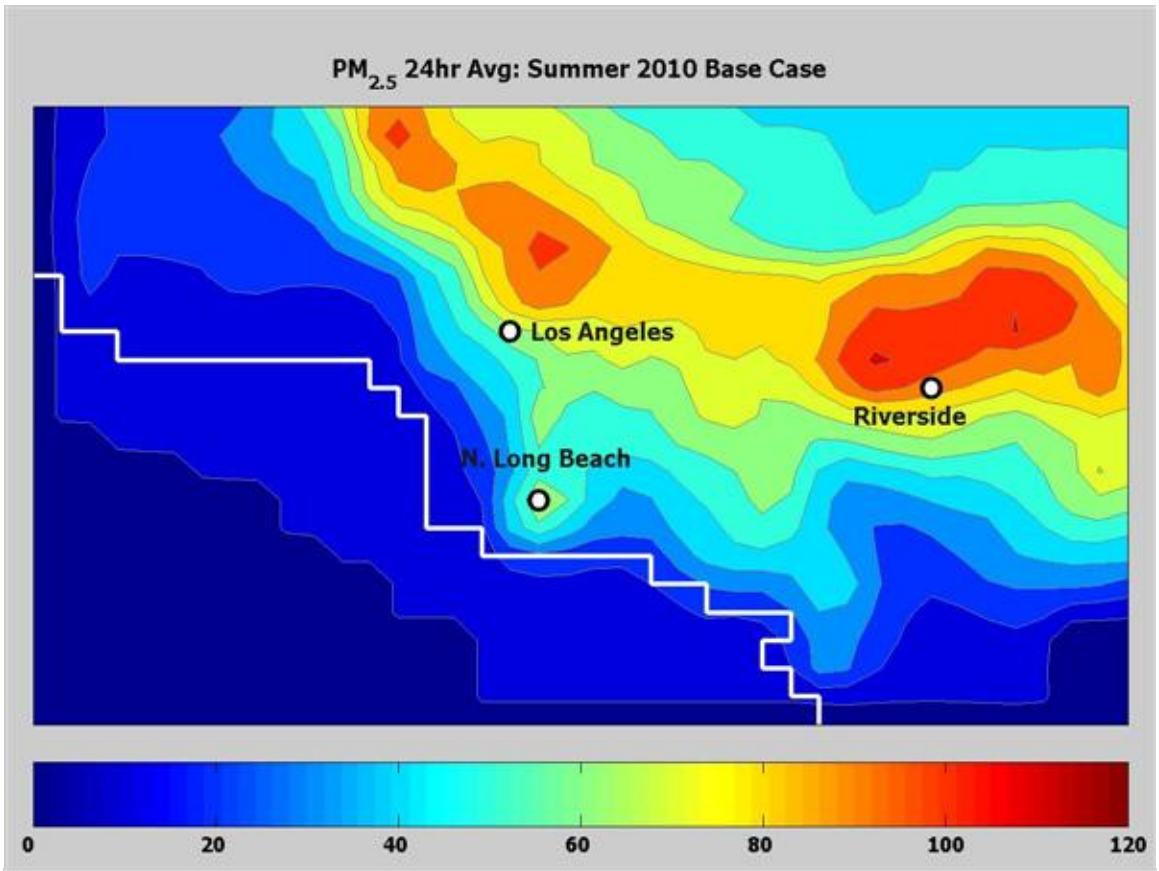
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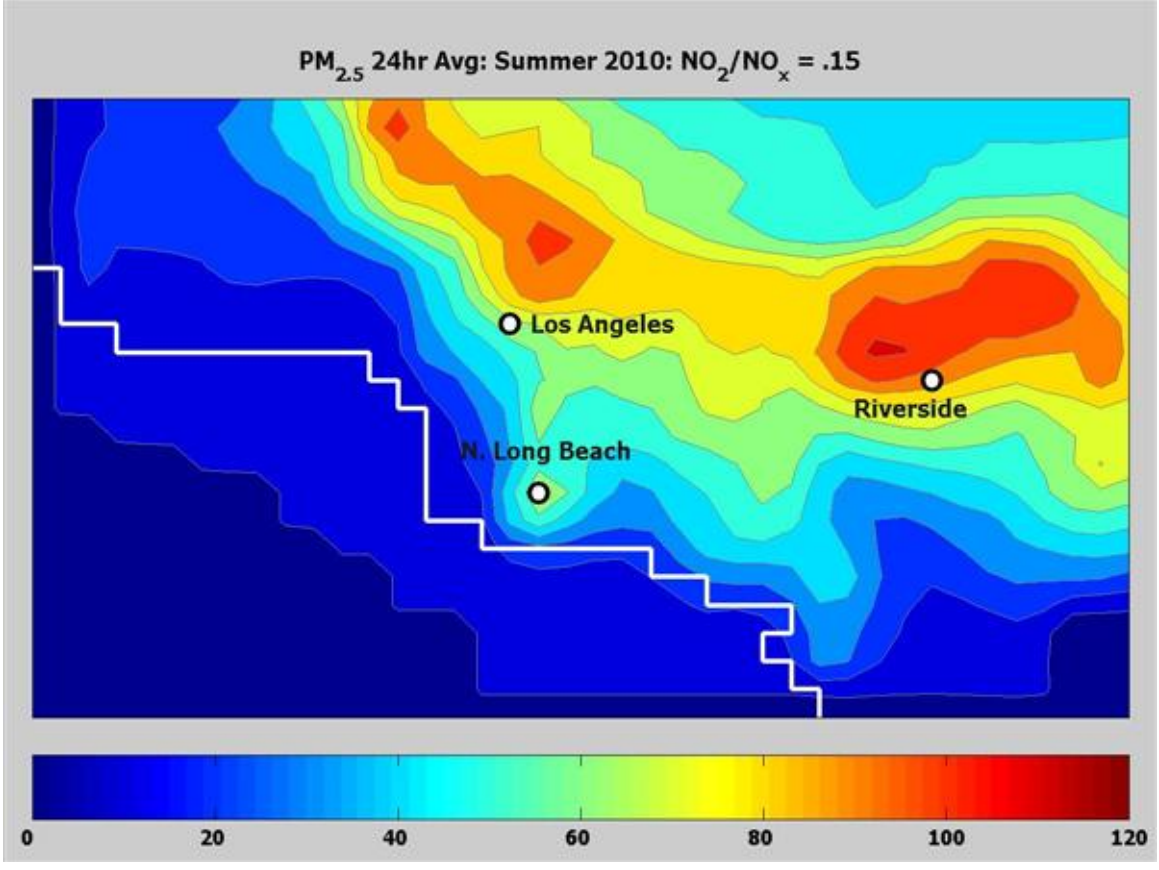
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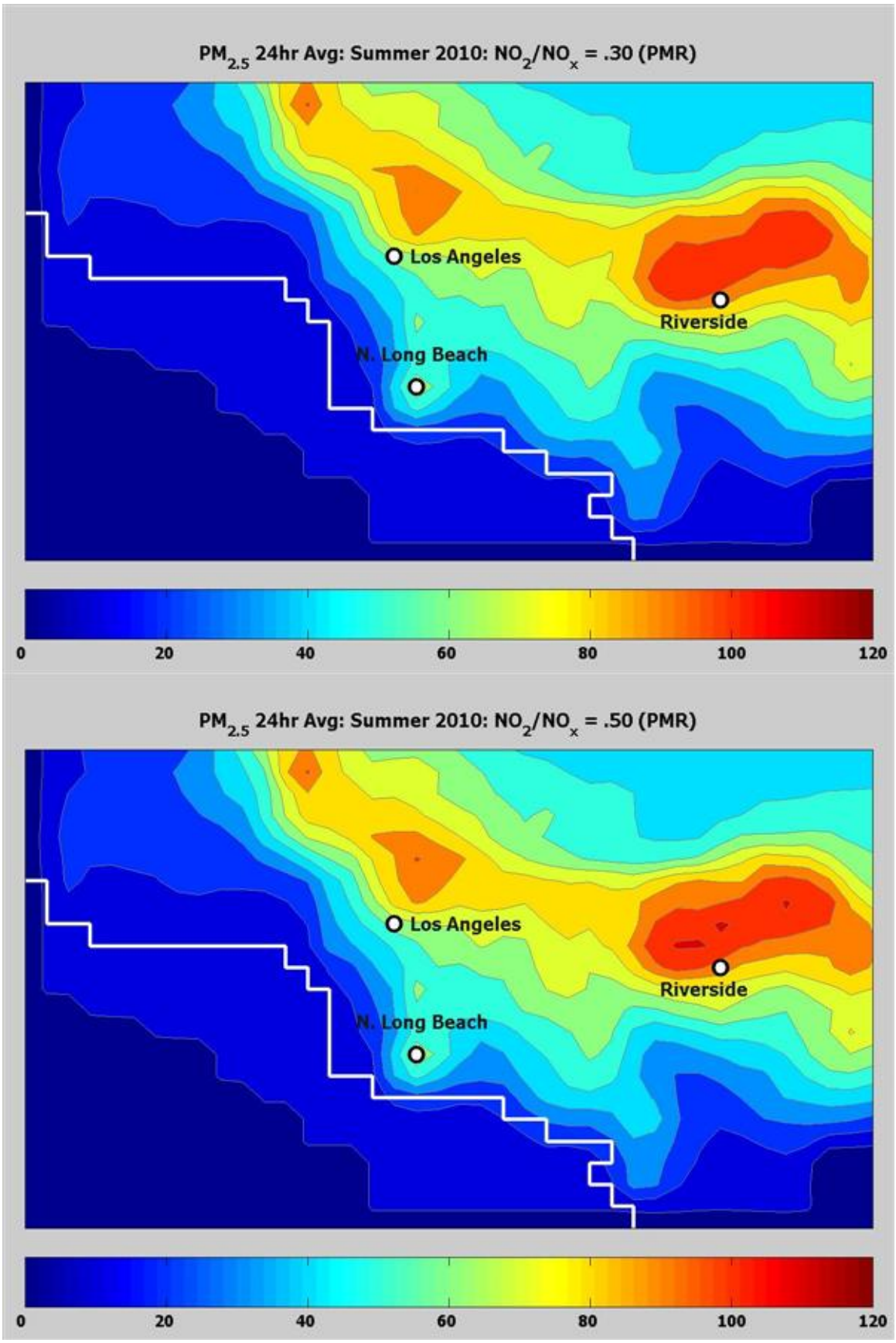
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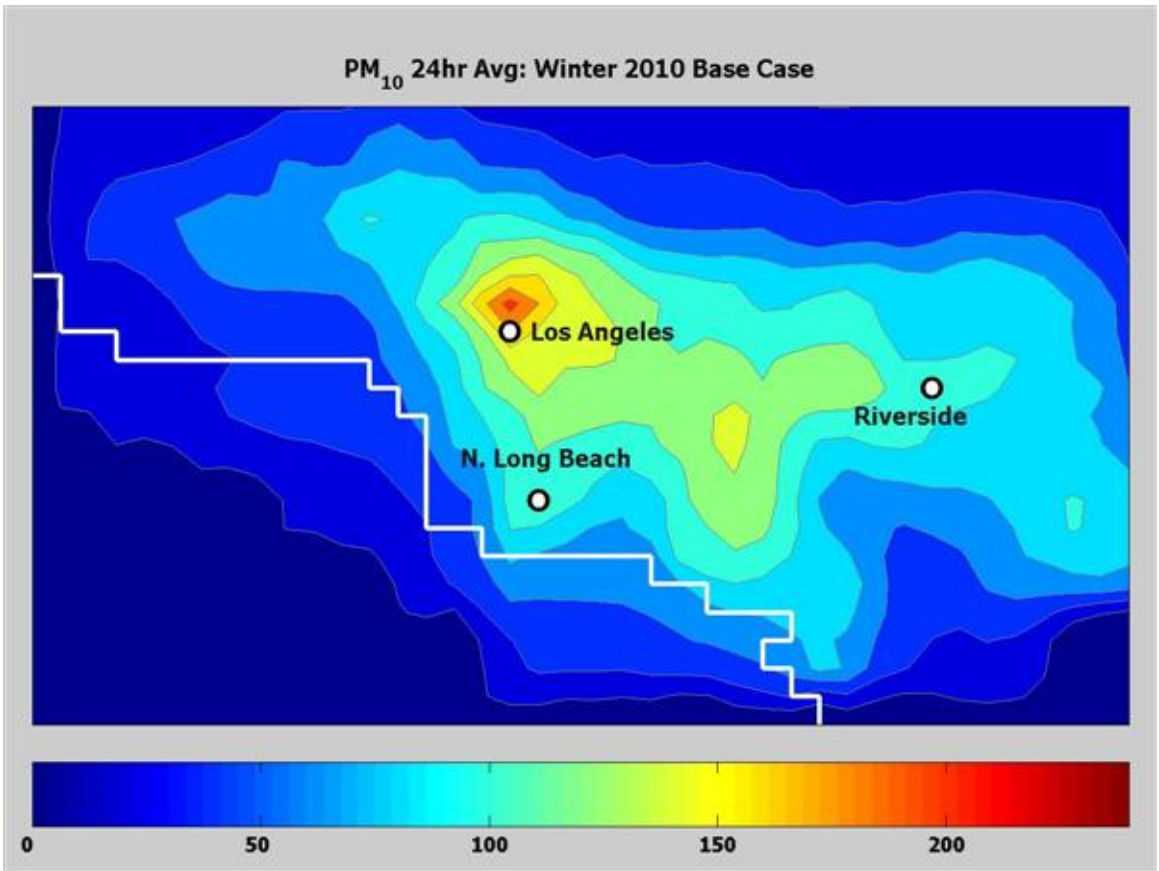
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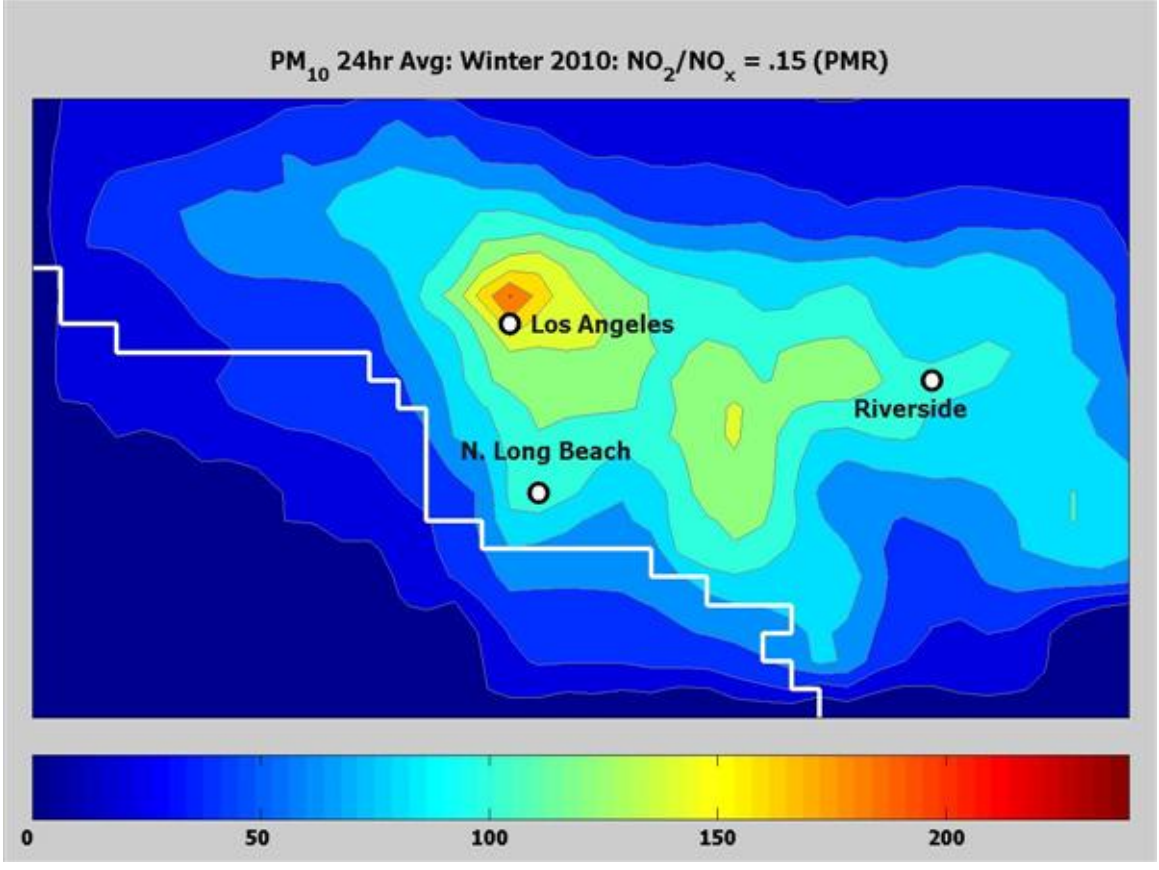
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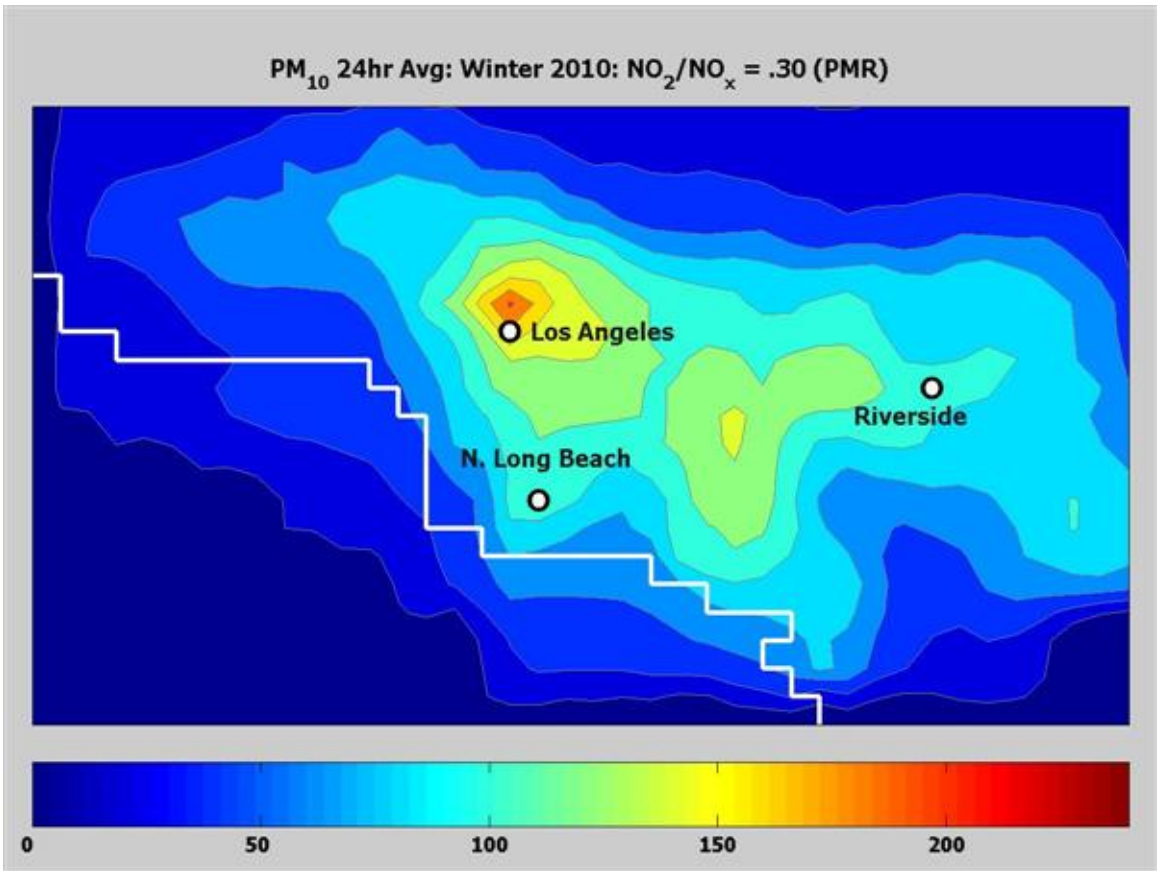
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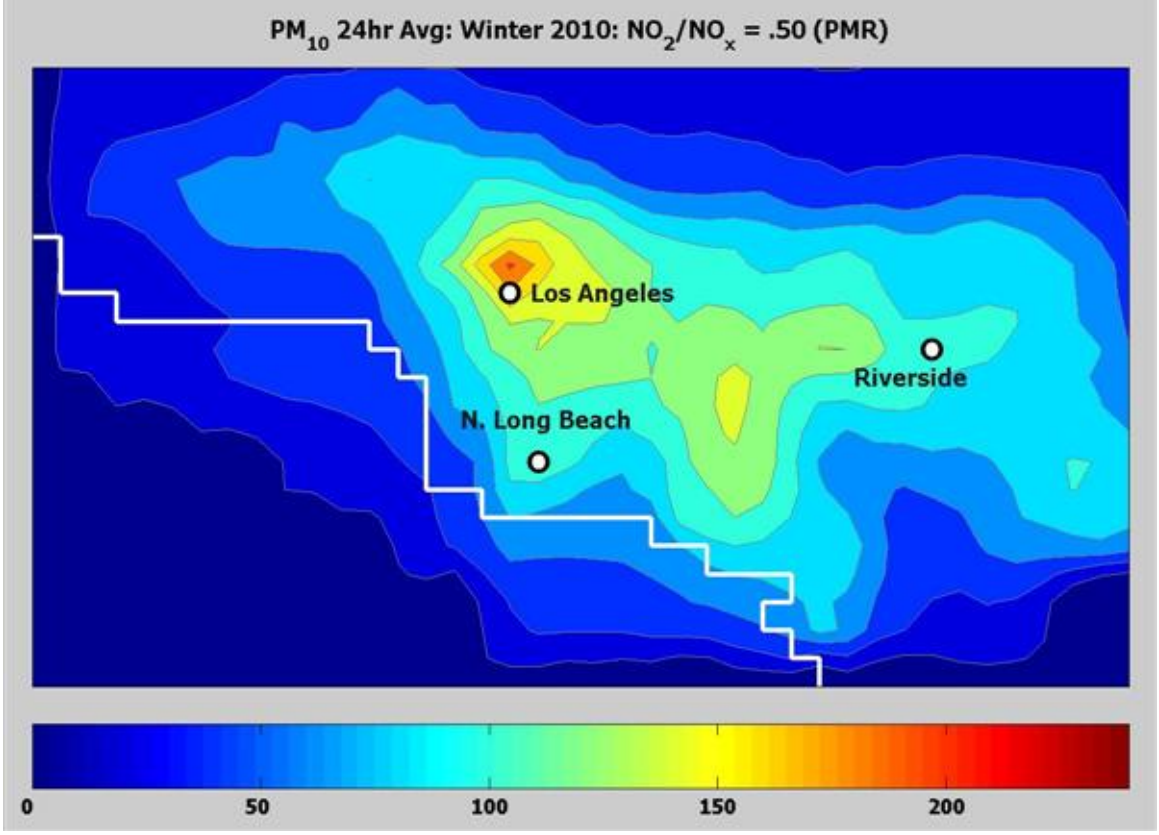
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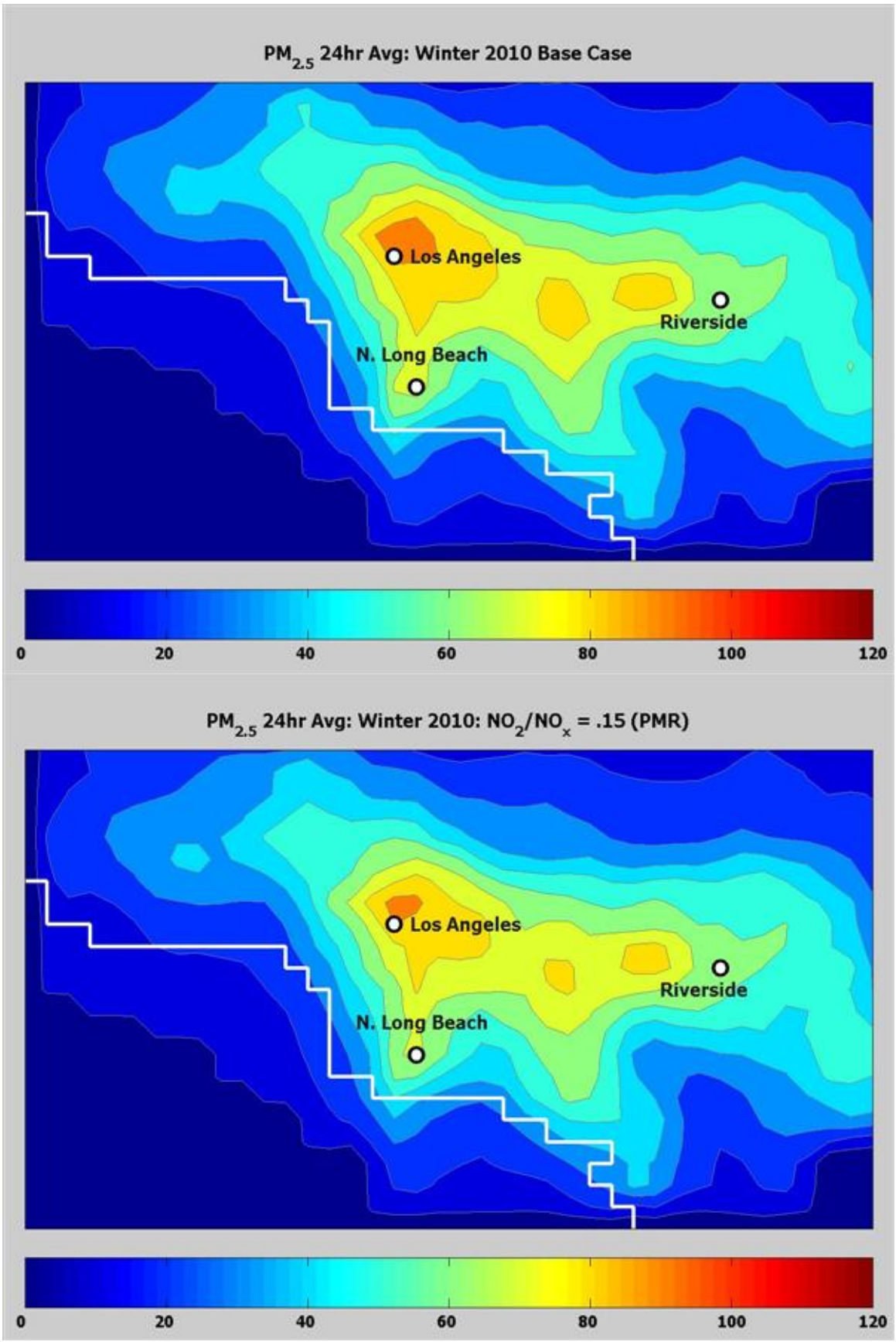
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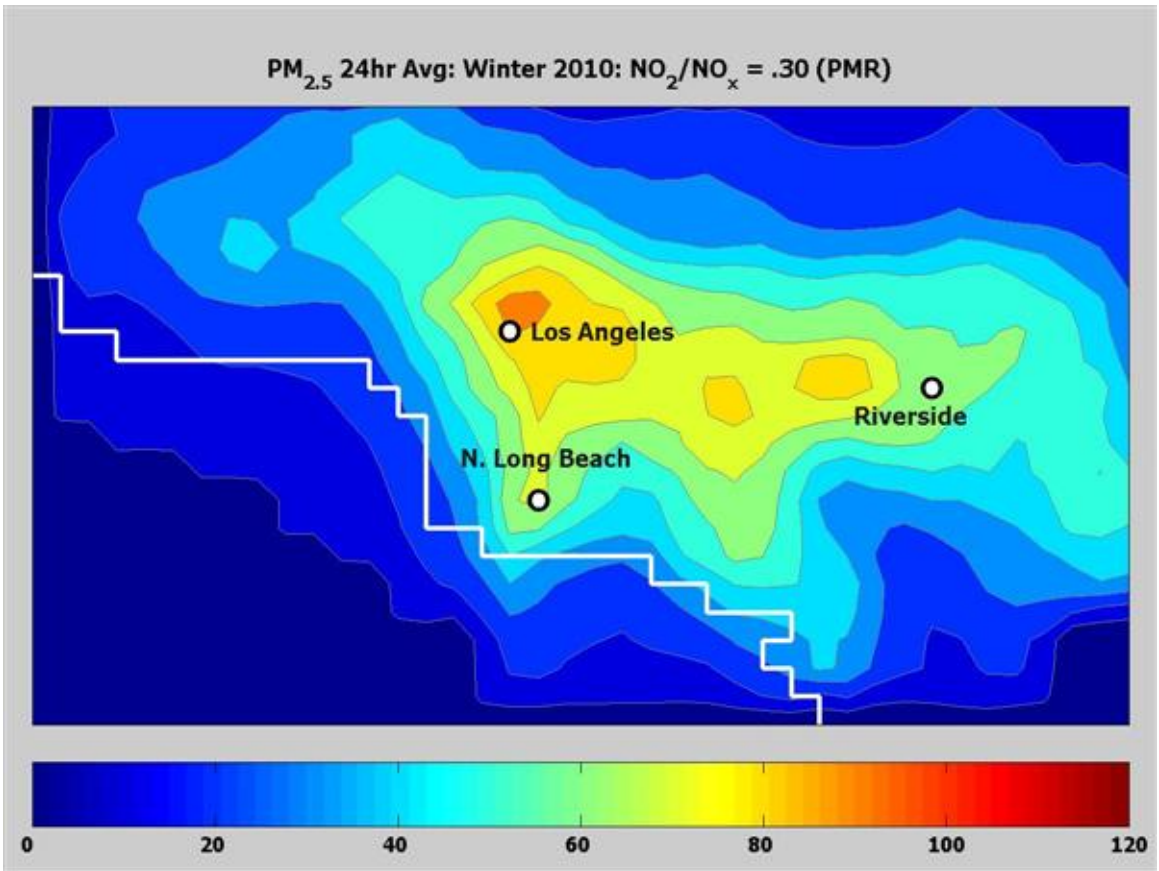
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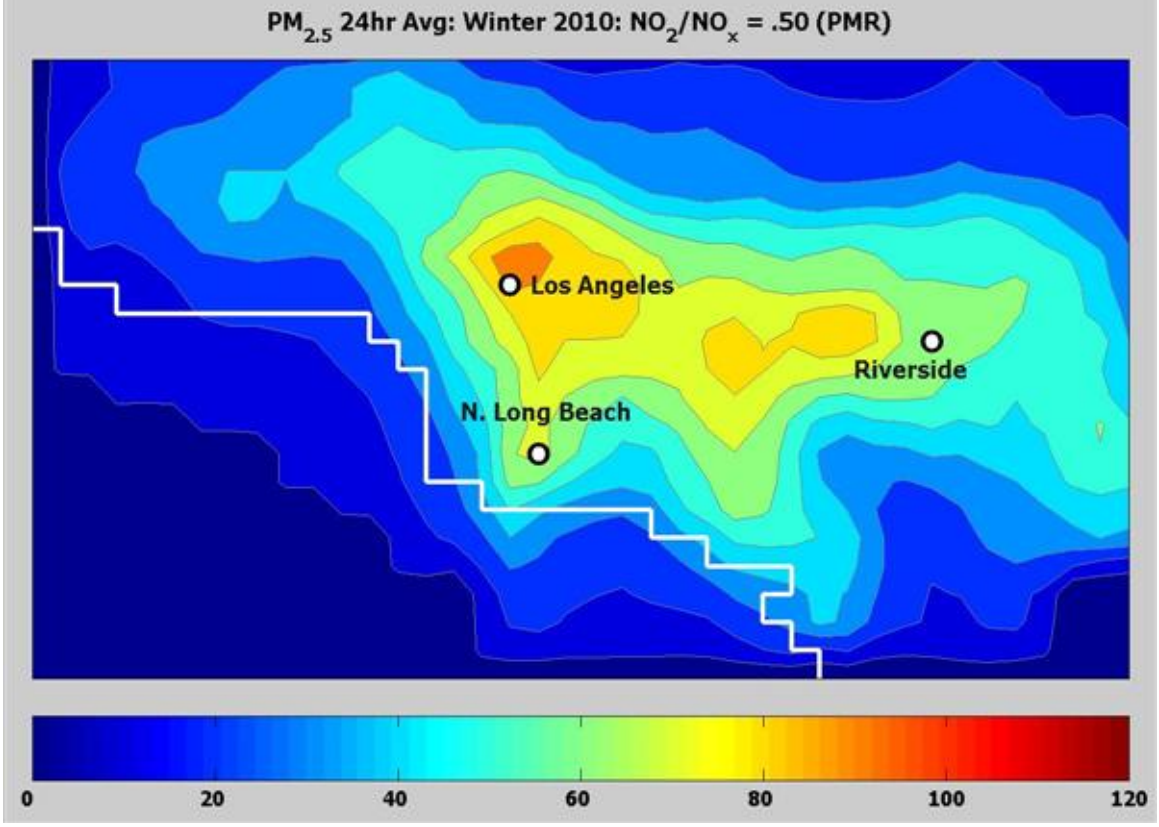
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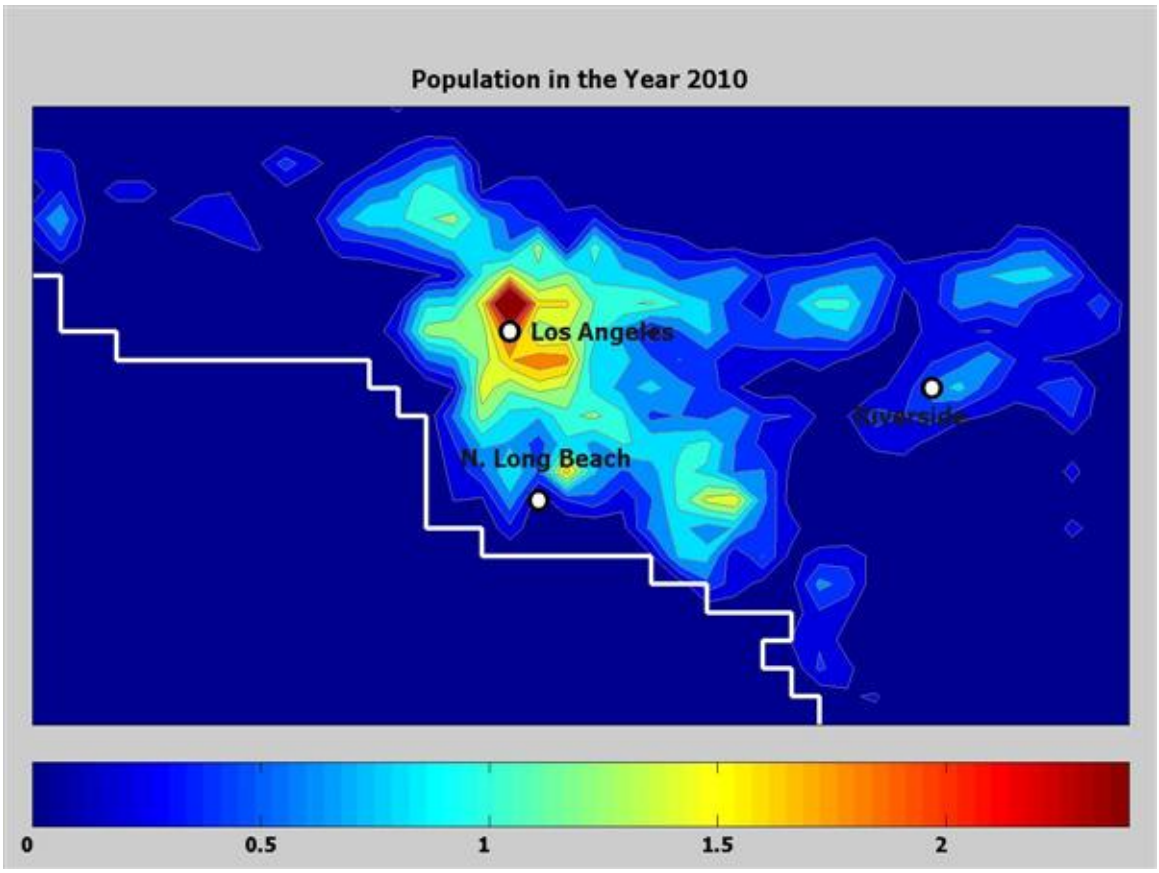
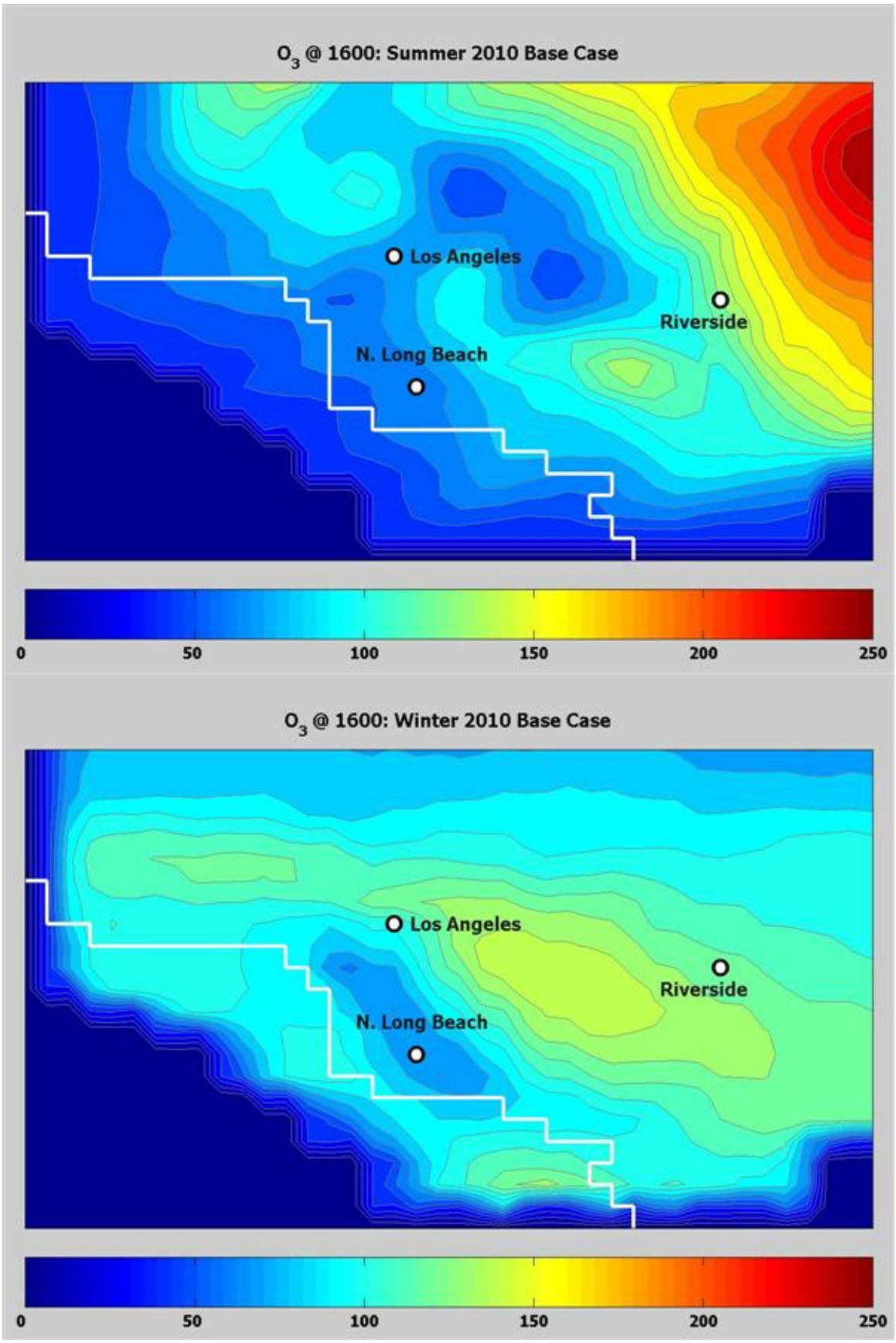


Population scale in 100,000 persons per cell (25 km2) = 4,000 persons/km2.
Each contour represents 20,000 persons per cell = 800 persons/km2.

Population Statistics:
Population of Master Domain: 20,423,802
Population of Computational Domain: 18,959,658

Approximately 93% of the population of the master domain (~20.4M) is contained in the computational domain (~19.0M).
The peak in Los Angeles exceeds the colorbar limit of 240,000 and has a value of 362,207. Only one cell, corresponding to this value, exceeds the colorbar limit.


O3 @ 1600: Summer 2010 Base Case
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O3 @ 1600: Winter 2010 Base Case
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4. Discussion

Tables 1 and 2 present the metrics for one-hour ozone and nitrogen dioxide concentrations predicted by the CIT Airshed Model simulations for the Summer and Fall 2010 scenarios, respectively. The higher peak ozone concentrations in the summer scenario are indicative of the hotter and more stagnant conditions experience during the SCAQS episode. In addition, higher ozone concentrations are predicted by the CIT Airshed Model than other photochemical models in response to a new numerical method applied to solve the hyperpbolic advection equation, the Quintic Splines Taylor Series Expansion (QSTSE) algorithm. The QSTSE algorithm is an Eulerian scheme that uses quintic splines to calculate derivatives in the spatial domain and a Taylor series expansion to progress in time. In application to the atmospheric advection equation, the algorithm maintains high accuracy and reduces the effect of numerical dissipation of peak gas-phase and aerosol concentrations [*Nguyen and Dabdub*, 2001].

The CIT Airshed Model calculates the extent of aerosol nitrate formation from its principal precursor, gas-phase nitric acid, throughout the domain. Aerosol nitrate exists primarily as ammonium nitrate in the proximity of the city of Riverside. Nonetheless, the model also considers formation of other nitrate salts, e.g. sodium nitrate, and direct condensation of nitric acid. Therefore, nitric acid levels predicted by the airshed model are much lower than those values predicted by other models due to partitioning to the particle phase. Maximum 24-hour average gas-phase HNO_3 concentrations are ~3.3 ppb and ~2.1 ppb for all Summer 2010 and Fall 2010 simulations.

Table 1: Summer 2010 sensitivity simulations – Gas-phase results for the SCAB domain using CIT Airshed Model

Simulation	1-Hr O_3 (ppb)			1-Hr NO_2 (ppb)		
	Max.	ΔMax.*	Max.Δ#	Max.	ΔMax.*	Max.Δ$
Baseline (Diesel NO_2/NO_x = 10%)	248.8			99.6		
Diesel NO_2/NO_x = 15%	248.8	~0.0 (~0.0%)	+4.8	102.6	+3.0 (+3.0%)	+6.8
Diesel NO_2/NO_x = 30%	249.5	+0.7 (+0.3%)	+5.5	110.6	+11.0 (+11.1%)	+21.4
Diesel NO_2/NO_x = 50%	250.5	+1.7 (+0.7%)	+10.2	125.9	+26.3 (+26.4%)	+39.7

* Change in maximum predicted concentration, i.e., in the cell with the peak predicted value.
# Maximum change in predicted ozone concentration from all grid cells with an ozone concentration above the California standard.
$ Maximum change in predicted NO_2 concentration from all grid cells. This is the largest change anywhere in the modeling domain, and is usually not from the grid cell with the peak predicted value.

Table 2: Fall 2010 sensitivity simulations – Gas-phase results for the SCAB domain using CIT Airshed Model

Simulation	1-Hr O_3 (ppb)			1-Hr NO_2 (ppb)		
	Max.	ΔMax.*	Max.Δ#	Max.	ΔMax.*	Max.Δ$
Baseline (Diesel NO_2/NO_x = 10%)	148.2			112.0		
Diesel NO_2/NO_x = 15%	148.1	–0.1 (–0.1%)	+1.0	114.0	+2.0 (1.8%)	+6.7
Diesel NO_2/NO_x = 30%	148.7	+0.5 (+0.3%)	+4.0	122.9	+10.8 (+9.7%)	+14.9
Diesel NO_2/NO_x = 50%	150.4	+2.2 (+1.5%)	+9.4	129.3	+26.5 (+15.4%)	+38.1

* Change in maximum predicted concentration, i.e., in the cell with the peak predicted value.
# Maximum change in predicted ozone concentration from all grid cells with an ozone concentration above the California standard.
$ Maximum change in predicted NO_2 concentration from all grid cells. This is the largest change anywhere in the modeling domain, and is usually not from the grid cell with the peak predicted value.

Altering the NO_x splits in emissions from diesel engines enhances the rate of nitric acid formation and subsequent partitioning to the aerosol phase. During daytime, the reaction rate of NO_2 and OH may be increased in regions where oxidation of nitric oxide by peroxy radicals may have limited the rate of NO_2 formation. At night, direct emission of NO_2 may increase the rate of nitrate radical formation via reaction with residual and background ozone. Nitrate radical reactions with volatile organics compounds may increase nitric acid levels. Furthermore, the reaction of the increased nitrate radical levels with increased NO_2 levels may yield higher concentrations of N_2O_5. The reaction of N_2O_5 with water may also elevate nitric acid levels and enhance aerosol nitrate production.

In contrast to simulations of the 1987 SCAQS episode [*Meng et al.*, 1988], year 2010 emission estimates shift the baseline PM peak from the Riverside area to the Central Los Angeles area. This shift supports studies of the effects of general VOC/NO_x controls on aerosol formation [*Nguyen and Dabdub*, 2002]. The shift represents a transformation from secondary ammonium-nitrate dominated peak aerosol concentrations to new peak aerosol concentrations dominated by dust, elemental carbon primarily-emitted organic species.

Table 3: Summer 2010 sensitivity simulations – PM results for the SCAB domain using CIT Airshed Model

Simulation	24-Hr PM_{10} (µg/m^3)			24-Hr $PM_{2.5}$ (µg/m^3)		
	Max.	ΔMax.*	Max.Δ#	Max.	ΔMax.*	Max.Δ$
Baseline (Diesel NO_2/NO_x = 10%)	198.3			111.9		
Diesel NO_2/NO_x = 15%	191.8	–6.4 (–3.2%)	+2.2	109.4	–2.5 (–2.2%)	+1.9
Diesel NO_2/NO_x = 30%	192.8	–5.5 (–2.8%)	+3.4	109.8	–2.0 (–1.8%)	+3.1
Diesel NO_2/NO_x = 50%	193.7	-4.6 (–2.3%)	+3.6	111.3	–0.5 (–0.5%)	+3.3

* Change in maximum predicted concentration, i.e., in the cell with the peak predicted value.
# Maximum change in predicted PM_{10} concentration from all grid cells with a PM_{10} concentration above the California standard.
$ Maximum change in predicted $PM_{2.5}$ concentration from all grid cells. This is the largest change anywhere in the modeling domain, and is usually not from the grid cell with the peak predicted value.

Table 4: Fall 2010 sensitivity simulations – PM results for the SCAB domain using CIT Airshed Model

Simulation	24-Hr PM_{10} (µg/m^3)			24-Hr $PM_{2.5}$ (µg/m^3)		
	Max.	ΔMax.*	Max.Δ#	Max.	ΔMax.*	Max.Δ$
Baseline (Diesel NO_2/NO_x = 10%)	209.5			99.8		
Diesel NO_2/NO_x = 15%	202.9	–6.6 (–3.2%)	+0.9	94.1	–5.7 (–5.7%)	+1.0
Diesel NO_2/NO_x = 30%	204.4	–5.1 (–2.5%)	+1.0	95.2	–4.6 (–4.6%)	+1.3
Diesel NO_2/NO_x = 50%	205.1	–4.4 (–2.1%)	+1.9	96.5	–3.3 (–3.3%)	+2.1

* Change in maximum predicted concentration, i.e., in the cell with the peak predicted value.
# Maximum change in predicted PM_{10} concentration from all grid cells with a PM_{10} concentration above the California standard.
$ Maximum change in predicted $PM_{2.5}$ concentration from all grid cells. This is the largest change anywhere in the modeling domain, and is usually not from the grid cell with the peak predicted value.

Tables 3 and 4 present the metrics for PM_{10} and $PM_{2.5}$ concentrations predicted by the CIT Airshed Model simulations for the Summer and Fall 2010 scenarios, respectively. The tables

show that the direct reductions in PM mass by the diesel trap offset the increase in PM mass due to the changes in the NOx splits, particularly in the $NO_2/NO_x = 0.15$ case. Although the peak PM mass is reduced in all cases, the CIT Airshed Model as currently developed cannot be used to infer any conclusions on the particle number concentrations, in particular within the ultrafine particle size range.

As the NO_2/NO_x emission ratio increases, the maximum change in PM levels in non-peak cells increase substantially due to enhancement in secondary aerosol nitrate formation. In order to determine the overall effect of the evaluated scenarios, estimates of total aerosol exposure and exposure above state and federal standards are provided on Tables 5 – 8.

Table 5: Summer 2010 population exposure and population exposure in excess of standards
Simulated 24-Hr average PM_{10} Exposure per Capita ($\mu g/m^3$)

PM_{10} Particulate Matter	**Exposure**	**Population Above State Standard**	**Excess PM Exposure (Exposed Population)**
Base Case	114.9	17,522,330	71.5
Diesel NO_2/NO_x = 15%	112.1	17,503,643	68.6
Diesel NO_2/NO_x = 30%	112.5	17,491,736	69.0
Diesel NO_2/NO_x = 50%	113.1	17,521,080	69.6

Table 6: Summer 2010 population exposure and population exposure in excess of standards
Simulated 24-Hr avg. $PM_{2.5}$ exposure per capita ($\mu g/m^3$)

$PM_{2.5}$ Particulate Matter	**Exposure**	**Population Above Federal Standard**	**Excess PM Exposure (Exposed Population)**
Base Case	66.1	9,910,725	20.0
Diesel NO_2/NO_x = 15%	63.8	9,320,397	18.1
Diesel NO_2/NO_x = 30%	64.1	9,364,421	18.4
Diesel NO_2/NO_x = 50%	64.6	9,460,797	18.9

Table 7: Fall 2010 population exposure and population exposure in excess of standards
Simulated 24-Hr average PM_{10} Exposure per Capita ($\mu g/m^3$)

Simulation	**Exposure**	**Population Above State Standard**	**Excess PM Exposure (Exposed Population)**
Base Case	108.4	17,731,975	63.7
Diesel NO_2/NO_x = 15%	105.7	17,718,717	60.9
Diesel NO_2/NO_x = 30%	106.3	17,723,907	61.5
Diesel NO_2/NO_x = 50%	107.1	17,729,459	62.3

Table 8: Fall 2010 population exposure and population exposure in excess of standards
Simulated 24-Hr avg. $PM_{2.5}$ exposure per capita ($\mu g/m^3$)

$PM_{2.5}$ Particulate Matter	**Exposure**	**Population Above Federal Standard**	**Excess PM Exposure (Exposed Population)**
Base Case	62.6	8,622,895	13.6
Diesel NO_2/NO_x = 15%	60.4	7,653,949	11.8
Diesel NO_2/NO_x = 30%	60.9	8,109,704	11.9
Desel NO_2/NO_x = 50%	61.5	8,715,546	11.9

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