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METAMODEL DEMONSTRATION: EFFECTS OF MOBILE SOURCE REDUCTIONS ON OZONE TRENDS IN THE NORTHEAST US

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Metamodel demonstration: effects of mobile source reductions on ozone trends in the Northeast US

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I. Introduction

A metamodel is a mathematical relationship between the inputs and outputs of a simulation experiment. They are used to calculate outputs for scenarios of interest without having to run new (presumably costly) experiments. In this report we apply a metamodel to two problems: (1) impact of changes in mobile source NOX emissions on temporal trends in ozone and (2) the ozone response to mobile source NOX emissions relative to other anthropogenic emissions.

The metamodel we are using is based on ozone observations that are fit to emissions and meteorology from a simulation experiment for the Northeastern US (NEUS) for the years 1993 to 2005. The model was estimated by first transforming model emissions and meteorology into their principal components. The observations were then fit to the principal components using stochastic kriging (SK). SK is a spatial interpolation technique in which emissions and meteorology (in this case their principal components) play the role of location coordinates. The model finds ozone values closest to a given set of emission and meteorological principal components.

This metamodel is a composite of two other metamodels previously developed for this project, namely projection onto latent structures (PLS) and stochastic kriging (SK). PLS uses principal components in a linear model framework, while SK is a nonlinear technique that operates on the original untransformed input variables. A shortcoming of PLS is that it is a linear model of a nonlinear phenomena. An issue with SK is that several of the emission sources are nearly collinear, making it difficult to discern their separate effects. By estimating an SK model with principal components we hope to take advantage of the strengths of both methods. In addition, the models in this report use observed ozone, eliminating the need for bias adjustments when CMAQ ozone is the dependent variable.

A metamodel that includes meteorological variables permits estimation of trends free from meteorological variability. When anthropogenic emissions are kept at their actual (emission inventory) levels and meteorology and biogenic emissions are fixed, the trend due to emissions becomes clear. To understand the influence of meteorology, anthropogenic emissions are fixed while meteorology (and biogenic sources) are allowed to vary. Similarly, the ozone response to mobile source emissions can be estimated by varying mobile source emissions while keeping meteorology (and biogenic emissions) and all other anthropogenic emissions fixed.

This study is motivated by the desire to estimate the impact of changes in mobile source NOX emissions on ozone concentrations and compliance with existing and proposed national ambient air quality standards (NAAQS) for ozone.

II. Methods

A. Model Setup

CMAQ (Northeastern US, 1988-2005, source Hogrefe et al, 2009)

Model:	MM5v3.7.2 CMAQv4.5.1, CB4, aero3, years 1988 B2005.
Emissions:	NEI1990, 1996-2001, OTC2002, OTC2009 (SMOKE).
Domain:	Northeastern U.S., 36 km / 12 km (details in Hogrefe et al, 2009) 95 * 65 grid cells for the inner 12 km domain

Hourly ozone, emissions and meteorological time series were provided (Hogrefe, 2013). Emissions were partitioned into NOX and VOCs from area, point, mobile, and biogenic sources. Meteorological variables included planetary boundary layer height, temperature, surface solar radiation, water vapor mixing ratio, and wind speed. From the hourly data, monthly averages of daily maximum 8-hr average ozone concentrations, meteorology and emissions were calculated.

B. Observations

Ozone observations were extracted from http://www.epa.gov/ttn/airs/airsaqs/detaildata/downloadaqsdata.htm. Sites with 80% completion for the 8 hour daily maximum for all summer months (1 May – 30 September) during the years 1993-2005 were used, yielding 133 sites for the northeast US model domain. Figure 1 displays the CMAQ model domain and the 133 ozone monitoring sites.

C. Metamodel description: stochastic kriging of principal components

Principal components analysis (PCA) is a technique for reducing the dimension of a problem and for creating an orthogonal set of independent variables. In this case, PCA is used to reduce the 95*65 grids * 65 month CMAQ dimension as follows:

$$\boldsymbol{XS} = (\boldsymbol{X} - \bar{\boldsymbol{X}}) * \boldsymbol{XL}\ , \qquad \boldsymbol{X} = \boldsymbol{XS} * \boldsymbol{XL'} + \bar{\boldsymbol{X}} \tag{1}$$

where X is the original data matrix (the 65 month time series for each of the eight (8) emission and five (5) meteorological variables at the 95*65 model grids). The XS are termed ‘scores’ and XL ‘loadings’. Scores are the representation of X in the principal component space and are orthogonal, while loadings are the coefficients (weights applied to X) that accomplish the transformation between X and XS. Dimension reduction occurs when a few ‘scores’ are able to explain nearly all the variability in X. In the applications described here 15 scores represented the gridded emissions and meteorology.

A mixed spatial model has the form:

$$\boldsymbol{Y_i = X_iB + GRF + \varepsilon_i} \qquad \textbf{(2)}$$

where GRF is a Gaussian random field. The GRF is estimated using kriging techniques, which means the mixed spatial model is an interpolation method for which emissions and/or meteorology have the role that location coordinates play in geostatistical estimation. Termed 'stochastic kriging' (SK, Ankeman et al, 2010) an interpolation estimate looks like:

$$\boldsymbol{\widehat{Y} = \mu + B_1Y_1 + B_2Y_2 + B_3Y_3 + B_4Y_4 + B_5Y_5 \,.\;\;.\;\;. + B_nY_n \quad + \quad \varepsilon_i} \qquad \textbf{(3)}$$

The Y_i are neighbors of an ozone value of interest (Y) in the sense that they are close to Y in terms of emissions and meteorology. The B_i are constants derived from the correlation between different ozone values as a function of their distance apart (again, distance in terms of emissions and/or meteorology)

Several of the emission variables are nearly collinear. For example, point source VOC and NOX emissions are very similar (downward trending step changes). Collinearity makes it difficult to distinguish the respective ozone responses to point source VOC and NOX emissions, hence the use of principal components which are independent of each other.

III. Results

A. Meteorological trend adjustment

Figure 2 shows the rate of exceedance of the current 75 and proposed 65 PPB standards by the annual 4th highest value (not the three year running mean of the 4th highest) over time for the 133 complete sites in the modeling domain (CMAQ values are taken from model grids with ozone monitors). Exceedance rates have declined over time, from more than 90% in 1993 to less than 5% in 2009, but the decline isn't smooth. For example, the exceedance rate in 2005 is greater than the 1994 rate. Under a 65 PPB standard, exceedance rates are above 65% for all years in this figure.

While the downward trend in exceedance rates can be attributed to reductions in emissions, year-to-year variability is due to meteorology. For instance, the increase in exceedance rates between 2004 (about 49%) and 2005 (about 68%) occurred during a period when emissions were not changing appreciably. In an effort to quantify the influence of meteorology on ozone trends, the metamodel was run with anthropogenic CMAQ emissions unchanged and meteorology and biogenic emissions fixed to a particular years' values. Figure 3 is an example for a single site of the metamodel estimate with meteorology fixed at 2005 values (blue) and varying meteorology (green). The fixed meteorology ozone closely matches the downward trend in anthropogenic emissions. Figure 4 displays metamodel ozone based on anthropogenic emissions fixed at 2005 levels and varying meteorology (blue), with varying emissions and meteorology (green). Given 2005 emissions, the year 1999 is seen to have the most ozone conducive meteorology at this site and 2000 the least.

Figure 5 displays the fraction of sites where a given years' meteorology led to the lowest or highest monthly mean ozone value (top and bottom panels, respectively). Using 2005 anthropogenic emissions, the years 2004 and 1999, respectively, had the least and most ozone conducive meteorology at the largest number of sites. As noted above, the rates of exceedance of the 75 PPB standard for those two years were about 49% and 68% (see Figure 2). The spatial distributions of 'least' and 'most' ozone conducive meteorology are shown in Figure 6. The 'least' ozone years appear in clusters and occurred, for example, in 2004 for eastern Ohio and in much of New Jersey. The 'most' ozone conducive meteorology occurred in 1999 for most of the domain, but for a cluster of sites in Ohio occurred in 1994.

B. Ozone trends

Linear trends were estimated at all sites for the month of July and time span 1993-2005 using actual observations and metamodel estimates of observations. Metamodel estimates were based on (1) varying meteorology and biogenic emissions and (2) meteorology and biogenic emissions fixed at a particular year. The fixed meteorology+biogenic emission estimates were further divided: (a) unaltered anthropogenic emissions, (b) NOX mobile source emissions fixed at 2005 levels, and (c) all anthropogenic emissions except NOX mobile fixed at 2005 levels. Mean trends across 133 sites are shown in Table 1. Trends estimated for observations and observations estimated from the metamodel were -0.46 and -0.44 PPB/year, respectively. Trends based on 'fixed meteorology' ranged from -0.20 to -0.44 PPB/year depending on which year's meteorology was used. Fixed meteorology trends tend to be smaller than those estimates which utilize all meteorology (compare the 'all' and 'fixed' column with -0.44 PPB/year).

Trend estimates for metamodel ozone with fixed and varying meteorology (and biogenic emissions) for all sites are shown in the upper left and upper right panels of Figure 7, respectively. The fixed meteorology and biogenic emission estimates (upper left panel) utilize 2005 meteorology. The ratio of trends (fixed/varying, lower left panel) tends to be less than 1.0 because variability has been reduced by fixing meteorology and biogenic emissions. Notice that the meteorologically-free time series in the lower right panel has eliminated the peaks and troughs seen in the time series with varying meteorology.

Figure 8 shows trends for all sites when NOX mobile sources match the CMAQ emission inventory (they vary from year to year) and all other anthropogenic emissions are fixed, in this case at 2005 levels. The trends are smaller than when all emissions follow the emission inventory each year (Figure 7), and more variability has been removed from the time series (see lower right panel). Figure 9 shows trends when NOX mobile sources, meteorology, and biogenic emissions are fixed, while the anthropogenic emissions vary from year to year. It is evident that much of the trend can be attributed to sources other than NOX mobile.

The scenarios depicted in Figures 7-9 are summarized for all meteorological years in Table 1. The meteorologically independent trends, averaged over 133 sites, range between -0.20 (1999 meteorology and biogenic emissions) and -0.44 (2005 meteorology and biogenic emissions) PPB/year, while the mean trend when all model inputs vary is -0.44 PPB/year. In addition, trends attributable to NOX mobile sources (last column on right) are smaller in magnitude than those attributable to other anthropogenic sources (2nd column from right).

Table 1. Ozone trends for July 1993-2005, PPB/year, mean for 133 sites

	meteorological year		anthropogenic emissions		
		varying	varying	fixed NOX mobile	fixed except NOX mobile
			meteorology and biogenic emissions		
		varying	fixed	fixed	fixed
observations		-0.46			
metamodel observations		-0.44			
	1993		-0.27	-0.26	-0.12
	1994		-0.38	-0.34	-0.14
	1995		-0.41	-0.36	-0.14
	1996		-0.26	-0.27	-0.09
	1997		-0.28	-0.30	-0.10
	1998		-0.21	-0.25	-0.11
	1999		-0.20	-0.20	-0.10
	2000		-0.24	-0.28	-0.15
	2001		-0.26	-0.29	-0.08
	2002		-0.21	-0.21	-0.10
	2003		-0.37	-0.32	-0.12
	2004		-0.38	-0.30	-0.12
	2005		-0.44	-0.39	-0.18

C. Effect of emission changes on ozone annual 4th highest values

Three emission reduction scenarios are played out in this section: (1) elimination of all mobile NOX source emissions, (2) elimination of all anthropogenic source emissions other than NOX mobile, and (3) elimination of all anthropogenic sources. All scenarios are carried out at constant meteorology.

Figure 10 is an example of all three scenarios using July 2005 meteorology and biogenic emissions. The upper left panel is monthly mean ozone (PPB) for the base case (other emission sources varying), the upper right panel is the result of eliminating all NOX mobile sources, the lower left is the result of eliminating all anthropogenic sources but NOX mobile sources, and the lower right is elimination of all anthropogenic sources.

Domain-wide mean ozone values for each scenario are shown for all meteorological years in Table 2. Reductions in ozone attributable to mobile NOX sources range from 1.6 PPB (1997 meteorology) to 3.3 PPB (1999 meteorology). Reductions in ozone due to changes in all other sources are larger, ranging from 3.8 (1997 meteorology) to 8.2 PPB (2004 meteorology).

What impact do emission reductions have relative to the NAAQS of 75 PPB? To address this question the monthly mean ozone values were converted to estimates of 4th highest values by multiplying by the ratio of the 4th highest to the monthly mean value found in the observations for each month and site. For example, if the metamodel monthly mean ozone is 50 PPB and the observed ratio of 4th highest to monthly mean were 90/45 for the same site, the metamodel 4th highest would be 100 (50x90/45). The ozone values in the example of Figure 10 transformed in this way are shown in Figure 11.

On the basis of the transformed values (i.e., Figure 11), domain-wide emission reductions result in modest reductions in the rate of exceedance of the 75 PPB standard (Table 3). Eliminating all anthropogenic emissions leaves more than 40% of the sites with values exceeding the standard for all meteorological years. Observed exceedance rates for years past the end of our simulation (2006-2011, a time of continuing though less dramatic declines in emission rates) for the set of 133 sites were [0.60 0.82 0.47 0.02 0.41 0.44]. The implication is that as emissions continue to fall, progress toward complete compliance is small. Considering the proposed 65 PPB standard, exceedance rates exceed 85% for all meteorological years (Table 4).

Table 2. Domain wide mean monthly ozone given emission reductions

	anthropogenic emissions			
	varying	NOX mobile = 0	all except NOX mobile = 0	all = 0
		meteorology and biogenic emissions		
year (also for fixed variables)	varying	fixed	fixed	fixed
1993	60.0	58.2	52.6	51.0
1994	58.0	55.5	51.5	50.1
1995	56.0	53.3	50.6	49.2
1996	60.2	57.4	52.6	51.3
1997	52.3	50.7	48.5	47.1
1998	59.1	56.2	52.4	50.8
1999	57.8	54.5	51.3	49.7
2000	58.8	55.6	51.9	50.6
2001	54.1	51.7	48.8	47.3
2002	58.5	55.8	52.2	50.7
2003	58.6	56.2	51.7	50.4
2004	61.7	59.6	53.5	52.3
2005	53.3	51.1	48.7	46.9

Table 3. Fraction of sites exceeding 4th highest limit of 75 PPB

	anthropogenic emissions			
	varying	NOX mobile = 0	all except NOX mobile = 0	all = 0
	meteorology and biogenic emissions			
year (also for fixed variables)	varying	fixed	fixed	fixed
1993	0.93	0.92	0.71	0.65
1994	0.95	0.86	0.68	0.63
1995	0.94	0.77	0.65	0.59
1996	0.92	0.90	0.71	0.69
1997	0.98	0.68	0.51	0.41
1998	0.95	0.85	0.71	0.67
1999	0.99	0.90	0.71	0.62
2000	0.88	0.89	0.74	0.67
2001	0.99	0.75	0.62	0.56
2002	1.00	0.86	0.70	0.67
2003	0.85	0.87	0.68	0.65
2004	0.73	0.94	0.73	0.69
2005	0.93	0.75	0.56	0.41

Table 4. Fraction of sites exceeding 4th highest limit of 65 PPB

	anthropogenic emissions			
	varying	NOX mobile = 0	all except NOX mobile = 0	all = 0
		meteorology and biogenic emissions		
year (also for fixed variables)	varying	fixed	fixed	fixed
1993	0.99	0.99	0.92	0.89
1994	0.99	0.98	0.91	0.91
1995	0.99	0.96	0.89	0.89
1996	0.99	0.99	0.93	0.92
1997	0.99	0.95	0.86	0.83
1998	0.99	0.98	0.92	0.91
1999	0.99	0.99	0.92	0.89
2000	0.99	0.98	0.93	0.93
2001	0.99	0.95	0.91	0.89
2002	1.00	0.99	0.92	0.91
2003	0.99	0.99	0.92	0.90
2004	0.99	0.99	0.92	0.93
2005	0.98	0.94	0.87	0.86

Summary

An ozone metamodel based on thirteen (13) years (1993-2005) of a CMAQ simulation for the northeast U.S. was developed. Independent variables were monthly mean emission inventory values for eight (8) sources (NOX and VOCs from area, point, mobile, and biogenic sources) and five meteorological variables (planetary boundary layer height, temperature, surface solar radiation, water vapor mixing ratio and wind speed). Dependent variables were observed monthly mean ozone values at 133 sites in the model domain.

The metamodel was used to estimate ozone values for scenarios that included constant meteorology and/or emissions. We were able to (1) identify years and sites with the least and most ozone conducive meteorology, (2) estimate meteorologically independent temporal trends in ozone, and (3) compare the impact of mobile sources with other anthropogenic emissions on ozone trends and exceedances of 75 PPB.

With constant meteorology, ozone time series mirror those of emissions and are therefore smoothly trending downward. Constant emissions, on the other hand, lead to identification of ozone conducive meteorology. Identification of the years1999 and 2000 as among the least/most ozone conducive meteorology years, respectively, explains the dip in ozone exceedance rates that occurred between the years 1999 and 2000.

The effect of changes in particular emission sources on trends and exceedance rates were studied by holding one or more sources constant (under constant meteorology). In this demonstration we find that trends due to reductions in mobile sources are smaller than those attributable to reductions in other emissions.

References

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Hogrefe, C., Lynn, B., Goldberg, R, Rosenzweig, C., Zalewsky, E., Hao, W., Doraswamy, P., Civerolo, K., Ku, J., Sistla, G., and P. Kinney. 2009. A combined model-observation approach to estimate historic gridded fields of PM2.5 mass and species concentrations, *Atmospheric Environment* **43**:2561-2570.

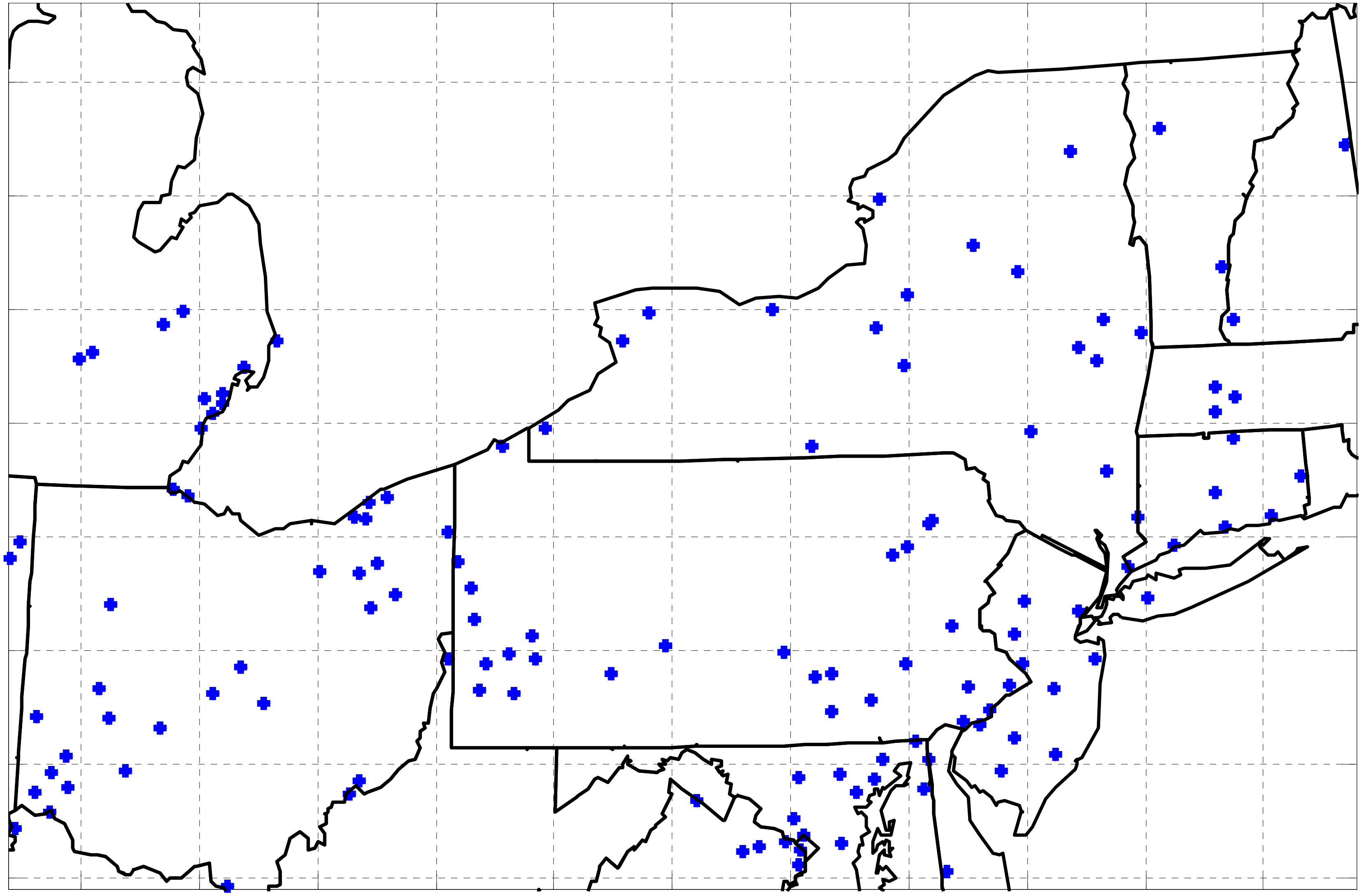

Figure 1. Monitor locations (80% complete)

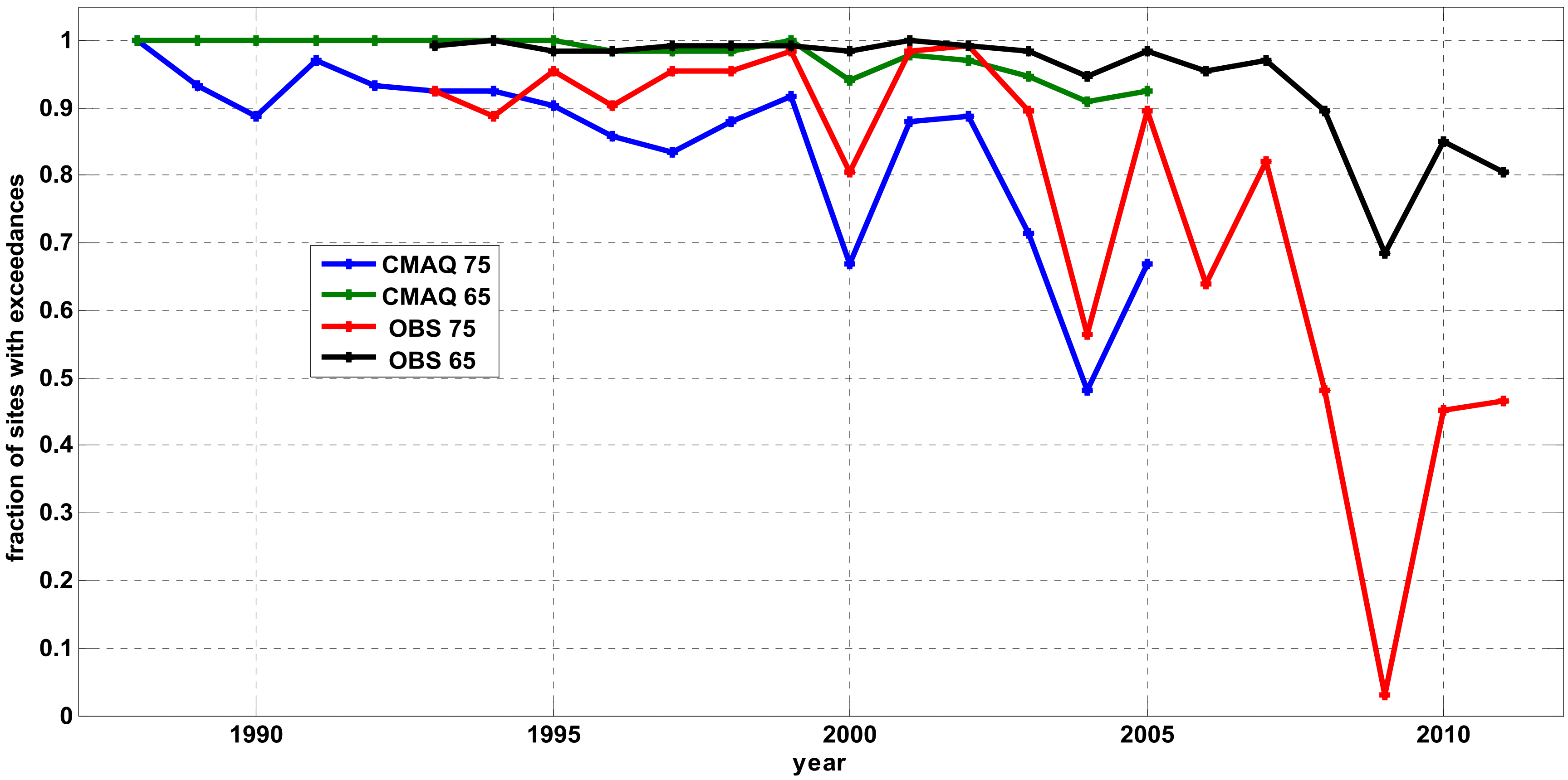

Figure 2. Observed and CMAQ exceedance rates for 133 complete sites in the NEUS domain using 75 and 65 ppb

Figure 3. Effect of emissions on July ozone trend at a single site; blue: fixed meteorology (2005), green: varying meteorology

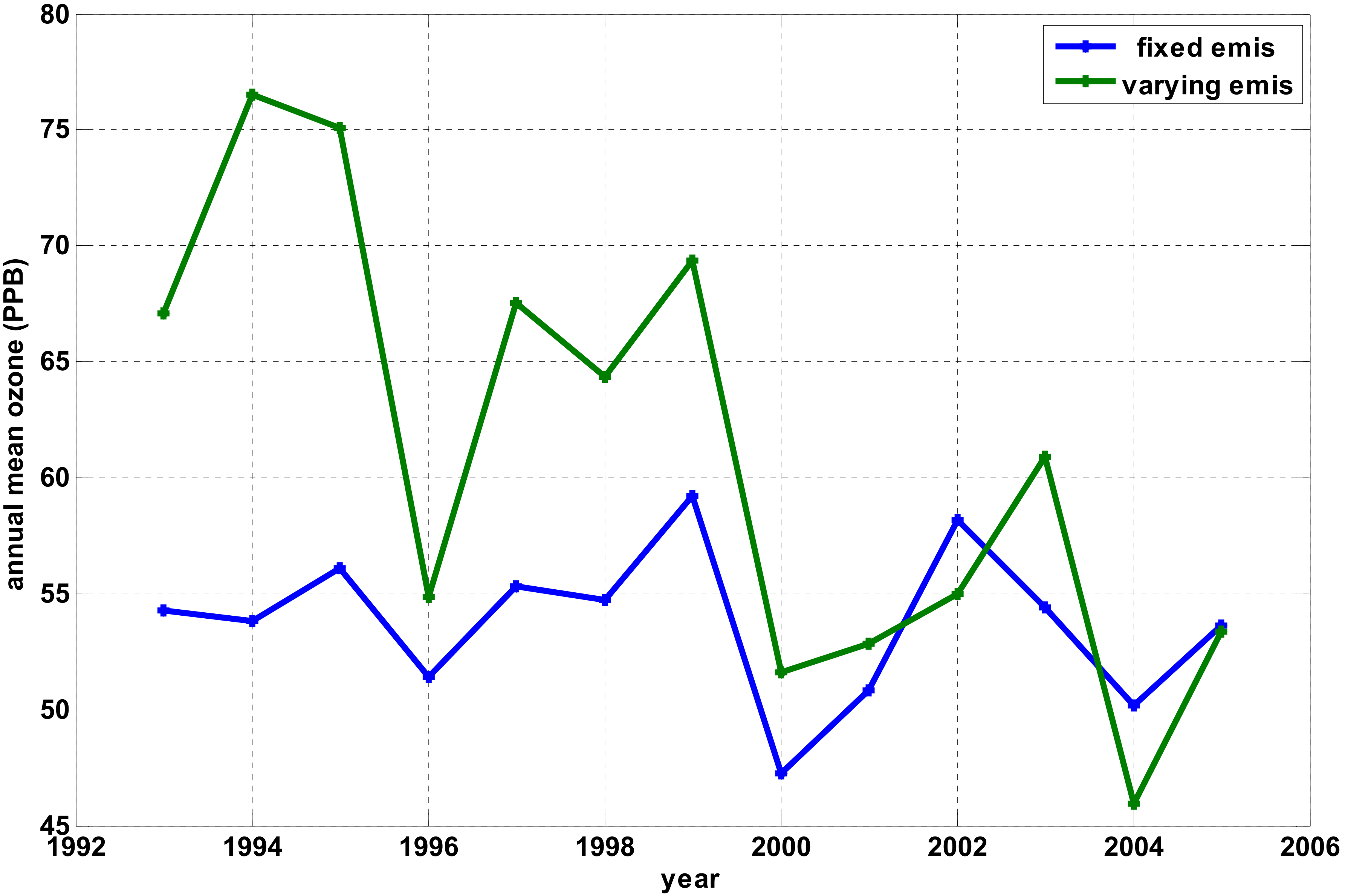

Figure 4. Metamodel identification of ozone conducive meteorology at a single site: fixed at 2005 emissions (blue), variable emissions (green), both with CMAQ meteorology. Fixed emissions indicate 1999 as having the most ozone conducive meteorology and 2000 the least.

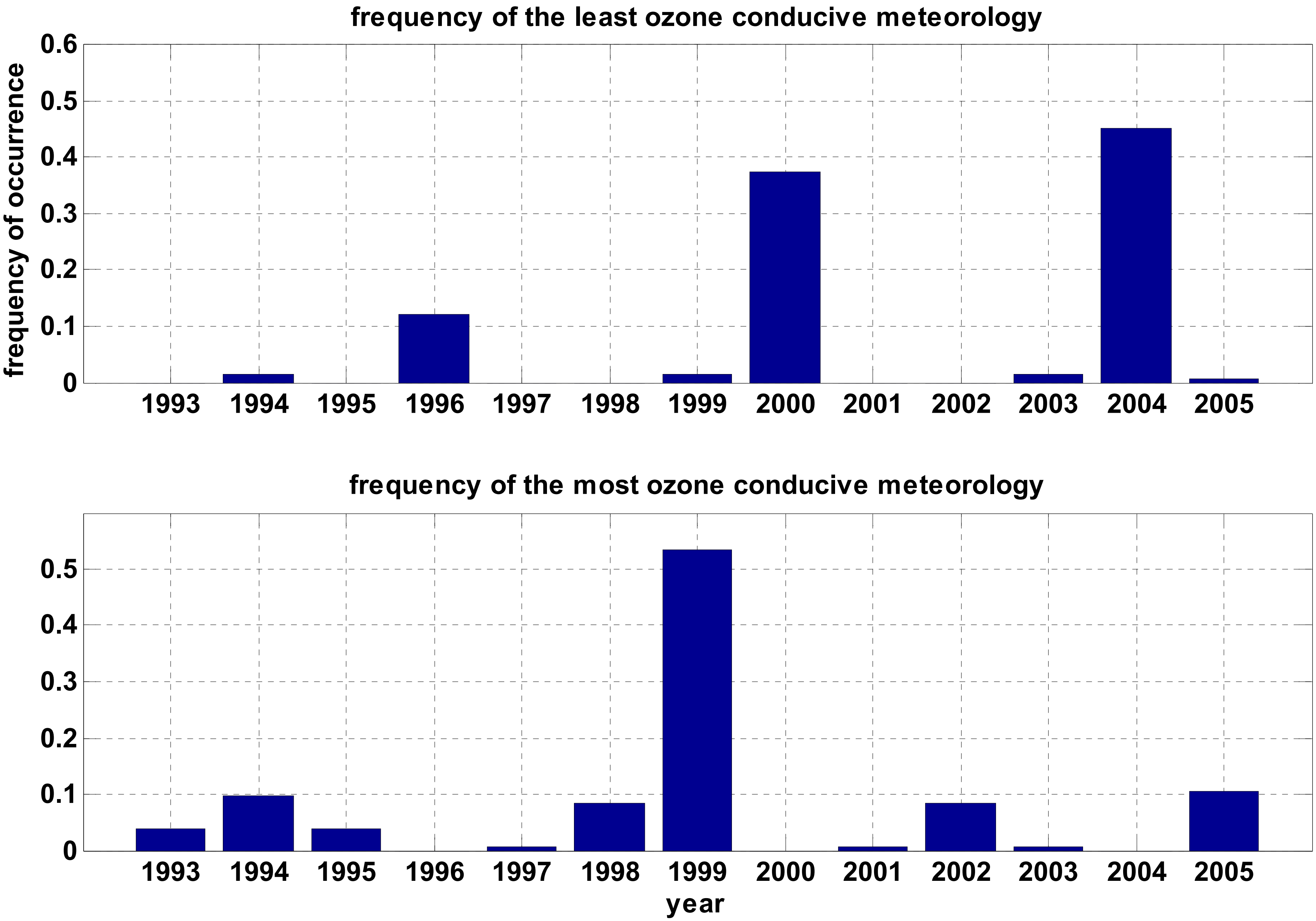

Figure 5. Frequency of occurrence of least (top panel) and most (bottom panel) ozone conducive years for 133 sites and emissions for 2005. The years 2004 (45%) and 1999 (53%) were most frequently the least and most ozone conducive years, respectively.

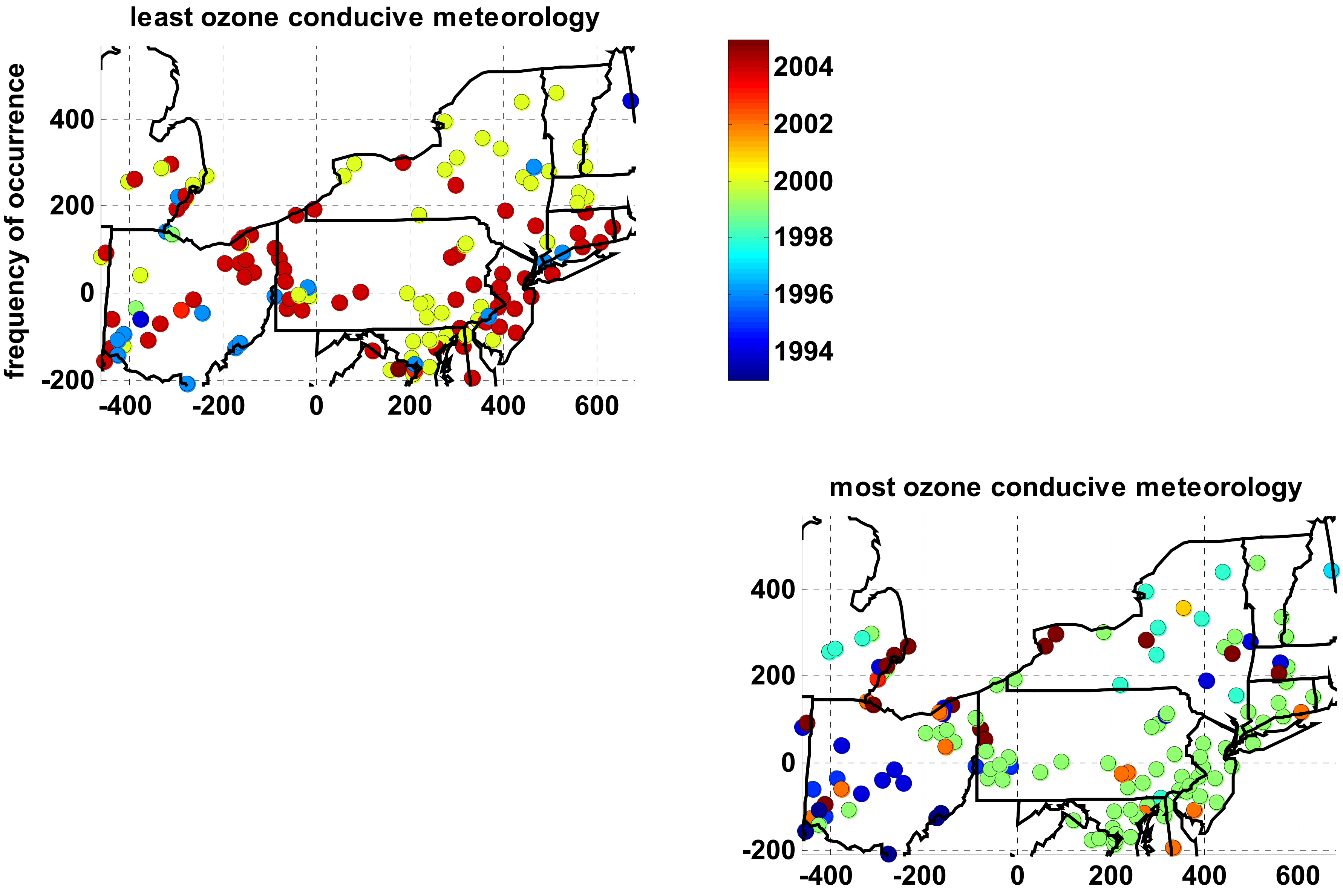

Figure 6. Year by site of least (upper left panel) and most (lower right panel) ozone conducive meteorology

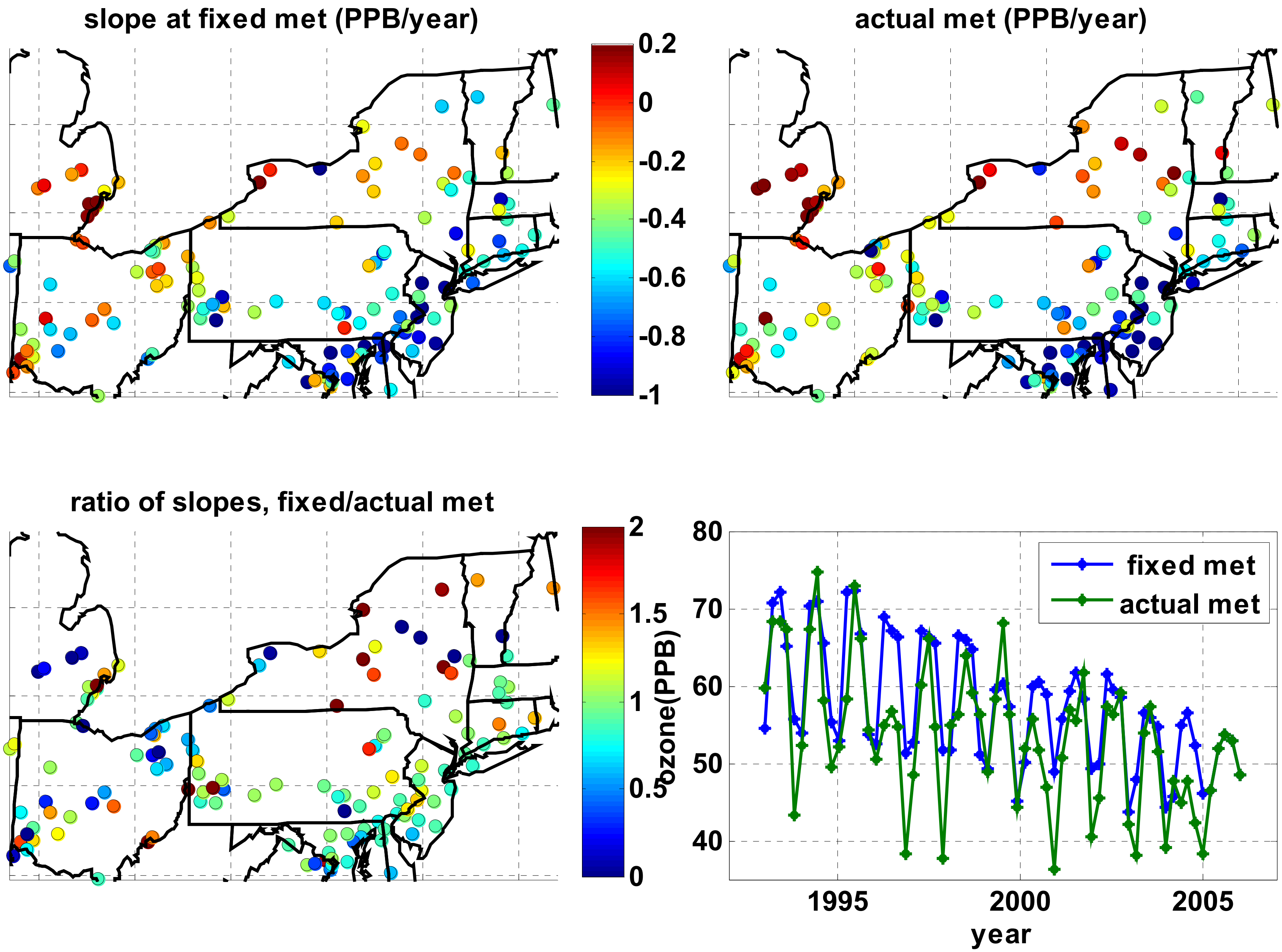

Figure 7. Ozone temporal trends for July with meteorology and biogenic emissions:

upper left:	fixed (2005 values)
upper right:	varying
lower left:	trend ratio, fixed/varying
lower right:	example time series for a single site

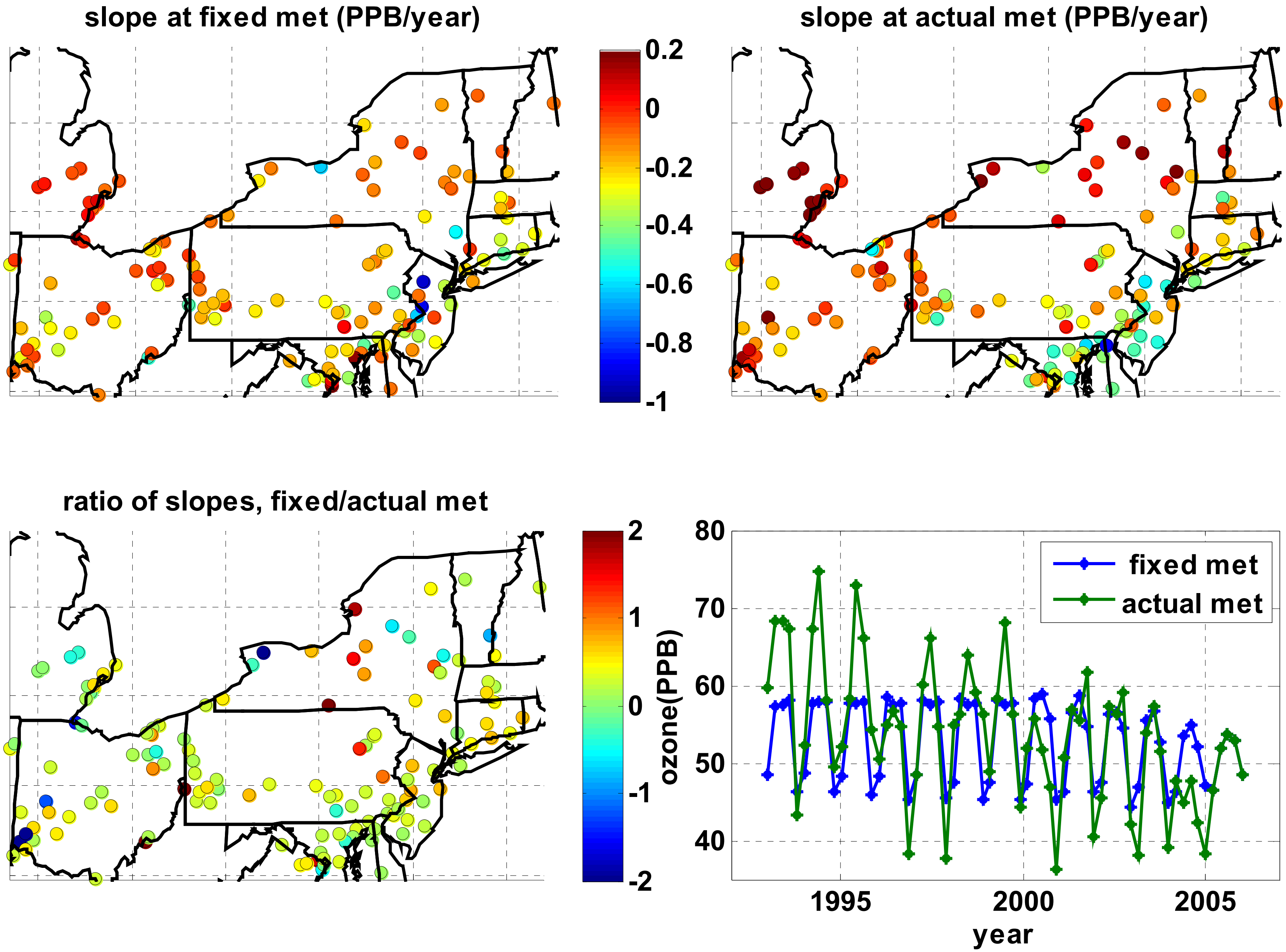

Figure 7. Ozone temporal trends for July with varying NOX mobile sources and all else constant.
upper left: trend (ppb/year) with 2005 meteorology,
upper right: trend with actual meteorology;
lower left: trend ratio, 2005 meteorology/actual meteorology,
lower right: example time series for a single site

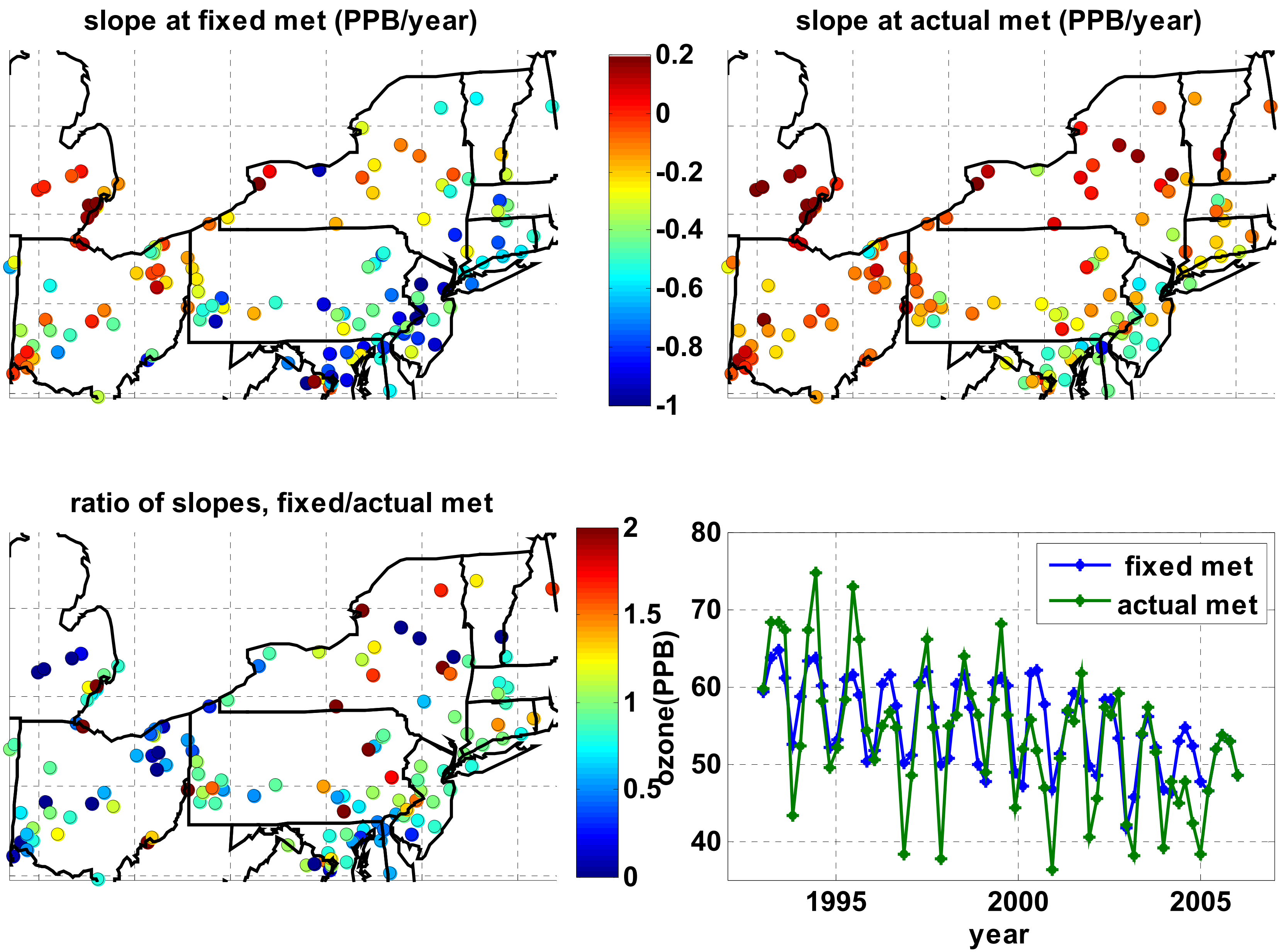

Figure 8. Ozone temporal trends for July with varying anthropogenic emissions except constant NOX mobile sources.
upper left: trend (ppb/year) with 2005 meteorology,
upper right: trend with actual meteorology;
lower left: trend ratio, 2005 meteorology/actual meteorology,
lower right: example time series for a single site

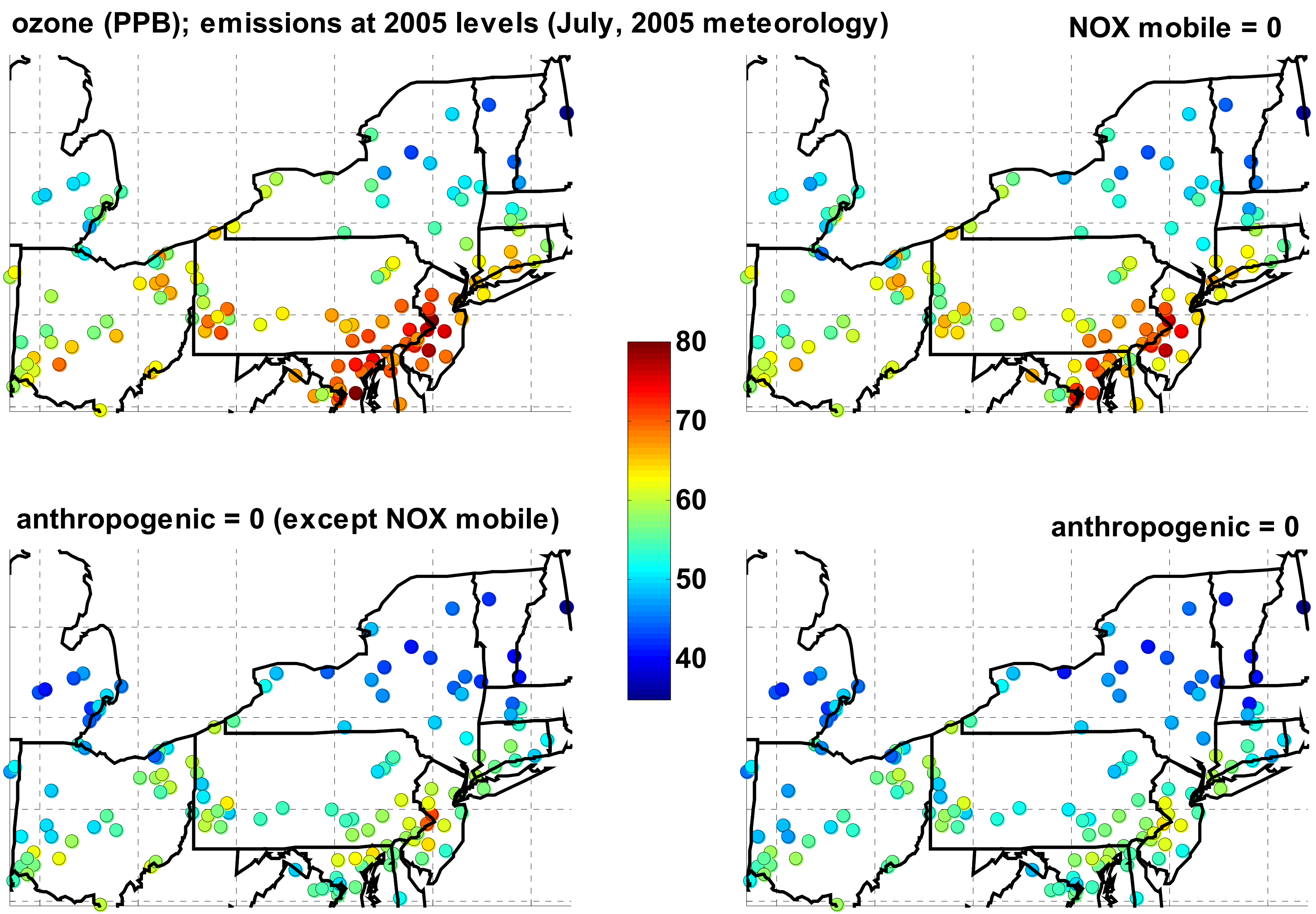

Figure 9. Monthly mean ozone (PPB) for July 2005, meteorology and biogenic sources fixed at 2005 values;
upper left: varying emissions (other than biogenic)
upper right: NOX mobile sources set to 0
lower left: anthropogenic (except NOX mobile) set to 0,
lower right: all anthropogenic set to 0,

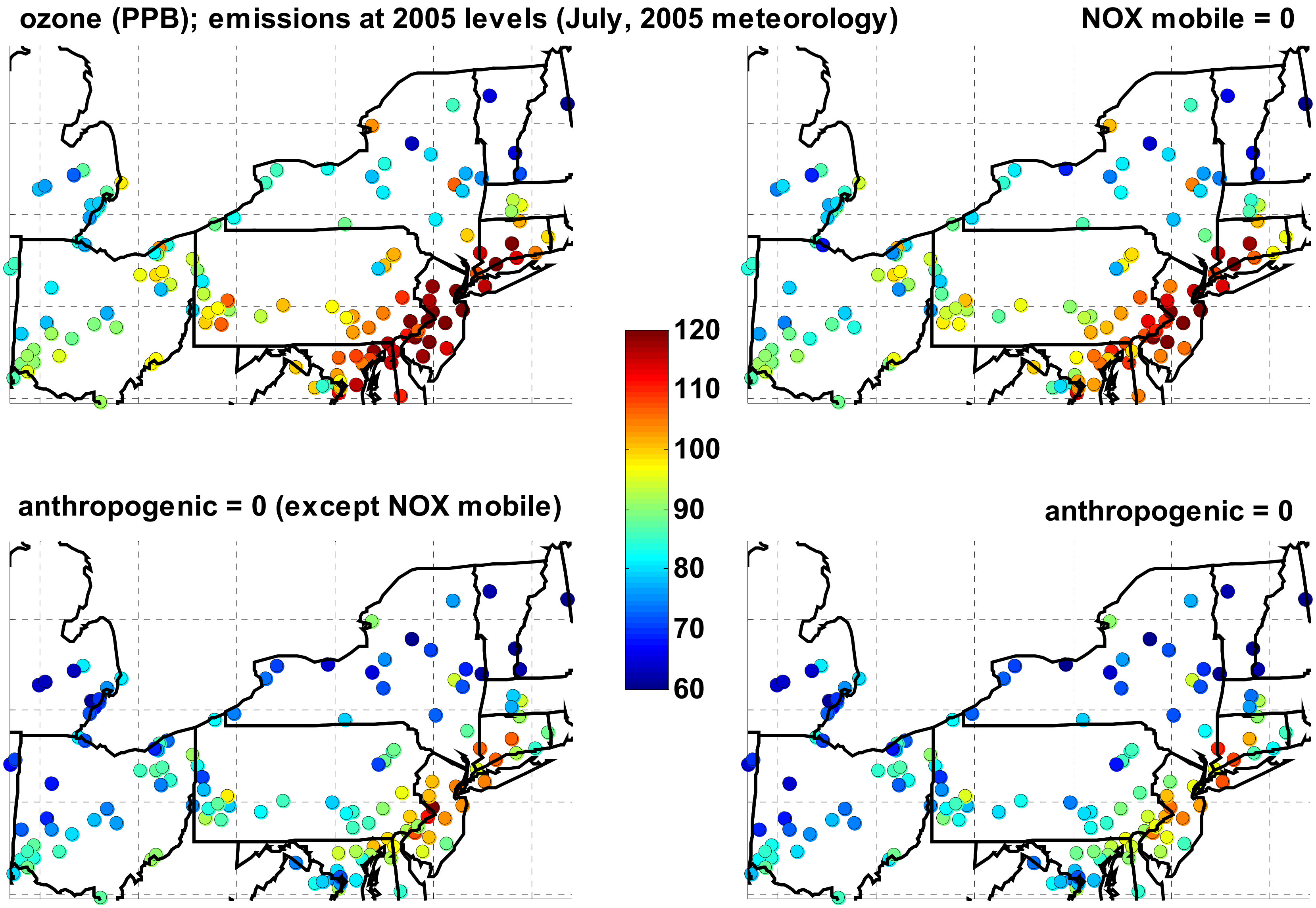

Figure 10. Same as figure 10 except adjusted to match annual 4th highest values (PPB) for 2005;

upper left: actual (CMAQ) emissions
upper right: NOX mobile sources set to 0
lower left: anthropogenic (except NOX mobile) set to 0,
lower right: all anthropogenic set to 0,