Source-Receptor Relationships Between Precursor Emissions and O_3 and $PM_{2.5}$ Air Pollution Impacts

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This supporting information document contains 23 pages with 1 equation, 9 tables, and 12 figures.

Equation S1. Linear regression equations relating distance with air quality estimates as published in Baker and Foley, 2011. Here, new source emissions are expressed in tpy, ammonia concentration at receptor grid cells in ppb, and distance between the source and downwind grid cell in km to predict O_3 (ppb) or $PM_{2.5}$ ($\mu g/m^3$) concentrations. The β4 term is zero unless estimating $PM_{2.5}$ nitrate ion. This equation is not used in PCAPS and is a separate modeling approach.

$$\text{Concentration} = \frac{\beta_1 * emissions + \beta_4 * ammonia}{1 + (\beta_2 * dist)^{\beta_3}}$$

Table S1. Total emission reductions for each of the emissions scenarios.

	Annual Total Emission Reductions (tons)		
Scenario	**NO_X**	**SO_2**	**$PM_{2.5}$**
Mobile (Tier 3)	348,467	13,132	8,518
EGU (Clean Power Plan Proposal)	424,237	426,529	63,192
Pulp & Paper	34,616	36,464	7,197
Cement Kilns	97,185	55,417	13,093
Refineries	34,982	16,422	3,932

Table S2. Definition of model performance metrics. Here, *M* refers to the reduced complexity model and *O* refers to observation data or photochemical grid model prediction depending on the type of evaluation.

Definitions of performance metrics.

Abbreviation	Term	Definition[a]
MB	Mean bias	$\frac{1}{N}\sum(M_i - O_i)$
ME	Mean error	$\frac{1}{N}\sum\lvert M_i - O_i\rvert$
FB	Fractional bias	$100\% \times \frac{2}{N}\sum\frac{(M_i - O_i)}{(M_i + O_i)}$
FE	Fractional error	$100\% \times \frac{2}{N}\sum\frac{\lvert M_i - O_i\rvert}{(M_i + O_i)}$
NMB	Normalized mean bias	$100\% \times \frac{\sum(M_i - O_i)}{\sum O_i}$

Table S3. Regression coefficients calculated for the nonlinear regression model (Baker and Foley, 2011) using the generic source training dataset described in this assessment.

Precursor	Pollutant	Release Type	beta1	beta2	beta3	beta4
Primary PM2.5	Annual average PM2.5	tall stack	1.26E-04	0.046	1.515	0.00E+00
Primary PM2.5	Annual average PM2.5	surface	1.56E-03	0.102	1.950	0.00E+00
PM Coarse Mass	Annual average PM2.5	tall stack	1.15E-04	0.050	1.566	0.00E+00
PM Coarse Mass	Annual average PM2.5	surface	1.35E-03	0.104	2.118	0.00E+00
SO2	Annual average PM2.5	tall stack	5.96E-06	0.031	1.071	0.00E+00
SO2	Annual average PM2.5	surface	1.66E-05	0.084	1.065	0.00E+00
NOX	Annual average PM2.5	tall stack	1.73E-06	0.013	1.478	5.85E-04
NOX	Annual average PM2.5	surface	4.80E-06	0.028	1.375	9.77E-04
NOX	Seasonal average MDA8 O3	tall stack	1.94E-04	0.042	1.409	
NOX	Seasonal average MDA8 O3	surface	2.35E-04	0.045	1.424	
VOC	Seasonal average MDA8 O3	tall stack	1.02E-05	0.027	1.399	
VOC	Seasonal average MDA8 O3	surface	9.24E-06	0.029	1.389	

Table S4. Performance metrics comparing the non-linear regression model (NLIN2) with photochemical model (CMAQ) predicted change in seasonal MDA8 O_3 with two complex emission control scenarios for each grid cell in multiple regions and the entire U.S. Modeled means and mean bias (MB) expressed in ppb. Normalized mean bias (NMB), fractional bias (FB), and fractional error (FE) expressed as a percent.

Seasonal MDA8 O3	Mobile Control Scenario							EGU Control Scenario						
Region	NLIN2 mean	CMAQ mean	MB	NMB	FB	FE	r	NLIN2 mean	CAMx mean	MB	NMB	FB	FE	r
Northeast	-0.34	-0.27	-0.071	26.5	23.4	29.8	0.82	-0.36	-0.26	-0.096	36.6	30.9	34.0	0.76
Northern Rockies	-0.16	-0.13	-0.022	16.3	15.0	26.4	0.78	-0.19	-0.16	-0.035	22.1	19.9	35.3	0.77
Northwest	-0.08	-0.12	0.033	-28.3	-32.9	46.7	0.41	-0.07	-0.05	-0.020	40.8	33.9	39.1	0.93
Ohio Valley	-0.58	-0.48	-0.099	20.7	18.8	21.3	0.47	-0.43	-0.42	-0.009	2.2	2.2	33.6	0.43
South	-0.36	-0.31	-0.045	14.6	13.6	16.8	0.86	-0.55	-0.58	0.035	-6.0	-6.1	27.5	0.86
Southeast	-0.54	-0.58	0.041	-7.1	-7.4	11.4	0.85	-0.52	-0.70	0.184	-26.1	-30.0	33.5	0.77
Southwest	-0.18	-0.21	0.033	-15.5	-16.8	23.7	0.49	-0.26	-0.27	0.008	-3.1	-3.1	26.1	0.66
Upper Midwest	-0.37	-0.27	-0.093	34.1	29.1	31.9	0.87	-0.35	-0.27	-0.079	28.8	25.2	27.4	0.28
West	-0.07	-0.07	0.0001	-0.1	-0.1	34.7	0.76	-0.10	-0.12	0.022	-18.2	-20.0	40.7	0.14
US	-0.2928	-0.27	-0.023	8.5	8.1	21.7	0.90	-0.33	-0.34	0.007	-2.1	-2.1	30.8	0.84

Table S5. Performance metrics comparing COBRA with photochemical model predicted annual average $PM_{2.5}$ for each grid cell in multiple regions and the entire U.S. Modeled means and mean bias (MB) expressed in $\mu g/m^3$. Normalized mean bias (NMB), fractional bias (FB), and fractional error (FE) expressed as a percent.

Annual PM2.5	Mobile Control Scenario							EGU Control Scenario						
Region	COBRA mean	CMAQ mean	MB	NMB	FB	FE	r	COBRA mean	CAMx mean	MB	NMB	FB	FE	r
Northeast	-0.029	-0.023	-0.006	25.0	22.3	35.7	0.83	-0.038	-0.102	0.064	-62.7	-91.4	91.4	0.75
Northern Rockies	-0.011	-0.011	0.000	-3.1	-3.1	56.1	0.84	-0.019	-0.035	0.016	-46.1	-60.0	71.2	0.93
Northwest	-0.008	-0.007	-0.002	24.2	21.6	75.3	0.16	-0.008	-0.004	-0.004	112.5	72.0	95.0	-0.13
Ohio Valley	-0.034	-0.062	0.028	-45.0	-58.0	61.3	0.38	-0.046	-0.144	0.098	-67.9	-102.7	105.1	0.08
South	-0.023	-0.029	0.006	-21.3	-23.8	46.0	0.55	-0.060	-0.144	0.084	-58.4	-82.5	83.7	0.63
Southeast	-0.034	-0.045	0.011	-23.6	-26.7	45.1	0.21	-0.060	-0.200	0.140	-70.0	-107.7	110.7	-0.14
Southwest	-0.014	-0.009	-0.005	57.9	44.9	65.2	0.57	-0.023	-0.032	0.008	-26.5	-30.5	49.3	0.52
Upper Midwest	-0.027	-0.050	0.023	-46.4	-60.3	69.1	0.40	-0.057	-0.117	0.060	-51.1	-68.6	79.6	0.11
West	-0.006	-0.002	-0.004	165.2	90.5	103.7	0.43	-0.015	-0.009	-0.007	72.9	53.4	81.6	0.48
US	-0.020	-0.026	0.006	-21.7	-24.4	55.6	0.71	-0.037	-0.088	0.051	-57.8	-81.4	89.6	0.58

Table S6. Performance metrics comparing the nonlinear regression model NLIN2 with photochemical model predicted annual average $PM_{2.5}$ for each grid cell in multiple regions and the entire U.S. Modeled means and mean bias (MB) expressed in $\mu g/m^3$. Normalized mean bias (NMB), fractional bias (FB), and fractional error (FE) expressed as a percent.

Annual PM2.5	Mobile Control Scenario							EGU Control Scenario						
Region	NLIN2 mean	CMAQ mean	MB	NMB	FB	FE	r	NLIN2 mean	CAMx mean	MB	NMB	FB	FE	r
Northeast	-0.021	-0.023	0.002	-9.4	-9.8	26.7	0.86	-0.104	-0.102	-0.002	2.3	2.3	11.3	0.95
Northern Rockies	-0.010	-0.011	0.001	-10.7	-11.4	49.9	0.91	-0.050	-0.035	-0.015	43.2	35.5	45.7	0.89
Northwest	-0.005	-0.007	0.002	-29.2	-34.2	70.7	0.69	-0.015	-0.004	-0.011	277.3	116.2	121.1	0.41
Ohio Valley	-0.040	-0.062	0.023	-36.1	-44.0	45.6	0.75	-0.148	-0.144	-0.004	3.0	3.0	21.2	0.34
South	-0.023	-0.029	0.006	-22.1	-24.9	33.6	0.89	-0.148	-0.144	-0.004	2.5	2.5	23.8	0.80
Southeast	-0.035	-0.045	0.010	-22.6	-25.5	32.9	0.79	-0.194	-0.200	0.006	-3.0	-3.0	13.6	0.76
Southwest	-0.012	-0.009	-0.003	38.0	31.9	60.2	0.79	-0.067	-0.032	-0.035	112.2	71.9	73.5	0.83
Upper Midwest	-0.027	-0.050	0.023	-45.4	-58.7	59.2	0.85	-0.132	-0.117	-0.015	13.2	12.4	22.5	0.94
West	-0.004	-0.002	-0.002	83.8	59.0	75.4	0.76	-0.033	-0.009	-0.024	264.6	113.9	114.4	0.81
US	-0.019	-0.026	0.006	-24.5	-27.9	43.9	0.91	-0.101	-0.088	-0.012	13.9	13.0	28.1	0.84

Table S7. Performance metrics comparing PCAPS with photochemical model predicted annual average $PM_{2.5}$ nitrate ion for each grid cell in multiple regions and the entire U.S. Modeled means and mean bias (MB) expressed in $\mu g/m^3$. Normalized mean bias (NMB), fractional bias (FB), and fractional error (FE) expressed as a percent.

PM2.5 nitrate ion	Mobile Control Scenario							EGU Control Scenario						
Region	PCAPS mean	CMAQ mean	MB	NMB	FB	FE	r	PCAPS mean	CAMx mean	MB	NMB	FB	FE	r
Northeast	-0.016	-0.013	-0.003	24.6	21.9	30.3	0.85	-0.019	-0.013	-0.006	48.2	38.8	58.3	0.63
Northern Rockies	-0.004	-0.006	0.002	-37.8	-46.5	57.4	0.97	-0.005	-0.009	0.004	-45.3	-58.5	77.6	0.90
Northwest	-0.003	-0.004	0.001	-25.9	-29.8	67.9	0.62	-0.001	-0.001	0.001	-43.1	-55.0	91.4	0.22
Ohio Valley	-0.029	-0.032	0.003	-10.2	-10.7	23.3	0.85	-0.020	-0.024	0.003	-14.1	-15.1	53.1	0.56
South	-0.010	-0.012	0.003	-20.8	-23.3	35.8	0.82	-0.017	-0.012	-0.006	48.4	39.0	69.4	0.57
Southeast	-0.022	-0.015	-0.007	44.3	36.3	44.8	0.47	-0.020	-0.004	-0.016	361.4	128.8	143.0	0.01
Southwest	-0.002	-0.003	0.000	-9.2	-9.6	62.3	0.79	-0.003	-0.001	-0.002	121.6	75.6	99.5	0.52
Upper Midwest	-0.021	-0.029	0.008	-27.5	-31.9	36.6	0.85	-0.019	-0.032	0.013	-41.9	-52.9	57.4	0.70
West	-0.001	-0.001	0.000	26.2	23.2	83.8	0.75	-0.002	-0.003	0.002	-48.4	-63.9	91.2	0.86
US	-0.011	-0.012	0.001	-9.2	-9.7	36.8	0.88	-0.011	-0.011	-0.001	8.5	8.2	73.1	0.58

Table S8. Performance metrics comparing PCAPS with photochemical model predicted annual average $PM_{2.5}$ sulfate ion for each grid cell in multiple regions and the entire U.S. Modeled means and mean bias (MB) expressed in $\mu g/m^3$. Normalized mean bias (NMB), fractional bias (FB), and fractional error (FE) expressed as a percent.

PM2.5 sulfate ion	Mobile Control Scenario							EGU Control Scenario						
Region	PCAPS mean	CMAQ mean	MB	NMB	FB	FE	r	PCAPS mean	CAMx mean	MB	NMB	FB	FE	r
Northeast	-3E-03	-6E-04	-2E-03	298.6	119.8	121.5	0.50	-0.048	-0.049	0.000	-0.9	-0.9	10.0	0.98
Northern Rockies	-4E-04	-3E-04	-2E-04	71.5	52.7	52.8	0.81	-0.010	-0.014	0.003	-24.5	-27.9	31.1	0.98
Northwest	-5E-04	-4E-04	-8E-05	19.1	17.5	35.4	0.61	-0.001	-0.001	0.000	21.9	19.8	25.2	0.96
Ohio Valley	-2E-03	-9E-04	-2E-03	182.2	95.3	95.7	0.04	-0.077	-0.068	-0.009	13.2	12.4	17.7	0.86
South	-1E-03	-1E-03	-8E-06	0.6	0.6	21.6	0.79	-0.072	-0.1	0.004	-4.6	-4.8	14.4	0.93
Southeast	-3E-03	-2E-03	-8E-04	40.8	33.9	35.9	0.35	-0.114	-0.108	-0.005	5.1	4.9	12.1	0.90
Southwest	-4E-04	-7E-04	3E-04	-42.8	-54.5	61.8	-0.06	-0.013	-0.015	0.002	-13.2	-14.2	20.9	0.86
Upper Midwest	-1E-03	2E-04	-2E-03	-735.1	274.8	274.5	-0.37	-0.033	-0.039	0.006	-16.2	-17.6	24.9	0.51
West	-2E-04	-2E-04	6E-05	-23.9	-27.1	35.6	0.72	-0.002	-0.002	0.000	-8.2	-8.6	21.3	0.77
US	-1E-03	-8E-04	-5E-04	64.2	48.6	65.1	0.52	-0.042	-0.042	0.001	-1.3	-1.3	15.9	0.96

Table S9. Performance metrics comparing PCAPS with photochemical model predicted annual average $PM_{2.5}$ elemental carbon for each grid cell in multiple regions and the entire U.S. Modeled means and mean bias (MB) expressed in $\mu g/m^3$. Normalized mean bias (NMB), fractional bias (FB), and fractional error (FE) expressed as a percent.

PM2.5 elem. carbon	Mobile Control Scenario							EGU Control Scenario						
Region	PCAPS mean	CMAQ mean	MB	NMB	FB	FE	r	PCAPS mean	CAMx mean	MB	NMB	FB	FE	r
Northeast	-6E-04	-6E-04	5E-05	-7.9	-8.2	15.4	0.94	-1E-03	-1E-03	-2E-04	23.2	20.8	26.8	0.91
Northern Rockies	-2E-04	-3E-04	9E-05	-29.4	-34.5	40.6	0.88	-2E-04	-2E-04	3E-06	-1.4	-1.4	21.8	0.87
Northwest	-2E-06	-2E-05	2E-05	-90.5	-165.4	77.4	0.66	-3E-05	-4E-05	6E-06	-18.3	-20.2	42.3	0.70
Ohio Valley	-2E-03	-2E-03	2E-04	-10.7	-11.3	18.5	0.92	-1E-03	-1E-03	-1E-04	14.3	13.4	26.7	0.90
South	-9E-04	-1E-03	2E-04	-21.6	-24.2	29.0	0.93	-1E-03	-1E-03	-1E-04	12.8	12.0	23.1	0.76
Southeast	-2E-03	-2E-03	3E-04	-14.1	-15.2	25.3	0.85	-3E-03	-2E-03	-7E-04	29.6	25.8	30.0	0.77
Southwest	-4E-04	-5E-04	1E-04	-23.5	-26.6	50.6	0.81	-5E-04	-5E-04	3E-06	-0.6	-0.6	27.6	0.84
Upper Midwest	-1E-03	-2E-03	3E-04	-16.5	-18.0	24.1	0.92	-1E-03	-1E-03	-2E-04	14.8	13.8	31.8	0.48
West	-9E-05	-1E-04	2E-05	-21.8	-24.4	62.5	0.70	-5E-05	-9E-05	3E-05	-37.8	-46.6	56.4	0.67
US	-8E-04	-9E-04	2E-04	-16.8	-18.3	27.4	0.92	-9E-04	-8E-04	-1E-04	16.4	15.1	27.6	0.70

Figure S1. The extent of the model domain used for PCAPS application. Location of generic sources tracked with photochemical model source apportionment used for the training dataset. Locations differ by precursor/pollutant/release height combination.

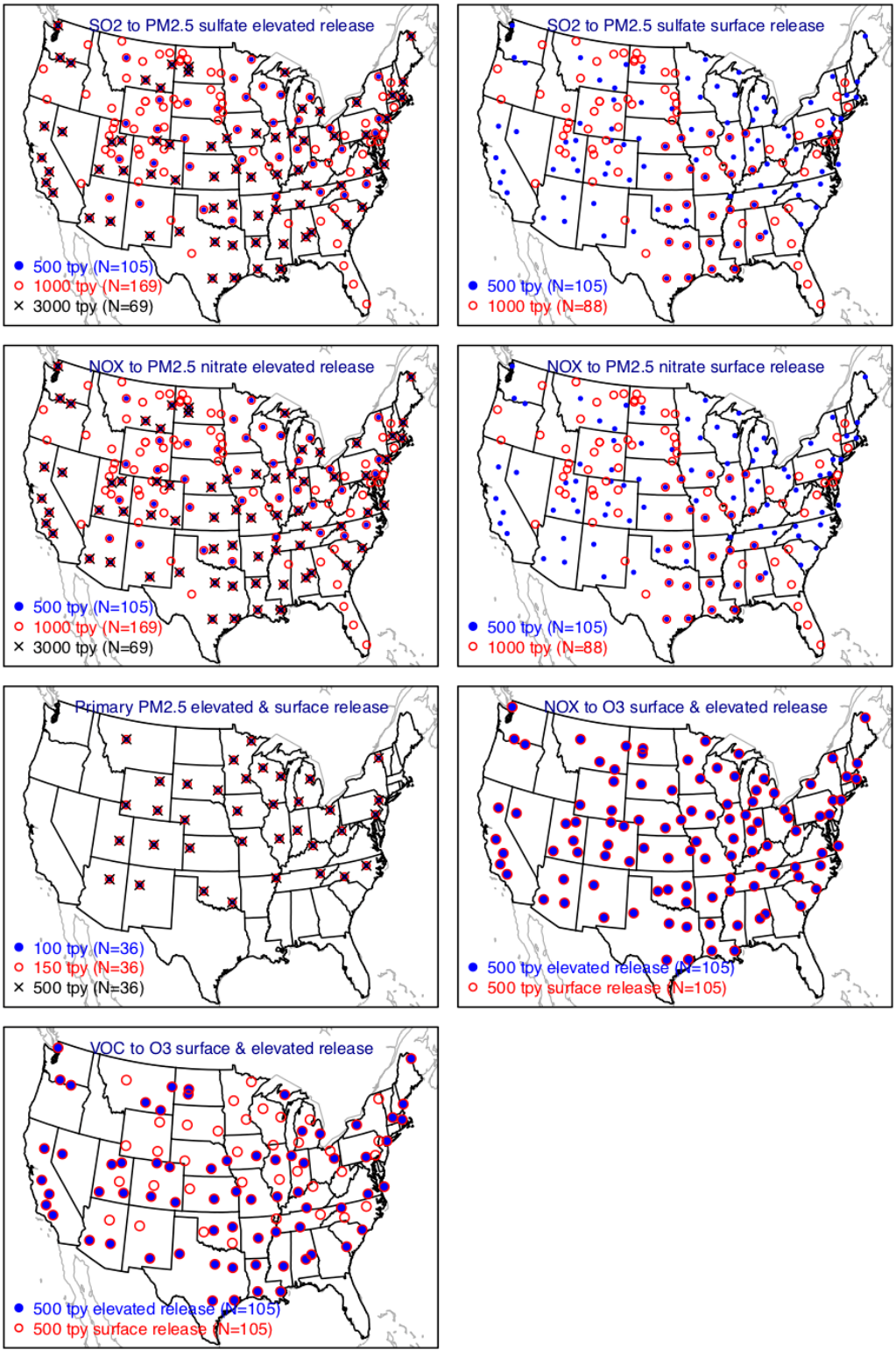


Figure S2. Areas where O_3 formation was typically NO_X limited (category 1) or NO_X saturated (category 2 and 3) for 2007 and 2016 based on photochemical grid modeling. Annual average ammonia predicted by the CMAQ model used as input for the nonlinear regression model is also shown.

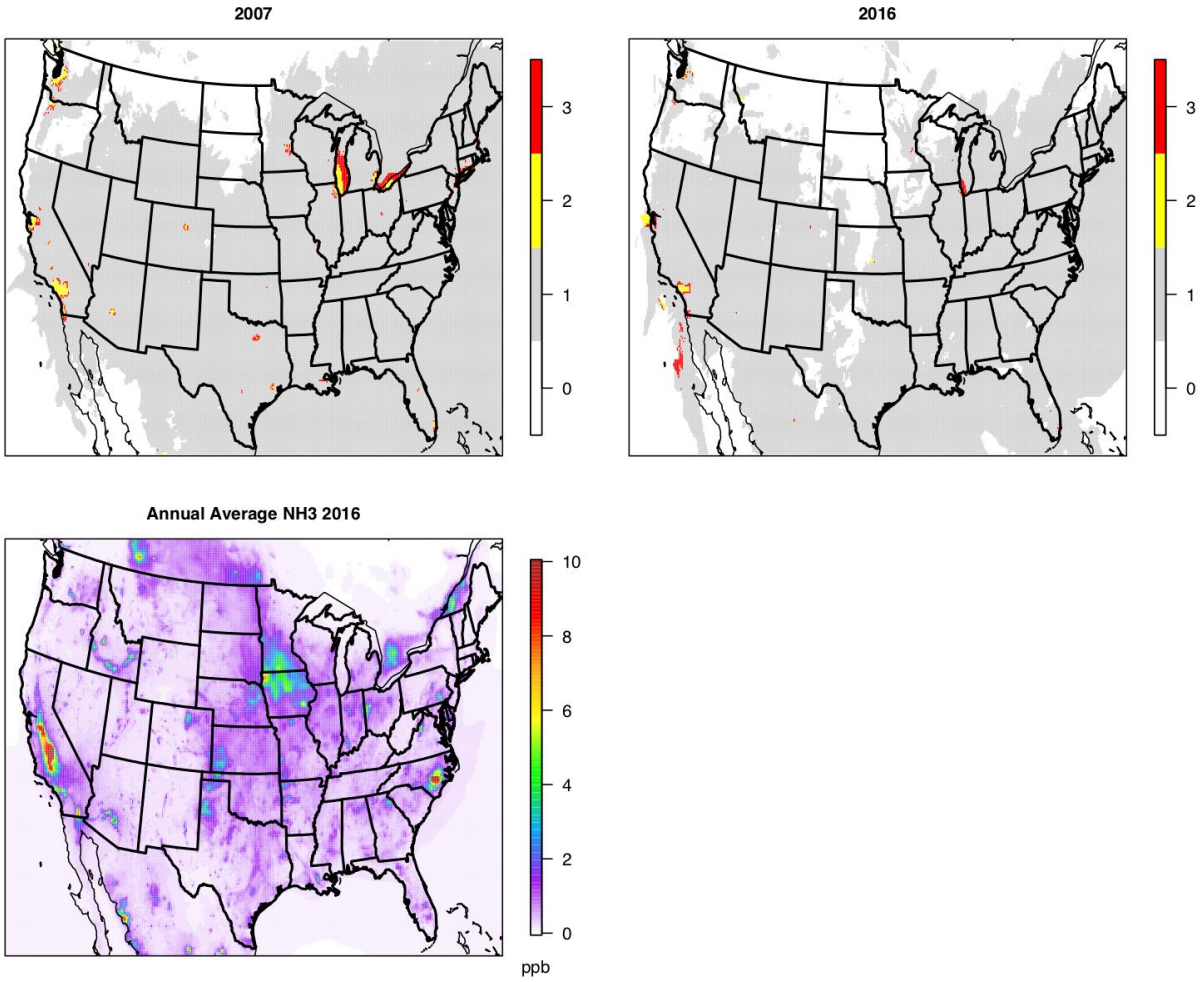


Figure S3. The change in emissions (tpy) is shown for the mobile emissions scenario NO_X (top left) and EGU emissions scenario SO_2 and NO_X, (middle and bottom left). The change in industrial sector scenario NO_X is shown in the right column. Cool colors represent a decrease in emissions due to the emissions scenario and warm represent an emissions increase.

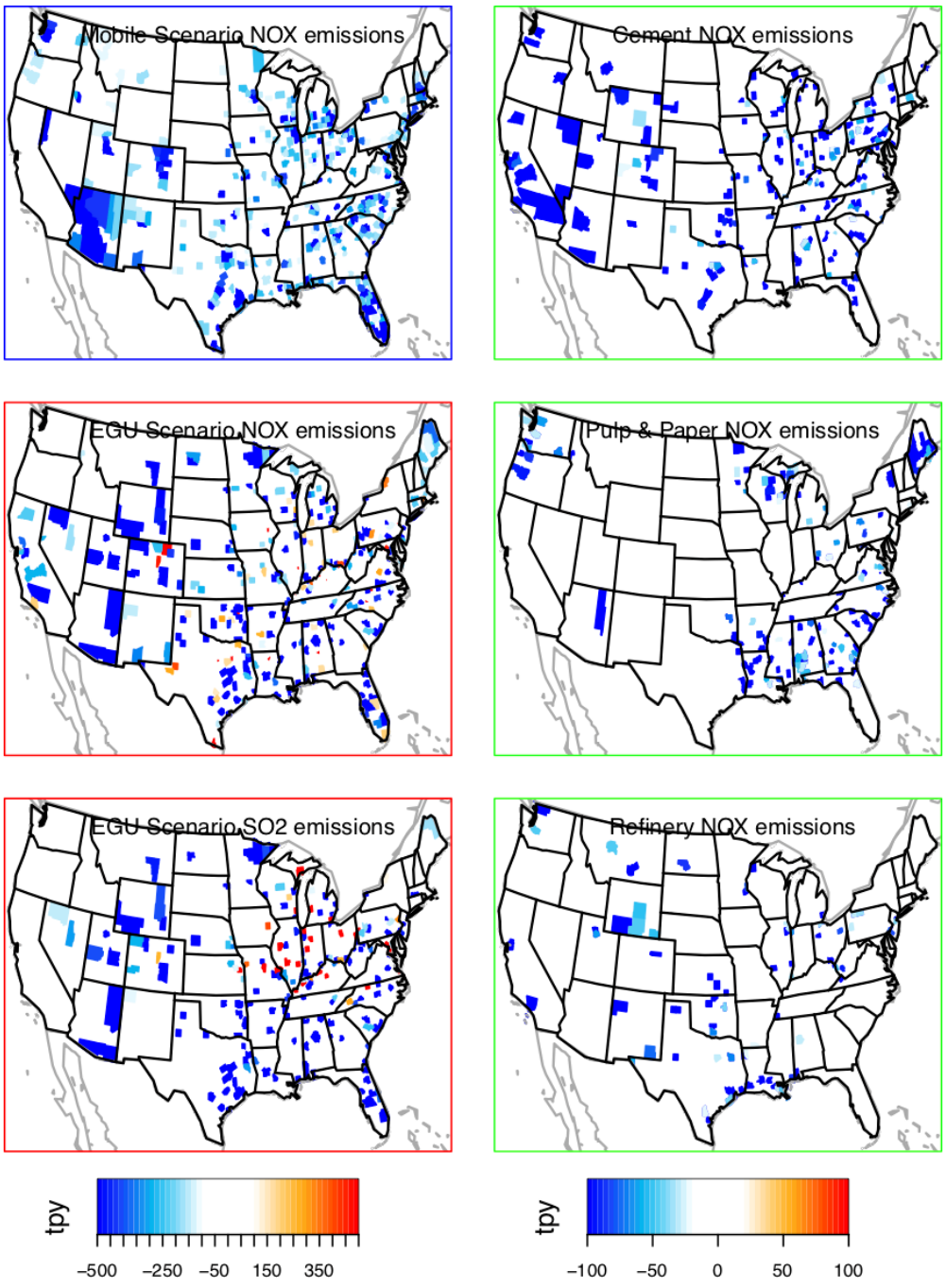


Figure S4. Spatial representation of photochemical (left panels) and nonlinear regression model (NLIN2) (center panels) model prediction of change in seasonal average MDA8 O_3 for multiple emission scenarios. The difference between predicted change in air quality between these models is also shown (right panels).

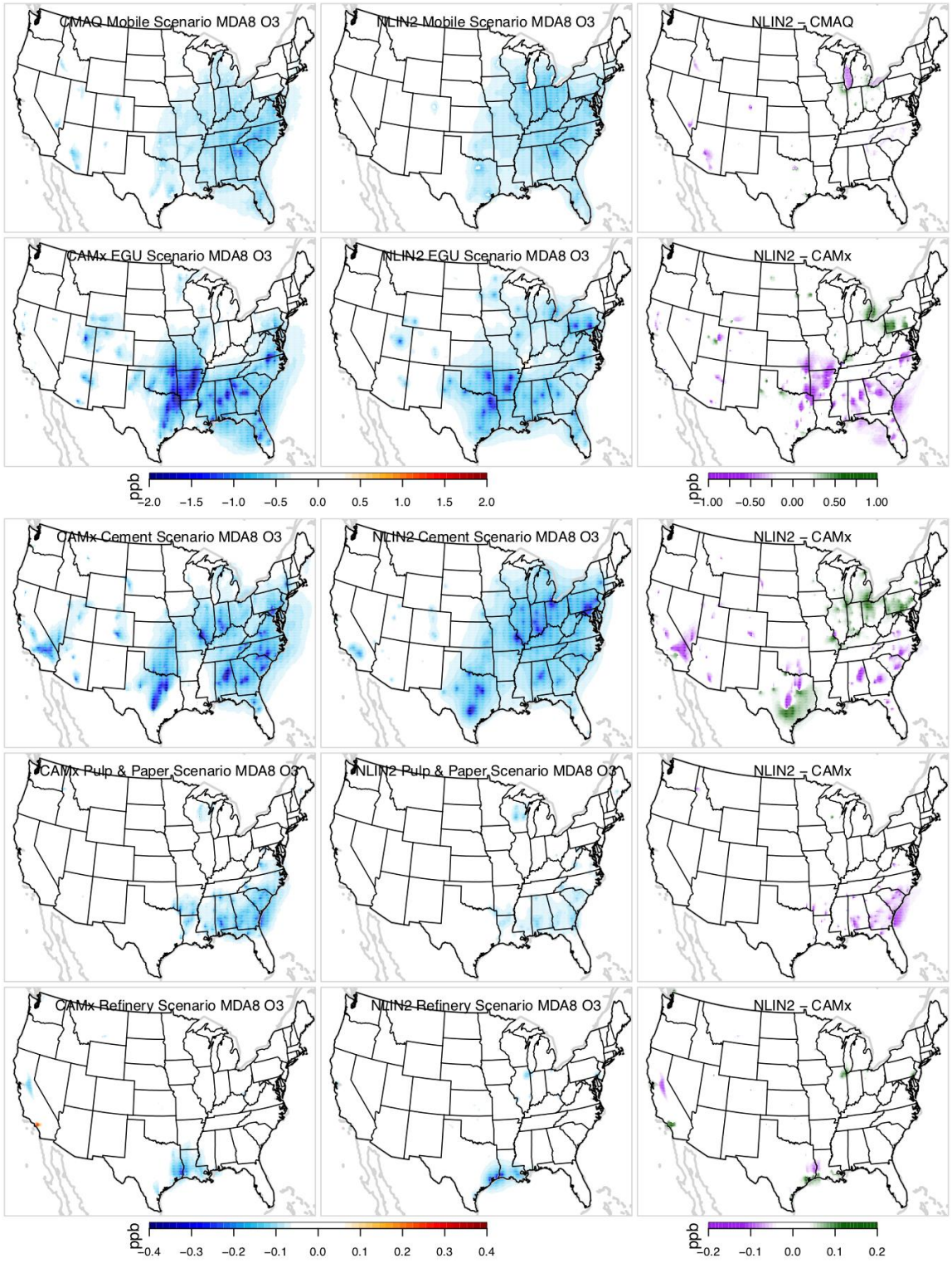


Figure S5. Spatial representation of photochemical (left panels) and COBRA (center panels) model prediction of change in annual average $PM_{2.5}$ for multiple emission scenarios. The difference between predicted change in air quality between these models is also shown (right panels).

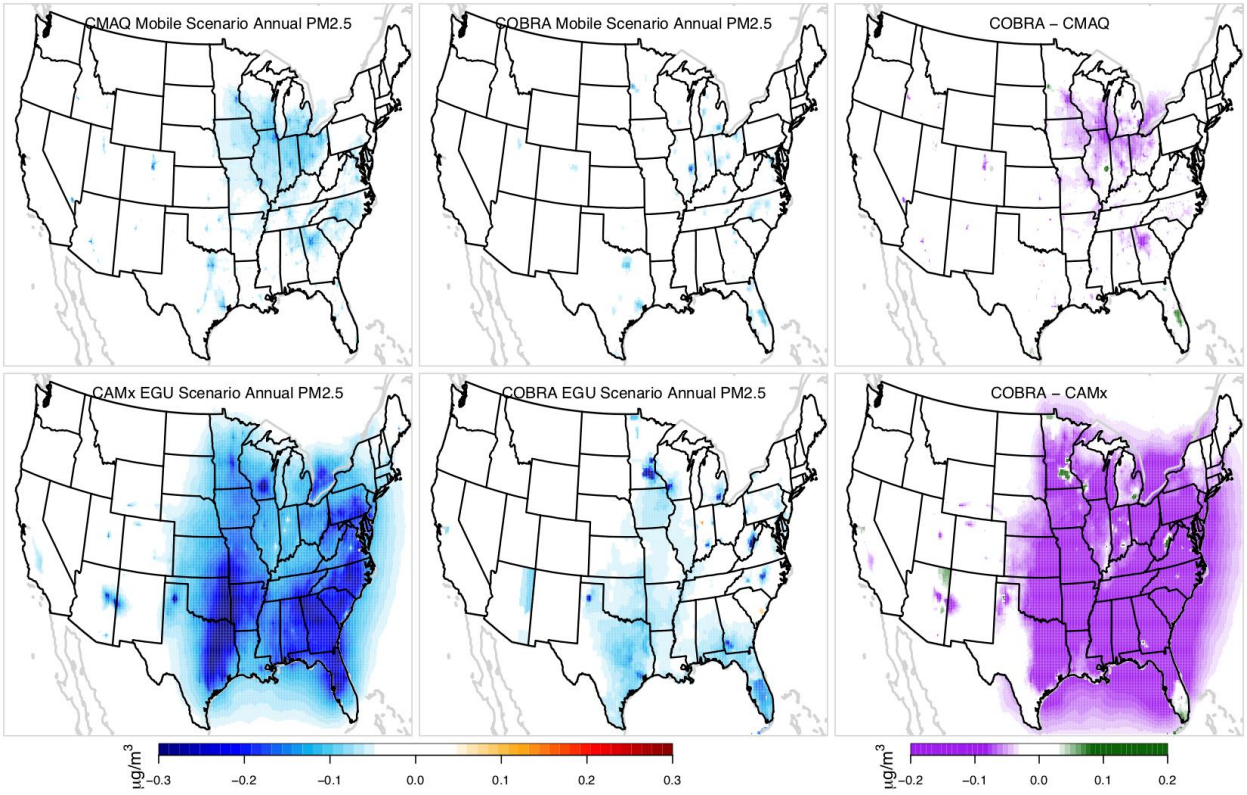


Figure S6. Spatial representation of photochemical (left panels) and nonlinear regression model (center panels) model prediction of change in annual average $PM_{2.5}$ for multiple emission scenarios. The difference between predicted change in air quality between these models is also shown (right panels).

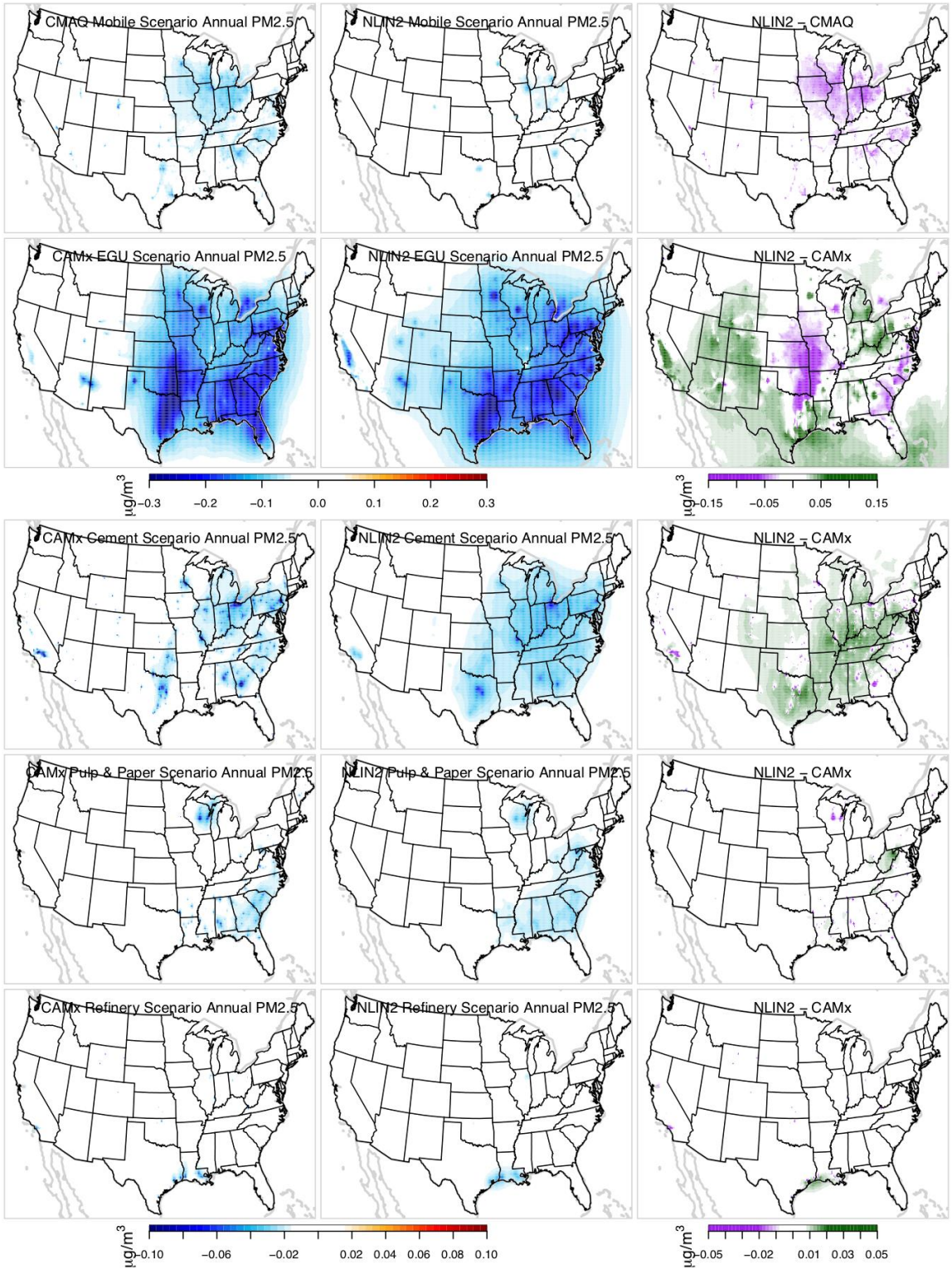


Figure S7. Comparison of photochemical model and PCAPS predicted change in $PM_{2.5}$ elemental carbon for both emission scenarios.

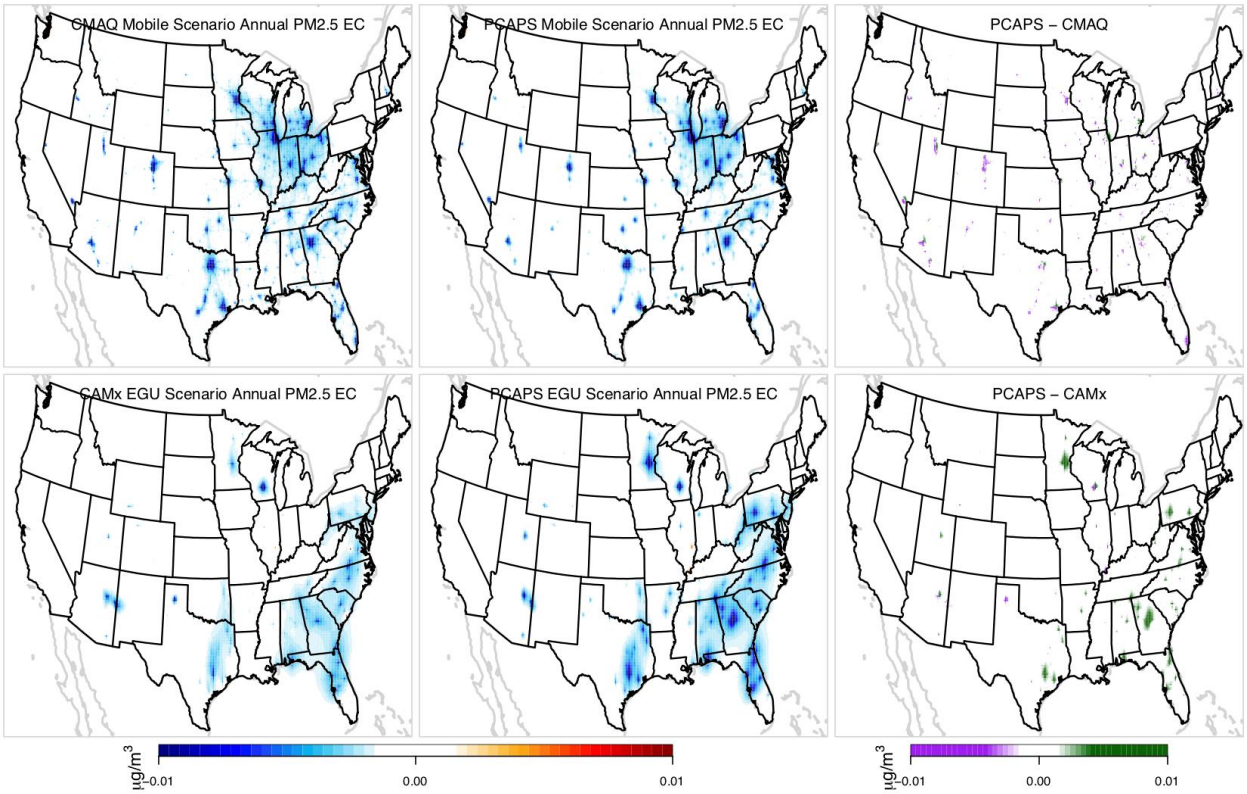
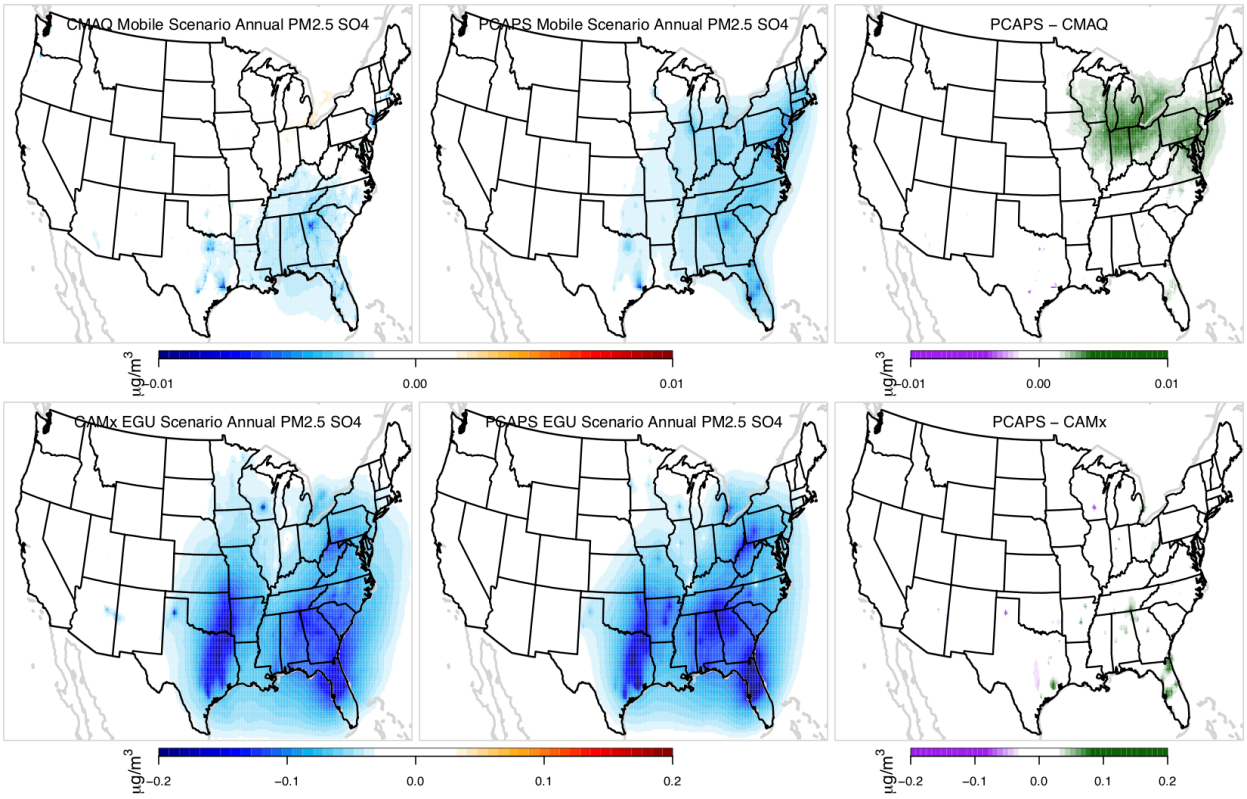


Figure S8. Comparison of photochemical model and PCAPS predicted change in $PM_{2.5}$ sulfate ion for both emission scenarios.



147 Figure S9. Comparison of photochemical model and PCAPS predicted change in $PM_{2.5}$ nitrate ion for both
148 emission scenarios.

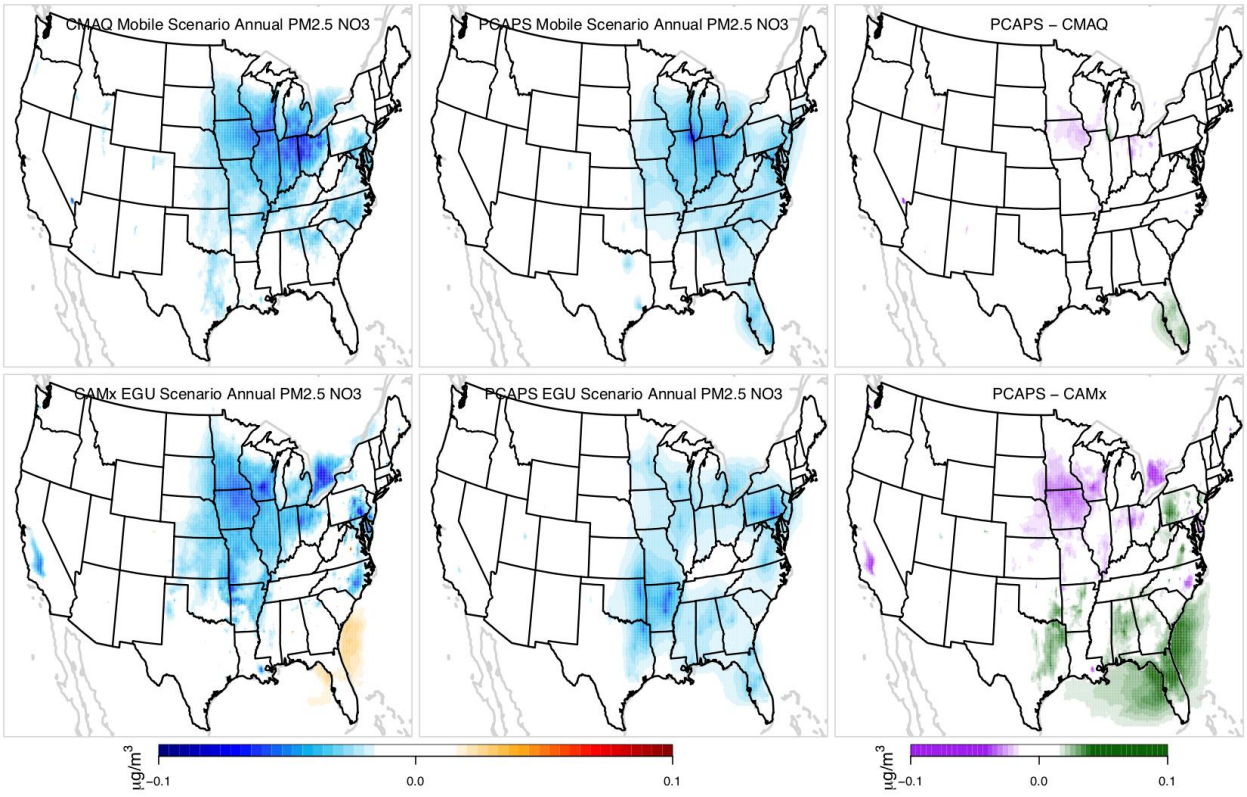


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Figure S10. Spatial representation of photochemical (left panels) and the nonlinear regression model NLIN2 (center panels) model prediction of change in annual average $PM_{2.5}$ elemental carbon for the mobile (top row) and EGU (bottom row) emission scenarios. The difference between predicted change in air quality between these models is also shown (right panels).

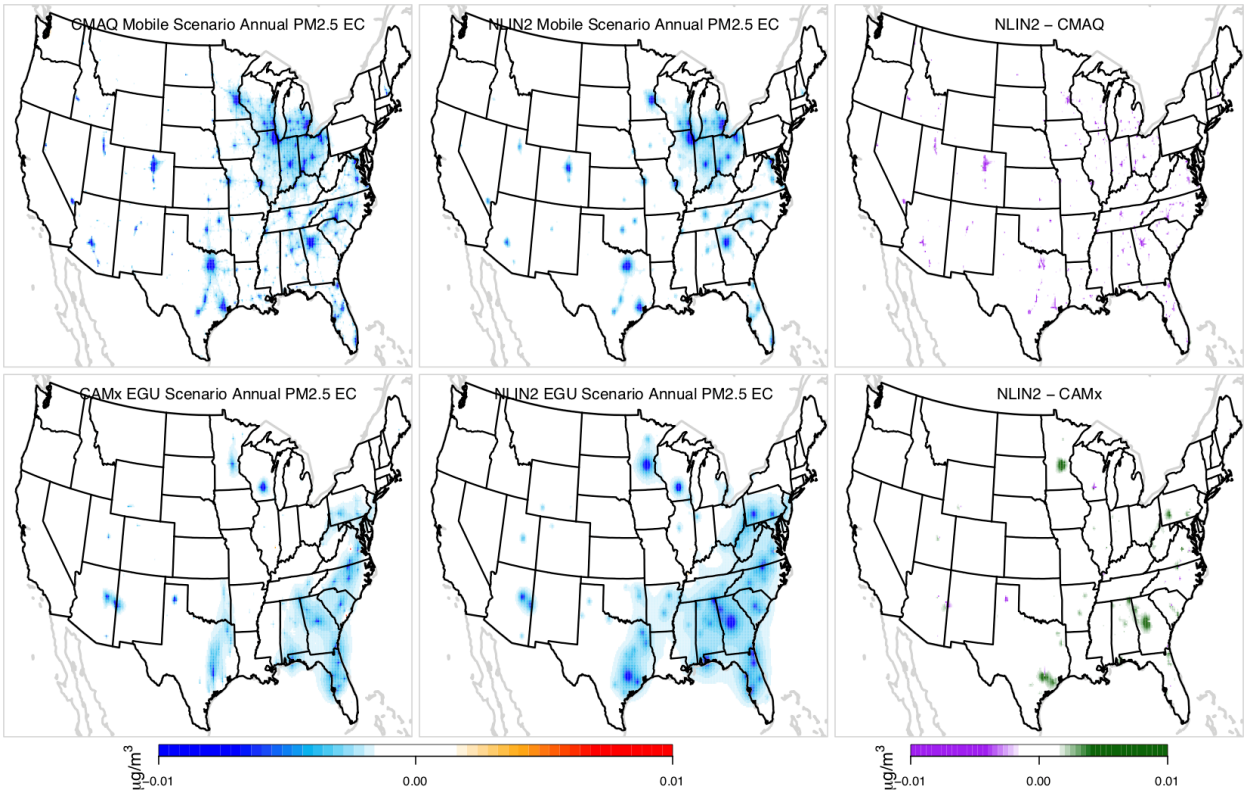

Figure S11. Spatial representation of photochemical (left panels) and the nonlinear regression model NLIN2 (center panels) model prediction of change in annual average $PM_{2.5}$ sulfate ion for the mobile (top row) and EGU (bottom row) emission scenarios. The difference between predicted change in air quality between these models is also shown (right panels).

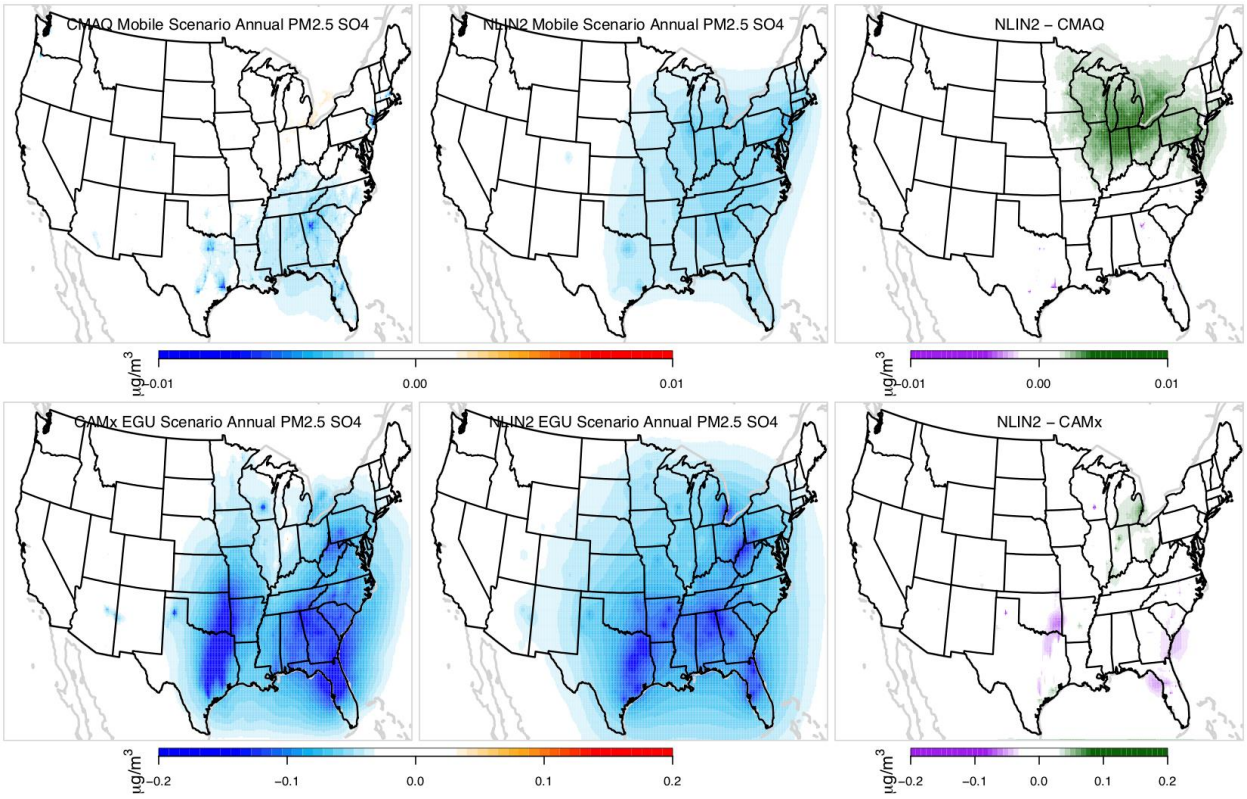

Figure S12. Spatial representation of photochemical (left panels) and the nonlinear regression model NLIN2 (center panels) model prediction of change in annual average $PM_{2.5}$ nitrate ion for the mobile (top row) and EGU (bottom row) emission scenarios. The difference between predicted change in air quality between these models is also shown (right panels).