



2017 National Emission Inventory Based Photochemical Modeling for Sector Specific Air Quality Assessments

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Quality Assessments

U.S. Environmental Protection Agency
Office of Air Quality Planning and Standards
Air Quality Assessment Division
Research Triangle Park, NC

BACKGROUND

This project is intended to update sector-specific air quality surfaces developed from the 2005 National Emission Inventory (NEI) that were used as input to the Benefits Mapping Analysis Program – Community Edition (BenMAP-CE) (U.S. Environmental Protection Agency, 2018a) to generate benefit-per-ton values (Fann et al., 2012) to support regulatory assessments in situations where photochemical modeling of specific rules was not feasible. The EPA periodically updates these benefit-per-ton values to account for changes in population (e.g. size and distribution) and economic factors (e.g., inflation, personal income) that each influence the size of the benefit per-ton value (U.S. Environmental Protection Agency, 2018b). However, these periodic updates do not account for changes over time in the number of facilities, distribution of facilities, and facility specific emissions of each emissions sector; these are each factors that influence the magnitude of the BPT value. The results of recently performed sector-specific modeling suggests that these factors should be updated to account for changes since 2005 (Industrial Economics Incorporated, 2019). Mobile source sector benefit estimates have been updated recently and described elsewhere (Wolfe et al., 2019).

This document presents an overview of EPA photochemical modeling of 2017 NEI based sector specific emissions on downwind O₃ and secondary PM_{2.5}. Ozone contributions were estimated using Ozone Source Apportionment Technology and PM_{2.5} contributions using Particulate Source Apportionment Technology as implemented in the CAMx photochemical model (Ramboll Environ, 2020). The contribution from each of these emissions sectors to model predicted O₃ and PM_{2.5} sulfate and nitrate ions were tracked using reactive tracers which track impacts of chemistry, atmospheric transport and deposition in the photochemical model (Kwok et al., 2015; Kwok et al., 2013; Ramboll Environ, 2020). Primary emitted PM_{2.5} was tracked with inert tracers which track impacts of atmospheric transport and deposition in the photochemical model. All precursor impacts on PM_{2.5} and O₃ are tracked separately (e.g. NO_x to O₃, VOC to O₃, etc.).

MODEL CONFIGURATION & APPLICATION

Emissions Sectors Tracked for Contribution

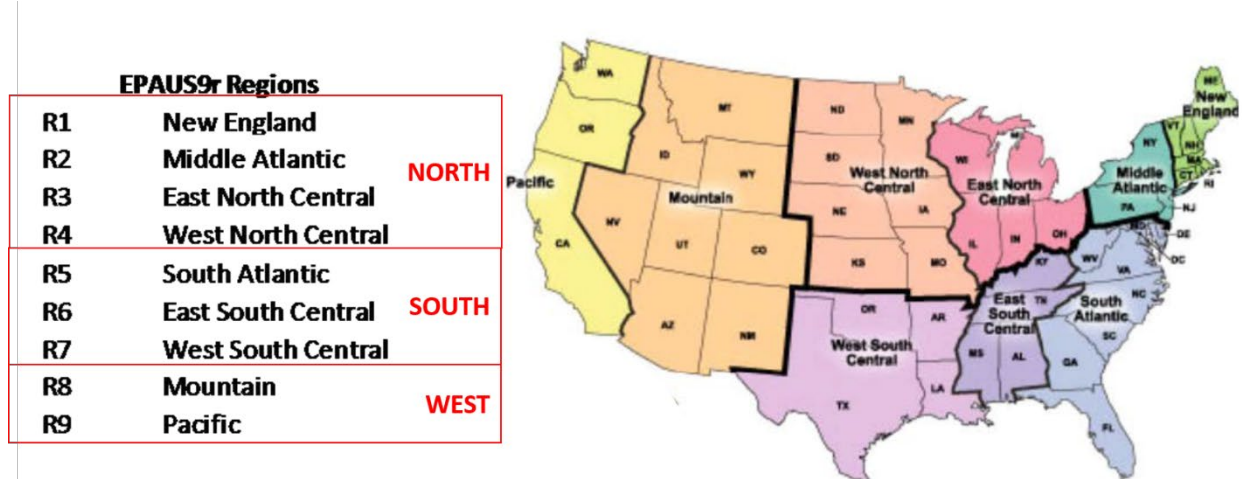
The emissions sectors tracked for contribution are shown in Table 1. These emissions sectors were selected based on a review of sectors that were the subject of past or planned future regulation that included a health benefits assessment with monetized impacts related to PM_{2.5} exposure. Sectors with very small amounts of precursor emissions were not included as part of this assessment.

Table 1. List of emissions sectors tracked for contribution as part of this project.

brick	oil and natural gas
cement kilns	oil and natural gas transmissions
coke ovens	paint stripping / misc surface coating
electric arc furnaces and argon	primary copper smelting
ferroalloys	pulp and paper
gasoline distribution bulk terminals	refineries
industrial boilers	residential woodstoves
integrated iron and steel	secondary lead smelters
internal combustion engines	synthetic organic chemical
iron and steel foundries	taconite mining

The industrial boilers and internal combustion engine sectors were tracked by state. All other sector contribution were tracked with a broader geographic source region delineation based on EPA’s U.S. Nine-region MARKAL Database (LeNO_x et al., 2013). A total of 3 regions will be used to track contribution and were defined to match up to MARKAL regions: 1) WEST = Pacific and Mountain, 2) NORTH = New England, Middle Atlantic, East North Central, and West North Central, and 3) SOUTH = South Atlantic, East South Central, and West South Central (Figure 1).

Figure 1. EPA USA9r Regions used to geographically group emission sectors in the U.S. Nine-region MARKAL database.



Annual emission totals in tons per year (tpy) for each of the sectors tracked for contribution by region is shown in Table 2. Emissions are provided for total primarily emitted PM_{2.5} (PM25PRI), primarily emitted organic aerosol PM_{2.5} (POA), primarily emitted elemental carbon (PEC), volatile organic compounds (VOC), ammonia (NH₃), sulfur dioxide (SO₂), and nitrogen oxides (NO_x). Emissions are shown for industrial boilers by State, offshore, and Tribal lands in Table 3 and internal combustion engines similarly in Table 4. Offshore emissions include emissions from state boundaries to the edge of the economic exclusion zone (EEZ). Sectors were defined based on North American Industrial Classification System (NAICS) and Source Classification Code (SCC). Some industrial boilers and internal combustion engine emissions may also be part of other 18 sectors tracked for contribution. These are the only 2 sectors that may have sector overlap in this assessment.

Table 2. Annual total emissions (tpy) for each sector tracked for contribution.

Sector Name - Region	NOX	SO2	NH3	VOC	PEC	POA
brick - NORTH	3,458	3,849	79	218	44	383
brick - SOUTH	2,539	5,552	22	702	71	569
brick - WEST	301	292	1	151	5	48
cement kilns - NORTH	36,224	16,432	820	1,755	54	320
cement kilns - SOUTH	45,537	9,378	325	2,464	45	274
cement kilns - WEST	22,818	1,929	554	659	14	84
coke ovens - NORTH	7,635	9,641	24	437	51	142
coke ovens - SOUTH	1,280	1,733	12	170	18	19
coke ovens - WEST	-	-	-	-	-	-
electric arc furnaces and argon - WEST	195	117	-	43	-	3
electric arc furnaces and argon- NORTH	843	591	-	523	1	8
electric arc furnaces and argon- SOUTH	1,752	1,041	-	775	3	36
ferroalloys - NORTH	1,021	2,027	-	175	120	91
ferroalloys - SOUTH	3,245	4,299	3	194	156	111
ferroalloys - SOUTH	-	-	-	-	-	-
gasoline distribution bulk terminals - NORTH	4	-	-	60,481	-	-
gasoline distribution bulk terminals - SOUTH	34	-	-	117,591	-	1
gasoline distribution bulk terminals - WEST	-	-	-	28,186	-	-
integrated iron and steel - NORTH	7,374	7,217	94	2,639	18	887
integrated iron and steel - SOUTH	4,677	1,967	33	865	4	263
integrated iron and steel - WEST	343	60	-	55	1	80
iron and steel foundries - NORTH	1,138	524	57	4,570	45	495
iron and steel foundries - SOUTH	675	246	26	2,058	26	167
iron and steel foundries - WEST	175	163	2	184	1	8
oil and natural gas - NORTH	158,632	13,750	1,790	687,867	191	1,850
oil and natural gas - SOUTH	488,506	45,686	63	1,357,120	699	4,948
oil and natural gas - WEST	149,057	12,933	222	499,533	271	2,448
oil and natural gas transmissions - NORTH	66,288	361	76	6,365	125	1,026
oil and natural gas transmissions - SOUTH	101,291	660	29	20,152	153	1,409
oil and natural gas transmissions - WEST	17,337	321	17	6,271	38	288
paint stripping / misc surface coating - NORTH	-	-	-	291,043	-	-
paint stripping / misc surface coating - SOUTH	-	-	-	261,702	-	-
paint stripping / misc surface coating - WEST	-	-	51	108,850	19	52
primary copper smelting - NORTH	5	141	-	15	-	1
primary copper smelting - SOUTH	3	-	-	-	-	-
primary copper smelting - WEST	245	25,012	3	8	-	7
pulp and paper - NORTH	7,282	1,687	550	4,933	27	170
pulp and paper - SOUTH	49,777	18,649	3,807	56,112	185	942
pulp and paper - WEST	5,388	2,003	466	3,579	28	129
refineries - NORTH	18,221	5,840	434	11,922	266	951
refineries - SOUTH	40,855	14,869	1,486	37,056	620	2,495
refineries - WEST	17,879	7,576	1,620	16,126	240	1,046
residential woodstoves - NORTH	8,195	1,257	3,094	60,605	2,661	42,824
residential woodstoves - SOUTH	5,443	847	2,421	55,948	2,162	34,792
residential woodstoves - WEST	3,663	564	1,582	40,536	1,597	25,702
secondary lead smelters - NORTH	429	3,425	-	65	-	-
secondary lead smelters - SOUTH	298	8,332	-	128	-	-
secondary lead smelters - WEST	-	-	-	-	-	-
synthetic organic chemical - NORTH	10,365	1,960	332	10,814	151	1,269
synthetic organic chemical - SOUTH	21,324	18,390	2,410	13,122	149	822
synthetic organic chemical - WEST	608	51	6	348	7	26
taconite mining - NORTH	38,192	5,090	24	402	124	1,146
taconite mining - SOUTH	-	-	-	-	-	-
taconite mining - WEST	-	-	-	-	-	-

Table 3. Industrial boiler annual total emissions (tpy) by group.

State	NOX	SO2	NH3	VOC	POA
Alabama	9,508	6,464	14	584	820
Arizona	132	1	1	8	6
Arkansas	10,198	15,207	40	354	524
California	5,706	845	312	581	390
Colorado	2,228	144	22	149	88
Connecticut	165	2	4	8	7
Delaware	833	150	23	27	12
District of Columbia	24	0	-	1	1
Florida	7,347	4,841	297	3,251	815
Georgia	10,397	6,511	7	703	762
Idaho	4,576	702	0	121	135
Illinois	6,386	13,482	194	241	270
Indiana	7,599	10,104	157	398	1,751
Iowa	3,583	3,122	154	239	142
Kansas	2,410	82	40	145	145
Kentucky	3,068	948	71	128	237
Louisiana	25,407	5,587	248	1,792	1,574
Maine	4,208	2,027	113	122	268
Maryland	1,695	8,595	1	25	24
Massachusetts	976	115	24	59	46
Michigan	5,115	3,545	98	212	243
Minnesota	7,601	3,336	175	510	230
Mississippi	4,595	257	0	1,305	575
Missouri	1,437	307	48	103	95
Montana	2,450	295	63	389	48
Nebraska	1,481	434	15	116	153
Nevada	212	16	-	38	46
New Hampshire	137	123	-	4	8
New Jersey	891	65	19	47	70
New Mexico	290	5	0	24	23
New York	3,818	9,005	39	143	145
North Carolina	9,250	4,140	38	733	644
North Dakota	4,915	6,478	122	197	309
Offshore to EEZ	243	4	8	13	8
Ohio	5,803	3,203	156	307	576
Oklahoma	3,221	1,424	15	104	196
Oregon	4,314	244	-	388	364
Pennsylvania	7,309	6,263	398	456	602
Puerto Rico	231	210	-	7	3
Rhode Island	114	12	3	7	5
South Carolina	7,418	5,540	263	497	644
South Dakota	242	83	29	43	43
Tennessee	10,330	13,107	97	319	274
Texas	13,458	7,686	239	1,074	1,072
Tribal Data	285	50	-	24	34
Utah	1,068	1,413	16	35	37
Vermont	45	4	-	7	12
Virginia	5,397	479	113	290	320
Washington	5,162	971	23	349	189
West Virginia	2,444	2,175	14	91	64
Wisconsin	7,826	9,816	33	358	311
Wyoming	5,614	4,628	3	115	58

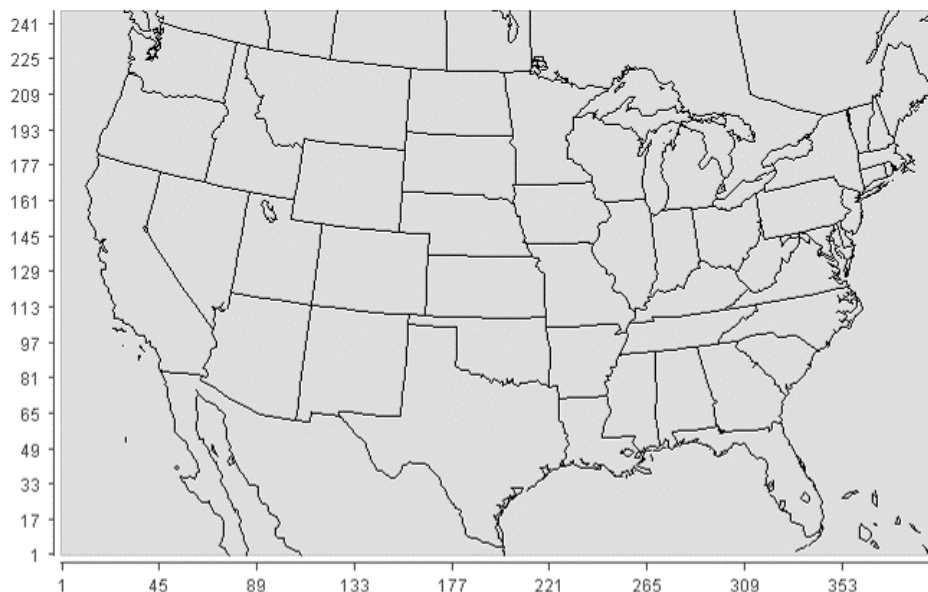
Table 4. Internal combustion endings annual total emissions (tpy) by group.

State	NOX	SO2	NH3	VOC	POA
Alabama	8,514	79	11	570	194
Arizona	2,109	20	59	51	49
Arkansas	5,444	13	2	302	59
California	4,121	211	599	598	365
Colorado	14,999	143	-	4,813	236
Connecticut	296	8	9	64	24
Delaware	65	19	0	13	14
Florida	7,999	136	26	522	141
Georgia	4,427	121	245	560	382
Idaho	1,140	7	-	34	11
Illinois	5,712	45	10	323	134
Indiana	3,810	22	0	210	40
Iowa	5,885	38	1	344	87
Kansas	23,675	35	58	1,403	190
Kentucky	9,468	15	0	632	174
Louisiana	28,027	235	757	2,118	754
Maine	86	1	0	4	1
Maryland	118	3	19	9	6
Massachusetts	669	71	22	109	23
Michigan	11,179	29	45	931	112
Minnesota	3,895	66	65	176	19
Mississippi	11,784	32	-	734	150
Missouri	3,882	20	0	156	40
Montana	1,682	17	0	544	54
Nebraska	3,507	4	0	277	42
Nevada	652	35	0	39	17
New Hampshire	27	1	-	1	1
New Jersey	424	13	5	101	21
New Mexico	14,348	106	103	2,118	189
New York	2,802	42	54	349	71
North Carolina	1,086	33	51	167	51
North Dakota	1,335	12	-	114	36
Offshore to EEZ	48,915	435	-	1,387	304
Ohio	10,072	32	8	630	201
Oklahoma	47,977	66	-	11,959	769
Oregon	325	4	-	4	4
Pennsylvania	5,155	47	47	830	232
Puerto Rico	4	3	-	0	0
Rhode Island	150	4	0	26	3
South Carolina	728	35	9	53	22
South Dakota	251	8	-	10	63
Tennessee	3,991	17	-	553	50
Texas	57,551	864	928	9,039	2,163
Tribal Data	5,358	22	-	801	37
Utah	2,329	13	14	110	46
Virginia	1,936	41	3	134	40
Washington	770	38	10	54	30
West Virginia	4,914	5	-	322	60
Wisconsin	773	1	9	45	10
Wyoming	11,212	406	15	7,959	556

Model Configuration

Annual 2017 photochemical model simulations were performed for a domain covering the contiguous United States with 12 km sized grid cells (Figure 2). Each simulation tracked a different combination of sectors and pollutants. All simulations were conducted using version 7.00 of the Comprehensive Air Quality Model with Extensions (CAMx) photochemical grid model (www.camx.com). This CAMx application includes ISORROPIA inorganic chemistry (Nenes et al., 1998), gas phase reactions based on the Carbon Bond (CB6r4) mechanism (Ramboll Environ, 2016), and aqueous phase reactions (Ramboll Environ, 2020). Chemical boundary inflow is extracted from a photochemical model simulation for 2017 with a larger geographic domain covering the northern hemisphere (U.S. Environmental Protection Agency, 2019). A total of 35 layers resolve the vertical atmosphere to 50 mb with thinner layers nearer the surface (the height of the layer closest to the surface is approximately 20 m). More details about the meteorological model simulation used to supply inputs to the emissions and CAMx model are available elsewhere (ref 2017 WRF TSD). Baseline emissions include anthropogenic sources based on the “2017gb” version of the 2017 National Emission Inventory (U.S. Environmental Protection Agency, 2020) and biogenic sources estimated with the Biogenic Emission Inventory System version 3.6.1 (Bash et al., 2016). Wildland fire emissions are day specific for 2017 (U.S. Environmental Protection Agency, 2020).

Figure 2. Photochemical model domain.



Model Application

The photochemical model was applied for the entire year of 2017 at 12 km grid resolution. Multiple annual model simulations were performed to capture precursor/pollutant impacts on ozone and PM_{2.5} for each sector and geographic source region. Each sector/source region combination is called a source apportionment “tag”.

Table 5 shows the relationship between precursor emissions and contribution to modeled primary and secondary pollutants. The model was applied so that primary and secondary precursors were tracked for

contribution to modeled PM_{2.5} components. NO_x emissions were tracked for contribution to PM_{2.5} nitrate ion, NH₃ emissions were tracked for contribution to PM_{2.5} ammonium ion, and SO₂ emissions were tracked for contribution to PM_{2.5} sulfate ion. Primarily emitted elemental carbon was tracked to model predicted PM_{2.5} elemental carbon. The contribution to PM_{2.5} nitrate does not include primarily emitted PM_{2.5} nitrate and the contribution to PM_{2.5} sulfate does not include primarily emitted PM_{2.5} sulfate.

Table 5. Relationship between emissions species and tracked primary and secondarily formed PM_{2.5} and also ozone in the modeling system.

Precursor	Tagged Pollutant
SO ₂	Secondarily formed PM _{2.5} sulfate ion
NO _x	Secondarily formed PM _{2.5} nitrate ion
NH ₃	Secondarily formed PM _{2.5} ammonium ion
Primary PM _{2.5} elemental carbon	Primary PM _{2.5} elemental carbon
Primary PM _{2.5} organic aerosol	Primary PM _{2.5} organic aerosol
VOC	Ozone
NO _x	Ozone

MODEL PERFORMANCE EVALUATION

Particulate Matter

An operational model performance evaluation for the speciated components of PM_{2.5} (e.g., sulfate, nitrate, elemental carbon, organic carbon, etc.) was conducted using 2017 monitoring data in order to estimate the ability of the modeling system to predict ambient concentrations. The evaluation of PM_{2.5} component species includes comparisons of predicted and observed concentrations of sulfate (SO₄), nitrate (NO₃), ammonium (NH₄), elemental carbon (EC), and organic carbon (OC). Chemically speciated PM_{2.5} ambient measurements for 2017 were obtained from the Chemical Speciation Network (CSN) and the Interagency Monitoring of PROtected Visual Environments (IMPROVE). The CSN sites are generally located within urban areas and the IMPROVE sites are typically in rural/remote areas. The measurements at CSN and IMPROVE sites represent 24-hour average concentrations. In calculating the model performance metrics, the modeled hourly species predictions were aggregated to the averaging times of the measurements.

Model performance statistics were calculated for observed/predicted pairs of all daily concentrations measured in 2017 (Simon et al., 2012). All daily average chemically speciated PM_{2.5} prediction-observation pairs are shown in Figure 3. Aggregated metrics and number (N) of prediction-observation pairs are shown by chemical specie in Table 6. PM_{2.5} ammonium ion is not measured at most IMPROVE monitors so metrics were not generated for that network. Model performance was compared to the performance found in recent regional PM_{2.5} model applications for other assessments. Overall, the mean bias (bias) and mean error (error) statistics are within the range or close to that found by other groups in recent applications (Kelly et al., 2019; Simon et al., 2012). The model performance results provide confidence that this application of CAMx provides a scientifically credible approach for estimating PM_{2.5} concentrations for the purposes of this assessment.

Table 6. Aggregated model performance metrics for speciated components of PM_{2.5} for the IMPROVE and CSN monitor networks.

Specie	Network	N	Mean Bias (µg/m ³)	Mean Error (µg/m ³)	Normalized Mean Bias (%)	Normalized Mean Error (%)	r ²
PM2.5 sulfate ion	CSN	13,523	0.37	0.56	39	59	0.32
PM2.5 sulfate ion	IMPROVE	16,542	0.28	0.40	44	63	0.47
PM2.5 nitrate ion	CSN	13,593	0.43	0.87	49	98	0.28
PM2.5 nitrate ion	IMPROVE	16,529	0.17	0.36	53	111	0.34
PM2.5 elemental carbon	CSN	13,041	-0.01	0.27	-2	47	0.29
PM2.5 elemental carbon	IMPROVE	16,666	-0.03	0.11	-16	55	0.17
PM2.5 organic carbon	CSN	13,066	0.64	1.15	31	56	0.29
PM2.5 organic carbon	IMPROVE	16,894	0.15	0.86	11	64	0.28
PM2.5 ammonium ion	CSN	11,419	0.49	0.60	126	155	0.17

Ozone

An operational model performance evaluation for eight-hour daily maximum (MDA8) ozone was conducted in order to estimate the ability of the modeling system to replicate the 2017 base year concentrations. Ozone measurements were taken from 2017 monitoring site data in the Air Quality System (AQS). The ozone metrics covered in this evaluation include eight-hour average daily maximum ozone bias and error (Simon et al., 2012). The evaluation principally consists of statistical assessments of model versus observed pairs that are paired in time and space. Aggregated metrics and number (N) of prediction-observation pairs are shown in Table 7. All MDA8 ozone prediction-observation pairs are shown in Figure 3 (bottom right panel).

Table 7. Aggregated model performance metrics for MDA8 O₃. Metrics are shown for all prediction-observation pairs, pairs where the model predictions exceed 60 ppb, and pairs where the observations exceed 60 ppb.

Specie	Network	N	Mean Bias (ppb)	Mean Error (ppb)	Normalized Mean Bias (%)	Normalized Mean Error (%)	r ²
MDA8O3	AIRS - ALL	215,245	-0.08	7.44	0	16	0.52
MDA8O3	AIRS - model > 60 ppb	24,834	5.57	9.17	9	15	0.22
MDA8O3	AIRS - obs > 60 ppb	23,783	-6.30	8.89	-9	13	0.29

Only prediction-observation pairs from April through September were included in the aggregated metrics. This ozone model performance includes all prediction-observation pairs, a subset of prediction-observation pairs where observed ozone exceeded 60 ppb, and a subset of prediction-observation pairs where predicted ozone exceeded 60 ppb. This cutoff was applied to evaluate the model on days of elevated ozone which are more policy relevant. Overall, the mean bias (bias) and mean error (error) statistics are within the range or close to that found by other groups in recent applications (Simon et al., 2012). The model performance results provide confidence that this application of CAMx provides a scientifically credible approach for estimating ozone mixing ratios for the purposes of this assessment.

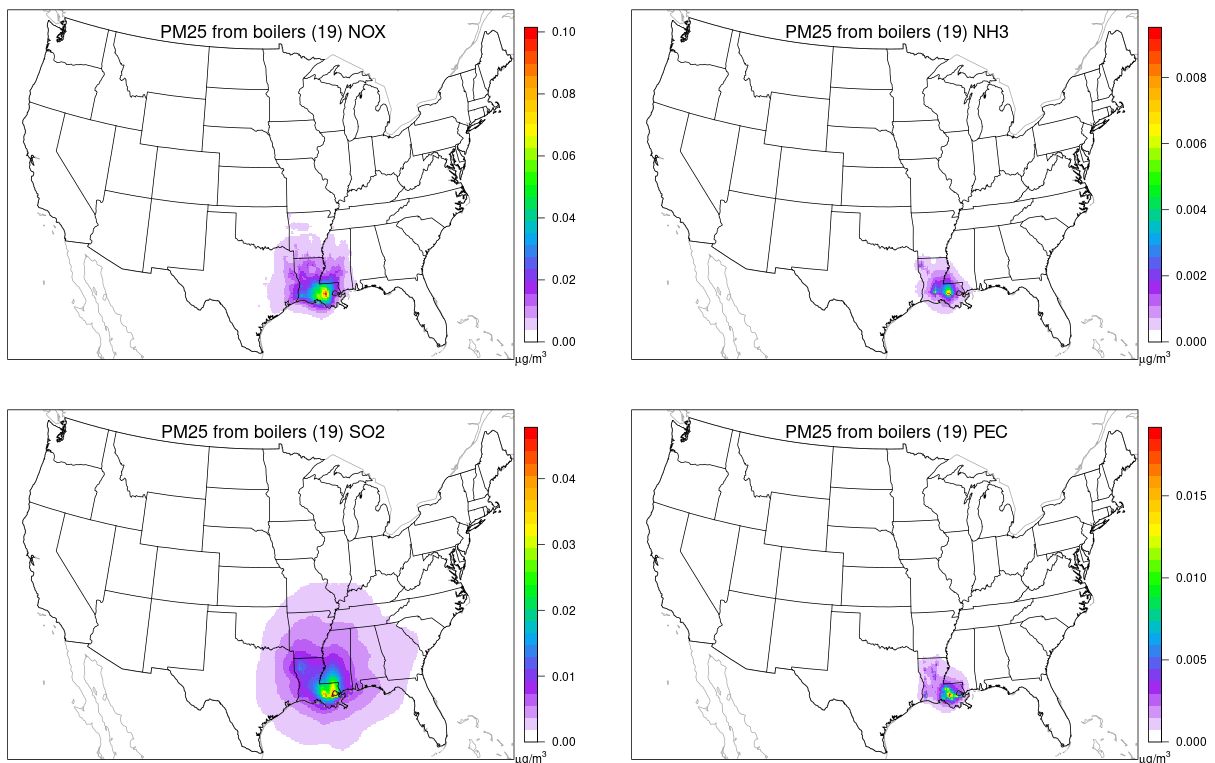
PRODUCTS

The photochemical model output was processed to be in the format for input to the BenMAP-CE tool. This requires temporal aggregation to convert hourly model output to annual average PM_{2.5} and ozone season (April through September) average of MDA8 ozone. BenMAP-CE input files were generated for the baseline simulation where all sources are included. Additionally, a set of BenMAP-CE input files

were generated representing air quality surfaces for which the contribution from specific sectors or state/sector combinations are removed from the baseline. The difference in air quality in the baseline and sector specific BenMAP-CE input files represent the health burden associated with that sector. A set of BenMAP-CE inputs were generated for annual average PM_{2.5} (sum of all chemical constituents of PM_{2.5}), and annual average PM_{2.5} chemical components: elemental carbon, sulfate ion, nitrate ion, and ammonium ion. BenMAP-CE inputs were also generated for multiple O₃ related metrics: 1) April-September MDA8, 2) June-August MDA8, 3) April-September MDA1, 4) May-October MDA1, and 5) April-October MDA8. The photochemical model output species were temporally aggregated but were not adjusted toward ambient measurement data in order to preserve the simulated emissions to ambient concentration relationship.

PM_{2.5} nitrate impacts were linked to secondary formation attributed to NO_x emissions only and therefore these outputs do not include the impacts from primarily emitted PM_{2.5} nitrate. PM_{2.5} sulfate impacts were linked to secondary formation attributed to SO₂ emissions only and similarly do not include the impacts from primarily emitted PM_{2.5} sulfate. PM_{2.5} ammonium impacts were linked to secondary formation attributed to NH₃ emissions only and do not include the impacts from primarily emitted PM_{2.5} ammonium.

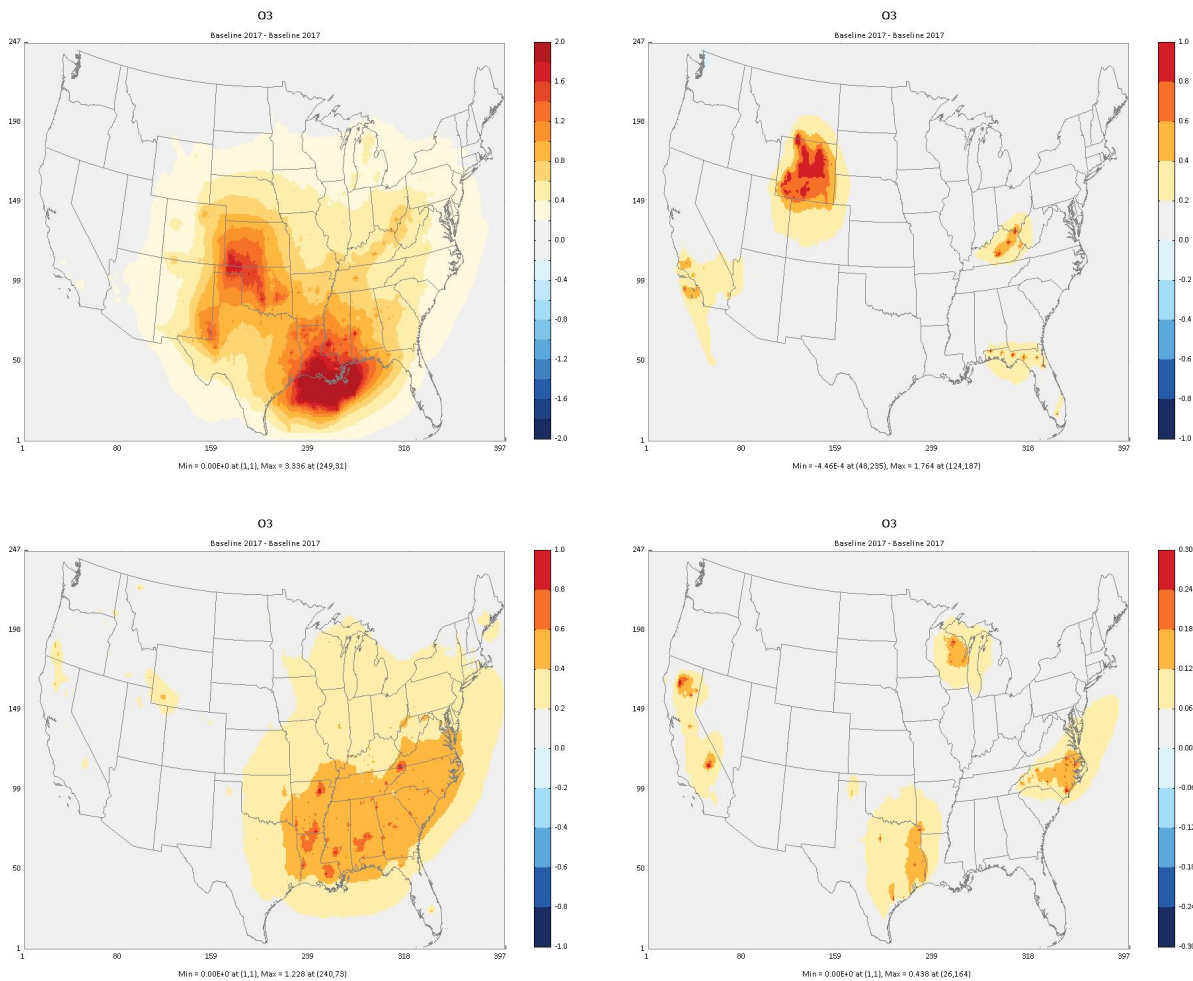
Figure 3. Contribution to PM_{2.5} from NO_x, SO₂, NH₃, and primarily emitted elemental carbon from industrial boilers in Louisiana.



The sum of PM_{2.5} elemental carbon and primarily emitted organic aerosol could be used as a surrogate for all primarily emitted PM_{2.5} emissions because those emissions and model concentrations do not have any secondary component and the emissions are considered more robust than many of the metals and ions that are highly variable spatially and generally more uncertain with respect to the underlying emission inventory. This approach is consistent with other approaches to represent primary PM_{2.5} impacts from photochemical model output (Heo et al., 2016). Separate attribution was done for primarily emitted PM_{2.5} sulfate ion and PM_{2.5} nitrate ion to differentiate primary and secondary forms of these pollutants.

Figure 3 shows the contribution to annual average PM_{2.5} from emissions of NO_x, SO₂, NH₃, and elemental carbon in Louisiana. The model shows very localized impacts of primarily emitted pollutants and NH₃ on annual PM_{2.5}. The PM_{2.5} impacts from NO_x and SO₂ extend further downwind due to chemical transformation over time.

Figure 4. Average ozone season MDA8 for IC engines (top left), state subset (Wyoming, Kentucky, California, and Florida) of IC engines (top right), industrial boilers (bottom left), and state subset (California, Texas, North Carolina, and Wisconsin) of industrial boilers (bottom right).



Precursor emissions of NO_x and VOC were separately tracked for contribution to MDA8 O₃ predictions. Figure 4 shows average O₃ season MDA8 NO_x contribution from the entirety of the internal combustion engines and boilers sectors tracked here and an example of state-level impacts for each. The left panels show the entirety of impacts from internal combustion engines (top left) and industrial boilers (bottom left) on seasonal average MDA8 O₃. The right panels show the same sectors but only impacts from a subset of states.

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