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Assessing Model Characterization of Single Source Secondary Pollutant Impacts Using 2013 SENEX Field Study Measurements

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Abstract

Aircraft measurements made downwind from specific coal fired power plants during the 2013 Southeast Nexus field campaign provide a unique opportunity to evaluate single source photochemical model predictions of both O₃ and secondary PM_{2.5} species. The model did well at predicting downwind plume placement. The model shows similar patterns of an increasing fraction of PM_{2.5} sulfate ion to the sum of SO₂ and PM_{2.5} sulfate ion by distance from the source compared with ambient based estimates. The model was less consistent in capturing downwind ambient based trends in conversion of NO_x to NO_y from these sources. Source sensitivity approaches capture near-source O₃ titration by fresh NO emissions, in particular subgrid plume treatment. However, capturing this near-source chemical feature did not translate into better downwind peak estimates of single source O₃ impacts. The model estimated O₃ production from these sources but often was lower than ambient based source production. The downwind transect ambient measurements, in particular secondary PM_{2.5} and O₃, have some level of contribution from other sources which makes direct comparison with model source contribution challenging. Model source attribution results suggest contribution to secondary pollutants from multiple sources even where primary pollutants indicate the presence of a single source.

Abstract

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Introduction

Impacts from specific sources have traditionally been estimated for pollutants with National Ambient Air Quality Standards through permit programs including New Source Review and Prevention of Significant Deterioration. However, little specific guidance exists in the 2005 version of the Guideline for Air Quality Models for single source air quality impact demonstrations for ozone (O₃) and secondary particulate matter less than 2.5 μm in diameter (PM_{2.5}) impacts to support permit applications under these programs. Traditional dispersion models (e.g., AERMOD) used to assess single source impacts for permit related programs do not contain either the plume chemistry or atmospheric chemistry and physics necessary to appropriately characterize O₃ and secondary PM_{2.5} impacts on the environment. The U.S. Environmental Protection Agency recently finalized changes to the Guideline for Air Quality Models and established new guidance that describes the type of models and methods used to assess single source secondary pollutant impacts for permit programs.(1) Public comment on this recent revision included requests that models for this purpose be further evaluated for suitability of estimating single source O₃ and secondary PM_{2.5} impacts.(1)

Photochemical grid modeling systems have been used extensively to estimate source specific impacts on O₃ and secondary PM_{2.5} with various techniques to differentiate those impacts from other sources.(2–6) Previous studies have shown that Eulerian photochemical grid models are able to replicate near-source secondary pollutant scavenging (e.g., titration) and downwind production of O₃.(2, 6) Some photochemical grid models have been instrumented with a Lagrangian subgrid plume model to provide source impacts at subgrid scales with the intent of more finely resolved spatial representation of plumes by not immediately diluting emissions into the grid volume.(5, 7–15) Emissions mass is typically tracked in the Lagrangian submodel until plume sizes are comparable to the size of the host model grid cell at which time the subgrid pollutant mass is transferred to the host grid cell.(7, 11) Past evaluations of subgrid plume model predictions of secondary pollutants in 3-dimensional photochemical models include comparisons against routine surface monitors which suggest differences in overall model performance with and without subgrid treatment for specific sources are usually insignificant.(8, 16) It is not clear whether the small differences in model performance are related to the different chemistry realized at the subgrid level or differences in the transport of primary and secondary pollutants by the subgrid plume treatment implementation.

Source oriented field measurements of ambient air dominated by a single facility provide an opportunity to evaluate air quality modeling systems that estimate single source impacts. In-plume measurements of O₃, O₃ precursors such as nitrogen oxides (NO_x) and volatile organic compounds (VOC), and other secondary pollutants have been sparse leading to limited comparisons with photochemical model predictions. Recent in-plume measurements of these same pollutants and secondary PM_{2.5} made during the 2013 Southeast Nexus (SENEX) field campaign in the southern United States provide the first opportunity to extend these earlier evaluations to include secondary PM_{2.5}.(17) Plume enhancements of particulate matter have been identified downwind of multiple single sources from this field campaign based on relationships in the ambient data.(18) Here, a photochemical transport model was applied coincident with the in-plume field study measurements downwind of four separate electrical generating units using source sensitivity and source apportionment methods to differentiate these sources from other local and regional sources. In addition, subgrid plume treatment was applied with the source sensitivity approach to better understand whether treating source emissions with a Lagrangian submodel results in better agreement with in-plume source measurements. Model estimates are compared with ambient estimates of single source impacts both in space and time to illustrate model skill in plume placement and also just time to emphasize chemical plume evolution recognizing that for some types of applications skill in near-source plume placement is less important than chemical production.

Materials and Methods

The Community Multiscale Air Quality (CMAQ) model (www.cmascenter.org/cmaq) version 5.0.2 was used to model the periods of 2013 coincident with in-plume measurements made as part of the SENEX field campaign: June 16 and 22 for Scherer and Harllee electrical generating unit (EGU) facilities in northern Georgia, June 26 for Independence power plant in northeast Arkansas, and July 3 and 8 for New Madrid power plant in

southeast Missouri (Table 1). The CMAQ model includes gas-phase chemistry using the Carbon Bond approach,(19) inorganic aerosol partitioning based on ISORROPIA II,(20) 2-product semivolatile organic aerosol partitioning,(21) and aqueous phase chemistry that includes sulfur oxidation.(22) CMAQ was applied with 3 different model domains using 4 km sized grid cells covering an area centered over field measurements in Arkansas, Missouri, and Georgia (Supporting Information (SI) Figure S1). The atmosphere is resolved with 35 layers from the surface (layer 1 height approximately 22 m) to the 50 mb top of the model with more layers in the boundary layer to better represent diurnal changes in mixing layer heights.

Anthropogenic emissions from area and mobile sources are based on the 2011 National Emission Inventory.(23) Wild and prescribed fires are day specific for 2013 and point sources are based on 2013 Continuous Emissions Monitoring information where available and 2011 otherwise. The sources modeled here for impacts are based on 2013 emissions. Hourly emissions from each of the 4 facilities tracked for contribution are shown in SI Figure S2. The Harlee Branch facility has the highest emissions due to the lack of emissions control equipment during 2013. Location and stack release characteristics for these facilities are shown in Table 1. Biogenic emissions are estimated using version 3.61 of the Biogenic Emission Inventory System model with Biogenic Emissions Landuse Database version 4 vegetation information.(24) Previous work shows good agreement between biogenic impacts and field study measurements in the southeast United States.(25) Meteorological inputs to CMAQ were generated using version 3.7 of the Weather Research & Forecasting model.(26) Previous applications of this model show generally good agreement with surface variables and mixing layer height.(27)

Multiple approaches were used to differentiate single source impacts on modeled primary and secondary pollutants. A source sensitivity approach estimates source impacts by difference between 2 CMAQ model simulations, one of which contains all sources and another which contains all sources except the source of interest (e.g., brute-force zero-out).(28) The Integrated Source Apportionment Method (ISAM) was also used to track the contribution of each source of interest through all chemical and physical processes in the model and estimate the contribution to total bulk model predictions for O₃(29) and PM_{2.5}.(30) Source sensitivity(2, 4–6) and source apportionment(2, 31) approaches have been used in the past to estimate single source impacts using photochemical grid models.

Advanced Plume Treatment (APT)(8) is a subgrid plume treatment approach integrated in CMAQ and was applied with the brute-force zero-out sensitivity method to differentiate source impacts. CMAQ-APT uses the Second-Order Closure Integrated puff model with CHEMistry (SCICHEM) to treat subgrid puffs within CMAQ.(32) SCICHEM uses overlapping 3-D puffs to represent plumes for emissions from a specified source. Puffs evolve on a subgrid scale, undergoing transport and various other plume dynamics (plume rise, dispersion, puff merging/splitting) which use information from the host grid cell but are not consistent with the host model advection and diffusion schemes. The subgrid chemical evolution uses an identical chemical mechanism and aerosol module as the parent grid model. Once puffs reach a similar size to the model grid, the puffs are “merged” with the grid, meaning the mass contained in the puff is added to the grid and the puff is no longer

tracked. Because CMAQ-APT does not support inline photolysis, which was used in CMAQ and CMAQ-ISAM simulations, photolysis look-up tables were used in CMAQ-APT. Other relevant CMAQ-APT parameters are summarized in SI Table S1. The average number of puffs in a domain per facility at a given time during these simulations was 60 with the maximum being 243. The average time between puff releases was 30 s with a maximum value of 100 s which is comparable to tolerances set in other subgrid plume treatment approaches.(2)

As a postprocessing step, the “merge concs” CMAQ-APT utility was used to merge CMAQ-APT puffs with gridded CMAQ-APT results. This technique adds puff mass to the model grid to allow consistent comparisons against traditional gridded CMAQ results (SI Figure S3). In practice, all puff mass would merge into the grid if enough time has elapsed for the puff size to reach the size of the grid. However, when comparing hourly gridded impacts without using “merge concs”, the grid-only impacts would exclude pollutants contained within puffs at that specific hour. Another CMAQ-APT postprocessing utility, “receptor concs” was used to assess subgrid scale impacts at aircraft measurement locations (SI Figure S3). These results represent subgrid scale impacts (i.e., point-based impacts) estimated as host grid cell concentrations plus subgrid puff concentrations. Here, CMAQ-APT results postprocessed using “merge concs” are referred to as merged or grid based while those postprocessed using “receptor concs” are referred to as point based.

Details regarding measurements used here to evaluate the model are provided elsewhere. (17) Briefly, aircraft based measurements were collected at time intervals ranging from every 1 s (for NO_x , O_3 , and SO_2) to every 10 s (for PM_{10} sulfate ion). Measurements used in this study include: submicron speciated PM measured using Aerosol Mass Spectrometry (AMS); (33) SO_2 measured by pulsed UV fluorescence; (34) and NO , NO_2 , NO_y , and O_3 measured by gas phase chemiluminescence. (34–36) Modeled $\text{PM}_{2.5}$, calculated as the sum of the Aitken and accumulation modes, was compared without adjustment to measured submicron PM_{10} . This approach introduces uncertainty into the comparison, but converting CMAQ $\text{PM}_{2.5}$ to match AMS PM_{10} would introduce different uncertainties since CMAQ sometimes overpredicts fine particle mean diameters (37, 38) and AMS transmission efficiency changes as a function of particle size. (39) A review of AMS PM_{10} sulfate ion and particle volume (SI Figure S4) for all flights examined here showed relationships consistent with those for the Georgia flights published elsewhere. (18) PM_{10} sulfate ion tends to follow temporal variation seen in the particle volume measurements and often will increase when volume increases.

To compare modeled single-source impacts to observations, model predictions and observations were matched in horizontal and vertical space and time. Ambient based source specific contribution were estimated by subtracting observed “background” concentrations, here defined as the median observed pollutant concentration on a flight-by-flight basis, from each transect measurement. (2) The median values for each flight day and pollutant are shown in SI Table S2. When comparisons of modeled and observed plume centerlines were made, modeled plume centerlines were adjusted horizontally such that the maximum modeled and observed NO_y were matched in space. Note that no adjustments were made vertically for centerlines. Flight days and transects were prioritized for use in this model

evaluation where multiple well oriented downwind transects were made from a large power plant and extra consideration was given for flight days and plants examined elsewhere.(18)

Results and Discussion

Conceptual Understanding of Source Contributions to Flight Days

Southerly winds transported the New Madrid plume toward the north during the day on July 8th (see Figure 1) and to the southeast during the July 3rd nighttime flight transects (SI Figure S5). Figure 1 shows the ambient based (measurements minus median value from flight) and CMAQ source apportionment estimates of July 8 daytime downwind impacts from the New Madrid facility, all other EGUs in the model domain, and all non-EGU point sources in the model domain. The additional source apportionment results are presented to help identify other local sources that may be contributing to the ambient based impacts. Figure 1 shows while the New Madrid contribution to SO₂ and PM_{2.5} sulfate ion is typically largest, a nearby industrial source (Noranda Aluminum) also contributed SO₂ and PM_{2.5} sulfate to the downwind transects along with nearby power plants (Sikeston and Joppa). Contributions from these facilities, especially Sikeston and Joppa, are also evident in the ambient enhancements downwind of those facilities (Figure 1).

Figure 2 shows downwind transect ambient and source apportionment modeled SO₂ and PM_{2.5}sulfate ion impacts from the Independence power plant and New Madrid power plant. Other local sources, in particular Noranda Aluminum and Sikeston Power, have notable modeled impacts on the nighttime transects made downwind of New Madrid on July 3. However, the nighttime flight has a large contribution from sources outside the model domain (or recirculation of sources inside the domain) which may be PM_{2.5} sulfate ion formed the previous day that is above the surface mixed layer. Source apportionment modeling showed little notable contribution from other local sources in transects made downwind to the northeast (southwesterly winds) of the Independence facility on June 22 (Figure 2 and SI Figure S6).

The model estimated plume tends to be slightly lower in altitude than the aircraft during the nighttime flight downwind of New Madrid (SI Figure S9). Plots of daytime modeled facility impacts show the plume to be well mixed through the boundary layer during the period of aircraft measurements (SI Figure S10). During the nighttime flight, the model does predict large SO₂ impacts in the vertical layers between the stack release height and mixing layer height that are not well mixed upward or downward suggesting that the stack release point is above the modeled surface mixing layer during the hours of the flight. This feature suggests the CMAQ vertical advection local closure scheme is dominant over the nonlocal closure mixing scheme, which allows mass to be transported in the vertical direction to many layers as opposed to just the layers immediately adjacent to the emissions.(40)

Downwind daytime transects were made from Harlee Branch and Scherer power plants in Georgia (June 16 and 22). The model was able to differentiate the impacts of Scherer and Harlee Branch from other sources on both flight days. Ambient impacts from these facilities are most distinguishable on June 16 (SI Figure S7) due to favorable winds and downwind transect arrangement but the impacts are more problematic to differentiate in the June 22 (SI

Figure S8) downwind transect measurements due to easterly winds. Other EGUs in the model domain have a notable contribution to O_3 and $PM_{2.5}$ sulfate ion at the transect measurements made downwind of Harlee Branch and Scherer.

Single Source Plume Comparison

Ambient based and modeled impacts are shown as a function of plume centerline, which is based on NO_Y , in Figure 3 for the Independence plant (and SI Figures S11–S13 for other plants). This analysis more clearly illustrates plume structure by distance from the source since spatial differences exist between the ambient and modeled plume due to the modeled representation of local transport. The modeled impacts are shown using source apportionment and source sensitivity with and without subgrid plume treatment.

Modeled single source SO_2 impacts are highest nearest the source and $PM_{2.5}$ sulfate ion impacts show less of a downwind gradient. Ambient based impacts of facility specific SO_2 are often narrower in horizontal spatial extent and larger in magnitude than what is estimated by the modeling system at transects in close proximity to the source. The spatial scale and magnitudes become closer at the transects farther from these sources. Plume structure is most notable in the downwind transects of the Independence plant (Figure 3). The point-based subgrid plume treatment did well to capture the observed SO_2 , but this did not translate to improved model performance farther downwind. Estimated $PM_{2.5}$ sulfate contribution is both higher and lower compared with ambient based estimates. Ambient based $PM_{2.5}$ sulfate ion plume estimates do not tend to show large centerline peak concentrations compared with SO_2 , but are sampled over a slightly longer time interval. Figure 3 shows a sharp centerline $PM_{2.5}$ sulfate ion peak predicted by the APT approach but not grid-based approaches. This feature is also not evident in the ambient data.

Similar to SO_2 , the modeling system tends to estimate lower NO_X contribution from these plants compared to ambient based estimates, especially at transects in closest proximity to the source. Typically, each of the methods resulted in similar NO_X contribution estimates downwind. One exception is the APT approach contribution estimates downwind of the Independence plant (Figure 3), which are notably larger than the grid-based approaches in the nearer transects. The source sensitivity approaches (brute-force and brute-force with APT) capture near-source NO titration of O_3 where indicated by ambient data although the model tends to not capture the magnitude of the O_3 decrease. APT is the only approach to capture notable near-source O_3 decreases due to titration from fresh NO emissions but this does not translate into better O_3 production estimates at transects farther downwind based on ambient data. The model often predicts smaller contribution compared to the ambient approach but did better at matching ambient based downwind O_3 when comparing near-peak 98th percentile estimates (see Table 2). It is important to note that it is particularly difficult to differentiate O_3 from specific sources in ambient data due to the regional nature of the pollutant and many local sources in these areas. The spatial and plume cross-section comparisons demonstrate model ability to capture single source primary and secondary pollutant impacts over time and space which is similar to that shown in other studies. (2)

Daytime Plume Chemical Ratios

Ratios, as opposed to absolute concentrations, provide a method of normalization across model and observed values to focus the interpretation of results on chemical processes and minimize differences due to pollutant transport or emissions. The $\text{PM}_{2.5}$ sulfate ion to SO_2 + $\text{PM}_{2.5}$ sulfate ion ratio is intended to provide information about how quickly SO_2 is converted to particulate sulfate in these plumes and shown averaged by transect for each facility in Figure 4. Table 3 shows the flight averaged ratio and bias between the ambient based ratio and those estimated with modeling approaches. Downwind particulate sulfate production is well characterized by all methods for the New Madrid transects (bias less than 2%). The ISAM approach tends to overestimate downwind sulfate production at Independence (bias of 7%) and Scherer (bias of 20%) but is the only approach to fully capture the peak downwind production at Harlee Branch (bias of 1%) and was the closest to peak downwind production at Scherer. The production of particulate sulfate in these downwind plumes was generally well represented by these approaches for isolating single source impacts with average ratio bias less than 8% except for overestimation by the ISAM approach for the closest transects downwind of Scherer.

The NO_X to NO_Y ratio provides a proxy for photochemical age,(41–43) or how quickly or slowly primary emissions are converted to secondary pollutants. All of the methods converted NO_X to NO_Y too quickly downwind of Scherer and at transects furthest from Harlee and New Madrid (SI Figure S14), which are noted in Table 3 as negative bias in the ratio. The conversion downwind of Independence is generally well characterized by the BF and ISAM approaches. However, the APT approaches, in particular the APT grid approach, estimated less chemical conversion compared to the ambient data. The APT-grid approach shows almost no chemical production downwind of either Independence or New Madrid which is inconsistent with ambient measurements and the other modeling approaches (SI Figure S14). The difference could be attributed to the use of photolysis lookup tables, subgrid plume treatment in APT, or other factors. However, sensitivity brute-force simulations using photolysis lookup tables in place of in-line photolysis actually decreased the ratio of NO_X to NO_Y by 6% at the 48 km transect downwind of the Independence facility suggesting the lower conversions with APT are likely attributable to subgrid plume treatment or the postprocessing approach of generating merged grid and puff estimates.

Finally, the NO_Y to SO_2 ratio is used to assess modeled emissions compared to observations (Figure S15). Good agreement with the modeled and observed ratio suggests the modeled emissions are well characterized. The one exception is the APT results at the New Madrid facility, which predicted less NO_Y producing a lower ratio that is inconsistent with ambient data. The contrast of grid and point-based APT results suggests that the postprocessing to merge puffs into grids may be placing puff mass into adjacent grid cells (either vertically or horizontally) leading to differences in adjacent grid cells and possibly previous and subsequent hours.

Modeled Contribution Estimate Comparisons

Figure 5 shows modeled contribution from the New Madrid power plant on July 8, 2013 to illustrate differences in methods. A morning period is chosen to illustrate differences in

subgrid puff placement and the afternoon to illustrate both chemical and physical differences in these approaches. ISAM estimated surface SO₂ contribution (Figure 5a) at 10 am shows the highest levels nearest the plant and decreasing contribution in the direction of prevailing winds to the northeast. Downwind contribution is similar using the BF approach (Figure 5b). The BF approach shows higher contribution than APT nearer the source and lower contribution starting at approximately 12–15 km downwind. This feature is related to APT keeping mass in subgrid puffs closer to the source then dumping that mass into the host grid cells farther downwind (Figure 5c). ISAM, BF, and APT estimated contribution of the power plant to surface layer NO_x and O₃ are shown for 2 pm. Negative contribution for the source sensitivity methods represents how O₃ levels would change in the absence of NO_x emissions which results in less O₃ due to titration by fresh NO emissions. Here, titration is more muted when APT is employed (Figure 5h, 5i) which is related to less grid-resolved NO_x compared to the BF method (Figure 5f). ISAM is designed to only track contribution to O₃ production meaning no contribution will be estimated when destruction processes dominate (Figure 5g).

For the transects downwind of the power plants shown here, the ISAM and BF approaches estimate similar contribution for each of the pollutants except situations where O₃ destruction outpaces production. The APT approach results in notable differences from the BF method but are not directionally systematic (SI Figure S16). ISAM tends to predict higher PM_{2.5} sulfate ion contribution compared to the sensitivity based approaches. However, it is not clear that this resulted in a systematic difference in bias compared to ambient based contribution estimates. The APT approach changes model estimated contributions through both chemical and physical treatment. A comparison is provided using a conserved tracer with little chemical reactivity (e.g., CO) to illustrate nonchemical impacts of subgrid plume treatment. SI Figure S17 shows the episode average CO estimates using the brute-force zero out approach with and without APT. For this source and time period the APT approach results in higher contribution aloft and lower at the surface. This tendency toward less mixing to the surface has been shown in another subgrid plume scheme implemented in a different host model.⁽⁷⁾ While the subgrid impacts on pollutant chemistry may be desired, the impacts on model estimates due to puff transport are notable and should not be discounted when interpreting results generated with APT or when comparing estimates with other approaches. It is possible that the incommensurate advection and diffusion between the subgrid and host model contribute to a physically less realistic outcome in terms of source impacts compared to using either modeling system singularly.

Each of these approaches for differentiating single source impacts tends to provide a reasonable representation of downwind secondary chemical production. However, particular approaches may be better suited for different types of assessments. Where understanding how much air quality might change due to changes in emissions then a source sensitivity approach may be best, especially in situations where highly nonlinear chemistry is anticipated. If the contribution to modeled pollutants is desired, then source apportionment would be appropriate. Finally, in situations where an emissions source and key receptors are within the same grid cell then subgrid plume treatment approaches would provide additional information.

Supplementary Material

Refer to Web version on PubMed Central for supplementary material.

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Figure 1.

SO₂, PM_{2.5} sulfate ion, NO_x, and O₃ contribution estimates downwind of the New Madrid power plant on July 8, 2013 based on measurements (left column) and a source apportionment (ISAM) photochemical model simulation. The ISAM approach was also used to estimate the contribution from all other EGUs in the model domain and non-EGU point sources in the model domain. Modeled contribution from the facility shown here is the maximum contribution between the top of the stack and top of the surface mixing layer.

Figure 2.

SO_2 and PM_{2.5} sulfate ion contribution estimates downwind of the Independence and New Madrid (night-time flights) power plants based on measurements and source apportionment photochemical model simulations. Modeled contribution from the facility shown here is the maximum contribution between the top of the stack and top of the surface mixing layer.

Figure 3.

Model and observed concentrations depicting plume centerlines (matched in space by adjusting max NO_y model results horizontally to match max NO_y observations) at various distances downwind of the New Madrid Plant on July 8, 2013. Model results include the advanced plume treatment grid-based results (APT Grid), point-based (i.e. receptor) APT results (APT Point), brute-force (BF), and integrated source apportionment method (ISAM).

Figure 4.

Average observed and modeled species ratio of particulate sulfate to the sum of SO_2 and particulate sulfate at multiple downwind distances from each source. Only the daytime transect information is included for New Madrid.

Figure 5. Model estimated contribution from New Madrid power plant on July 8, 2013 to SO₂ (top row), NO_x (middle row), and O₃ (bottom row).

Table 1.

Stack Release Characteristics for the Facilities Modeled for Contribution Assessment

Facility Name	Stack Height (m)	Stack Diameter (m)	Exit Temperature (C)	Exit Flow Rate (m ³ /s)	Exit Velocity (m/s)	Longitude	Latitude
Scherer	305	8	128	1283	24	-83.8064	33.0613
	305	8	137	1234	23	-83.8074	33.0595
	258	10	56	1463	17	-83.8064	33.0634
New Madrid	244	6	157	690	24	-89.5683	36.5136
	244	6	177	623	21	-89.5617	36.5147
	244	6	162	606	21	-89.5683	36.5136
Independence	305	8	161	1322	27	-91.4078	35.6782
	305	8	161	1322	27	-91.4078	35.6782
Harllee	305	9	127	1435	23	-83.2997	33.1945
	305	7	121	920	25	-83.2997	33.1945

Table 2.

Source Contribution to Ambient Measurements (Measured–Median of Flight Segment) and Modeled Contribution Using Multiple Methods

pollutant	flight day	related facility	units	98th percentile estimate				bias (OBS-MODEL)		
				OBS	ISAM	BF	APT	ISAM	BF	APT
SO ₂	130616	Scherer	ppb	5.1	3	1.8	1.6	-2.2	-3.3	-3.6
PM _{2.5} sulfate	130616	Scherer	ug/m ³	1.4	1.5	0.5	0.5	0.1	-0.9	-0.9
NO _x	130616	Scherer	ppb	1.7	1.7	0.1	0.1	0	-1.6	-1.6
O ₃	130616	Scherer	ppb	10.5	2.5	1.2	1.5	-7.9	-9.2	-9.0
SO ₂	130616	Hartlee Branch	ppb	0.7	0.3	19.4	12.1	-0.4	18.7	11.4
PM _{2.5} sulfate	130616	Hartlee Branch	ug/m ³	0.3	0.4	3.3	2.1	0.1	3	1.8
NO _x	130616	Hartlee Branch	ppb	0.2	0.2	5.5	3.1	0	5.2	2.9
O ₃	130616	Hartlee Branch	ppb	2.3	0.7	6.9	5.4	-1.5	4.6	3.1
SO ₂	130626	Independence	ppb	7	3.8	3.8	3	-3.2	-3.2	-4.0
PM _{2.5} sulfate	130626	Independence	ug/m ³	0.6	1.5	0.9	0.3	0.9	0.3	-0.3
NO _x	130626	Independence	ppb	1.9	2.2	2.1	1.6	0.3	0.2	-0.3
O ₃	130626	Independence	ppb	7.8	2.6	2.2	1.7	-5.2	-5.6	-6.1
SO ₂	130703	New Madrid	ppb	20.6	6.3	6.4	0.9	-14.3	-14.1	-19.7
PM _{2.5} sulfate	130703	New Madrid	ug/m ³	4.1	0.4	0.4	0.1	-3.7	-3.7	-4.0
NO _x	130703	New Madrid	ppb	13.9	8.6	8.5	1.2	-5.3	-5.4	-12.7
O ₃	130703	New Madrid	ppb	14.8	0	0.1	0.1	-14.8	-14.6	-14.7
SO ₂	130708	New Madrid	ppb	13.9	3.6	3.6	2.7	-10.3	-10.3	-11.2
PM _{2.5} sulfate	130708	New Madrid	ug/m ³	5.6	2.7	1.6	1.7	-2.9	-4.0	-4.0
NO _x	130708	New Madrid	ppb	4.3	5.7	4.9	3.2	1.4	0.6	-1.1
O ₃	130708	New Madrid	ppb	8.6	7.5	8.2	9.2	-1.1	-0.4	0.6

Table 3.

Average Observed and Modeled Species Ratio over All Transects of (1) Particulate Sulfate to the Sum of SO₂ and Particulate Sulfate and (2) NO_x to NO_y for Each Source

ratio		plant	average ratio					bias (MODEL - OBS)			
			OBS	ISAM	BF	APT	APT Point	ISAM	BF	APT	APT Point
Sulfur Ratio		Hartlee Branch	0.14	0.15	0.10	0.09	0.09	1.3	-4.1	-4.4	-4.6
		Independence	0.02	0.09	0.06	0.03	0.02	7.2	4.1	0.9	0.1
		New Madrid	0.16	0.17	0.15	0.18	0.16	1.1	-1.6	1.8	-0.2
		Scherer	0.18	0.38	0.13	0.13	0.12	19.5	-5.1	-5.6	-6.1
NO _x :NO _y Ratio		Hartlee Branch	0.61	0.54	0.49	0.48	0.50	-7.3	-12.2	-13.4	-10.8
		Independence	0.79	0.86	0.82	1.00	0.91	7.2	3.4	21.0	11.6
		New Madrid	0.70	.63	.51	1.00	0.48	-6.3	-18.9	29.9	-22.2
		Scherer	0.50	0.21	0.17	0.16	0.17	-29.5	-33.3	33.7	-33.0