



# Interagency Workgroup on Air Quality Modeling Phase 3 Summary Report: Near-Field Single-source Secondary Impacts

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**Interagency Workgroup on Air Quality Modeling Phase 3 Summary Report: Near-Field  
Single-source Secondary Impacts**

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## Executive Summary

The Interagency Workgroup on Air Quality Modeling (IWAQM) was originally formed in 1991 to provide a forum for development of technically sound regional air quality models for regulatory assessments of pollutant source impacts on Federal Class I areas. The IWAQM process largely concluded in 1998 with the publication of the Interagency Workgroup on Air Quality Modeling (IWAQM) Phase 2 Summary Report and Recommendations for Modeling Long-range transport Impacts (EPA-454/R-98-019) (U.S. Environmental Protection Agency, 1998). The IWAQM Phase 2 process provided a series of recommendations concerning the application of the CALPUFF model for use in long-range transport (LRT) modeling and informed the promulgation of that model for such regulatory purposes in 2003. The IWAQM process was reinitiated in June 2013 to inform EPA's commitment to update the "Guideline on Air Quality Models" (Appendix W to CFR Part 51), hereafter referred to as Appendix W, to address chemically reactive pollutants in near-field and long-range transport applications (U.S. Environmental Protection Agency, 2012a). This report provides information and recommendations from the "Phase 3" effort focused on near-field single-source impacts of secondary pollutants. A separate report provides information and recommendations on long-range transport for air quality related values (AQRVs) and deposition (U.S. Environmental Protection Agency, 2015).

This document describes chemical and physical processes important to the formation of ground-level O<sub>3</sub> and PM<sub>2.5</sub> in the context of modeled near-field assessments to support permit review programs. Chemical transport models that characterize these processes include both Lagrangian which typically only have a single-source included in the model and photochemical grid models which include some representation of all anthropogenic, biogenic, and geogenic sources. Modeling systems appropriate for the purposes of estimating single-source near-field secondary impacts are described and recommendations are made with respect to the use of certain types of modeling systems for this type of application. Model evaluation is important to ensure that a particular system is fit for the purpose of estimating near-field single-source secondary impacts. In addition to establishing a modeling system is generally appropriate for this purpose, project-specific evaluations that compare model-estimated meteorology and chemical estimates with measurements near the project source and key receptors is also an important model evaluation component.

An illustrative example is provided showing hypothetical single-source impacts in two different urban areas: Atlanta and Detroit. A photochemical grid model was applied with baseline emissions and subsequent additional simulations where a new hypothetical source was included with a fixed precursor emission rate. The rates used here are illustrative and not reflective of any specific policy or programs. The simulations with the additional hypothetical source are compared with the baseline simulation where the hypothetical source is not included (e.g. brute-force difference) and single-source impacts are estimated for O<sub>3</sub> and secondary PM<sub>2.5</sub> sulfate and nitrate. Downwind impacts from these hypothetical sources tend to increase as precursor emissions increase. Impacts tend to be highest near the source and decrease as distance from the source increases. However, there is variability in downwind impacts directionally from each of these sources due to differences in meteorology and available oxidants and neutralizing agents.

Finally, a review of existing research published between 2005 and 2015 relating single-source precursor emissions and downwind impacts on O<sub>3</sub> and secondary PM<sub>2.5</sub> is summarized. Downwind O<sub>3</sub> impacts from these studies show a general increase as NO<sub>x</sub> emissions increase. Downwind impacts for O<sub>3</sub> and secondary PM<sub>2.5</sub> in the studies reviewed tend to be largest nearest the source and decrease as distance

from the source increases. Approaches for developing reduced-form or screening versions of more refined modeling tools such as photochemical transport models are also reviewed. Where appropriately developed, relationships between hypothetical source precursor emissions and downwind O<sub>3</sub> and secondary PM<sub>2.5</sub> impacts could be used to provide credible information about single-source secondary pollutant impacts before applying more rigorous modeling techniques. This type of approach is more commonly called a Tier 1 demonstration tool or Modeled Emission Rates for Precursors (MERPS).

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## 1 Background: IWAQM Phase 3 process

The Interagency Workgroup on Air Quality Modeling (IWAQM) was originally formed in 1991 to provide a forum for development of technically sound regional air quality models for regulatory assessments of pollutant source impacts on Federal Class I areas. Meetings were held with personnel from participating Federal agencies: the Environmental Protection Agency (EPA), the U.S. Forest Service (USFS), the U.S. Fish and Wildlife Service (USFWS), and the National Park Service (NPS). The original purpose was to review respective modeling programs, develop an organizational framework, and formulate reasonable objectives and plans for single-source model applications. The IWAQM process largely concluded in 1998 with the publication of the Interagency Workgroup on Air Quality Modeling (IWAQM) Phase 2 Summary Report and Recommendations for Modeling Long-range transport Impacts (EPA-454/R-98-019) (U.S. Environmental Protection Agency, 1998). The IWAQM Phase 2 report provided a series of recommendations concerning the application of the CALPUFF model for use in long-range transport (LRT) modeling and informed the promulgation of that model for such regulatory purposes in 2003. Draft updates to the IWAQM Phase 2 report were released in 2009 to better reflect the state-of-the-practice of long-range transport modeling techniques based on experience gained since the early 2000s.

The IWAQM process was reinitiated in June 2013 to inform EPA's commitment to update the "Guideline on Air Quality Models" (Appendix W to CFR Part 51), hereafter referred to as Appendix W, to address chemically reactive pollutants in near-field and long-range transport applications (U.S. Environmental Protection Agency, 2012a). Comments received from the 10<sup>th</sup> Modeling Conference (March 2012) from stakeholders support this interagency collaborative effort to provide additional guidance for modeling single-source impacts on secondarily formed pollutants in the near-field and for long-range transport. Stakeholder comments also support the idea of this collaborative effort working in parallel with separate stakeholder efforts to further model development and evaluation.

This "Phase 3" effort includes the establishment of 2 separate working groups, one focused on long-range transport of primary and secondary pollutants and the other on near-field single-source impacts of secondary pollutants. A separate report provides information and recommendations on long-range transport for air quality related values (AQRVs) and deposition (U.S. Environmental Protection Agency, 2015). While many of the objectives are similar for each of these groups, the focus and regulatory endpoints are different. It is expected the "Phase 3" effort will continue with future efforts related to reviewing and responding to comments given on the 2015 proposed changes to Appendix W related to single-source impact assessments for O<sub>3</sub> and secondary PM<sub>2.5</sub>. IWAQM3 near-field impacts team members (affiliated with U.S. Environmental Protection Agency unless noted otherwise) include James Kelly, George Bridgers, Andy Hawkins, Randall Robinson, Jaime Julian, Rebecca Matichuk, Robert Kotchenruther, Rynda Kay, and Richard Monteith. Additional participation was provided by Erik Snyder, Robert Elleman, and Bret Anderson (U.S. Department of Agriculture).

## 2 Regulatory Motivation

Pursuant to 40 CFR part 51.166 and 52.21, subsections (k)(1)(i) and (k)(1)(ii), new or modified sources emitting in significant amounts (see 40 CFR part 51.166 and 52.21, subsection (b)(23)(i)) are required to demonstrate that the source under review does not cause or contribute to a violation of any applicable National Ambient Air Quality Standards (NAAQS) ((k)(1)(i)) or maximum allowable increases over a baseline concentration ((k)(1)(ii)). The relevant permitting authority administers the NAAQS and increments component of the air quality analysis.

### 3 Model Selection

This section describes the types of air quality impacts that need to be assessed and the tools that are best suited for this purpose. For a variety of regulatory programs, impacts on secondary pollutants such as O<sub>3</sub> and PM<sub>2.5</sub> need to be assessed at two spatial scales (near-source and long-range transport). It is important that modeling systems used for these assessments be fit for this purpose and be evaluated for skill in replicating meteorology and atmospheric chemical and physical processes that result in secondary pollutants and deposition.

#### 3.1 Secondary Pollutant Formation: O<sub>3</sub> and PM<sub>2.5</sub>

PM<sub>2.5</sub> and O<sub>3</sub> are closely related to each other in that they are formed in the atmosphere from chemical reactions with similar precursors (U.S. Environmental Protection Agency, 2005). Air pollutants formed through chemical reactions in the atmosphere are referred to as secondary pollutants. For example, ground-level ozone (O<sub>3</sub>) is predominantly a secondary pollutant formed through nonlinear photochemical reactions driven by emissions of nitrogen oxides (NO<sub>x</sub>) and volatile organic compounds (VOCs) in the presence of sunlight. Warm temperatures, clear skies (abundant levels of solar radiation), and stagnant air masses (low wind speeds) increase ozone formation potential (Seinfeld and Pandis, 2012). PM<sub>2.5</sub> can be either primary (i.e. emitted directly from sources) or secondary (formed in the atmosphere). The fraction of PM<sub>2.5</sub> which is primary versus secondary varies by location and season. In the United States, PM<sub>2.5</sub> is dominated by a variety of chemical species: ammonium sulfate, ammonium nitrate, organic carbon (OC) mass, elemental carbon (EC), and other soil compounds and oxidized metals. PM<sub>2.5</sub> elemental (black) carbon and soil dust are both directly emitted into the atmosphere from primary sources. Organic carbon particulate is directly emitted from primary sources but also has a secondary component formed by atmospheric reactions of VOC emissions. PM<sub>2.5</sub> sulfate, nitrate, and ammonium ions are predominantly the result of chemical reactions of the oxidized products of sulfur dioxide (SO<sub>2</sub>) and NO<sub>x</sub> emissions and direct ammonia (NH<sub>3</sub>) emissions (Seinfeld and Pandis, 2012).

#### 3.2 Air Quality Models for Secondary Pollutants

Single-source impacts on secondary pollution including ozone and PM<sub>2.5</sub> are becoming increasingly important for facility permit reviews under the Prevention of Significant Deterioration (PSD) program as well as New Source Review (NSR) and other regulatory programs. Gaussian dispersion models such as AERMOD have been used to quantify the near-field (less than 50 km) impacts of primary PM<sub>2.5</sub> emissions from new or modified sources (Perry et al., 2005; U.S. Environmental Protection Agency, 2005, 2014). However, these types of models cannot treat the important chemical and physical processes of O<sub>3</sub> and secondary PM<sub>2.5</sub>.

Chemical transport models treat atmospheric chemical and physical processes such as gas and particle chemistry, deposition, and transport. There are two types of chemical transport models which are differentiated based on a fixed frame of reference (Eulerian grid based) or a frame of reference that moves with parcels of air between the source and receptor point (Lagrangian) (McMurry et al., 2004). Photochemical grid models are three-dimensional grid-based models that treat chemical and physical processes in each grid cell and use Eulerian diffusion and transport processes to move chemical species to other grid cells (McMurry et al., 2004). These types of models are appropriate for assessment of near-field and regional scale reactive pollutant impacts from specific sources (Baker and Foley, 2011; Baker

and Kelly, 2014; Bergin et al., 2008; Zhou et al., 2012) or all sources (Chen et al., 2014; Russell, 2008; Tesche et al., 2006). Photochemical transport models have been used extensively to support State Implementation Plans and explore relationships between inputs and air quality impacts in the United States and beyond (Cai et al., 2011; Civerolo et al., 2010; Hogrefe et al., 2011).

### 3.2.1 Lagrangian models

Quantifying secondary pollutant formation requires simulating chemical reactions and thermodynamic partitioning in a realistic chemical and physical environment. Some Lagrangian models treat in-plume gas and particulate chemistry. These models require as input background fields of time and space varying oxidant concentrations, and in the case of PM<sub>2.5</sub> also neutralizing agents such as ammonia, because important secondary impacts happen when plume edges start to interact with the surrounding chemical environment (Baker and Kelly, 2014; ENVIRON, 2012c). These oxidant and neutralizing agents are not routinely measured, but can be generated with a three-dimensional photochemical transport model and subsequently be input to a Lagrangian modeling system. Photochemical models simulate a more realistic chemical and physical environment for plume growth and chemical transformation (Baker and Kelly, 2014; Zhou et al., 2012), but simulations may sometimes be more resource intensive than Lagrangian or dispersion models.

### 3.2.2 Photochemical transport models

Publically available and documented Eulerian photochemical grid models such as the Comprehensive Air Quality Model with Extensions (CAMx) (ENVIRON, 2014) and the Community Multiscale Air Quality (CMAQ) (Byun and Schere, 2006) model treat emissions, chemical transformation, transport, and deposition using time and space variant meteorology. These modeling systems include primarily emitted species and secondarily formed pollutants such as O<sub>3</sub> and PM<sub>2.5</sub> (Chen et al., 2014; Civerolo et al., 2010; Russell, 2008; Tesche et al., 2006). Even though single-source emissions are injected into a grid volume, photochemical transport models have been shown to adequately capture single-source impacts when compared with downwind in-plume measurements (Baker and Kelly, 2014; Zhou et al., 2012). Where set up appropriately for the purposes of assessing the contribution of single-sources to primary and secondarily formed pollutants, photochemical grid models could be used with a variety of approaches to estimate these impacts. These approaches generally fall into the category of source sensitivity (how air quality changes due to changes in emissions from a specific source) and source apportionment (how specific source emissions contribute to air quality levels under modeled atmospheric conditions).

The simplest source sensitivity approach (brute-force change to emissions) would be to simulate 2 sets of conditions, one with all emissions and one with the source of interest changed from the baseline simulation (e.g. post-construction conditions) (Cohan and Napelenok, 2011). The difference between these simulations provides an estimate of the air quality change related to the change in emissions from the project source. Another source sensitivity approach to identify the impacts of single-sources on changes in model-predicted air quality is the decoupled direct method (DDM), which tracks the sensitivity of an emissions source through all chemical and physical processes in the modeling system (Dunker et al., 2002). Sensitivity coefficients relating source emissions to air quality are estimated during the model simulation and output at the resolution of the host model.

Some photochemical models have been instrumented with source apportionment, which tracks emissions from specific sources through chemical transformation, transport, and deposition processes

to estimate a contribution to predicted air quality at downwind receptors (Kwok et al., 2015; Kwok et al., 2013). Source apportionment has been used to differentiate the contribution from single-sources on model predicted ozone and PM<sub>2.5</sub> (Baker and Foley, 2011; Baker and Kelly, 2014). DDM has also been used to estimate O<sub>3</sub> and PM<sub>2.5</sub> impacts from specific sources (Baker and Kelly, 2014; Bergin et al., 2008; Kelly et al., 2015) as well as the simpler brute-force sensitivity approach (Baker and Kelly, 2014; Bergin et al., 2008; Kelly et al., 2015; Zhou et al., 2012). Limited comparison of single-source impacts between models (Baker et al., 2013) and approaches to identify single-source impacts (Baker and Kelly, 2014; Baker et al., 2013) show generally similar downwind spatial gradients and impacts.

Near-source in-plume aircraft-based measurement field studies provide an opportunity for evaluating model estimates of (near-source) downwind transport and chemical impacts from single stationary point sources (ENVIRON, 2012c). Photochemical grid model source apportionment and source sensitivity simulation of single-source downwind impacts compare well against field study primary and secondary ambient measurements made in Tennessee and Texas (ENVIRON, 2012c). This work indicates photochemical grid models and source apportionment and source sensitivity approaches provide meaningful estimates of single-source impacts. However, additional evaluations are needed for longer time periods and more diverse environments, both physical and chemical, to generate broader confidence in these approaches for this purpose. In particular, it is important to ensure that adequate model performance is achieved in areas with complex terrain and meteorology.

### 3.3 Recommendations for estimating single-source O<sub>3</sub> and secondary PM<sub>2.5</sub> impacts using photochemical grid models

Photochemical transport models are suitable for estimating single-source O<sub>3</sub> and secondary PM<sub>2.5</sub> impacts since important physical and chemical processes related to the formation and transport of both are realistically treated. Source sensitivity and apportionment techniques implemented in photochemical grid models have evolved sufficiently and provide the opportunity for estimating potential secondary pollutant impacts from one or a small group of emission sources. Photochemical grid models using meteorology output from prognostic meteorological models have demonstrated skill in estimating source-receptor relationships in the near-field (Baker and Kelly, 2014; ENVIRON, 2012c) and over long distances (ENVIRON, 2012b).

In situations of close proximity between the source and receptor, a photochemical model instrumented with sub-grid plume treatment and sampling could potentially represent these relationships. However, the simplest approach to better representing the spatial gradient in source-receptor relationships when they are in close proximity would be to use smaller sized grid cells. Sub-grid plume treatment extensions in photochemical models typically solve for in-plume chemistry and use a set of physical and chemical criteria for determination of when puff mass is merged back into the host model grid (Baker et al., 2014). Sub-grid plume (puff) sampling or sub-grid puff merging with host grid cell estimates is necessary because inherently in this type of system (sub-grid plume treatment in a photochemical grid model) some of the source's impacts on air quality are resolved in puffs at the sub-grid scale and some have been resolved in the 3-dimensional grid space. Just extracting sub-grid plume information or just 3-dimensional model output would omit some of the source's contribution to air quality. In practice, some type of source apportionment or source sensitivity (e.g. brute-force difference) would be necessary to track in the grid resolved source contribution in addition to sub-grid plume treatment to fully capture source contribution when using sub-grid plume treatment.

Previous research has shown that photochemical grid models applied without “sub-grid plume treatment” do capture the initial stage of plume chemistry (e.g. O<sub>3</sub> titration) based on single-source sensitivity simulations at multiple grid resolutions (Cohan et al., 2005) and also when comparing modeled single-source impacts against near-source in-plume measurements (Baker and Kelly, 2014; Zhou et al., 2012). Given the complexities in fully determining project source impacts in both the grid model and sub-grid puffs (Baker et al., 2014) and the tendency for puffs to stay aloft compared to grid-resolved mass (Baker et al., 2014; Kelly et al., 2015), the use of sub-grid plume treatment for the purposes of estimating project source impacts for PSD/NSR would typically not be recommended. Additionally, these tools sometimes exacerbate numerical instability that infrequently might occur in inorganic and aqueous chemical reactions (Kelly et al., 2015).

## 4 Model evaluation

There are multiple components to model evaluation for the purposes of assessing single-source secondary pollutant impacts. First, an alternative modeling system as defined in Appendix W must meet certain criteria for this purpose (Appendix W Section 3.2.2.e). One type of evaluation is to show that the modeling system is theoretically fit for purpose. A second evaluation component involves comparison to ambient measurements to assess whether the modeling system and generated inputs are appropriate for a specific project application.

Since PM<sub>2.5</sub> and O<sub>3</sub> impacts may be estimated for single-sources as part of a permit review process, it is important that a modeling system be able to capture single-source primary (e.g. precursors) and secondary impacts. Near-source in-plume measurements are useful to develop confidence that a modeling system captures secondarily formed pollutants from specific sources. These types of assessments are typically only done occasionally when a modeling system has notably changed from previous testing or has never been evaluated for this purpose. This type of assessment is discussed in more detail in section 4.1.

A second type of evaluation fulfills the need to determine whether inputs to the modeling system for a particular scenario are adequate for the specific conditions of the project impact assessment (Appendix W Section 3.2.2.e). This type of evaluation usually consists of comparing model predictions with observation data that coincides with the episode being modeling for a permit review assessment. One of the most important questions in an evaluation concerns whether the prognostic or diagnostic meteorological fields are adequate for their intended use in supporting the project model application demonstration. Sections 4.2 and 4.3 cover project-specific evaluation approaches that develop confidence that a particular model application is appropriate for the project source and key downwind receptors. It is important to emphasize that a broad evaluation of a model platform’s skill in estimating meteorology or chemical measurements may not sufficiently illustrate the appropriateness of that platform for specific projects that will be focused on a narrow subset of the larger set of model inputs and outputs. Therefore, broad model platform evaluations should be supplemented with focused evaluation and discussion of the appropriateness of model inputs for specific project assessments.

### 4.1 Fit for Purpose Evaluations

Near-source in-plume aircraft-based measurement field studies provide an opportunity for evaluating model estimates of (near-source) downwind transport and chemical impacts from single stationary point sources (ENVIRON, 2012c). Since single-source impacts in the near-field are assessed in each direction

from a source at evenly distributed receptor locations, model system skill in plume placement is not emphasized. Ideally, these modeling systems will capture near-source plume placement to best match plume evolution with the surrounding heterogeneous chemical environment. Model system skill in capturing secondary impacts is important in near-field permit related assessments and in-plume field measurements provide the best opportunity for evaluating model skill in capturing secondary impacts from a specific source. Often when comparing modeled and measured in-plume pollutants the model impacts are shifted spatially to match the location of the measured plume, meaning the comparison is paired in time but not space and therefore emphasizing secondary pollutant formation over plume placement.

Photochemical grid model source apportionment and source sensitivity simulation of single-source downwind impacts compare well against field study primary and secondary ambient measurements made in Tennessee and Texas (Baker and Kelly, 2014; ENVIRON, 2012c). This work indicates photochemical grid models and source apportionment and source sensitivity approaches provide meaningful estimates of single-source impacts. However, additional evaluations are needed for longer time periods and more diverse environments to generate broader confidence in these approaches for this purpose.

## 4.2 Model evaluation: meteorology

It is important to determine whether and to what extent confidence may be placed in a prognostic meteorological model's output fields (e.g., wind, temperature, mixing ratio, diffusivity, clouds/precipitation, and radiation) that will be used as input to models. Currently there is no bright line for meteorological model performance and acceptability. There is valid concern that establishment of such criteria, unless accompanied with a careful evaluation process might lead to the misuse of such goals as is occasionally the case with the accuracy, bias, and error statistics recommended for judging model performance. In spite of this concern, there remains nonetheless the need for some statistical performance metrics against which to compare new prognostic and diagnostic model simulations. A significant amount of information (e.g. model performance metrics) can be developed by following typical evaluation procedures that will enable quantitative comparison of the meteorological modeling to other contemporary applications and to judge its suitability for use in modeling studies.

Development of the requisite meteorological databases necessary for use of photochemical transport models should conform to recommendations outlined in Guidance on the Use of Models and Other Analyses for Demonstrating Attainment of Air Quality Goals for Ozone, PM<sub>2.5</sub>, and Regional Haze (U.S. Environmental Protection Agency, 2014). Demonstration of the adequacy of prognostic or diagnostic meteorological fields can be established through appropriate diagnostic and statistical performance evaluations consistent with recommendations provided in the appropriate model guidance (U.S. Environmental Protection Agency, 2014).

## 4.3 Model evaluation: chemistry

An operational evaluation is used to assess how accurately the model predicts observed concentrations. Therefore, an operational evaluation can provide information about model performance and identify model limitations and uncertainties that require diagnostic evaluation for further model development/improvement. An operational evaluation for PM<sub>2.5</sub> is similar to that for ozone. Some important differences are that PM<sub>2.5</sub> consists of many components and is typically measured with a 24-

hour averaging time. The individual components of PM<sub>2.5</sub> should be evaluated individually. In fact, it is more important to evaluate the components of PM<sub>2.5</sub> than to evaluate total PM<sub>2.5</sub> itself. Apparent “good performance” for total PM<sub>2.5</sub> does not indicate whether modeled PM<sub>2.5</sub> is predicted for “the right reasons” (the proper mix of components). If performance of the major components is good, then performance for total PM<sub>2.5</sub> should also be good. Databases that contain ambient O<sub>3</sub>, PM<sub>2.5</sub>, and key precursors are noted in section 4.4. Section 4.4 is not intended to provide an exhaustive review of all ambient databases but provide an initial set of data that could be used for this purpose.

Regardless of the modeling system (e.g. photochemical transport or Lagrangian puff model) used to estimate secondary impacts of ozone and/or PM<sub>2.5</sub>, model estimates should be compared to observation data to generate confidence that the modeling system is representative of the local and regional air quality. For ozone related projects, model estimates of ozone should be compared with observations in both time and space. For PM<sub>2.5</sub>, model estimates of speciated PM<sub>2.5</sub> components (such as sulfate ion, nitrate ion, etc.) should be matched in time and space with observation data in the model domain. Model performance metrics comparing observations and predictions are often used to summarize model performance. These metrics include mean bias, mean error, fractional bias, fractional error, and correlation coefficient (Simon et al., 2012). There are no specific levels of any model performance metric that indicate “acceptable” model performance. Model performance metrics should be compared with similar contemporary applications to assess how well the model performs (Simon et al., 2012).

Accepted performance standards for speciated and total PM<sub>2.5</sub> and ozone for photochemical models used in attainment demonstrations may not be applicable for single-source assessments. Since the emissions and release parameters for the project source are well known, a direct connection between general photochemical model performance and the ability of the modeling system to characterize the impacts of the project source would be difficult to make. It is important that any potential approaches for photochemical model performance for the purposes of single-source assessments for PSD and NSR use an approach that would be universally applicable to any single-source modeling system, which includes the Lagrangian models described above.

#### 4.4 Model performance evaluation data sources

Provided below is an overview of some of the various ambient air monitoring networks currently available that provide relevant data for model evaluation purposes. Network methods and procedures are subject to change annually due to systematic review and/or updates to the current monitoring network/program. Please note, there are other available monitoring networks which are not mentioned here and more details on the networks and measurements should be obtained from other sources.

AQS: The Air Quality System (AQS) is not an air quality monitoring network. However it is a repository of ambient air pollution data and related meteorological data collected by EPA, state, local and tribal air pollution control agencies from tens of thousands of monitors. AQS contains all the routine hourly gaseous pollutant data collected from State and Local Air Monitoring Stations (SLAMS) and National Air Monitoring Stations (NAMS) sites. SLAMS is a dynamic network of monitors for state and local directed monitoring objectives (e.g., control strategy development). A subset of the SLAMS network, the NAMS has an emphasis on urban and multi-source areas (i.e., areas of maximum concentrations and high population density). The AQS database includes criteria pollutant data (SO<sub>2</sub>, NO<sub>2</sub>, O<sub>3</sub>, and PM<sub>2.5</sub>) and speciation data of particulate matter (SO<sub>4</sub>, NO<sub>3</sub>, NH<sub>4</sub>, EC, and OC), and meteorological data. The data are

measured and reported on an hourly or daily average basis. An overview of the AQS can be found at <https://www.epa.gov/aqs>.

IMPROVE: The Interagency Monitoring of PROtected Visual Environments (IMPROVE) network began in 1985 as a cooperative visibility monitoring effort between EPA, federal land management agencies, and state air agencies (IMPROVE, 2000). Data are collected at Class I areas across the United States mostly at National Parks, National Wilderness Areas, and other protected pristine areas. Currently, there are approximately 160 IMPROVE rural/remote sites that have complete annual PM<sub>2.5</sub> mass and/or PM<sub>2.5</sub> species data. The website to obtain IMPROVE documentation and/or data is <http://vista.cira.colostate.edu/improve/>.

STN: The Speciation Trends Network (STN) began operation in 1999 to provide nationally consistent speciated PM<sub>2.5</sub> data for the assessment of trends at representative sites in urban areas in the U.S. The STN was established by regulation and is a companion network to the mass-based Federal Reference Method (FRM) network implemented in support of the PM<sub>2.5</sub> NAAQS. As part of a routine monitoring program, the STN quantifies mass concentrations and PM<sub>2.5</sub> constituents, including numerous trace elements, ions (sulfate, nitrate, sodium, potassium, ammonium), elemental carbon, and organic carbon. In addition, there are approximately 181 supplemental speciation sites which are part of the STN network and are SLAMS sites. The STN data at trends sites are collected 1 in every 3 days, whereas supplemental sites collect data either 1 in every 3 days or 1 in every 6 days. Comprehensive information on the STN and related speciation monitoring can be found at <https://www3.epa.gov/ttnamti1/speciepg.html>.

CASTNet: Established in 1987, the Clean Air Status and Trends Network (CASTNet) is a dry deposition monitoring network where data are collected and reported as weekly average data (U.S. EPA, 2002b). Relevant CASTNet data includes weekly samples of inorganic PM<sub>2.5</sub> species and ground-level ozone. More information can be obtained through the CASTNet website at <http://www.epa.gov/castnet/>.

SEARCH: The South Eastern Aerosol Research and CHaracterization (SEARCH) monitoring network was established in 1998 and is a coordinated effort between the public and private sector to characterize the chemical and physical composition as well as the geographical distribution and long-term trends of PM<sub>2.5</sub> in the Southeastern U.S. SEARCH data are collected and reported on an hourly/daily basis. Background information regarding standard measurement techniques/protocols and data retrieval can be found at <http://www.atmospheric-research.com/studies/SEARCH/index.html>.

NADP: Initiated in the late 1970s, the National Acid Deposition Program (NADP) monitoring network began as a cooperative program between federal and state agencies, universities, electric utilities, and other industries to determine geographical patterns and trends in precipitation chemistry in the U.S. NADP collects and reports wet deposition measurements as weekly average data (NADP, 2002). The network is now known as NADP/NTN (National Trends Network) and measures sulfate, nitrate, hydrogen ion (measure of acidity), ammonia, chloride, and base cations (calcium, magnesium, potassium). Detailed information regarding the NADP/NTN monitoring network can be found at <http://nadp.sws.uiuc.edu/>.

## 5 Illustrative example of near-field single-source impacts on O<sub>3</sub> and PM<sub>2.5</sub>

Photochemical grid models have been used with a variety of approaches to isolate secondary pollutant impacts from specific sources, including brute-force sensitivity (Baker and Kelly, 2014; Bergin et al., 2008; Kelly et al., 2015), direct decoupled method (DDM) (Baker and Kelly, 2014; Kelly et al., 2015), and source apportionment (Baker and Foley, 2011; Baker and Kelly, 2014). Here, downwind impacts of ozone and PM<sub>2.5</sub> are described for hypothetical single-sources placed in the Atlanta and Detroit metropolitan areas. These illustrative hypothetical single-source impacts are based on CMAQ model simulations done for two different urban areas using 4 km sized grid cells. Impacts are estimated on ozone and PM<sub>2.5</sub> from a hypothetical emissions source of SO<sub>2</sub>, NO<sub>x</sub>, and VOC using the brute-force sensitivity approach. The approach taken for this assessment is not intended to be a prescriptive approach recommended by this process or EPA. The emission rates used here are illustrative and do not have any policy or regulatory implications.

### 5.1 Model application approach for estimating these illustrative example single-source impacts

CMAQ version 5.0.1 ([www.cmaq-model.org](http://www.cmaq-model.org)) was applied for the entire year of 2007 to estimate PM<sub>2.5</sub> and ozone. Aerosol chemistry is based on the AERO6 option that includes ISORROPIAII inorganic partitioning and chemistry (Fountoukis and Nenes, 2007), aqueous phase chemistry that includes sulfur and methylglyoxal oxidation (Sarwar et al., 2013), and organic aerosol partitioning (Carlton et al., 2010). Gas phase chemistry is represented with the Carbon-Bond 05 gas phase chemical mechanism with toluene updates (Sarwar et al., 2011).

Two separate model domains were used covering the Detroit and Atlanta metropolitan areas with 4 km sized grid cells (Figure 5-1). The vertical domain extends to 50 mb using 25 layers (surface layer height is ~20 m) with most resolution in the boundary layer to capture important diurnal variation in mixing height. The Weather Research and Forecasting model (WRF), Advanced Research WRF core (ARW) model version 3.3 (Skamarock et al., 2008) was applied with a horizontal grid resolution of 4 km and 35 vertical layers. Additional details regarding photochemical and meteorological model application and evaluation are provided elsewhere (U.S. Environmental Protection Agency, 2013a, b).

Anthropogenic and biogenic emissions are processed for CMAQ input using the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system (<http://www.cmascenter.org/smoke/>). Stationary, point, and area sources are based on version 2 of the 2008 National Emissions Inventory (NEI) (U.S. Environmental Protection Agency, 2012b). Mobile source emissions are day-specific for the model simulation period based on data submitted to the NEI and generated with SMOKE-MOVES (<http://cmasceneter.org/smoke/>). Hourly WRF estimated solar radiation and temperature are input to the Biogenic Emission Inventory System (BEIS) version 3.14 to generate emissions estimates of speciated VOC and nitric oxide (Carlton and Baker, 2011). Hourly boundary inflow from a coarser domain covering the continental United States with 12 km sized grid cells account for emissions from sources outside the 4 km model domain.

In addition to the full set of anthropogenic and biogenic emissions for this model domain, new hypothetical emissions sources are added to illustrate single-source impacts on the Atlanta and Detroit

areas. VOC (Table 5-1) and NO<sub>x</sub> (90% NO and 10% NO<sub>2</sub>) speciation are based on average speciation profiles for non-EGU point sources in these areas. The location of the fictitious sources are shown in Figure 5-1. The same set of stack parameters were used for each fictitious source location: stack height 19 m, stack diameter 1.2 m, exit temperature 424 K, and exit velocity 14 m/s. Separate photochemical model simulations were done for each hypothetical source location and precursor emission rate: 100 tpy of VOC, 100 tpy of NO<sub>x</sub>, 100 tpy of SO<sub>2</sub>, 300 tpy of VOC, 300 tpy of NO<sub>x</sub> and 300 tpy of SO<sub>2</sub>. This resulted in a total of 6 simulations for 2 different hypothetical source locations or 12 total simulations with hypothetical sources in addition to 2 baseline simulations (1 for each area without any hypothetical source).

Table 5-1. Hypothetical source VOC speciation

<b>Carbon Bond Specie</b>	<b>Fraction</b>	<b>Carbon Bond Specie</b>	<b>Fraction</b>
ALD2	0.0152	MEOH	0.0054
ALDX	0.0155	NVOL	0.0008
ETH	0.0324	OLE	0.1143
ETHA	0.0094	PAR	0.4057
ETOH	0.0090	TERP	0.0170
FORM	0.0757	TOL	0.1148
IOLE	0.0088	UNR	0.1080
ISOP	0.0007	XYL	0.0674

## 5.2 Illustrative single-source impact results for O<sub>3</sub> and PM<sub>2.5</sub>

Annual maximum 24-hr average PM<sub>2.5</sub> sulfate ion impacts are shown spatially in Figure 5-1 and by distance from the source in Figure 5-2 for hypothetical sources emitting 100 and 300 tpy of SO<sub>2</sub> in the Detroit and Atlanta areas. Impacts are generally highest nearest the source and decrease as distance from the source increases. However, visual examination of the spatial extent of maximum concentrations for each source shows that peak secondary impacts are not always coincident with the location of the emissions release. Occasional increases in downwind secondary impacts are generally related to single-source precursor emissions reaching an area of increased oxidant availability, neutralizing agents, differences in terrain, mixing layer, or some combination of these influences.

The magnitudes and patterns of downwind impacts vary between these two areas and even within areas. This is likely due to differences in terrain features, available oxidants, and neutralizing chemicals such as ammonia. Different magnitudes and spatial patterns between these different source locations are more evident when looking at maximum 24-hr impacts compared to annual average. Maximum impacts tend to be dominated by conducive meteorology and nearby chemical environment on fewer days compared to the longer term average impacts, which is expected.

Figure 5-1. Annual maximum 24-hr PM<sub>2.5</sub> sulfate ion impacts from a hypothetical source emitting 100 and 300 tpy of SO<sub>2</sub> at a location in Atlanta (top row) and Detroit (bottom row).

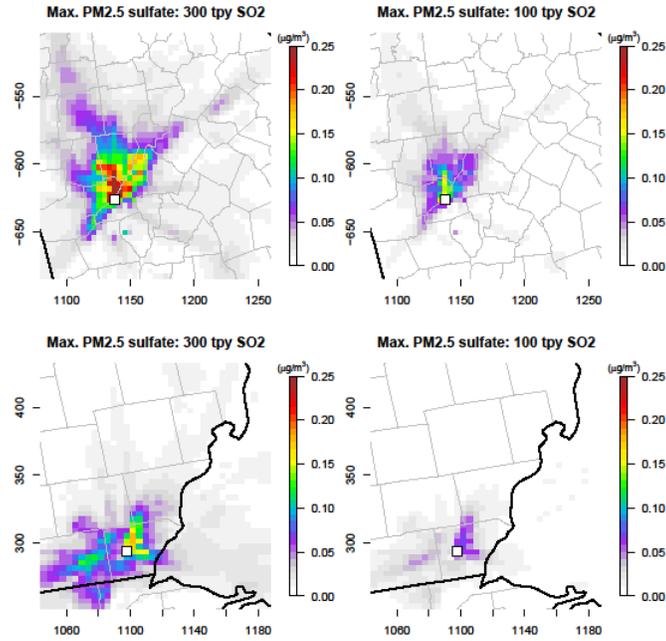
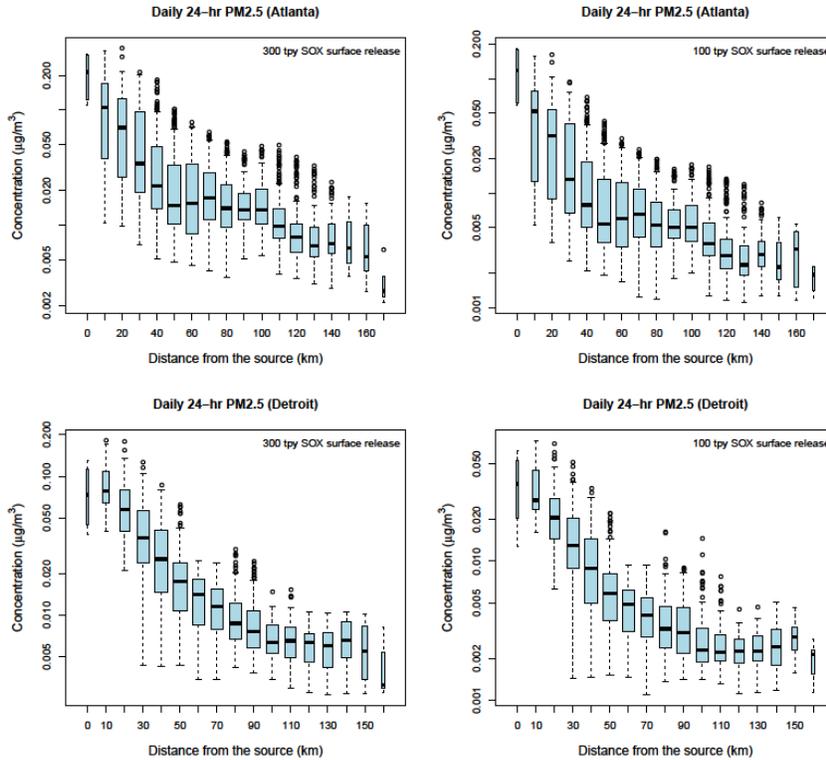


Figure 5-2. Maximum 24-hr PM<sub>2.5</sub> sulfate ion impacts from a hypothetical source emitting 100 and 300 tpy of SO<sub>2</sub> at a location in Atlanta (top row) and Detroit (bottom row) by distance from the source.



Daily maximum 8-hr O<sub>3</sub> impacts over all days in the ozone season are shown as a function of distance from the hypothetical source emitting NO<sub>x</sub> in Figure 5-3 and spatially in Figure 5-4. Similar information is provided in Figures 5-5 and 5-6 for hypothetical source emissions of VOC. Ozone impacts tend to be highest in grid cells adjacent to the hypothetical source and contributions generally decrease as distance from the source increases. Emissions of nitrogen oxides are concentrated enough in the 4 km grid cell containing the source that titration often dominates over production in that grid cell. For these particular urban areas and VOC emission mixtures, the hypothetical sources emitting NO<sub>x</sub> emissions tended to form more O<sub>3</sub> compared to when emitting similar amounts of VOC emissions. Ozone from the hypothetical source placed in Detroit shows notable impacts over Lake Erie. This is more prominent for the scenario of VOC emissions rather than NO<sub>x</sub> emissions. It is possible that VOC from this hypothetical source encounters a favorable combination of available NO<sub>x</sub> emissions from commercial marine sources and low boundary layer heights resulting in larger downwind O<sub>3</sub> contribution than in other directions from the hypothetical source.

Figure 5-3. Distribution of ozone season highest daily 8-hr maximum O<sub>3</sub> by distance from the hypothetical source NO<sub>x</sub> emissions at a location in Atlanta (top row) and Detroit (bottom row).

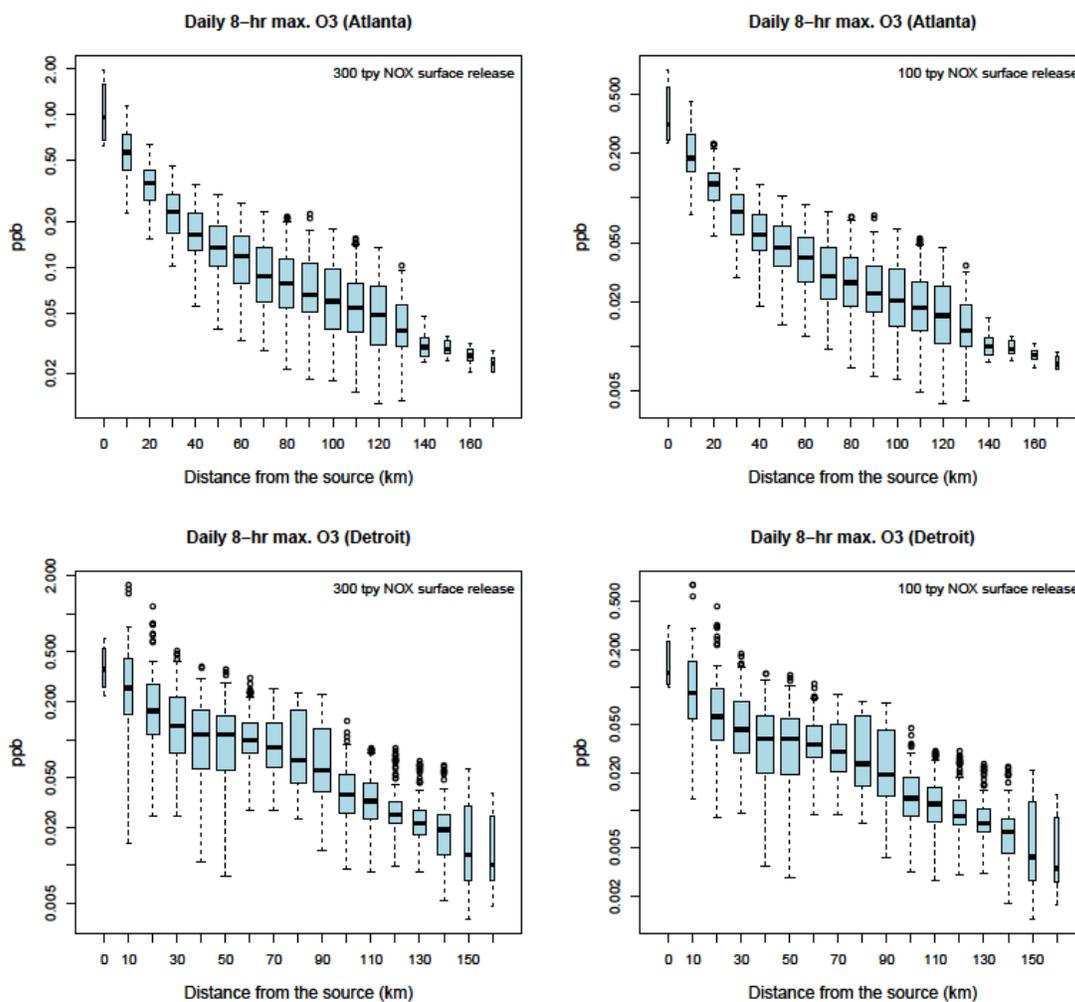


Figure 5-4. Spatial plot of ozone season highest daily 8-hr maximum O<sub>3</sub> from the hypothetical source NO<sub>x</sub> emissions at a location in Atlanta (top row) and Detroit (bottom row).

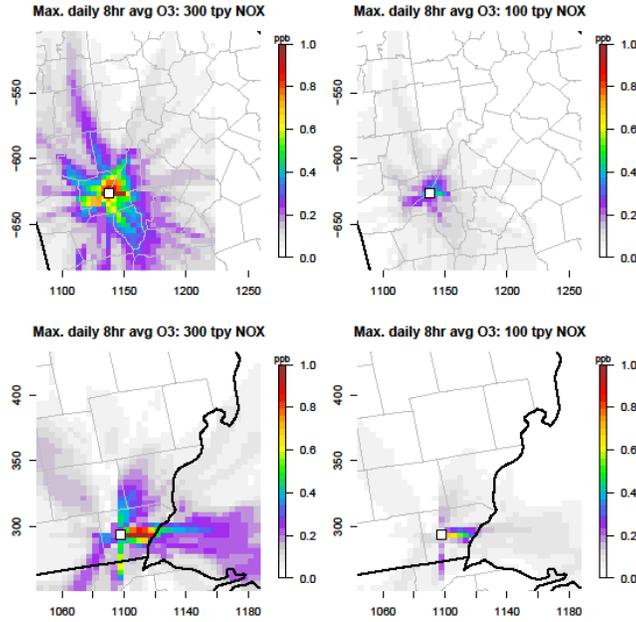


Figure 5-5. Distribution of ozone season highest daily 8-hr maximum O<sub>3</sub> by distance from the hypothetical source VOC emissions at a location in Atlanta (top row) and Detroit (bottom row).

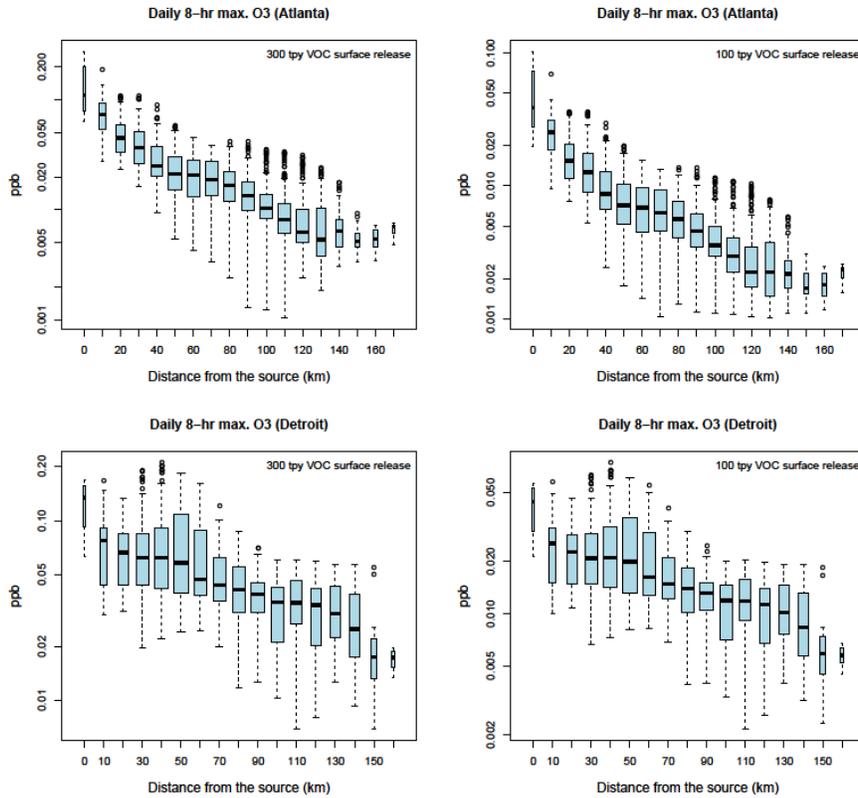
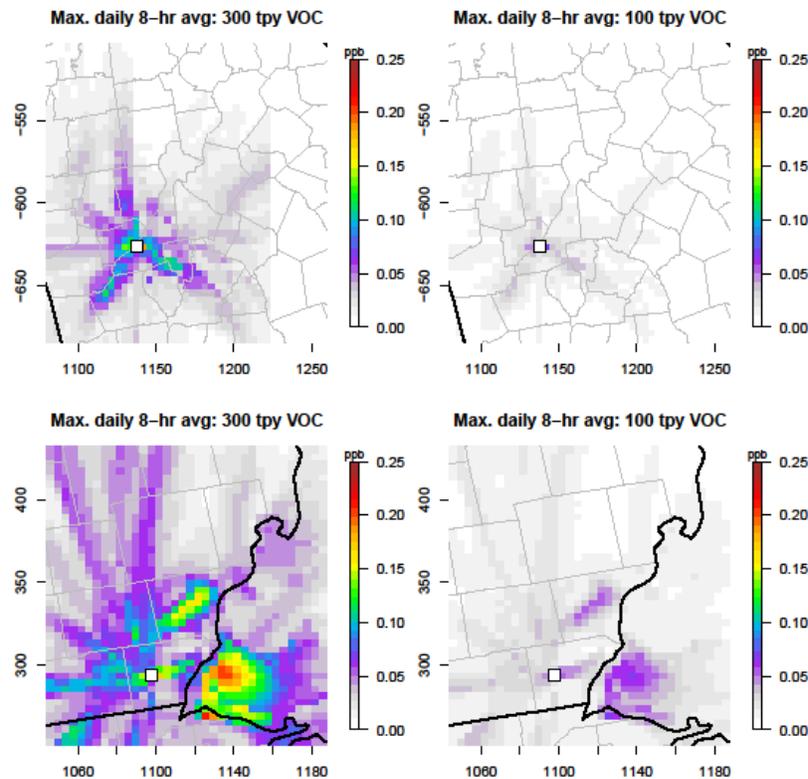


Figure 5-6. Spatial plot of ozone season highest daily 8-hr maximum O<sub>3</sub> from the hypothetical source VOC emissions.



## 6 Review of published single-source impacts on O<sub>3</sub> and PM<sub>2.5</sub>

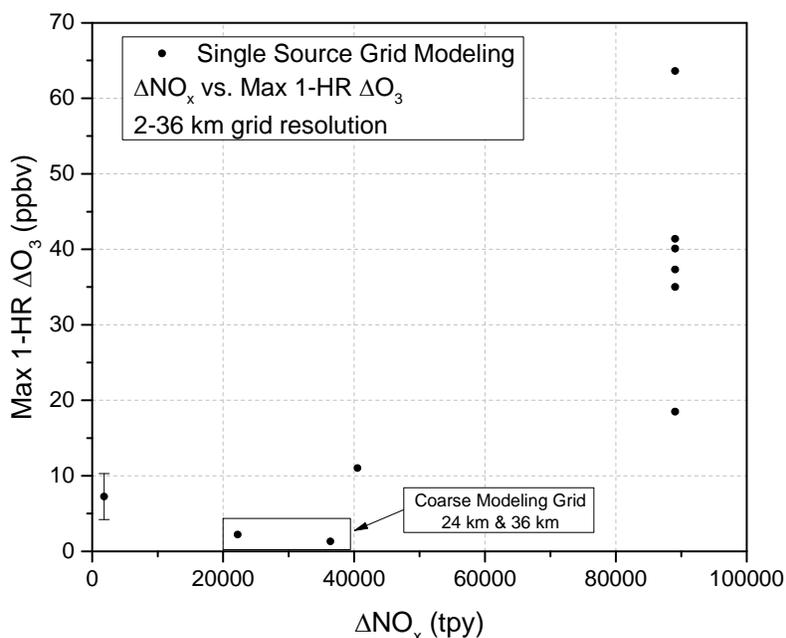
Published literature between 2005 and 2015 relating single-source emissions with downwind O<sub>3</sub> and secondary PM<sub>2.5</sub> impacts has been collected and summarized. This information reflects currently understood relationships between precursors and secondary pollutants and provides context for future model applications. The assessments reviewed here may not reflect every study done between 2005 and 2015. The primary criteria for inclusion in this report is a published study that presents both the emissions rate of a specific source and downwind impacts on O<sub>3</sub> or secondary PM<sub>2.5</sub> from that same source. While these published studies provide useful information, additional assessments of single-source impacts on secondary pollutants are still needed to provide a more comprehensive assessment of different source types and source environments.

### 6.1 Single-source ozone impacts

Figure 6-1 presents the results from studies that quantified the 1-hr average maximum downwind O<sub>3</sub> from a single-source NO<sub>x</sub> emissions perturbation using photochemical grid models (Baker et al., 2015). Figure 6-2 shows the results from studies that quantified single-source downwind 8-hr average O<sub>3</sub> impacts (Baker et al., 2015). For the studies estimating downwind 1-hr O<sub>3</sub> contributions, there appears

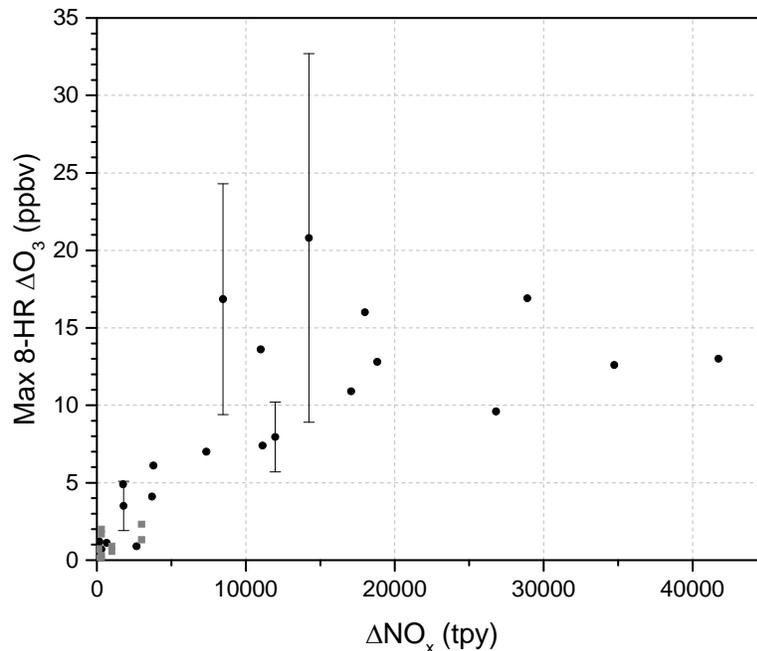
to be no clear pattern between  $\text{NO}_x$  emissions and maximum downwind  $\text{O}_3$ . A relationship is not evident even if results from studies with coarser model resolution (24 km, 36 km;  $N=2$ ) are removed. However, Figure 6-2 shows a clearer relationship between  $\text{NO}_x$  emissions and 8-hr  $\text{O}_3$ . This may be due to the longer averaging time smoothing out some of the conditions that cause high variability in the 1-hr results. Another explanation for the notable relationship between emissions and secondary impacts for 8-hr  $\text{O}_3$  is that most of the elements in Figure 6-2 are from a single publication (ENVIRON, 2012a) that presented multiple source-impact relationships, meaning the consistent relationships are likely due to consistent model application and post-processing for each modeled source. Overall, peak 8-hr average  $\text{O}_3$  impacts reported in literature range up to 33 ppbv, which is a reported impact modeled from a large  $\text{NO}_x$  source ( $\sim 14,000$  tpy) over multiple high ozone episodes in the Louisiana/eastern Texas area (ENVIRON, 2005) using 4 km grid resolution. The results for single-source VOC releases show notable variability in maximum downwind  $\text{O}_3$  impacts due to large differences in ozone forming potential and OH reactivity of the VOC released (ENVIRON, 2005).

Figure 6-1. Published single-source  $\text{NO}_x$  emissions impacts on downwind hourly  $\text{O}_3$  estimated using photochemical grid modeling.



Publications reporting results from observational field studies provide additional context to the model-based studies for ozone production from point source emissions (Luria et al., 2003; Ryerson et al., 2001; Springston et al., 2005; Zhou et al., 2012). In these studies, in-plume observations related to specific sources were collected with aircraft and the sources examined were either power plants or petrochemical facilities publications (Luria et al., 2003; Ryerson et al., 2001; Springston et al., 2005; Zhou et al., 2012). Many of these studies focused on quantifying ozone production efficiency from precursor emissions and typically did not provide key information to discern a relationship between source emissions and downwind  $\text{O}_3$  impacts: a well-defined  $\Delta\text{O}_3$  (in plume  $\text{O}_3$  minus an estimate of ambient background  $\text{O}_3$ ) and facility precursor emissions. In some instances the study did not isolate impacts from a single facility plume but looked at some aggregate of nearby sources.

Figure 6-2. Published single-source NO<sub>x</sub> emissions impacts on downwind 8-hr average O<sub>3</sub> estimated using photochemical grid modeling.



One observation-based study analyzed data from a field campaign that sampled plumes via helicopter downwind of the Tennessee Valley Authority Cumberland power plant on four summer days in 1998 and 1999 (Luria et al., 2003). These four days represented different NO<sub>x</sub> emissions rates and meteorology. Three of the four days were conducive to ozone production, with one day having cooler temperatures where no positive delta-O<sub>3</sub> was observed at the farthest measured distance downwind. The three days with positive delta-O<sub>3</sub> reported the following maximum observed hourly delta-O<sub>3</sub> and corresponding NO<sub>x</sub> emissions: 36 ppb O<sub>3</sub> (140,643 TPY NO<sub>x</sub>), 39 ppb O<sub>3</sub> (71,697 TPY NO<sub>x</sub>), and 24 ppb O<sub>3</sub> (115,681 TPY NO<sub>x</sub>). While these NO<sub>x</sub> emissions rates are generally higher than those of most of the modeling studies reported in Figure 6-1 (1-hr O<sub>3</sub>), the measured change in O<sub>3</sub> appears to be in reasonable agreement with modeled estimates compiled from studies published in literature. Also, these are likely not maximum plume impacts since these measurements are transects that only sampled some portion of the plume in space and time.

## 6.2 Single-source PM<sub>2.5</sub> impacts

A number of studies examined the effect of regional scale emissions on PM<sub>2.5</sub> concentrations (Simon et al., 2012). Fewer studies have attempted to quantify the effects of single-sources on downwind PM<sub>2.5</sub> concentrations, and fewer still that report estimated secondary PM<sub>2.5</sub> enhancements from these single-sources (Baker and Foley, 2011; Baker and Kelly, 2014; ENVIRON, 2012a; National Association of Clean Air Agencies, 2011). Synthesizing the results of these limited studies is difficult due to differences in modeling (e.g., averaging timescales, PM<sub>2.5</sub> species reported, etc), geographic area, emission profile and rates, stack height, near-source and regional NH<sub>3</sub> availability, and meteorology. Here, we summarize

four studies which provide sufficient information on precursor emissions and secondary PM<sub>2.5</sub> enhancements from single-sources.

The NACAA Workgroup Final Report (National Association of Clean Air Agencies, 2011) provided a test case where PM<sub>2.5</sub> impacts from different sources are assessed. The Minnesota case study presented predicted PM<sub>2.5</sub> ammonium sulfate and ammonium nitrate from a full photochemical grid model simulation (CAMx) applied at 12 km grid resolution with sub-grid plume treatment and 200 m sub-grid plume sampling (National Association of Clean Air Agencies, 2011). Four individual stacks over Minnesota were chosen to reflect varying emission scenarios and background conditions. Emissions ranged from 400 to 13,000 tpy NO<sub>x</sub> and 500 to 15,000 tpy SO<sub>2</sub>, each with varying stack height. In these case study simulations all precursor emissions are co-emitted by each source (National Association of Clean Air Agencies, 2011). Over all cases, 24-hour maximum 98th percentile concentrations of secondary formation PM<sub>2.5</sub> accounted for up to 1 µg/m<sup>3</sup>. These sources had stack release points well above ground level and had surface level peak impacts typically within 10 km of the source.

One published approach (Baker and Foley, 2011) use Particulate Matter Source Apportionment Technology (PSAT) applied with CAMx using 12 km grid resolution to estimate annual average secondarily formed PM<sub>2.5</sub> sulfate and nitrate from precursor emissions. The study selected facilities representing the top 5% emitters of primary PM<sub>2.5</sub>, NO<sub>x</sub>, and SO<sub>x</sub> from all stationary point sources located east of -97° longitude over midwest, mid-Atlantic, and southeast modeling domains (NO<sub>x</sub> >7000 tpy, SO<sub>x</sub> >20,000 tpy, and PM<sub>2.5</sub> > 1100 tpy based on 2005 inventory). This study showed maximum annual average PM<sub>2.5</sub> values of 0.385 µg/m<sup>3</sup> and 0.018 µg/m<sup>3</sup> for PM<sub>2.5</sub> sulfate ion and PM<sub>2.5</sub> nitrate ion respectively. Impacts were typically highest nearest the source and decrease as distance from the source increases (Baker and Foley, 2011).

Secondary PM<sub>2.5</sub> was estimated for the Hunter EGU emitting 18,800 tpy of NO<sub>x</sub> and 7,300 tpy of SO<sub>2</sub> in eastern Utah (ENVIRON, 2012). The CAMx model was applied with PSAT at 12 km resolution for an entire year. Predicted 24-hour (annual) maximum values were 3.44 µg/m<sup>3</sup> (0.11 µg/m<sup>3</sup>) and 0.53 µg/m<sup>3</sup> (0.05 µg/m<sup>3</sup>) of PM<sub>2.5</sub> nitrate ion and PM<sub>2.5</sub> sulfate ion respectively. Again, the highest secondary PM<sub>2.5</sub> impacts tended to be closest to the source (ENVIRON, 2012).

A case-study examined the impact of a single EGU on downwind O<sub>3</sub> and PM<sub>2.5</sub> sulfate ion using several photochemical grid model-based source impact assessment approaches applied with the CMAQ model: brute force emission adjustments, DDM, and PSAT (Baker and Kelly, 2014). This case study examined emissions from the TVA Cumberland facility located in western Tennessee (48,000 tpy NO<sub>x</sub>, 8,300 tpy SO<sub>2</sub>) during a high pollution episode focusing on July 6, 1999. Maximum modeled enhancements range up to 1.5 µg/m<sup>3</sup> of PM<sub>2.5</sub> sulfate ion. The different approaches for estimating single-source impacts generally have similar spatial patterns.

## 7 Reduced-form approaches for estimating single-source secondary impacts

Predicting downwind secondary pollutant concentrations from point source emissions necessitates accounting for the interaction of the plume with ambient levels of oxidants, neutralizing agents, meteorology and potential nonlinear chemistry. State-of-the-science approaches involve employing photochemical transport models like CMAQ and CAMx. There have been recent efforts to develop reduced-form models that maintain the state of the science approach at their base, but provide a

screening tool that is faster and cheaper to use. Ideally, screening level information would be an approximation of secondary impacts based on photochemical modeling of the single-source, to take advantage of the state of the science treatment of multi-phase chemistry and deposition. This includes a realistic chemical and physical environment for single-source impacts (Baker and Kelly, 2014).

## 7.1 Review of reduced-form approaches for estimating O<sub>3</sub> single-source impacts

One example of a reduced-form O<sub>3</sub> modeling approach that incorporates a state of the science chemical transport model at its foundation has been identified. This approach was developed for the New South Wales (NSW) Greater Metropolitan Region in Australia (Yarwood et al., 2011). Briefly described, the Australian NSW approach involves a photochemical modeling analysis performed for several ozone seasons that includes hypothetical new emissions sources tracked using the higher order Decoupled Direct Method (HDDM) (Dunker et al., 2002) to calculate sensitivity coefficients for O<sub>3</sub> to the additional of NO<sub>x</sub> and VOC emissions from the new hypothetical sources. The resulting O<sub>3</sub> sensitivity coefficients then allow O<sub>3</sub> impacts to be estimated for other NO<sub>x</sub> and/or VOC sources within the same metropolitan area (Yarwood et al., 2011). While new sources or sources making modifications may not match the exact location, stack release characteristics, or emissions rates of the hypothetical sources in that analysis, options exist to pick the modeled source that best matches the new or modified source or even choose the highest impact from any of the modeled sources as a conservative approach. An existing set of relationships between modeled impacts and precursor emissions are sometimes referred to as Modeled Emission Rates for Precursors (MERPs). MERPs are a Tier 1 demonstration tool and provide a simple way to relate maximum downwind impacts with a critical air quality threshold. MERPs are intended to relate a specific precursor to regulated pollutant and are not intended to provide a single demonstration for all NAAQS pollutants. For example, separate MERPs will relate VOC to O<sub>3</sub>, NO<sub>x</sub> to O<sub>3</sub>, SO<sub>2</sub> to secondary PM<sub>2.5</sub>, and NO<sub>x</sub> to secondary PM<sub>2.5</sub>.

## 7.2 Review of reduced-form approaches for estimating PM<sub>2.5</sub> single-source impacts

Simplified techniques for secondary PM<sub>2.5</sub> include the emissions divided by distance metric (Q/D) and the 100% conversion assumption. For the Q/D metric, allowable total emissions (Q) in tons per year are divided by distance to key receptors (D). This approach allows for a relative comparison of a variety of sources, but does not directly relate emission to concentrations for comparison to regulatory impact levels nor does it account for the variability in secondary PM<sub>2.5</sub> formation. Under the 100% conversion assumption, NO<sub>x</sub> and SO<sub>2</sub> emissions are assumed to convert entirely to ammonium nitrate and ammonium sulfate. A modeling study conducted with multiple case studies found that the 100% conversion approach was overly conservative, yielding physically unrealistic estimates (National Association of Clean Air Agencies, 2011).

One approach (Baker and Foley, 2011) developed a nonlinear regression model relating large single-source emissions over the eastern United States (N=99) to predicted annual average primary and secondarily formed PM<sub>2.5</sub> sulfate and nitrate as a function of emissions and distance. Individual regression models are developed for primary PM<sub>2.5</sub>, PM<sub>2.5</sub> sulfate ion, PM<sub>2.5</sub> nitrate ion under favorable conditions, and PM<sub>2.5</sub> nitrate ion under unfavorable conditions (Baker and Foley, 2011). This approach, a more physically realistic improvement to the Q/D approach, could be used to develop shorter-timescale (e.g., 24-hr), region- and season-specific regression models of PM<sub>2.5</sub>. This nonlinear regression approach has been applied to facilities in other countries to provide information about the downwind long term impacts of large point sources (Myllyvirta, 2014).

Inter-pollutant offset ratios have been used to estimate secondary PM<sub>2.5</sub> formation from single-source SO<sub>2</sub> and NO<sub>x</sub> emissions. In the case study of 4 EGUs in Minnesota described above, (National Association of Clean Air Agencies, 2011) estimate primary PM<sub>2.5</sub> concentrations using AERMOD, then secondary concentrations were either added from CAMx results or using standard SO<sub>2</sub> and NO<sub>x</sub> to primary PM<sub>2.5</sub> offset ratios in EPA's New Source Review implementation rule for PM<sub>2.5</sub> (73 FR 28321). The report concludes standard offset ratios lead to an over prediction of secondary PM<sub>2.5</sub> and suggest a downward revision of offset ratios for the region. The report suggests new studies could be conducted to develop region, and season-specific offsets for use in the regulatory permitting context if that approach is used.

The photochemical grid model CAMx was used to examine the effects of distance, season, grid resolution, emission rate and stack height on predicted offset ratios for the Port Washington coal-fired power plant in Georgia (Boylan and Kim, 2012). The study suggests maximum ratios for this facility are found near the source and vary most strongly with season and distance from the source. More recent work (Boylan and Kim, 2014) expanded on that study to investigate the spatial variability in seasonal offset ratios by modeling Port Washington emissions at 8 different locations in Georgia. Offset ratios varied by up to a factor of 7 as a function of season or location, illustrating the sensitivity of secondary PM<sub>2.5</sub> formation on meteorology and the local chemical environment.

Several of the studies reviewed presented promising techniques for developing regional scale reduced-form models to predict the impact of single-sources on secondary pollutants. These approaches ranged from region-specific ratios to more advanced regression models. Generalizing these techniques for areas not included in the original assessment is a difficult challenge but will be desired by many in the regulating and regulated communities. A Tier 1 demonstration tool as described in the 2015 proposed revision to the Guideline for Air Quality Modeling (Appendix W) consists of technically credible air quality modeling done to relate precursor emissions and peak secondary pollutant impacts from specific or hypothetical sources. Permit applicants should provide a narrative explanation describing how project source post-construction emissions relate to the information provided as part of the Tier 1 demonstration tool. It should be made clear how the chemical and physical environments modeled as part of an existing set of information included in the Tier 1 demonstration tool are relevant to the area of the source and key receptors. The existing set of relationships between modeled impacts and precursor emissions are also sometimes referred to as Modeled Emission Rates for Precursors (MERPs). MERPs are a generic term for a Tier 1 demonstration tool based on existing credible air quality modeling that meets the requirements in the 2015 revision to the Guideline for Air Quality Modeling (Appendix W). MERPs provide a simple way to relate maximum downwind impacts with a critical air quality thresholds.

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