UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
RESEARCH TRIANGLE PARK, NC 27711

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OFFICE OF
AIR QUALITY PLANNING
AND STANDARDS

MEMORANDUM

SUBJECT: Use of Photochemical Grid Models for Single-Source Ozone and secondary $PM_{2.5}$ impacts for Permit Program Related Assessments and for NAAQS Attainment Demonstrations for Ozone, $PM_{2.5}$ and Regional Haze

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TO: EPA Regional Modeling Contacts

The EPA recently revised the *Guideline on Air Quality Modeling*, also referred to as Appendix W or the *Guideline*, to recommend a two tiered screening approach for permit related program demonstrations rather than establishing a single preferred model (U.S. Environmental Protection Agency, 2017). As detailed in Section 5 of the *Guideline*, both of these tiers involves the use of chemical transport models (*e.g.*, photochemical grid models). The recommended approach for Tier 1 demonstrations would utilize such models to provide sensitivity estimates (either through existing modeling work or new projects) of responsiveness to precursor emissions in developing screening tools or methods (U.S. Environmental Protection Agency, 2016a). The recommended approach for Tier 2 demonstrations would directly utilize such models to estimate the impacts of the new or modifying sources (U.S. Environmental Protection Agency, 2016b). As stated in the preamble to the 2017 revisions (U.S. Environmental Protection Agency, 2017),the EPA believes that use of photochemical models for such purposes is scientifically appropriate and practical to implement. The purpose of this memorandum is to provide an alternative model demonstration for specific photochemical transports models establishing their fit for purpose in PSD compliance demonstrations for ozone and $PM_{2.5}$ and in NAAQS attainment demonstrations for ozone, $PM_{2.5}$ and Regional Haze.[1] This document provides for their general applicability; however, it does not replace the need for such demonstrations to provide model protocols describing model application choices or the evaluation of model inputs and baseline predictions

[1] These specific photochemical models are the Comprehensive Air Quality Model with Extensions (CAMx) and the Community Multiscale Air Quality (CMAQ).

against measurements relevant for their specific use by permit applicants and state, local, tribal air agencies.

Photochemical grid models have been used extensively for decades to support both scientific and regulatory air quality assessments for primary and secondarily formed pollutants. These models have been traditionally applied to support urban to continental scale multi-source assessments but have increasingly been used to understand air quality impacts from specific sectors and sources. The United States Environmental Protection Agency (US EPA) has used photochemical grid models to support interstate transport rules including Clean Air Interstate Rule (U.S. Environmental Protection Agency, 2005b), Cross-State Air Pollution Rule (U.S. Environmental Protection Agency, 2011a); criteria pollutant impacts of the Mercury and Air Toxics Standard (U.S. Environmental Protection Agency, 2011c); reviews of National Ambient Air Quality Standard (U.S. Environmental Protection Agency, 2014c); and federal rulemakings related to the mobile sources (U.S. Environmental Protection Agency, 2011b, 2014a). US EPA has used photochemical grid models to provide generalized relationships about precursor emissions from specific emissions sectors (*e.g.* pulp & paper, residential wood combustion, coke ovens, electric arc furnaces, etc.) to model estimated ozone and $PM_{2.5}$ and subsequent health benefit analysis (Fann et al., 2012). State and local agencies have used photochemical grid models to support NAAQS attainment demonstrations for non-attainment areas, Regional Haze rule reasonable progress demonstrations, county-specific contribution analysis to support nonattainment area proposals (U.S. Environmental Protection Agency, 2012), source impacts for exceptional events demonstrations (Kansas Department of Health and Environment, 2012), and single-source related demonstrations (ENVIRON, 2005).

The *Guideline on Air Quality Modeling* outlines multiple criteria that need to be satisfied to provide a satisfactory alternative model demonstration that the modeling system is fit for the purpose of supporting permit related program technical demonstrations or NAAQS attainment demonstration plans (U.S. Environmental Protection Agency, 2005a, 2015). For situations where there is no EPA preferred model, Section 3.2.2(e) includes specific elements which are listed below.

1) The model or technique has received a scientific peer review;
2) The model or technique can be demonstrated to be applicable to the problem on a theoretical basis;
3) The databases which are necessary to perform the analysis are available and adequate;
4) Appropriate performance evaluations of the model or technique have shown that the model or technique is not inappropriately biased for regulatory application; and
5) A protocol on methods and procedures to be followed has been established.

The remainder of this memorandum provides information about the Comprehensive Air Quality Model with Extensions (CAMx) (ENVIRON, 2016) and the Community Multiscale Air Quality

(CMAQ) (Byun and Schere, 2006) model systems relevant for each of these elements. This document is not intended to provide a demonstration for the appropriateness of other chemical transport models to support single source permit program related assessments nor NAAQS attainment demonstrations.

Element 1: Peer Review

Publicly available and documented Eulerian photochemical grid models such as the Comprehensive Air Quality Model with Extensions (CAMx) (ENVIRON, 2016) 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 ozone, $PM_{2.5}$, and regional haze (Chen et al., 2014; Civerolo et al., 2010; Russell, 2008; Tesche et al., 2006).

Both modeling systems are open source and freely available on the internet, have full documentation, and have been peer-reviewed. Information about the location of the freely available code and documentation is provided in the table below.

Acronym	**Name**	**Internet location for source code and documentation**
CAMx	Comprehensive Air Quality Model with eXtensions	http://www.camx.com
CMAQ	Community Multiscale Air Quality Model	http://www.epa.gov/cmaq

The Comprehensive Air Quality Model with extensions (CAMx) has been extensively peer-reviewed for estimating O_3 and $PM_{2.5}$ (Boylan and Russell, 2006; Morris et al., 2006; Nopmongcol et al., 2012; Tesche et al., 2006). Further, the modeling system has been peer reviewed specifically toward estimating the impacts of single sources on secondary pollutants (Baker and Foley, 2011; Baker et al., 2014; Baker et al., 2015).

The Community Multiscale Air Quality (CMAQ) model has also been extensively peer-reviewed for estimating O_3 and $PM_{2.5}$ (Appel et al., 2012; Appel et al., 2017; Foley et al., 2010). The CMAQ modeling system has also been peer-reviewed for application of estimating single source impacts on secondary pollutants (Baker and Kelly, 2014; Baker and Woody, 2017; Bergin et al., 2008; Zhou et al., 2012).

Element 2: Theoretically Applicable

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). Photochemical models have been used to support single source assessments for O_3 and secondary $PM_{2.5}$ and also to support NAAQS attainment demonstrations for O_3 and $PM_{2.5}$ and reasonable progress demonstrations for the Regional Haze Rule.

Single Source Permit Related Assessments

Photochemical 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). Since $PM_{2.5}$ and O_3 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. Photochemical grid models including CAMx and CMAQ appropriately treat single source impacts on O_3 and secondarily formed $PM_{2.5}$ because these modeling systems include emissions from all source sectors and treat the subsequent chemical and physical fate of pollutants using gas, aerosol, and aqueous phase chemistry and wet and dry deposition processes. The approaches used to model these chemical and physical processes are based on state of the science (Seinfeld and Pandis, 2012). In addition to characterizing the physical and chemical evolution of plumes from specific sources, these models provide a realistic 3D chemical and physical environment for these plumes so that when these plumes interact with the surrounding environment secondary formation of pollutants such as O_3 and $PM_{2.5}$ can take place (Baker and Kelly, 2014; Baker and Woody, 2017; Kelly et al., 2015).

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. Even though single source emissions are injected into a grid volume, photochemical transport models have been shown to capture single source impacts when compared with downwind in-plume measurements (Baker and Kelly, 2014; Baker and Woody, 2017; Zhou et al., 2012). Specific to single-source applications for PSD, near-source in-plume aircraft based measurement field studies provide an approach for evaluating model estimates of (near-source) downwind transport and chemical impacts from single stationary point sources (ENVIRON, 2012). Photochemical grid model source apportionment and source sensitivity simulation of a single source downwind impacts compare well against field study primary and secondary ambient measurements (*e.g.* O_3) made in Tennessee and Texas

(ENVIRON, 2012). This work indicates photochemical grid models and source apportionment and source sensitivity approaches provide meaningful estimates of single source impacts. Assessments comparing photochemical grid model estimates of single source impacts with ambient measurements do not show a systematic tendency toward over-estimation (Baker et al., 2014; Baker and Kelly, 2014; Baker and Woody, 2017; ENVIRON, 2012; Zhou et al., 2012).

Where set up appropriately for the purposes of assessing the contribution of multiple or 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) and source apportionment (how 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 removed from the simulation (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 $PM_{2.5}$ (Baker and Foley, 2011; Baker and Kelly, 2014; Baker and Woody, 2017). DDM has also been used to estimate O_3 and $PM_{2.5}$ 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; Baker and Woody, 2017; 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; Baker and Woody, 2017) show generally similar downwind spatial gradients and impacts.

NAAQS Attainment Demonstration Assessments

Photochemical transport models have been used extensively to support State Implementation Plans (SIPs) 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). Both CMAQ and CAMx have been used extensively to estimate O_3 and both primary and secondarily formed $PM_{2.5}$ on local to continental scales (Appel et al., 2012; Appel et al., 2017; Byun and Schere, 2006; Cai et al., 2011; Foley et al., 2010; Morris et al., 2006; Pun et al., 2007; Russell, 2008; Simon et al., 2012; Tesche et al., 2006). Both modeling systems contain chemistry and physics designed for the purposes of estimating O_3 and $PM_{2.5}$ based on precursor emissions, transport, chemical evolution, and physical removal processes.

Some examples of the use of photochemical models to support SIPs include:

- The California Air Resources Board used CMAQ to support a $PM_{2.5}$ attainment demonstration for the San Joaquin Valley: http://www.valleyair.org/Air_Quality_Plans/docs/PM25-2015/2015-PM2.5-Plan_Bookmarked.pdf
- Alaska used CMAQ as part of a $PM_{2.5}$ Impracticability Demonstration for Fairbanks: http://dec.alaska.gov/air/anpms/comm/fbks_pm2-5_moderate_SIP.htm
- The South Coast Air District in southern California used the CMAQ model to support a $PM_{2.5}$ attainment demonstration and to project 8-hr O3 design values: http://www.aqmd.gov/docs/default-source/clean-air-plans/air-quality-management-plans/2012-air-quality-management-plan/final-2012-aqmp-(february-2013)/appendix-v-final-2012.pdf
- LADCO used the CAMx model to support an O_3 attainment demonstration for Chicago: http://www.ladco.org/reports/ozone/post08/LADCO%20Ozone%20TSD%20FINAL%20(Feb%203%202017).pdf
- The state of Georgia applied CMAQ to support a technical demonstration of the Regional Haze Rule: https://epd.georgia.gov/air/sites/epd.georgia.gov.air/files/related_files/document/appendixd.pdf

Element 3: Databases for Application

EPA works to continually develop photochemical grid model platforms that generally support both CMAQ and CAMx systems. These platforms are regularly updated and tend to follow the cycle of updates to the National Emission Inventory and include gridded hourly meteorology inputs for a baseline meteorology year, gridded hourly emissions from all source types matching the meteorological year, and projected future year emissions to support potential rulemakings, and sets of initial and boundary conditions. These platforms are regularly distributed to multi-jurisdictional organizations and also to specific interested groups or organizations interested in using the EPA model platform as a starting point for scientific assessments and regulatory demonstrations. EPA also makes scripts and inputs for processing emissions publically available so that other groups can reprocess emissions for different grid projections, subsets of the modeling domain, or with updated spatial, temporal, or speciation allocations appropriate for their specific application. Further, the meteorological and photochemical model simulations done to support these periodic modeling platforms are compared with ambient data and broad model performance evaluations are available. An example platform evaluation is the technical support document for the 2011 EPA modeling platform used for the Cross State Air Pollution Rule update (U.S. Environmental Protection Agency, 2016d).

In addition to data being available from EPA, other organizations have made photochemical model inputs and outputs (i.e, model platform) freely available to interested users. For instance, model-ready inputs for both CAMx and CMAQ for the entire year of 2011 are available at http://views.cira.colostate.edu/tsdw/. Further, multi-jurisdictional organizations typically either have existing photochemical grid model inputs or can direct those interested to other groups/organizations in the same region that may have suitable data. A brief list of multi-jurisdictional organizations with experience in the application of photochemical grid models such as CMAQ and CAMx is provided in the table below with an internet location for more information about that organization including contacts. The appropriateness of any data for a specific regulatory demonstration necessitate the development of a modeling protocol and agreement by the regulating authority.

Organization	**Region of the country**	**Internet site**
CENSARA	Central U.S.	http://www.censara.org
LADCO	Upper Midwest	http://www.ladco.org
MARAMA	Mid-Atlantic	http://www.marama.org
NESCAUM	Northeast U.S.	http://www.nescaum.org
NW-AIRQUEST	Northwestern U.S.	http://lar.wsu.edu/airpact
SESARM	Southeast U.S.	http://www.metro4-sesarm.org/content/metro-4sesarm-partnership
WESTAR/WRAP	Western U.S.	https://www.wrapair2.org

Element 4: Model Evaluation

The results of a model performance evaluation should be considered prior to using modeling to support a regulatory assessment. The objective of a model performance evaluation is to demonstrate that the baseline model scenario specific to the application can simulate observed pollution concentrations during historical episodes of elevated pollution. Both CAMx and CMAQ models have been shown to display generally similar performance features with respect to matching historical periods of primary and secondarily formed pollutants. A recent literature review (Simon et al., 2012) summarized photochemical model performance for applications published in the peer-reviewed literature between 2006 and 2012. This review may serve as a useful resource for identifying typical model performance for state of the science modeling applications. The remainder of this section provides more information relevant for evaluating photochemical models used for single source permit related assessments and NAAQS attainment demonstrations. Information about meteorological model performance evaluation for both purposes is also provided.

Models used for single source permit related demonstrations need routine evaluation of model estimates compared to routine surface measurements to provide general confidence that the modeling system is appropriately replicating historical pollution episodes. This is a more systematic evaluation as compared to the fit for purpose evaluation done to show whether the modeling system can replication single source plumes compared to in-plume or near-source field measurements that are infrequently available. This 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 modeled for a permit review assessment. 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 focused on the specific locations and time periods of interest.

Model evaluation is used to assess how accurately the model predicts observed concentrations and can provide a benchmark for model performance and identify model limitations that require diagnostic evaluation for further model development and improvement. The evaluation should be done for $PM_{2.5}$ and ozone. Some additional considerations for a $PM_{2.5}$ evaluation are that $PM_{2.5}$ consists of many components and is typically measured with a 24-hour averaging time. The individual components of $PM_{2.5}$ should be evaluated individually. In fact, it is more important to evaluate the components of $PM_{2.5}$ than to evaluate total $PM_{2.5}$ itself. Apparent "good performance" for total $PM_{2.5}$ does not indicate whether modeled $PM_{2.5}$ is predicted for "the right reasons" (the proper mix of components). If performance of the major components is good, then performance for total $PM_{2.5}$ should also be good.

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 hourly average ozone and daily maximum 8-hour ozone should be compared with observations in both time and space. For $PM_{2.5}$, model estimates of speciated 24-hour average $PM_{2.5}$ components (such as sulfate ion, nitrate ion, etc.) should be matched in time and space with observation data in the model domain. Modeled concentrations should not be averaged in space or averaged over multiple days/weeks/months before being compared to measurements as this averaging may mask errors that occur on shorter time-scales or at specific locations. 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). Evaluation of the photochemical transport models used to support NAAQS attainment demonstrations should conform to recommendations outlined in EPA guidance (U.S. Environmental Protection Agency, 2014b).

Meteorological Model Evaluation

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. 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. 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. Evaluation of the requisite meteorological databases necessary for use of photochemical transport models should conform to recommendations outlined in EPA guidance (U.S. Environmental Protection Agency, 2014b).

Element 5: Model Protocol

Per section 9.2.1 of the *Guideline*, the development of a modeling protocol is critical to a successful modeling assessment and that "Every effort should be made by the appropriate reviewing authority (paragraph 3.0(b)) to meet with all parties involved in either a SIP submission or revision or a PSD permit application prior to the start of any work on such a project." A modeling protocol is intended to communicate the scope of the analysis and generally includes (1) the types of analysis performed, (2) the specific steps taken in each type of analysis, (3) the rationale for the choice of modeling system, (4) names of organizations participating in preparing and implementing the protocol, and (5) a complete list of model configuration options. This protocol should detail and formalize the procedures for conducting all phases of the modeling study, such as describing the background and objectives for the study, creating a schedule and organizational structure for the study, developing the input data, conducting model performance evaluations, interpreting modeling results, describing procedures for using the model to demonstrate whether regulatory levels are met, and producing documentation to be submitted for review and approval.

Protocols should include the following elements at a minimum.

1. Overview of Modeling/Analysis Project
    - Participating organizations
    - Schedule for completion of the project
    - Description of the conceptual model for the project source/receptor area
    - Identification of how modeling and other analyses will be archived and documented
    - Identification of specific deliverables to the review authority

2. Model and Modeling Inputs
    - Rationale for the selection of air quality, meteorological, and emissions models
    - Modeling domain specifications
    - Horizontal resolution, vertical resolution and vertical structure
    - Episode selection and rationale for episode selection
    - Description of meteorological model setup
    - Description of emissions inputs
    - Specification of initial and boundary conditions
    - Methods used to quality assure emissions, meteorological, and other model inputs

3. Model Performance Evaluation
    - Identification of relevant ambient data near the project source and key receptors; provide relevant performance near the project source and key receptor locations
    - List evaluation procedures
    - Identification of possible diagnostic testing that could be used to improve model performance

4. Model Outputs
    - Description of the process for extracting project source impacts including temporal aggregation and in the case of $PM_{2.5}$ chemical species aggregation

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