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Support Document for Alternative Model Demonstrations for Using the SCICHEM Lagrangian Photochemical Model in Single-Source Ozone and Secondary $PM_{2.5}$ Impact Assessments

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Technical Update, December 2021

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ABSTRACT

On January 17, 2017, the United States Environmental Protection Agency (USEPA) published revisions to the Guideline on Air Quality Modeling, also referred to as *Appendix W* or the *Guideline*, in the Federal Register that were effective May 22, 2017. One of the updates in the revised Guideline was the approach for treating ozone and secondary fine particulate matter ($PM_{2.5}$) impacts from proposed new or modified sources under the Prevention of Significant Deterioration (PSD) permitting program. The Guideline recommended a two-tiered screening approach for permit-related program demonstrations rather than establishing a single preferred model.

This report is a support document that provides guidance for alternative model demonstrations for the SCICHEM (Second-order Closure Integrated puff model with CHEMistry) Lagrangian photochemical CTM that establishes the suitability of SCICHEM applications in PSD compliance demonstrations for ozone and secondary $PM_{2.5}$. This support document establishes the general applicability of SCICHEM for this purpose; however, it does not replace the need for SCICHEM PSD compliance demonstrations to include modeling protocols that describe model application choices, evaluation of model inputs, and evaluation of baseline air quality predictions against measurements.

Keywords
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PRIMARY AUDIENCE: Applicants and reviewers of air quality modeling compliance demonstrations.

KEY RESEARCH QUESTION

This document addresses the question of suitability of the SCICHEM (Second-order Closure Integrated puff model with CHEMistry) Lagrangian chemical transport model for use in compliance demonstrations for ozone and secondary $PM_{2.5}$.

RESEARCH OVERVIEW

This report describes the SCICHEM Lagrangian chemical transport model, including its history of development over two decades, evaluation of model performance with available data, and its applications for single source assessments. The report discusses the regulatory guidelines for satisfactory alternative model demonstrations and shows how SCICHEM fulfils each of these guidelines.

KEY FINDINGS

- SCICHEM is a peer-reviewed Lagrangian photochemical model that treats emissions, chemical transformation, transport, and deposition using time and space varying or constant meteorology. SCICHEM simulates both the primary emitted species and secondary pollutants including ozone and PM2.5.
- SCICHEM is an open source model and is freely available on the internet, with full documentation and pre-processors and post-processors.
- SCICHEM is theoretically applicable, with a state-of-the-science dispersion and chemistry modules.
- Background concentrations to use as one of the model inputs can be derived from available photochemical grid model (PGM) databases using provided processors.
- SCICHEM has been extensively evaluated and results published in the peer-reviewed literature, technical reports, and presented at modeling conferences.
- SCICHEM has been used for evaluating single-source assessments for ozone and PM2.5 and the results have been compared with those from established PGMs.

WHY THIS MATTERS

SCICHEM provides an alternative to more resource-intensive PGMs for single-source air quality modeling applications.

LEARNING AND ENGAGEMENT OPPORTUNITIES

- Training on SCICHEM will be offered after model releases and may also be offered at air quality modeling conferences.

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INTRODUCTION

1.1 Background

On January 17, 2017, the United States Environmental Protection Agency (USEPA) published revisions to the Guideline on Air Quality Modeling (USEPA, 2017), also referred to as *Appendix W* or the *Guideline*, in the Federal Register that were effective May 22, 2017. One of the updates in the revised Guideline was the approach for treating ozone and secondary fine particulate matter ($PM_{2.5}$) impacts from proposed new or modified sources under the Prevention of Significant Deterioration (PSD) permitting program. The Guideline recommended a two-tiered screening approach for permit-related program demonstrations rather than establishing a single preferred model (USEPA, 2017). As detailed in Section 5 of the Guideline, both tiers involve the use of Chemical Transport Models (CTMs), including photochemical grid models (PGMs) and other models with state-of-the-science photochemistry.

The recommended approach for Tier 1 demonstrations would use CTMs to provide sensitivity estimates (from existing or newly performed modeling) of ozone or secondary $PM_{2.5}$ responsiveness to precursor emissions (USEPA, 2016a). To facilitate the Tier 1 qualitative assessment of single-source ozone and secondary $PM_{2.5}$ impacts, USEPA has published draft guidance for using modeled emission rate precursors (MERPs) for Tier 1 screening of single-source NOx, SO_2, and volatile organic compounds (VOC) emission contributions to ozone and secondary $PM_{2.5}$ (USEPA, 2016a). The draft MERP guidance document performed screening modeling using a PGM to estimate the magnitude of single-source NOx, SO_2, or VOC emissions that would produce ozone or $PM_{2.5}$ impacts below the significant impact levels (SILs).

The recommended approach for Tier 2 demonstrations would directly use CTMs to develop a quantitative estimate of the impacts of a new or modified source (USEPA, 2016b). As stated in the preamble to the 2017 revised Guidelines (USEPA, 2017), USEPA believes that the use of photochemical CTMs for such purposes is scientifically appropriate and practical to implement. On August 4, 2017, USEPA published a Memorandum that performed an alternative model demonstration that justified the use of two specific PGMs for Tier 2 modeling analysis: the Community Multiscale Air Quality (CMAQ; USEPA, 2016c) and the Comprehensive Air Quality Model with extensions (CAMx; Ramboll, 2016), for use in single-source ozone and $PM_{2.5}$ assessments for permit-related assessments and for demonstrating attainment for ozone, $PM_{2.5}$, and regional haze (Fox, 2017).

1.2 Purpose

The purpose of this support document is to provide guidance for alternative model demonstrations for the SCICHEM (Second-order Closure Integrated puff model with CHEMistry) Lagrangian photochemical CTM (EPRI, 2021a,b) that would establish that SCICHEM is fit for purpose in PSD compliance demonstrations for ozone and secondary $PM_{2.5}$. This support document establishes the general applicability of SCICHEM for this purpose; however, it does not replace the need for SCICHEM PSD compliance demonstrations to include

modeling protocols that describe model application choices, evaluation of model inputs, and evaluation of baseline air quality predictions against measurements.

1.3 SCICHEM Alternative Model Demonstration Approach

This support document for alternative model demonstrations for SCICHEM follows the procedures used in EPA's alternative model demonstration Memorandum for CMAQ and CAMx (Fox, 2017). The Guideline on Air Quality Modeling (USEPA, 2017) outlines multiple criteria that need to be fulfilled to provide a satisfactory alternative model demonstration that a modeling system is fit for the purpose of supporting permit-related program technical demonstrations or NAAQS attainment demonstration plans (USEPA, 2005a; 2017). For situations in which there is no EPA preferred model, the Guideline Section 3.2.2(e) specifies the following five criteria to be satisfied:

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

This support document provides information about the SCICHEM modeling system relevant to each of these five elements. To introduce the support document for SCICHEM alternative model demonstrations, we document the history of the SCICHEM model development to provide context.

2
HISTORY OF SCICHEM DEVELOPMENT

The SCICHEM Lagrangian photochemical CTM is based on the Second-Order Closure Integrated Puff (SCIPUFF) dispersion model. Essentially, photochemical mechanisms used in CMAQ and CAMx have been added to SCIPUFF to develop SCICHEM. Therefore, the development of SCICHEM is intricately linked to the development of SCIPUFF.

2.1 Development of the SCIPUFF Model

SCIPUFF is a Lagrangian puff dispersion model using Gaussian puffs to represent an arbitrarily complex, three-dimensional, time-dependent plume from one or more sources (Sykes et al., 1988; 1996; 1997). The diffusion parameterization is based on the second-order turbulence closure theories of Donaldson (1973) and Lewellen (1977). The parameterization provides a prediction of the dispersion rate in terms of the measurable turbulent velocity statistics of the wind field. This generalized approach provides a unified parameterization for modeling dispersion at all ranges from laboratory to continental scales. The explicit representation of diffusion in terms of velocity statistics also provides a rational basis for the assessment of time-averaging effects. The generality of the turbulence closure scheme provides a dispersion representation for a wide range of conditions. The closure model has been applied on local scales up to 50-km range (Sykes et al., 1988) and on continental scales up to 3000-km range (Sykes et al., 1993; USEPA, 2012). Gabruk et al. (1999) showed that the second-order closure algorithm provided better model performance than either empirical algorithms—such as the Pasquill-Gifford-Turner (PGT) method—or first-order closure algorithms that use similarity theory to relate dispersion coefficients to micrometeorological variables.

Technical capabilities of the SCIPUFF model include the following:

- Suitable for short-range and long-range transport assessments
- Emission of gaseous and particulate pollutants
- Emission from continuous, instantaneous, moving, and stack sources
- Buoyant and non-buoyant emission releases
- Mass-consistent wind fields that account for complex terrain effects
- Fixed winds, surface or profile observations, or gridded meteorological input accepted
- Accurate treatment of wind shear, including puff-splitting in response to wind shear
- Puff-merging when similar puffs overlap substantially to improve model efficiency
- Pollutant removal by dry deposition
- Wet deposition and gravitational settling of particles
- Optional first-order decay of released (primary) pollutants
- Time-history concentration sampling capability (that is, receptors)
- Estimates of the uncertainty in tracer concentrations

SCIPUFF was originally developed to describe emission dispersion from tall stacks under the sponsorship of the Electric Power Research Institute (EPRI) (Sykes et al., 1989). Under the sponsorship of the Defense Threat Reduction Agency, SCIPUFF has been greatly extended to describe different material properties as they affect dispersion over a wide range of scales. The turbulence closure diffusion framework has been extended to describe long-range transport, using the mesoscale turbulence representation of Gifford (1988), and has been compared with the continental-scale dispersion data from the Across North American Tracer Experiment (ANATEX) experiment (Sykes et al., 1993) as well as the European Tracer Experiment (ETEX) and Cross-Appalachian Tracer Experiment (CAPTEX) tracer experiments (USEPA, 2012).

In July 2000, a public domain version of SCIPUFF (version 1.2PD) was submitted to EPA as an EPA alternative model with associated documentation.[1] Although the July 2000 SCIPUFF version is obsolete, the model was approved as an alternative dispersion model that could be used in regulatory applications with case-by-case justification to the Reviewing Authority under Section 3.2 of Appendix W. The latest version of SCIPUFF available in SCICHEM incorporates additional enhancements for puff dispersion, such as the addition of skewed turbulence to accurately capture dispersion in the convective boundary layer (Chowdhury et al., 2015).

2.2 Development of the SCICHEM Model

The SCICHEM model was originally developed as a state-of-the-science reactive plume model by adding the carbon bond mechanism (CBM-IV; Gery et al., 1989) to SCIPUFF to simulate ozone photochemistry (Karamchandani et al., 2000). The model was evaluated against helicopter-based measurements of the Cumberland power plant plume (Karamchandani et al., 2000). Initial applications of SCICHEM for single sources focused on short-period (1 to 2 days) simulations for model evaluation purposes.

After the initial development and evaluation of the stand-alone version of SCICHEM, the model was implemented as the advanced plume treatment (APT) plume-in-grid module in the CMAQ PGM to investigate sub-grid-scale effects, associated with NOx emissions from large elevated point sources, on O_3 formation (Karamchandani, et al., 2002). Subsequent updates were made to both the stand-alone and APT versions of the model simultaneously to address $PM_{2.5}$ and mercury. SCICHEM and CMAQ-APT were first updated to include a state-of-the-science treatment of $PM_{2.5}$ (Karamchandani et al., 2006). This treatment was based on a condensed version of the Model of Aerosol Dynamics, Reaction, Ionization, and Dissolution (MADRID) of Zhang et al. (2004). The MADRID treatment includes modules for the thermodynamics of inorganic species (ISOROPPIA; Nenes et al., 1999), the condensed secondary organic aerosol (SOA) representation of Pun et al. (2004), and aerosol dynamics using a sectional size representation. It also includes aqueous-phase chemistry and equilibrium modules to treat the scavenging of soluble gases and aerosols and the oxidation of SO_2 to sulfate in clouds.

Most SCICHEM applications and development activity from 2000 to 2010 focused on plume-in-grid simulations using CMAQ-APT (Karamchandani et al., 2002; 2006; 2009; 2010a; 2010b; Vijayaraghavan et al., 2006; 2008; 2009). SCICHEM was also implemented as a plume-in-grid module in WRF-Chem (Karamchandani et al., 2012a) and more recently in CMAQ 5.01

[1] https://www3.epa.gov/scram001/7thconf/information/scipuff.pdf

(Karamchandani et al., 2014). Major improvements and updates to the dispersion component (SCIPUFF) during this period were not carried forward to SCICHEM, except for minor bug fixes.

Since 2010, attention has focused once more on developing a stand-alone version of SCICHEM that can be applied for single-source applications over longer time periods to calculate long-term impacts. As part of this effort, SCICHEM was synchronized with SCIPUFF so that all improvements to SCIPUFF after the initial development of SCICHEM were incorporated in SCICHEM. An early beta version, referred to as *SCICHEM 3.0 Public Beta 1*, was released by EPRI in June 2013 on SourceForge. This version was suitable for short-range impacts, with a compact chemistry scheme for near-source NO and NO_2 impacts.

The chemistry modules in SCICHEM were subsequently updated to more recent versions (CB05 gas-phase chemistry, the CMAQ AERO5 aerosol module with modal size distribution, CMAQ aqueous-phase chemistry corresponding to AERO5 species). Model instabilities discovered during long-term (annual) simulations were addressed. The second public beta release (SCICHEM 3.0 Public Beta 2) was made available on SourceForge in June 2014. This version was suitable for both short-range and long-range impacts, including secondary ozone and $PM_{2.5}$ formation.

Additional SCICHEM improvements and bug fixes continued after the second beta release in response to testing by the model developers and comments from beta testers. The model was evaluated with aircraft measurements of power plant plumes (Chowdhury et al., 2015) and tested for robustness. This version (SCICHEM 3.0) was released as an open source software package on SourceForge in August 2015.

The next public release of the model was SCICHEM 3.1, released in April 2017 on GitHub[2] along with associated documentation (User's Guide, Technical Description, Read Me files), test cases, background concentrations for several regions of the United States, and post-processors. Science updates in SCICHEM 3.1 included the Zhang et al. (2003) dry deposition scheme for gas-phase species (previous versions of SCICHEM used constant user-specified dry deposition velocities) and the latest version of ISORROPIA, referred to as *ISORROPIA II* (Fountoukis and Nenes, 2007). Earlier versions of ISORROPIA introduced instabilities in SCICHEM in calculating $PM_{2.5}$ nitrate concentrations. The background concentrations provided with the model are for 2011 and are derived from a CONUS simulation with CAMx using the EPA 2011 modeling platform. These background concentration fields are generally at the state level.

SCICHEM 3.3, released in December 2021, is the latest publicly available version of SCICHEM. It can be downloaded from GitHub and includes updated User Documentation, as well as a pre-processor that allows users to develop their own background concentration fields for user-defined regions from available PGM outputs. This provides the flexibility of having a more representative background specific to the region of interest for the modeling application than the state-level background concentrations provided with the software package.

[2] https://github.com/epri-dev/SCICHEM/releases

SCICHEM 3.3 has been extensively tested and applied for single-source applications in four different geographical regions. Annual simulations for the four regions were conducted for a hypothetical source (a coal-fired power plant). Source impacts on ozone and secondary $PM_{2.5}$ were calculated and compared with corresponding impacts calculated by two PGMs: CMAQ and CAMx. The model comparison study is described in a peer-reviewed journal paper (Karamchandani et al., 2020).

3
SUPPORT FOR SCICHEM ALTERNATIVE MODEL DEMONSTRATIONS

This section describes each of the five elements in the Guideline (USEPA, 2017) that needs to be fulfilled to provide a satisfactory alternative model demonstration for using SCICHEM for single-source ozone and secondary $PM_{2.5}$ assessments.

3.1 Element 1: Peer Review

The SCICHEM photochemical CTM is a peer-reviewed Lagrangian photochemical model that treats emissions, chemical transformation, transport, and deposition using time and space varying or constant meteorology. SCICHEM simulates primary emitted species and secondary pollutants including ozone and $PM_{2.5}$ (EPRI, 2021b).

The SCICHEM modeling system is open source and freely available on the internet and has full documentation, including a User's Guide (EPRI, 2021a) and a Technical Description (EPRI, 2021b). Information about the location of the freely available SCICHEM code and documentation is provided in Table 3-1.

Table 3-1
Location of the freely available SCICHEM code

Acronym	Name	Internet location for source code and documentation
SCICHEM	Second-order Closure Integrated puff model with CHEMistry, Version 3.3	https://github.com/epri-dev/SCICHEM/releases

The stand-alone and plume-in-grid versions of SCICHEM have been extensively peer-reviewed for estimating ozone and $PM_{2.5}$ concentrations and other pollutants (Chowdhury et al., 2015; Karamchandani et al., 2000; 2002; 2006; 2009; 2010a,b; 2011a; 2012a,b; 2014; 2015b; Kelly et al, 2015; Vijayaraghavan et al., 2006; 2008; 2009; 2010).

3.2 Element 2: Theoretically Applicable

CTMs treat atmospheric chemical and physical processes such as gas and particle chemistry, deposition, and transport. The two fundamental types of CTMs are differentiated by their frame of reference (McMurry et al., 2004). Eulerian CTMs, including CMAQ and CAMx, employ a fixed frame of reference (grid based) that is anchored to the earth's surface. Lagrangian CTMs, including SCICHEM, employ a moving frame of reference that travels with parcels of air.

PGMs, such as CMAQ and CAMx, are Eulerian models that divide a modeling domain into a 3-D array of grid cells. PGMs treat emissions from all sources within the domain, perform transport and diffusion using 3-D meteorological fields, and perform detailed photochemistry for ozone and secondary $PM_{2.5}$. Because PGMs treat emissions from all sources, single-source impacts can be obtained from the difference between two PGM simulations with and without the source (referred to as the *brute force approach*) or by using instrumented tools (source

apportionment and/or source sensitivity) available in some PGMs. CMAQ and CAMx have been optimized to run efficiently on powerful multiprocessor workstations. However, conducting PGM simulations requires a significant amount of computer resources and extensive model setup.

Lagrangian models, such as SCICHEM, are inherently well-suited to simulating impacts from a single source because they follow the downwind transport, dispersion, and chemistry of the emissions. SCICHEM represents a plume as a sequence of puffs and can calculate plume impacts in a single run without having to simulate all sources. Lagrangian model setup tends to be simpler than for PGMs. However, because Lagrangian models do not simulate all sources, they depend on information about background concentrations in the atmosphere that influence the chemical transformation of the single-source emissions. Most Lagrangian models have highly simplified chemical transformation algorithms without photochemistry (for example, AERMOD and CALPUFF), which simplifies the requirement for background concentrations but restricts ability to simulate ozone and secondary $PM_{2.5}$. SCICHEM is a more advanced Lagrangian model and includes full-science photochemistry and other chemistry algorithms that are comparable to those in CMAQ and CAMx. SCICHEM can use temporally and spatially varying background concentrations to more realistically simulate the chemistry of pollutants emitted from single sources. The background concentrations for SCICHEM can be generated by running a PGM or using existing PGM outputs if available. SCICHEM accounts for chemical interactions among puffs that overlap one another. An important benefit of explicitly treating puff overlap is that co-located puffs share the available background concentrations of oxidants and ammonia, which avoids over-estimating chemical transformation rates due to double-counting the influence of the background.

3.2.1 Using SCICHEM for Single-Source Permit-Related Assessments

SCICHEM is appropriate for assessing near-field and far-field reactive pollutant impacts from user-specified sources (Chowdhury et al., 2015; Karamchandani et al, 2000; 2011a; 2012b; 2013; 2015a, b; Kelley et al., 2015). Because $PM_{2.5}$ and ozone 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 and secondary impacts. SCICHEM appropriately treats single-source impacts on ozone and secondary $PM_{2.5}$ for two reasons: 1) it includes photochemical interactions of the single-source emissions with background concentrations that represent emissions from all other sources and 2) it treats the subsequent chemical and physical fate of the single-source 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 the same state-of-the-science algorithms (for example, Seinfeld and Pandis, 2012) as used in CMAQ and CAMx. In addition to characterizing the physical and chemical evolution of plumes from specific sources, the 3-D input data to SCICHEM can provide a realistic chemical and physical environment for simulating ozone and secondary $PM_{2.5}$ formation.

Near-source, in-plume measurements are useful for building confidence that a modeling system captures secondary formation of pollutants from a specific source. For PGMs, even though single-source emissions are immediately diluted to grid volume, the 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). Earlier versions of SCICHEM were implemented in a plume-in-grid version of the CMAQ PGM, referred to as CMAQ with

Advanced Plume Treatment (APT). Single-source assessments using CMAQ with and without APT (that is, essentially comparing a PGM vs. SCICHEM single-source impact) were generally comparable with differences attributable to variations in transport path or SCICHEM's more accurate representation of near-source chemistry better resolving the NOx inhibition of ozone and secondary $PM_{2.5}$ formation near the source (for example, Karamchandani et al., 2002; Karamchandani et al., 2010a,b).

Specific to single-source applications for PSD, near-source in-plume aircraft-based measurement field studies provide data for evaluating model estimates of (near-source) downwind transport and chemical impacts from single-point sources (ENVIRON, 2012a). When initially developed, SCICHEM was extensively evaluated against in-plume aircraft observations of large power plant plumes in Tennessee (Karamchandani et al., 2000) and demonstrated good agreement with the observed ozone, SO_2, NO_X, and NO_Y concentrations. In a multi-model intercomparison study, the SCICHEM simulation of single-source downwind impacts compared well against field study primary and secondary pollutant measurements (for example, O_3) for sources in Tennessee and Texas (ENVIRON, 2012a). SCICHEM 3.0 was recently evaluated against other power plant plume measurements of ozone and other gas-phase pollutants (Chowdhury et al., 2015). These studies indicate that SCICHEM estimates of single-source impacts are comparable to in-plume field study measurements and other models and that SCICHEM is not overly biased toward over- or under-estimation tendencies.

These in-plume chemistry evaluations indicate the successful addition of chemistry to SCIPUFF, an EPA-recommended alternative model for puff dispersion and transport from single sources. Therefore, SCICHEM is an appropriate model for single-source ozone and $PM_{2.5}$ impact assessments. This issue is discussed in more detail under Element 4: Model Evaluation.

3.3 Element 3: Databases for Application

SCICHEM inputs are simpler than those for PGMs and more flexible for modeling single-source impacts. SCICHEM can be run in several different modes depending on the single-source application. For example, for near-source 1-hour NO_2 impacts, it may be appropriate to run SCICHEM using meteorological data from a single site and using only inorganic photochemical reactions (Karamchandani et al., 2012b). In contrast, for long-range transport to address ozone and secondary $PM_{2.5}$, fully 3-D meteorological input data and complete photochemistry are appropriate (Karamchandani et al., 2013; 2015a, b; 2017).

There are three main inputs for SCICHEM:

- Source emission inputs
- Meteorological inputs
- Background concentration inputs

3.3.1 Source Emission Inputs

The emissions for the single source being modeled by SCICHEM are critically important for an assessment of its ozone and secondary $PM_{2.5}$ impacts. SCICHEM is quite flexible in the types of emission sources it can accommodate and is capable of handling instantaneous and continuous sources, including point, volume, and area source types. Line sources may also be modeled as a string of volume sources or as elongated area sources. Source emission rates and stack

characteristics (for example, stack exit velocity or stack temperature) can be constant or variable throughout the modeling period. Emission rates may be specified for a single source or for several sources. The SCICHEM emissions input file is in ASCII (text) format and can be easily viewed and modified by the model user.

For secondary ozone and impacts, where full photochemistry calculations are required, emissions must be provided using the model species names of the photochemical mechanism. SCICHEM 3.3 uses the latest carbon bond chemical mechanism (CB6) which represents VOCs as structural groups (named PAR, OLE, TOL, and so on). Species mappings from specific VOCs to CB6 model species (for example, from toluene to TOL) are available from emission processing systems for PGMs (such as SMOKE or EPS3). The emission processing systems also include source profiles to assign total VOC emissions from specific emission categories (for example, diesel exhaust, fugitive natural gas) to CB6 model species. Data from the emission processing tools for PGMs can be used to speciate criteria pollutant emissions for SCICHEM. Similar to the methods described for VOC, NOx emissions can be speciated into NO and NO_2, SOx emissions into SO_2 and sulfate, and primary $PM_{2.5}$ into chemical components (sulfate, carbon, and so on).

3.3.1.1 Availability of Source Emission Inputs

The preparation of single-source emission inputs for SCICHEM is comparable to other single-source models (for example, AERMOD) and an expected, routine task for a single-source modeler. The permit applicant should characterize its source well because he or she will not be allowed to deviate greatly from the parameters provided once the permit is issued without conducting new permit modeling. If the source is an existing one, information may be available from the National Emissions Inventory (NEI; https://www.epa.gov/air-emissions-inventories/national-emissions-inventory-nei). As mentioned, before using SCICHEM for secondary pollutant impacts, the criteria pollutant emission rates must be mapped to SCICHEM model species. This component of emissions preparation for SCICHEM is comparable to the speciation requirements for PGMs but can be accomplished using simpler tools (such as spreadsheets) that use mappings from criteria pollutants (NOx, SOx, VOC, $PM_{2.5}$) to SCICHEM model species using speciation data applicable to the single source.

3.3.2 Meteorological Inputs

SCICHEM meteorological requirements are also quite flexible, and SCICHEM can handle a variety of inputs from standard observations to gridded meteorological fields. Processors are available to convert routine meteorological data and meteorological outputs from the Weather Research Forecast (WRF) meteorological model or the legacy Fifth-Generation Penn State/NCAR Mesoscale Model (MM5) to SCICHEM inputs. For near-source applications, SCICHEM can also use certain AERMET meteorological outputs (that is, inputs to AERMOD). Additional details are provided next.

3.3.2.1 Observed Meteorological Inputs

The SCICHEM package includes a meteorological pre-processor, referred to as *METSCI*, which can read upper air files in FSL format and surface files in TD-3505 or ISD format to create surface and profile meteorological input files for SCICHEM. These routine data can be downloaded easily, as documented in the SCICHEM User's Guide (EPRI, 2021a) and discussed next. METSCI is comparable to the AERMET pre-processor for AERMOD, and it is functionally equivalent to running only Stage 1 of AERMET. METSCI extracts only the basic

observations and does not perform any boundary layer modeling as is done in AERMET processing for AERMOD. The boundary layer calculations are conducted within SCICHEM as described in the SCICHEM Technical Document (EPRI, 2021b). Although SCICHEM can directly use certain types of AERMET files, it is recommended that the supplied processor—METSCI—be used to create input files in standard SCICHEM format because METSCI reads the same input files as AERMET to create surface and upper air inputs.

SCICHEM 3.3 can directly read Automated Surface Observing System (ASOS) 1-minute data files. However, the quality of the ASOS 1-minute data is quite variable. There may be extended gaps, invalid data, and duplicate times with disparate observations. SCICHEM outputs cautionary messages in its log file if there are large periods of missing or invalid data.

3.3.2.2 WRF Meteorological Inputs

USEPA has developed the Mesoscale Model Interface Program (MMIF, Version 3.4, 2018-07-18; Brashers and Emery, 2018) that can process MM5 and WRF output to develop 3-D hourly varying meteorological files in SCICHEM format (referred to as the *MEDOC* format, where *MEDOC* stands for *Multiscale Environmental Dispersion Over Complex terrain*). MMIF can alternatively create "pseudo-observation" files for AERMET or AERMOD that could be used as SCICHEM inputs. However, all SCICHEM applications to date with WRF outputs have used the 3-D hourly output from MMIF.

3.3.2.3 Availability of SCICHEM Meteorological Inputs

SCICHEM meteorological inputs based on observations are available throughout the world. Tutorials in the SCICHEM User's Guide (EPRI, 2021a) provide an example of downloading surface and upper air data for a case study. The NCDC DS-3505 data sets can be downloaded from ftp://ftp.ncdc.noaa.gov/pub/data/noaa while FSL5 upper air data can be obtained from http://esrl.noaa.gov/raobs. Higher time resolution surface data (ASOS 1-minute) can also be obtained from the NCDF ftp site (ftp://ftp.ncdc.noaa.gov/pub/data/noaa). As mentioned, SCICHEM 3.3 can directly read ASOS 1-minute meteorological data. However, it is necessary to concatenate the monthly data available from the NCDC ftp site when conducting simulations for periods longer than a month because SCICHEM can read only one file per measurement location.

EPA routinely performs WRF meteorological simulations that are readily available for generating SCICHEM meteorological inputs either as hourly single-site or hourly 3-D inputs. For example, EPA has run WRF at 12-km grid resolution on the continental United States (CONUS2) domain for the years 2011–2016 (and previous years as well, for example, 2002, 2007, and 2008) that can be acquired for use with SCICHEM (Gilliam, 2010; USEPA, 2014a). WRF output is also available from several multi-jurisdictional organizations (MJOs) (for example, WRAP for 2011 and 2014; UNC and ENVIRON, 2015; Bowden et al., 2016), states, and academic institutions (such as Zhang et al., 2014). Any of these WRF output databases can be easily turned into SCICHEM meteorological inputs using the MMIF processor (Brashers and Emery, 2018).

Table 3-2 lists websites for EPA and several organizations that may have WRF meteorological data available for use as SCICHEM meteorological inputs. As discussed in the next section, they

may also have PGM (for example, CMAQ and/or CAMx) model outputs that can be used for SCICHEM background concentration inputs.

Table 3-2
Multi-jurisdictional organizations, other organizations, and USEPA may have WRF model output for SCICHEM meteorological inputs and/or PGM model outputs for SCICHEM background concentration inputs

Organization	Region of Country	Website
CENSARA	Central U.S.	http://www.ceensara.org
LADCO	Upper Midwest	http://www.ladco.org
MARAMA	Mid-Atlantic	http://marama.org
NESCAUM	Northeast U.S.	http://nescaum.org
NW-AIRQUEST	Pacific Northwest	http://lar.wsu.edu/airpact
SESARM	Southeast U.S.	http://metro4-sesarm.org
WESTAR/WRAP	Western U.S.	http://www.wrapair2.org
EPA/OAQPS	Continental U.S.	https://www3.epa.gov/airquality/modeling.html

3.3.2.4 Background Concentration Inputs

Background concentration fields are important inputs to SCICHEM because the amount of ozone and secondary $PM_{2.5}$ formed from emissions from a single source will depend on the reactivity of the background air—for example, ozone formation can depend on background VOC concentrations interacting with a NOx plume, and background ammonia concentrations can determine formation of particulate nitrate in a NOx plume. Therefore, it is important to specify realistic and representative background concentration inputs for the region being modeled.

SCICHEM is flexible in the specification of background concentrations for a single-source application. It can use a single set of background concentrations (that is, constant over space and time) or hourly varying 3-D background concentrations from a PGM, such as CMAQ or CAMx. The latter data provide spatial and temporally varying chemically balanced realistic background concentration values with which the SCICHEM single-source puffs can interact to provide credible single-source ozone and $PM_{2.5}$ impacts. The PGM output may be processed spatially and/or temporally to provide regionally representative realistic background concentrations. The current SCICHEM 3.3 release[3] includes monthly average hourly background concentrations with vertical variation (18 layers up to about 3.5 km) for several different regions of the United States (generally at the state level with multiple regions for larger states like California and Texas) processed from a 2011 CONUS simulation using CAMx. In addition, SCICHEM 3.3, includes a pre-processor that can be used to extract background concentrations from either CAMx or CMAQ for any region of interest (in the CONUS domain). The modeler will be able to specify the CONUS subdomain for which background values are required.

[3] https://github.com/epri-dev/SCICHEM

3.3.2.5 Availability of SCICHEM Background Concentration Inputs

As noted, the current SCICHEM 3.3 release includes diurnally varying (hourly) monthly average background concentrations for each state in the continental United States with the two largest states (that is, California and Texas) split into multiple sub-regions. These concentrations were obtained by processing outputs from CAMx simulations of the CONUS domain for 2011. The simulation used EPA's CAMx 2011 version 6.2 modeling platform that was used in the Cross-State Air Pollution Rule (CSAPR) update for the 2008 ozone NAAQS (USEPA, 2016c,d). SCICHEM 3.3 also includes a pre-processor that can be used to develop background concentrations for any domain of interest using CMAQ or CAMx outputs. As discussed in the meteorology data availability sub-section, such outputs may be available from EPA or from the MJOs.

3.4 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 determine whether a baseline model scenario specific to the application can simulate observed pollution concentrations during historical episodes of elevated pollution. To demonstrate that the performance of the SCICHEM model is sufficiently good for single-source ozone and $PM_{2.5}$ modeling, we break the model evaluation into three components:

1. Past SCICHEM model performance evaluations demonstrating that SCICHEM is suitable for single-source ozone and $PM_{2.5}$ modeling
2. Past demonstrations of SCICHEM single-source ozone and $PM_{2.5}$ impacts and comparisons against the CMAQ or CAMx PGMs, which EPA has determined are suitable for single-source ozone and $PM_{2.5}$ assessments (Fox, 2017)
3. SCICHEM model evaluations that should be conducted for each single-source application on a case-by-case basis

3.5 Previous SCICHEM Model Evaluations for Single-Source Applications

SCICHEM and its dispersion and transport component (SCIPUFF) are specifically designed for single-source air quality assessments. The SCICHEM Lagrangian puff modeling framework is more efficient for single-source simulation than PGMs because SCICHEM can better resolve the large variation in size of a single-source plume from near-source to far-field. In contrast, PGMs face a computational challenge of requiring fine resolution grids to resolve near-source impacts but then needing numerous grid cells to capture far-field impacts. However, because SCICHEM is simulating only a single source, or group of sources, it is more difficult to evaluate SCICHEM predictions against ambient air quality observations that include impacts from all emission sources, as is done for PGMs (Simon et al., 2012; Emery et al., 2017). Thus, SCICHEM model evaluation can be broken down into the two major components needed by an air quality model to simulate single-source ozone and secondary $PM_{2.5}$ impacts:

- Evaluation of the transport and dispersion component of the SCICHEM model (that is, SCIPUFF) that can be accomplished using ambient field study tracer test experiments or alternatively using ambient monitoring of inert or semi-inert pollutant dispersion from fairly isolated sources.

- Evaluation of the chemistry component of SCICHEM through comparisons of SCICHEM modeling results with in-plume measurements of reactive pollutants or identifiable point source plume impacts at surface monitoring sites.

3.5.1 Evaluation of the Transport and Dispersion Component of SCICHEM

The SCIPUFF/SCICHEM model has been subjected to numerous evaluations studies that validate its ability to accurately simulate the transport and dispersion of emissions from single sources or groups of sources at many scales:

- An early version of SCIPUFF based on second-order closure theory was developed to predict plume transport out to ranges of about 50 km and was extensively evaluated with data from EPRI plume model validation experiments (Lewellen et al., 1988).
- The model of Lewellen et al. (1988) was adapted to simulate long-range transport and dispersion and was evaluated against the 1987 ANATEX (Sykes et al., 1993). ANATEX provides a high-quality, extensive database for dispersion over thousands of kilometers.
- Deng et al. (2004) evaluated the MM5-SCIPUFF system for interregional transport using surface measurements of tracer concentrations during the 1983 CAPTEX study.
- Lee et al. (2009) extended the analysis of Deng et al. (2004) to improve model performance for CAPTEX by augmenting the meteorological inputs to SCIPUFF with meteorological ensemble-uncertainty parameters from an ensemble of Numerical Weather Prediction (NWP) simulations.
- Anderson and Brode (2010) conducted an evaluation of four Lagrangian models against measurements from the CAPTEX and ETEX field studies. SCIPUFF was found to have the second best overall performance of the four models studied.
- USEPA conducted a massive evaluation of long-range transport (LRT) models using multiple tracer test field study data (USEPA, 2012). SCIPUFF was one of six LRT models evaluated against the 1983 CAPTEX releases no. 3 and 5 (CTEX3 and CTEX5) that evaluate models in the northeastern United States at distances of 100 to 1,100 km downwind of the tracer release. SCICHEM was also one of the models evaluated against the 1994 ETEX that evaluated models at distances of 100–1000 km downwind. For CTEX3, SCIPUFF was clearly the second best performing LRT model of the six evaluated and, for CTEX5, SCIPUFF was the third or fourth best performing LRT model of the six evaluated. For the ETEX tracer experiment, SCIPUFF essentially tied for second best performing LRT model of the five evaluated (USEPA, 2012).
- Chowdhury et al. (2013) evaluated an early version of SCICHEM 3.0 (referred to as *SCICHEM-2012* at that time) using AERMOD tracer and a semi-inert pollutant (for example, SO_2) databases (Perry et al., 2005). SCICHEM-2012 was updated to include a treatment of skewed turbulence to accurately capture dispersion in the convective boundary layer (Chowdhury et al., 2015). SCICHEM-2012 was evaluated using six test cases from the AERMOD evaluation database: the Kincaid field study, the Baldwin field study, the Clifty Creek study, the Martins Creek study, the Tracy field study, and the Bowline field study. The AERMET meteorological files for AERMOD were used directly in SCICHEM. SCICHEM performance was comparable to or better than AERMOD performance for four of the six cases. For the Kincaid database, SCICHEM tended to predict higher concentrations than AERMOD or the observations. Better performance for SCICHEM was obtained for the

Kincaid database when SCICHEM conducted its own boundary layer calculations based on upper air soundings rather than using the default AERMET values.

- SCICHEM 3.0 was evaluated against nine SF6 tracer releases in Copenhagen, Denmark (Chowdhury et al., 2015). SCICHEM's prediction of tracer dispersion and transport is fairly accurate, with the new implementation of the skewed turbulence modeling resulting in significantly improved performance for the Copenhagen test cases compared to previous versions of the model.

3.5.2 Evaluation of the Chemistry Component of SCICHEM Against In-Plume Measurements

The chemistry component of SCICHEM has been evaluated by comparing model estimates against aircraft measurements of reactive pollutants in plumes from power plant and petrochemical sources. These studies are summarized next in chronological order. Only stand-alone SCICHEM evaluation studies are given, but SCICHEM has also been evaluated as the plume-in-grid component of CMAQ in several studies, as discussed previously.

1. The first evaluation of SCICHEM as a reactive puff model was conducted by Karamchandani et al. (2000) after its initial development. The model was tested using helicopter measurements of several power plant plumes during the 1995 Southern Oxidants Study (SOS) Nashville/Middle Tennessee Ozone Study. The model was applied for six days in June and July of 1995, and the model's ability to estimate physical and chemical plume characteristics—such as plume width and reactive species concentrations—was evaluated using the helicopter measurements. The study showed that the model performed best when the meteorology and background chemistry were well-characterized—for example, on July 7, 1995, a day on which emissions from the Cumberland power plant were transported steadily to the Southeast over rural regions with little interaction with other point source plumes or urban emissions.
2. Vijayaraghavan et al. (2010) evaluated SCICHEM using aircraft measurements of the Dolet Hills power plant plume conducted during the Northeast Texas Air Care (NETAC) 2005 air quality study. This evaluation was repeated with SCICHEM 3.0 (Chowdhury et al., 2015) as discussed later below.
3. For the Oklaunion power plant in north Texas, SCICHEM was evaluated against NOAA P3 in-plume aircraft measurements for nighttime ozone, NO_Y, and SO_2 concentrations and next-day ozone formation (Karamchandani et al., 2011a). SCICHEM performance was also compared against the CAMx PGM (ENVIRON, 2012a).
4. The ability of SCICHEM to estimate near-source 1-hour NO_2 concentrations was evaluated using observed concentrations for a power plant in Wainwright on the North Slope of Alaska and for a natural gas generator in Washington and the results compared against AERMOD (Karamchandani, 2012b; 2013).
5. SCICHEM 3.0 was evaluated against aircraft measurements of ozone and NOx within plumes from two NOx sources: 1) the TVA Cumberland power plant in Tennessee that had high NOx emissions (11–15 tons per hour) and 2) the Dolet Hills power plant in Louisiana that had lower NOx emissions (~1 ton per hour). Peak NOx increments in the Cumberland plume were over 100 ppb at 20-km downwind, compared to peak increments of less than 18 ppb in the Dolet Hills plume at 18-km downwind. This resulted in ozone titration in the Cumberland plume near the source with ozone production starting at distances beyond 50

km. In contrast, O_3 production in the Dolet Hills plume began closer to the source. These phenomena were successfully predicted by the model. Model performance for the Dolet Hills plume was better than for the Cumberland plume. SCICHEM predicted a wider plume than observed for Cumberland and consequently lower ozone and NOx peaks. For Dolet Hills, the plume width and peaks were better predicted but with some lateral displacement attributable to limited wind observation data (Chowdhury et al., 2015).

6. In a particularly challenging test of the model, SCICHEM 3.0 was evaluated for sources in the Houston Ship Channel that emit both highly reactive volatile organic compounds (HRVOC) and NOx against NASA DC-8 in-plume aircraft measurements of the ship channel plume collected as part of the 2013 SEAC^{4}RS field study. SCICHEM was able to reproduce ozone, NOx, aldehyde (for example, HCHO) and other pollutants within the HRVOC plumes at several downwind distances (40, 80, and 100 km) (Karamchandani et al., 2015b).
7. SCICHEM 3.3 is currently being evaluated against power plant plume measurements taken by the NOAA WP-3 aircraft in June and July 2013 in the recent Southern Oxidants and Aerosol Study/Southeast Nexus (SOAS/SENEX) as part of the Southeast Atmosphere Study (SAS). The WP-3 aircraft measured several trace gas species and aerosol chemical composition. SCICHEM 3.0 was previously evaluated against this database, and the results of the evaluation are provided in Knipping et al. (2016).

3.6 Demonstration of SCICHEM Applications for Single-Source Assessments and Comparisons Against PGM Results

The stand-alone version of SCICHEM has been applied for numerous single-source applications to test the robustness of the model and to compare the SCICHEM single-source ozone and $PM_{2.5}$ impacts with those produced by PGMs that USEPA has determined suitable for single-source assessments (Fox, 2017). In addition, SCICHEM—as the APT plume-in-grid component of CMAQ—has been used in calculating source impacts and compared against CMAQ without using the APT. These applications are summarized as follows:

- SCICHEM is implemented as an APT plume-in-grid model within the CMAQ PGM. CMAQ-APT is a hybrid Eulerian/Lagrangian model. CMAQ and CMAQ-APT were both used to calculate ozone impacts of selected sources in the eastern United States, and the model outputs were compared (this essentially provides a comparison of single-source SCICHEM assessments against the CMAQ PGM). CMAQ and CMAQ-APT produced nearly identical ozone model performance, but CMAQ-APT produced lower ozone and nitric acid impacts than CMAQ without APT when the impacts from 30 point sources in the eastern United States were evaluated. The lower ozone and nitric acid impacts using CMAQ-APT compared to the CMAQ PGM were attributed to the plume model more accurately simulating chemical formation in the early stages of the plume than using CMAQ with a 12-km grid resolution (Karamchandani et al., 2002).
- CMAQ-APT (that is, SCICHEM) was extended to treat secondary $PM_{2.5}$ and tested for January and July 2002 for 14 coal-fired power plants in the southeastern United States with the results compared against ambient measurements from the SEARCH network. Although overall model performance of CMAQ and CMAQ-APT was similar for $PM_{2.5}$ and its components (such as sulfate and nitrate), CMAQ-APT better replicated power plant plume impacts identified at SEARCH monitoring sites than CMAQ without APT and produced slightly lower sulfate and nitrate concentrations (Karamchandani et al., 2006).

- CMAQ and CMAQ-APT were applied to central California with the top 10 NOx emitters selected for treatment by SCICHEM in CMAQ-APT. The model performance for ozone and other species was nearly identical for the CMAQ PGM and CMAQ-APT. However, the differences in predicted impacts on ozone concentrations between the CMAQ and CMAQ-APT models were much smaller than seen in the eastern United States. This was attributed to the fact that the highest NOx emitters in California had NOx emissions approximately an order of magnitude lower than those in the eastern United States (Vijayaraghavan et al., 2006).
- The CMAQ PGM and CMAQ-APT (referred to as *AMSTERDAM*) were compared for 150 power plants in the eastern United States. Both CMAQ and AMSTERDAM produced essentially identical model performance when compared to ambient air quality observations. However, when the SCICHEM module in AMSTERDAM was used to treat emissions from the 150 power plants, smaller ozone and $PM_{2.5}$ impacts were predicted than with the CMAQ PGM. This was attributed to a more accurate simulation of the early chemical evolution of point source plumes with SCICHEM. The higher NOx concentrations in the SCICHEM-simulated plumes in AMSTERDAM inhibited ozone and $PM_{2.5}$ formation whereas the CMAQ PGM instantaneously diluted point source across a 12-km grid cell—leading to lower near-source NOx concentrations in the CMAQ PGM (Karamchandani et al., 2010a,b).
- SCICHEM is implemented as a plume-in-grid treatment in a special version of the WRF-Chem coupled meteorological and chemical transport model. The plume-in-grid version (referred to as *WRF-Chem PinG*) and the WRF-Chem PGM were used to simulate downwind impacts of eight large coal-fired power plants in the eastern United States. As in previous studies with CMAQ, the PGM and plume-in-grid versions of WRF-Chem had nearly identical model performance, but the spatial distributions of the ozone and secondary $PM_{2.5}$ concentrations exhibited differences attributable to 1) the different near-source chemistry and transport paths when SCICHEM was used to simulate the point source plume and 2) differences in meteorology resulting from feedback of simulated secondary $PM_{2.5}$ concentrations to the WRF meteorological simulation (Karamchandani et al., 2012a).
- In 2012, EPA conducted single-source proof-of-concept modeling using the CAMx PGM and CALPUFF for several sources (ENVIRON, 2012b). One of the same databases was also used to demonstrate SCICHEM for single-source far-field ozone, secondary $PM_{2.5}$, and visibility assessments. SCICHEM provided comparable impacts to those predicted by the CAMx and CALPUFF models (Karamchandani, et al. 2013).
- SCICHEM is implemented in a more recent version of CMAQ (v5.02) as a plume-in-grid treatment (CMAQ-APT), and the CMAQ PGM and CMAQ-APT were used to calculate the impacts of 18 large NOx sources in the eastern United States. While the two models performed essentially identically for ozone and $PM_{2.5}$ concentrations when compared against ambient measurements, CMAQ-APT produced lower ozone and secondary $PM_{2.5}$ (sulfate and nitrate) impacts than CMAQ due to NOx inhibition of chemical formation processes that was better resolved in the SCICHEM-simulated plumes (Karamchandani et al., 2014).
- Prior to the public release of SCICHEM 3.0 in August 2015, the model was subjected to a comprehensive test of its robustness for single-source modeling using several diverse source types (for example, tall stack power plant, low stack flare VOC sources, and a petrochemical complex) and regions (Northwest, central California, Southwest, intermountain west, west

Texas, Southeast, and northeast United States) representing different atmospheric conditions (Karamchandani et al., 2015a).

- Kelley et al. (2015) evaluated the single-source impacts of hypothetical sources in California using the CMAQ model with three approaches: 1) emissions zero-out (brute force), 2) emissions sensitivity using the decoupled direct method (DDM), and 3) CMAQ-APT (SCICHEM). They found good agreement among the three approaches for NOx source contributions to ozone and SO_2 source contributions to $PM_{2.5}$ sulfate, but the three methods diverged in their estimates of the contributions of NOx sources to $PM_{2.5}$ nitrate.
- SCICHEM 3.2, released in June 2019, was used to calculate single-source impacts of hypothetical coal-fired power plants in four regions of the United States (western, southwestern, southeastern, and northeastern United States) on ozone and secondary $PM_{2.5}$ concentrations. The source impacts modeled by SCICHEM were compared with those modeled by CMAQ (using zero-out) and CAMx (using zero-out and the CAMx source apportionment tools) as well as with impacts calculated by USEPA (2016a) for the guidance on the development of MERPs. The comparisons showed both similarities and differences in the predicted impacts from different approaches. The results of the study are described in a peer-reviewed journal paper (Karamchandani et al., 2020).

3.7 Element 5: Model Protocol

As identified in Section 9.2.1 of the Guideline (USEPA, 2017), a modeling protocol is critical to a successful modeling assessment: "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."

The modeling protocol is intended to communicate the scope of the analysis and generally includes 1) the types of analysis to be 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. The modeling protocol should detail and formalize the procedures for conducting all phases of the modeling study, such as describing the study background and objectives, 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 regulated pollutant levels are met or exceeded, and producing documentation to be submitted for review and approval. Modeling protocols should include the following elements at a minimum:

- 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

- Model and modeling inputs
  - Rationale for the selection of air quality (background), meteorological, and emission models and/or data
  - Modeling domain specifications
  - Horizontal resolution, vertical resolution, and vertical structure of the meteorological fields
  - Episode selection and rationale for episode selection
  - Description of meteorological model setup
  - Description of emissions inputs
  - Specification of background concentrations
  - Methods used to ensure quality of emissions, meteorological, and other model inputs
- Model performance evaluation
  - Identify relevant ambient data near the project source and key receptors; provide relevant performance near the project source and key receptor locations
  - List evaluation procedures
  - Identify possible diagnostic testing that could be used to improve model performance
- 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

4
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