

# PM2.5 Precursor Demonstration Guidance

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# Acronyms Used in this Guidance

BACT	Best Available Control Technology
CAA	Clean Air Act
CAMx	Comprehensive Air Quality Model with Extensions
CI	Confidence Interval
CMAQ	Community Multiscale Air Quality model
CSN	Chemical Speciation Network
СТМ	Chemical transport model
DDM	Direct Decoupled Method
DV	Design Value
EC	Elemental carbon
EGU	Electric Generating Units
EPA	Environmental Protection Agency
FEM	Federal Equivalent Method
FRM	Federal Reference Method
IMPROVE	Interagency Monitoring of Protected Visual Environments
LAER	Lowest Achievable Emissions Rate
NNSR	Nonattainment New Source Review
NSR	New Source Review
OM	Organic matter
PM	Particulate matter
PM <sub>10</sub>	Particulate matter with diameter 10 microns or less
PM <sub>2.5</sub>	Particulate matter with diameter 2.5 microns or less
PSD	Prevention of Significant Deterioration
RACM	Reasonably Available Control Measures
RACT	Reasonably Available Control Technology
RFP	Reasonable Further Progress
RRF	Relative response factor
SANDWICH	Sulfate, adjusted nitrate, derived water, inferred carbonaceous balance
SILs	Significant Impact Levels
SIP	State Implementation Plan
SMAT	Software for the Modeled Attainment Test
SOA	Secondary Organic Aerosol
VOC	Volatile Organic Compound

# 1.0 Introduction

In 2016, the Environmental Protection Agency (EPA) finalized the fine particulate matter (PM<sub>2.5</sub>) State Implementation Plan (SIP) Requirements Rule,<sup>1</sup> which contains details on planning requirements that apply to areas designated nonattainment for any PM<sub>2.5</sub> national ambient air quality standard (NAAQS). The PM<sub>2.5</sub> SIP Requirements Rule addresses the statutory SIP requirements for state, local and tribal air agencies (hereafter known as "air agencies") such as: general requirements for attainment plan due dates and attainment dates; emissions inventories; attainment demonstrations; provisions for demonstrating reasonable further progress (RFP); quantitative milestones; contingency measures; and nonattainment New Source Review (NNSR) permitting programs.

The PM<sub>2.5</sub> SIP Requirements Rule identifies the four main PM<sub>2.5</sub> precursor pollutants (sulfur dioxide (SO<sub>2</sub>), nitrogen oxides (NO<sub>x</sub>), volatile organic compounds (VOC), and ammonia ( $NH_3$ )) that are required to be addressed in all  $PM_{2.5}$  nonattainment area SIPs. The rule establishes that PM<sub>2.5</sub> precursors must be evaluated for potential control measures in any PM<sub>2.5</sub> attainment plan and any NNSR program. The rule does not include any national presumption that excludes sources of emissions of a particular precursor from further analysis for attainment plan or NNSR control requirements. However, the rule indicates that air agencies may choose to submit an optional precursor demonstration designed to show that for a specific PM<sub>2.5</sub> nonattainment area, emissions of a particular precursor from sources within the nonattainment area do not or would not contribute significantly to PM<sub>2.5</sub> levels that exceed the standard. If the EPA approves the demonstration, the attainment plan for a particular  $PM_{2.5}$  nonattainment area may exclude that precursor from certain control requirements under the Clean Air Act (CAA or Act) (e.g., reasonably available control measures [RACM], reasonably available control technology [RACT], RFP, NNSR), depending on the type of demonstration provided.

This guidance document is designed to assist air agencies that may wish to submit PM<sub>2.5</sub> precursor demonstrations as allowed by the PM<sub>2.5</sub> SIP Requirements Rule. This guidance is intended for use by air agencies; the EPA Headquarters and Regional offices; and the public. This document does not substitute for provisions or regulations of the CAA, nor is it a regulation itself. As the term "guidance" suggests, it provides recommendations or guidelines, as authorized under CAA section 189(e), that will be useful to air agencies in developing the precursor demonstrations by which the EPA can ultimately determine whether sources of one or more precursors contribute significantly to PM<sub>2.5</sub> levels that exceed the standard in a particular nonattainment area. Thus, it does not impose binding, enforceable requirements on any party, nor does it ensure that the EPA will approve a precursor demonstration in all instances where the guidance is followed, as

<sup>&</sup>lt;sup>1</sup> See Fine Particulate Matter National Ambient Air Quality Standards: State Implementation Plan Requirements (PM<sub>2.5</sub> SIP Requirements Rule), 81 FR 58009 (Aug. 24, 2016).

the guidance may not apply to a particular situation based upon the facts and circumstances of a particular nonattainment area.

Where appropriate, and consistent with the requirements of the PM<sub>2.5</sub> SIP Requirements Rule, air agencies retain the discretion to develop precursor demonstrations on a caseby-case basis that differ from this guidance. Final decisions by the EPA to approve a particular precursor demonstration as part of a plan submission will only be made based on the requirements of the statute and applicable regulations, and will only be made following an air agency's final submission of the precursor demonstration to the EPA, and after appropriate notice and opportunity for public review and comment. Interested parties may raise comment about the appropriateness of the application of this guidance to a particular nonattainment area during the approval process for a SIP submittal that includes a precursor demonstration. The EPA and air agencies should consider whether or not the recommendations in this guidance are appropriate for each situation.

### 1.1 Precursor Demonstrations

The PM<sub>2.5</sub> SIP Requirements Rule permits states to submit precursor demonstrations to exclude sources of one or more precursors from control requirements under either the attainment plan or the NNSR program. Below are brief descriptions of comprehensive and major stationary source precursor demonstrations (collectively referred to as attainment plan precursor demonstrations) and NNSR precursor demonstrations.

#### 1.1.1 Comprehensive and Major Stationary Source Precursor Demonstrations

For any Moderate or Serious area plan<sup>2</sup>, an air agency could choose to provide an optional precursor demonstration showing that existing emissions of a particular precursor "do not contribute significantly to PM<sub>2.5</sub> levels that exceed the standard in the area."<sup>3</sup> In the preamble to the PM<sub>2.5</sub> SIP Requirements Rule, the EPA described two potential steps in this analytical process (a concentration-based analysis, and a sensitivity analysis).

*Concentration-Based Analysis*. The first step of the analysis would be to determine whether all emissions of the relevant precursor "contribute significantly" to total  $PM_{2.5}$  concentrations (a "concentration-based analysis"). This can be in the form of (1) a "comprehensive precursor demonstration," in which the state would need to show that emissions of a particular  $PM_{2.5}$  precursor from all existing emissions sources , do not contribute significantly to  $PM_{2.5}$  levels that exceed the standard in the area; or (2) a "major stationary source precursor demonstration," which the state would need to

<sup>&</sup>lt;sup>2</sup> Such plans may include an attainment demonstration or an impracticability demonstration. *See* 40 CFR 51.1011(a)(4)(i) and 40 CFR 51.1011(a)(4)(ii).

<sup>&</sup>lt;sup>3</sup> See 40 CFR 51.1006(a)(1).

show that emissions of a particular precursor from all existing major stationary sources located in the nonattainment area, do not contribute significantly to PM<sub>2.5</sub> levels that exceed the standard in the area. This analysis can be documented through the assessment of recent air quality monitoring data for PM<sub>2.5</sub> component species in the area, emissions inventory information, and/or air quality modeling.

Sensitivity-Based Analysis. If the concentration-based analysis does not support a finding of insignificant contribution, then the air agency could still choose to conduct an optional "sensitivity-based analysis."<sup>4</sup> Through air quality modeling, this sensitivity analysis can either evaluate the effect of reducing emissions of the precursor (by a certain percentage) from all existing emissions sources of the precursor on PM<sub>2.5</sub> levels in the area, or it can evaluate the effect of reducing emissions from only existing major stationary sources on PM<sub>2.5</sub> levels in the area.

If the EPA approves a comprehensive precursor demonstration for a particular nonattainment area, the air agency would not be required to control emissions of the relevant precursor, for any existing source, in the attainment plan for the area.<sup>5</sup> If the EPA approves a major stationary source precursor demonstration for a particular nonattainment area, the air agency would not be required to control emissions of the relevant precursor from existing major stationary sources in the attainment plan for the area.<sup>6</sup>

#### 1.1.2 Nonattainment NSR Precursor Demonstration

*NNSR Analysis*. Under the final rule, a separate optional analysis is available for air agencies that seek to demonstrate that new or modified major stationary sources of a particular precursor would not contribute significantly to PM<sub>2.5</sub> levels that exceed the standard in the nonattainment area.<sup>7</sup> For this demonstration, an air agency would need to provide a separate NNSR precursor demonstration that evaluates "the sensitivity of PM<sub>2.5</sub> levels in the nonattainment area to an increase in emissions of a particular precursor in order to determine whether the resulting air quality changes are significant."<sup>8</sup> If the EPA approves this type of demonstration for a particular nonattainment area, the air agency would be able to exempt such new major stationary sources and major modifications at existing sources from the NNSR requirements for that PM<sub>2.5</sub> precursor in 40 CFR 51.165.<sup>9</sup>

<sup>&</sup>lt;sup>4</sup> See 40 CFR 51.1006(a)(1)(ii) and 51.1006(a)(2)(ii).

<sup>&</sup>lt;sup>5</sup> See 40 CFR 51.1006(a)(1)(iii).

<sup>&</sup>lt;sup>6</sup> See 40 CFR 51.1006(a)(2)(iii).

<sup>&</sup>lt;sup>7</sup> See 40 CFR 51.1006(a)(3).

<sup>&</sup>lt;sup>8</sup> See 40 CFR 51.1006(a)(3)(i).

<sup>&</sup>lt;sup>9</sup> See 40 CFR 51.1006(a)(3)(ii).

This guidance document contains additional details on the recommended procedures for completing each of the three types of PM<sub>2.5</sub> precursor demonstrations defined in the final rule, including techniques for conducting these analyses and recommended contribution thresholds for this purpose. See the PM<sub>2.5</sub> SIP Requirements Rule for more information on these precursor demonstrations, including details on the specific SIP elements that do not need to be addressed based on the approval of a particular precursor demonstration.<sup>10</sup>

<sup>&</sup>lt;sup>10</sup> See PM<sub>2.5</sub> SIP Requirements Rule at 81 FR 58017.

# **Policy Guidance**

## 2.0 Overview

As discussed above, the PM<sub>2.5</sub> SIP Requirements Rule establishes that SO<sub>2</sub>, NO<sub>x</sub>, VOC, and NH<sub>3</sub> are precursors for which sources are to be presumptively evaluated for potential control measures in an attainment plan or any NNSR program for any PM<sub>2.5</sub> nonattainment area. The rule also indicates that an air agency may choose to submit an optional precursor demonstration designed to show that, for a particular PM<sub>2.5</sub> nonattainment area, emissions of one or more precursors from sources within the nonattainment area do not or would not contribute significantly to PM<sub>2.5</sub> levels that exceed the standard. This section discusses the factors that EPA recommends using to determine the degree of impact that reflects a significant contribution on annual and 24-hour PM<sub>2.5</sub> concentrations. Later sections of the guidance describe specific details about how to conduct recommended technical analyses for the three types of precursor demonstrations (attainment plan--comprehensive; attainment plan--major stationary source; and NNSR) included in the final rule.

# 2.1 Interpretation of "Contribute Significantly" in Section 189(e) of the Clean Air Act and the PM<sub>2.5</sub> SIP Requirements Rule

Section 189(e) of the CAA requires that control requirements "for major stationary sources of PM<sub>10</sub> shall also apply to major stationary sources of PM<sub>10</sub> precursors, except where the Administrator determines that such sources do not contribute significantly to PM<sub>10</sub> levels which exceed the standard in the area." Consistent with the decision of the United States Court of Appeals for the District of Columbia Circuit (D.C. Circuit) in *NRDC v. EPA*, 706 F.3d 428 (2013), this provision also applies to the regulation of sources of PM<sub>2.5</sub> precursors in designated PM<sub>2.5</sub> SIP Requirements Rule permits states to submit precursor demonstrations intended to exclude sources of one or more precursors from control requirements under either the attainment plan or the NNSR program. <sup>11</sup> Consistent with the statute, regulatory language at 40 CFR 51.1006 states that an attainment plan precursor demonstration must show that sources "do not contribute

<sup>&</sup>lt;sup>11</sup> See PM<sub>2.5</sub> SIP Requirements Rule, 81 FR 58009 (August 24, 2016). Page 58018 states: "Even though CAA section 189(e) only explicitly contemplates exceptions to control requirements for PM<sub>2.5</sub> precursors from major stationary sources in nonattainment areas, the EPA believes that by analogy it has authority to promulgate regulations that allow states to determine that it is not necessary to regulate PM<sub>2.5</sub> precursors from other sources in nonattainment areas as well, under appropriate circumstances."

significantly to PM<sub>2.5</sub> levels that exceed the standard in the area."<sup>12</sup> In addition, an NNSR precursor demonstration must show that sources will not "contribute significantly to PM<sub>2.5</sub> levels that exceed the standard in the nonattainment area."<sup>13</sup>

The phrase "contribute significantly" and the included terms "contribute" and "significantly" are not defined in section 189, section 302 or any other part of the CAA. Courts have observed that the absence of a statutory definition does not by itself establish that a term is ambiguous. *NRDC v. EPA*, 489 F.3d 1250, 1258 (D.C. Cir. 2007). In the absence of a definition, the ordinary meaning of a term should govern. *Petit v. Dep't of Education*, 675 F.3d 769, 781 (D.C. Cir. 2012). But courts have also observed that the meaning of a statutory term depends on the context in which it is used. *Bell Atlantic Telephone Co. v. FCC*, 131 F.3d 1044, 1047 (D.C. Cir. 1997). EPA's regulations likewise do not include a definition of the term "contribute significantly."<sup>14</sup>

One federal appeals court has recognized, based in part on competing dictionary definitions, that the term "contribute" does not itself have a consistent, ordinary meaning. *Catawba County, N.C. v. EPA*, 571 F.3d 20, 39 (D.C. Cir. 2009). In two different contexts under the CAA, the United States Court of Appeals for the District of Columbia Circuit has observed that the term "contribute" is ambiguous with respect to the degree of air quality effect to which it applies. *Id.* at 38-39; *EDF v. EPA*, 82 F.3d 451, 459, amended by 92 F.3d 1209 (D.C. Cir. 1996).

In the Catawba County case, the court considered the use of this term in section 107(d) of the CAA, which governs EPA actions to designate specific areas as in attainment or nonattainment with the NAAQS. Under this provision, a nonattainment area must include any area that does not meet the NAAQS or "that contributes to ambient air quality in a nearby area that does not meet" the NAAQS. The Petitioners argued that the EPA was required to interpret the word "contribute" in this context to require a "significant causal relationship" in order to include a nearby area in a nonattainment area. The Petitioners also argued that the EPA must establish a quantified amount of impact that gualifies as a contribution before the EPA could include a nearby area in a nonattainment area. Id. The court held that "section 107(d) is ambiguous as to how EPA should measure contribution and what degree of contribution is sufficient to deem an area nonattainment." In doing so, the court noted the Petitioners' citation of one dictionary definition and the EPA's citation of other dictionary definitions of the term "contribute" and concluded that "[t]his alone suggests an ambiguity." Catawba County, 571 F.3d at 39. Consequently, the court held that the EPA was not compelled to apply the Petitioners' preferred meaning of the term "contribute" in the context of section 107(d). The court recognized that the EPA had the discretion to interpret the term

<sup>&</sup>lt;sup>12</sup> See 40 CFR 51.1006(a)(1) and 51.1006(a)(2).

<sup>&</sup>lt;sup>13</sup> See 40 CFR 51.1006(a)(3)(i).

<sup>&</sup>lt;sup>14</sup> EPA's New Source Review Permitting regulations contain a definition of the term "significant," but this definition does not modify the term "contribute" and applies in a different context. *See e.g.*, 40 CFR 51.166(b)(2), (b)(23), (j)(2)-(3).

"contribute" in section 107(d) of the CAA to mean "sufficiently contribute" and that EPA could use a multi-factor test, rather than a quantified threshold, to determine when a nearby area contributed to a NAAQS violation. Likewise, in another case, the court reasoned that "contribute to" in section 176(c) of the CAA is ambiguous and "leaves wide open the question of how large a reduction in emissions must be to constitute a contribution." *EDF v. EPA*, 82 F.3d 451, 459, amended by 92 F.3d 1209 (D.C. Cir. 1996).

Section 189(e) is one of several provisions in the CAA that uses the term "contribute" or similar forms of this term. The reasoning of the *Catawba County* opinion supports the view that EPA has the discretion under section 189(e) to exercise judgment to determine the degree of impact that "contributes" to adverse air quality conditions based on the particular context in which the term "contribute" is used in the CAA. *See* 571 F.3d at 39.<sup>15</sup> Furthermore, this opinion supports EPA's discretion to identify qualitative or quantitative criteria or factors that may be used to determine whether something "contributes," as long as the Agency provides a reasoned basis to justify using such criteria or factors to represent a "contribution."

Although there is ambiguity regarding the degree of impact that "contributes" to an air quality condition, Congress has provided at least some direction regarding the degree of contribution that is required under section 189(e) of the CAA. In this provision, Congress included the term "significantly" after the word "contributes." This indicates that Congress intended to allow for the exemption of sources of a PM<sub>2.5</sub> precursor from control requirements even where there is an impact greater than a simple "contribution," but how much greater is not specified.

The D.C. Circuit has also observed that the term "significant" is ambiguous and may be subject to different meanings in different contexts. *Michigan v. EPA*, 213 F.3d 663, 677-(D.C. Cir. 2000). In this case, the court considered the use of this term in section 110(a)(2)(D)(i)(I) of the CAA, which requires state plans to prohibit those emissions which "contribute significantly" to nonattainment of a NAAQS in a downwind state. The EPA defined the amount of emissions from each state that "contribute significantly" to nonattainment as those emissions exceeding a specified threshold and which could be reduced using "highly cost-effective controls." *Id.* at 675. Petitioners challenged the EPA's reliance on cost effectiveness to define the level of upwind state contribution that qualified as "significant." Petitioners presented conflicting arguments to the court as to whether the statute permitted any consideration of cost, and, as such, the court determined that it could, therefore, discern no clear congressional intent to preclude the consideration of cost. *Id.* at 676-77. The court explained that "[t]he term 'significant' does not itself convey a thought that significance should be measured only in one

<sup>&</sup>lt;sup>15</sup> See also Environmental Defense v. Duke Energy Corp., 549 U.S. 561 (2007) (where the term "modification" and its definition appear, by cross-reference, in two places in the CAA, the EPA may interpret the term differently in the two contexts, so long as it does so in a reasonable manner consistent with the statutory definition).

dimension – here, in the petitioners' view, health alone." *Id.* at 677. Rather, the court explained that the meaning of "significant" may depend on its context and can, in some contexts, "beg a consideration of costs." *Id.* Thus, the court held that "nothing in the text, structure, or history of [section] 110(a)(2)(D) . . . bars EPA from considering costs in its application." *Id.* at 679. Consistent with the reasoning in *Michigan*, the use of the term "significant" in section 189(e) is ambiguous and is subject to a reasonable interpretation based on the context of the term's use. Thus, it is within the Agency's discretion to identify additional qualitative or quantitative criteria or factors to determine whether a contribution is "significant," as long as the Agency provides a reasoned basis to justify using such additional criteria or factors.

#### 2.2 Criteria for Identifying a Contribution

This guidance document on optional precursor demonstrations for the PM<sub>2.5</sub> SIP Requirements Rule describes the factors that the EPA recommends that states consider when seeking to demonstrate that sources of PM<sub>2.5</sub> precursors "do not contribute significantly" to PM<sub>2.5</sub> levels that exceed the NAAQS, for the specific purpose of attainment plan and NNSR program implementation for nonattainment areas. These factors include quantitative "contribution" values based on the Agency's April 17, 2018, memorandum titled "Guidance on Significant Impact Levels for Ozone and Fine Particles in the Prevention of Significant Deterioration Program" (USEPA, 2018a). These "significant impact levels" were derived from a statistical analysis described in the EPA document, "Technical Basis for the EPA's Development of Significant Impact Thresholds for PM<sub>2.5</sub> and Ozone" (USEPA, 2018b), hereafter referred to as the "Technical Basis Document."

The EPA first began developing these quantitative threshold values for use in the Prevention of Significant Deterioration (PSD) permitting program to implement section 165(a)(3) of the CAA, which requires that an applicant for a PSD permit demonstrate that the proposed source will not "cause or contribute" to a violation of any NAAQS or PSD increment. The statistical methods and analysis detailed in the Technical Basis Document focus on using the concept of statistical significance to identify levels of change in air quality concentrations that are not considered to represent a contribution to air quality degradation. The EPA believes the values derived through this method may be used as quantified levels of air quality change that would not "cause or contribute" to an exceedance of the NAAQS. Conversely, an impact above any such level may be viewed as a change that would contribute to an exceedance of the NAAQS.

Since section 189(e) of the CAA also uses the term "contribute," these values may also have relevance in this context. However, as discussed above, in section 189(e) of the CAA the term "contribute" is modified by the term "significantly." As a result, the EPA believes that, for purposes of the PM<sub>2.5</sub> precursor demonstration, other factors may be considered in determining whether an air quality change or impact would "contribute significantly" to PM<sub>2.5</sub> levels that exceed the applicable NAAQS in an area. Under the PM<sub>2.5</sub> SIP Requirements Rule, the significance of a precursor's contribution is to be

determined "based on the facts and circumstances of the area."<sup>16</sup> This section of the guidance document discusses how a state may determine whether emissions of a precursor would "contribute" to a violation of the NAAQS, and section 2.3 discusses factors that may inform a determination of whether a contribution should be treated as significant.

The discussion that follows in this section considers the concept of "statistical significance" that the EPA has used to evaluate whether an impact on ambient air quality should be considered to be a "contribution" under the statute. We strive to promote clarity when applying the results of this statistical analysis within the context of statutory provisions that use the terms "contribute" and "contribute significantly." This guidance document uses the term "contribution" to describe a degree of change in air quality that EPA's statistical analysis shows to be more than "negligible" or "trivial" and thus can be regarded as an impact that "contributes" to air quality concentrations.<sup>17</sup> This is not to be confused with the use of the term "contribute significantly" in the CAA, which the EPA interprets to encompass considering additional factors beyond those used to identify a "contribution." Given that Congress gave more specific direction that we consider whether precursor emissions "contribute significantly" in the context of CAA section 189(e), we have endeavored in this guidance to use the term "contribute significantly" or "significant contribution" only when discussing whether the criteria in section 189(e) for a precursor exemption has been satisfied.

The concept of statistical significance is well established, with a basis in commonly accepted scientific and mathematical theory. The Technical Basis Document notes that the statistical methods and data reflected in that analysis may be applicable for multiple regulatory applications where EPA seeks to identify a level of change in air quality that is either significant or insignificant. As described below, EPA believes a precursor demonstration for a PM<sub>2.5</sub> SIP is another regulatory application where the analysis EPA conducted in the PSD context can be applied. However, this analysis is only the first step of developing quantitative thresholds to initially determine whether there is a "contribution" before looking at other factors to determine if the contribution is "significant."

The Technical Basis Document describes that compliance with the NAAQS is determined by comparing the measured "design value" (DV) at an air quality monitor to the level of the NAAQS for the relevant pollutant.<sup>18</sup> The EPA believes that an insignificant change in ambient air quality can be defined and quantified based on characterizing the observed variability of ambient air quality levels. The Technical Basis Document analysis has been designed to take into account the ambient data used to determine DVs for both the

<sup>&</sup>lt;sup>16</sup> See 40 CFR 51.1006.

<sup>&</sup>lt;sup>17</sup> Here we use "contribution" to be analogous to the term "significant impact" in the PSD permitting program.

<sup>&</sup>lt;sup>18</sup> A design value is a statistic that describes the air quality status of a given location to be compared to the level of the NAAQS. More information may be found at <u>https://www.epa.gov/air-trends.</u>

annual and 24-hour PM<sub>2.5</sub> NAAQS. The EPA's technical approach, referred to as the "Air Quality Variability" approach, relies upon the fact that there is spatial and temporal variability in the observed ambient data and then uses statistical theory and methods to identify a level of change in DVs that is not statistically discernible from the original DV, thereby representing an "insignificant" change in air quality.

Based on these observed ambient data, the EPA has identified changes in air quality levels of PM<sub>2.5</sub> that may be considered an insignificant impact through applying a wellestablished statistical technique known as bootstrapping. Bootstrapping is a method that allows one to determine the accuracy of sample statistics (*e.g.*, mean, percentiles) for a population of data (Efron, 1979 and 2003). The bootstrap approach applied in the Technical Basis Document uses a non-parametric, random resampling with replacement, which recreates the sample dataset (*e.g.*, in this case, the ambient data underlying the DVs), resulting in many resampled datasets. This approach allows one to determine measures of accuracy of sample statistics based on these resampled datasets when the underlying distribution of the statistic is not known (Efron, 1993).

The bootstrap technique, as applied in the air quality variability analysis, quantifies the degree of air quality variability in an area and then allows one to determine appropriate confidence intervals (CIs), *i.e.*, statistical measures of the variability associated with the monitor-based DVs, to inform the degree of air quality change that may be considered "insignificant." This approach for quantifying a degree of impact that contributes to PM<sub>2.5</sub> air quality is fundamentally based on the concept that an anthropogenic perturbation of air quality that is within a specified CI may be considered indistinguishable from the inherent variability in the measured atmospheric concentrations and is, from a statistical standpoint, *not significant* at the given confidence interval. (USEPA, 2018b)

Specifically, the analysis in the Technical Basis Document uses 17 years (2000-2016) of nationwide ambient PM<sub>2.5</sub> measurement data to generate a large number of resampled datasets for PM<sub>2.5</sub> DVs at each monitor. These resampled datasets were used to determine statistical CIs that provide a measure of the inherent variability in air quality at the monitor location. This variability may be driven by the frequency of various types of meteorological and/or emissions conditions affecting a particular location. The analysis estimates a range of CIs for each monitor. In the analysis for the PSD permitting program, EPA selected the 50 percent CI to quantify the level of air quality change that can be considered "insignificant" for the purposes of meeting requirements under that program. The Agency's April 2018 memorandum (USEPA, 2018a) explains the analysis design and describes how the results are applied to develop Significant Impact Levels (SILs) for use in the PSD program.

We believe the air quality variability analysis described in the PSD memorandum (and documented in more detail in the Technical Basis Document) is also suitable for determining in the first instance whether emissions of a PM<sub>2.5</sub> precursor "contribute" to PM<sub>2.5</sub> levels that exceed the NAAQS, as part of a precursor demonstration under the PM<sub>2.5</sub> SIP Requirements Rule. The concept of significance as expressed in the Technical

Basis Document is that an anthropogenic perturbation of air quality that is less than the inherent variability in the measured atmospheric concentration is, from a statistical standpoint, not significant. The statistical analysis of ambient air quality variability is not dependent on the source of the anthropogenic perturbation (e.g., a single stationary source, versus multiple sources across an area). The analysis is based on the variability in ambient data measurements, which is driven by the variability in meteorology and emissions from all sources. This includes near source and long-range impacts from single sources and groups of sources (including major stationary sources, cars, minor sources, etc.). Accordingly, the analysis EPA initially conducted for PSD purposes is equally applicable to a number of circumstances. In this case, PM<sub>2.5</sub> precursor demonstrations attempt to show that a particular perturbation in anthropogenic emissions does not contribute significantly to PM<sub>2.5</sub> levels which exceed the standard in the area. The derived insignificance level from the statistical analysis is not specific to the PSD program. The analysis examines and defines a perturbation in ambient air measurements. EPA used the statistical analysis to define an air quality threshold, below which is considered an insignificant impact. Because the threshold is an ambient airbased value that defines a contribution, it is similarly applicable to both PSD analyses and PM<sub>2.5</sub> precursor demonstrations. This includes both comprehensive demonstrations (examining the impacts from all emissions sources) and major stationary source demonstrations (examining the impacts from only major stationary sources).

As noted above, the 50 percent CI was selected to quantify the level of air quality change that can be considered "insignificant" for the purposes of meeting requirements under the PSD program. The 50 percent level was chosen as a protective (low) level, below which would clearly represent an insignificant impact on air quality. We believe the same logic applies to identifying an impact that "contributes" in the context of precursor demonstrations and, therefore, we recommend use of the same 50 percent CI (and numerical thresholds) for precursor demonstrations. The threshold can be considered a value below which air quality impacts (from both emissions decreases and increases) are not significant or meaningful and thus, do not represent a contribution and, therefore, do not "contribute significantly" to PM<sub>2.5</sub> concentrations that exceed the standard. Note however that merely exceeding the threshold does not necessarily mean that the precursor contributes significantly, additional analysis may be required to make that determination. (*See* section 2.3)

In addition, the statistical significance analysis calculates the inherent variability in the ambient data both above and below the median observed concentrations. In this way, the variability analysis is equally applicable in examining the impact of both emissions *increases* (which would generally lead to higher observed or modeled concentrations) and emissions *decreases* (which would generally lead to lower observed or modeled concentrations), relative to a base case.

The Agency's April 2018 memorandum (USEPA, 2018a) recommends specific concentration values that represent the change in PM<sub>2.5</sub> air quality that can serve to quantify air quality impacts that "contribute" to PM<sub>2.5</sub> concentrations in each area. As

explained in more detail above, even though PM precursor demonstrations and the PSD program serve different purposes, the definition of an air quality "contribution" is viewed in the same manner, using the same ambient data based statistical analysis. Therefore, consistent with the April 2018 memorandum and the accompanying Technical Basis Document analysis, the EPA recommends using the following values for this purpose as part of an optional precursor demonstration under the PM<sub>2.5</sub> SIP Requirements Rule:

- $\geq 0.2 \ \mu g/m^3$  for the annual PM<sub>2.5</sub> NAAQS, and
- $\geq$  1.5 µg/m<sup>3</sup> for the 24-hour PM<sub>2.5</sub> NAAQS.<sup>19</sup>

The EPA believes that these recommended thresholds are appropriate guidelines for identifying an air quality impact level that below which is "insignificant" and thus, for purposes of the precursor demonstration, does not "contribute" to PM<sub>2.5</sub> concentrations subject to the current PM<sub>2.5</sub> NAAQS.<sup>20</sup>

Depending on the type of precursor demonstration conducted, the "perturbation" in air quality can be represented in different ways: as the precursor's impact on ambient PM<sub>2.5</sub> levels due to emissions from all sources or all major stationary sources in the nonattainment area; a decrease in precursor emissions from all sources or all major stationary sources in the nonattainment area; or, in the case of an NNSR demonstration, as an increase in precursor emissions from major stationary sources. As explained above, the thresholds should be appropriate for interpreting the significance of the perturbation for each of these analyses, regardless of whether the evaluation involves the impact of one or more new sources intending to locate in the nonattainment area, or examining the combined impact on PM<sub>2.5</sub> concentrations from multiple existing sources of emissions.

 $<sup>^{19}</sup>$  The recommended 24-hour NAAQS threshold for PM<sub>2.5</sub> precursor demonstrations is 1.5  $\mu g/m^3$ , which is the 50 percent CI value from the air quality variability analysis documented in the technical basis document. However, due to the fact that 40 CFR 51.165(b)(2) still lists 1.2  $\mu g/m^3$  as the significance level for the 24-hour PM<sub>2.5</sub> NAAQS for PSD purposes, it is EPA's intent to apply the 40 CFR 51.165(b)(2) threshold for PSD actions covered by that rule pending further evaluation.

 $<sup>^{20}</sup>$  As described in the Technical Basis Document, the monitoring site variability is first calculated as a percentage of the measured PM<sub>2.5</sub>. Then the median percent variability from all sites is multiplied by the level of the NAAQS to get the threshold concentrations. Therefore, these thresholds represent a percentage of the 2006 24-hour NAAQS (35  $\mu$ g/m<sup>3</sup>) and the 2012 annual NAAQS (12  $\mu$ g/m<sup>3</sup>). Different thresholds may be applicable to other levels and/or forms of the NAAQS (either past or future).

# 2.3 Evaluating Whether a Contribution is "Significant"- Considering Additional Information

An approvable precursor demonstration must show that the air quality change at relevant locations (as described in section 2.4 below) does not "contribute significantly" to  $PM_{2.5}$  levels that exceed the standard. The EPA generally expects that a precursor demonstration will be adequate to support exempting sources of a precursor from control requirements if the analysis shows that the air quality impact at all relevant locations does not exceed the recommended contribution thresholds (*i.e.*, 0.2 µg/m<sup>3</sup> for the annual  $PM_{2.5}$  NAAQS, and 1.5 µg/m<sup>3</sup> for the 24-hour  $PM_{2.5}$  NAAQS).<sup>21</sup>

If the estimated air quality impact is greater than or equal to the recommended contribution threshold, this fact does not necessarily preclude approval of the precursor demonstration. There may be cases where it could be determined that precursor emissions have an impact above the recommended contribution thresholds, yet "do not contribute *significantly*" to levels that exceed the standard in the area (pursuant to section 189(e), emphasis added). Under the PM<sub>2.5</sub> SIP Requirements Rule, the significance of a precursor's contribution is to be determined "based on the facts and circumstances of the area."

Air agencies may thus provide the EPA with information related to other factors they believe should be considered in determining whether the contribution of emissions of a particular precursor to levels that exceed the NAAQS is "significant" or not. Such factors may include: the amount by which a precursor's impact exceeds the recommended contribution threshold(s); the amount by which the cumulative impact from all modeled precursors exceeds the recommended threshold(s); the severity of nonattainment at relevant monitors and/or grid cell locations in the area; whether an area is measuring clean data and the amount by which the current DV is below the NAAQS;<sup>22</sup> the percent of emissions reduction analyzed; source characteristics (*e.g.*, source type, stack height, location); anticipated growth or loss of sources; analyses of speciation data and precursor emission inventories; chemical tracer studies; special intensive measurement

<sup>&</sup>lt;sup>21</sup> The criteria pollutant of concern is total PM<sub>2.5</sub>, for which there are multiple precursors that impact PM<sub>2.5</sub> concentrations. Therefore, if a precursor demonstration is submitted that intends to show that multiple precursors do not contribute significantly to PM<sub>2.5</sub> levels that exceed the standard in the area, the individual impact and the cumulative impact of all modeled precursors should be calculated and documented. A cumulative precursor impact that is above the recommended threshold may be an important consideration in assessing, on a case-by-case basis, if one or more precursors does not "contribute significantly" to PM<sub>2.5</sub> levels that exceed the standard in the area.

<sup>&</sup>lt;sup>22</sup> Note that some areas remain designated nonattainment, even though recent DVs may be below the NAAQS. While NNSR permitting requirements still apply until the area is formally redesignated to attainment, the fact that recent measured DVs are close to or even below the NAAQS can be used as a factor in considering precursor impacts.

studies to evaluate specific atmospheric chemistry in the area; or trends in ambient speciation data and precursor emissions.

We are not recommending one particular approach to evaluating additional factors, and the air agency may provide other information not listed here as well. Any air agency providing additional information should provide a clear rationale explaining how such information supports their claim that the precursor does or does not contribute significantly to PM<sub>2.5</sub> levels that exceed the standard. The EPA will consider such additional information and evaluate each demonstration on a case-by-case basis.

## 2.4 Locations at Which to Evaluate Air Quality Changes

For the comprehensive or major stationary source precursor demonstrations, the EPA believes that air quality changes of concern should be evaluated at existing or relevant historical PM<sub>2.5</sub> monitor locations (*i.e.*, as part of an air quality modeling analysis) because it is at those locations where NAAQS compliance will be determined. The evaluation of air quality changes at monitor locations for attainment plan precursor demonstrations is consistent with the PM<sub>2.5</sub> SIP Requirements Rule's treatment of monitor locations for modeled attainment demonstrations for PM<sub>2.5</sub> nonattainment areas.<sup>23</sup>

For an NNSR precursor demonstration, the EPA believes that the analysis should evaluate the projected air quality change from potential future major stationary sources in all parts of the nonattainment area (*i.e.*, all grid cells in an air quality modeling analysis) rather than just at existing monitor locations. While a monitor-based analysis is appropriate for nonattainment area planning, where the existing PM<sub>2.5</sub> ambient monitoring network is designed to represent air quality based on the geographic orientation and magnitude of existing sources, this contrasts with NNSR, where new major stationary sources might locate in parts of the nonattainment area that are not currently well represented by the current monitoring network. The overall objective of the NSR program is to prevent future violations. Therefore, it is important to examine the sensitivity of the entire nonattainment area to potential increases in precursor emissions to support a request to exempt sources of that precursor from NNSR permitting. This recommendation is consistent with how new major stationary sources are treated in modeling analyses required to be conducted for the PSD program (USEPA, 2014).

<sup>&</sup>lt;sup>23</sup> See PM<sub>2.5</sub> SIP Requirements Rule at 81 FR 58051.

# **Technical Guidance**

# 3.0 Concentration-Based Analysis

If an air agency chooses to perform a precursor demonstration for an attainment plan (either a comprehensive or major stationary source analysis), the final rule requires that the demonstration must include a concentration-based analysis.<sup>24</sup> This demonstration can consist of analyses using ambient data or it could optionally include air quality modeling. The goal of the comprehensive plan analysis is to examine the overall impact on PM<sub>2.5</sub> air quality in the nonattainment area as a result of emissions of a particular precursor from all existing sources (including stationary, area, and mobile sources). A major stationary source analysis examines the overall impact on PM<sub>2.5</sub> air quality from emissions of a particular precursor from all existing major stationary sources.

The recommended starting point for such an analysis is an evaluation of all available ambient air quality monitoring data for the area (and possibly nearby areas). The EPA recommends an examination of total PM<sub>2.5</sub> data (in the form of Federal Reference Method (FRM) measurements, Federal Equivalent Methods (FEM) measurements, Interagency Monitoring of Protected Visual Environments (IMPROVE) data, and/or other special study or research data), and ambient PM<sub>2.5</sub> speciation data, which characterizes the composition of total mass. PM<sub>2.5</sub> species data are critical for this analysis, since they allow for an accounting of ambient secondary PM<sub>2.5</sub> concentrations and provide a way to link precursor emissions to secondary PM<sub>2.5</sub> components.<sup>25</sup> See details on PM<sub>2.5</sub> species components and accounting for the various measured species in section 3.1, below. Additional analyses and information, including emissions inventory data and modeling can also be used to support a concentration-based analysis. This may be particularly important for major stationary source analyses since in most cases it is difficult to estimate major stationary source impacts solely from ambient data. See sections 3.1.7 and 3.2 for more details.

## 3.1 Ambient Data Analysis of Secondarily-Formed PM<sub>2.5</sub>

PM<sub>2.5</sub> is a complex and highly variable mixture, but the majority of PM<sub>2.5</sub> mass is comprised of five constituents: (i) organic matter (OM); (ii) elemental carbon (EC); (iii) crustal material; (iv) ammonium sulfate ((NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>); and (v) ammonium nitrate (NH<sub>4</sub>NO<sub>3</sub>) (Hand, 2012) (Seinfeld, 2006). In general, EC and crustal PM<sub>2.5</sub> are considered "primary" components (*i.e.*, they are emitted directly from sources and are not the product of chemical reactions of precursor gases in the atmosphere). (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub> and NH<sub>4</sub>NO<sub>3</sub> are considered "secondarily formed" PM<sub>2.5</sub> components because they are the

<sup>&</sup>lt;sup>24</sup> See 40 CFR 51.1006(a)(1)-(2).

<sup>&</sup>lt;sup>25</sup> Ambient data, including PM speciation data can be found at EPA's AQS Data Mart: <u>https://aqs.epa.gov/aqsweb/documents/data\_mart\_welcome.html.</u>

product of chemical reactions of precursor gases in the atmosphere.<sup>26</sup> OM can have both primary and secondary components. Since this guidance addresses precursors to secondary  $PM_{2.5}$ , we will focus the discussion on the most common secondary  $PM_{2.5}$  components.

A large number of possible chemical reactions, often non-linear in nature, can convert the gases SO<sub>2</sub>, NO<sub>x</sub>, VOC and NH<sub>3</sub> to PM<sub>2.5</sub>. Thus, these gases are precursors to PM<sub>2.5</sub>. OM is the fraction of ambient PM<sub>2.5</sub> with the most diverse chemical composition, containing potentially thousands of different organic compounds (*i.e.*, those compounds containing carbon) composed primarily of carbon, hydrogen, oxygen and nitrogen. Both primary particles and secondary particles contribute to ambient OM concentrations. Secondary OM particle formation involves oxidation of both anthropogenic and biogenic (plant-derived) VOC, and can involve other, more complex chemical reactions. Sulfate (SO<sub>4</sub>), nitrate (NO<sub>3</sub>) and ammonium (NH<sub>4</sub>), react in the ambient air to form ammonium sulfate ((NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>) and ammonium nitrate (NH<sub>4</sub>NO<sub>3</sub>). If there is not enough NH<sub>3</sub> in the ambient air to neutralize fully the available sulfate, ammonium bi-sulfate (NH<sub>4</sub>HSO<sub>4</sub>) or sulfuric acid (H<sub>2</sub>SO<sub>4</sub>) may also form. In addition, particle-bound water is often also associated with measured sulfate and nitrate PM<sub>2.5</sub>. A brief discussion of SO<sub>4</sub>, NO<sub>3</sub> and Secondary Organic Aerosol (SOA) formation, as well as the role of NH<sub>3</sub> in their formation, follows.

#### 3.1.1 Ammonium Sulfate

SO<sub>2</sub> is a gas-phase species emitted mostly from the combustion of fossil fuels (the largest source is coal combustion from electric utility boilers). When SO<sub>2</sub> oxidizes, it forms aerosol sulfuric acid. In the presence of NH<sub>3</sub>, however, sulfuric acid will react to form ammonium sulfate [(NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>], a less acidic compound and one of the five major components of PM<sub>2.5</sub>. If there is not enough NH<sub>3</sub> present to fully neutralize the sulfuric acid, part of it may convert to ammonium bi-sulfate (NH<sub>4</sub>HSO<sub>4</sub>), which is more acidic than ammonium sulfate [(NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>], but less so than sulfuric acid. All three products [H<sub>2</sub>SO<sub>4</sub>, NH<sub>4</sub>HSO<sub>4</sub>, and (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>] solely reside as particle-phase (or aqueous-phase) species in the atmosphere. There is a large amount of emerging scientific evidence that SO<sub>2</sub> may also contribute to the formation of SOA from biogenic VOC emissions (*see* section later on SOA). Sulfate levels in the ambient air peak in summer months due to increased SO<sub>2</sub> emissions, generally from electric generating units (EGUs), and from meteorological conditions that are conducive to sulfate formation.

#### 3.1.2 Ammonium Nitrate

The main sources of NO<sub>x</sub> emissions are combustion of fossil fuel in boilers (*e.g.*, electric utility boilers) and internal combustion engines (*e.g.*, cars and trucks). NO<sub>x</sub> reacts in the

<sup>&</sup>lt;sup>26</sup> There is a small primary component to both sulfate and nitrate ions, but the vast majority of measured sulfate and nitrate is secondary in nature.

atmosphere to form nitric acid. In the presence of NH<sub>3</sub>, nitric acid converts to ammonium nitrate, one of the five main components of PM<sub>2.5</sub>. Low temperatures and high relative humidity create ideal conditions for the formation of ammonium nitrate, typically leading to higher atmospheric levels in winter months and lower levels in summer months (Hand, 2012). At high temperatures and low relative humidity, particulate nitrate (most commonly in the form of ammonium nitrate) converts back into its component species of nitric acid (HNO<sub>3</sub>) and ammonium ion (NH<sub>4</sub>). Therefore, nitrate ion (NO<sub>3</sub>) cannot exist in particulate form without being neutralized by NH<sub>3</sub> or another neutralizing cation.<sup>27</sup> Similarly, NH<sub>3</sub> would not exist in particle form if not for the presence of acidic species (sulfate or nitrate) with which it can combine to form a particle.

#### 3.1.3 Secondary Organic Aerosols

VOCs (both anthropogenic and biogenic) are key precursors to the SOA component of PM<sub>2.5</sub>. The relative importance of these compounds in the formation of organic particles varies between geographic areas, depending upon local emission sources, atmospheric chemistry and season of the year. It should be further noted that not all inventoried VOC might be contributing to the formation of organic particles. For example, chemical reactions involving VOC are generally accelerated in warmer temperatures, and, for this reason, studies show that SOA typically comprises a higher percentage of PM<sub>2.5</sub> in the summer than in the winter (Pandis, 1992).

Anthropogenic sources of VOC include mobile sources, petrochemical manufacturing, oil and gas emissions and solvents (USEPA, 2016a). In addition, some biogenic VOC, emitted by vegetation such as trees, can contribute significantly to SOA formation, especially in heavily forested areas, such as the Southeast U.S. It should be noted, however, that anthropogenic impacts on SOA are likely highest in the wintertime when biogenic SOA levels are lower; conversely, in the summertime, the influence of biogenic emissions on SOA is likely higher (Carlton, 2010a). Despite significant progress in understanding the origins and properties of SOA, it remains the least understood component of PM<sub>2.5</sub> and continues to be a significant topic of research and investigation.

#### 3.1.4 Role of NO<sub>x</sub> and SO<sub>2</sub> in Secondary PM Chemistry

In addition to influencing secondary particulate nitrate formation, NO<sub>x</sub> also reacts with anthropogenic and biogenic VOC to enhance the secondary formation of sulfate and organic compounds that make up SOA (Carlton, 2010b). NO<sub>x</sub> is thus involved in all secondary PM chemistry, not just in particulate nitrate formation. Similarly, recent

<sup>&</sup>lt;sup>27</sup> If ammonia is not available, nitric acid can also be neutralized by calcium (Ca) or sodium (Na) (if available) to form calcium nitrate  $[Ca(NO_3)_2]$  and sodium nitrate  $(NaNO_3)$ , respectively. Unlike ammonium nitrate,  $Ca(NO_3)_2$  and  $NaNO_3$  do not convert back to the gas phase at higher temperatures.

research has indicated that  $SO_2$  can impact SOA formation (Surrat, 2010). One recent study found that chemical reactions involving  $SO_2$  and  $NO_x$  combined may be responsible for up to 70 percent of the total measured organic aerosol in the Southeast U.S. in the summer (Xu, 2015). Consequently, when  $NO_x$  or  $SO_2$  emissions are decreased or increased in the atmosphere, there can be impacts on all secondary  $PM_{2.5}$  species, including ammonium ion, nitrate ion, sulfate ion, and SOA.

#### 3.1.5 Assigning PM<sub>2.5</sub> Species to Precursors - Summary

Ambient PM<sub>2.5</sub> species data are generally measured and reported as OM, EC, crustal, nitrate, sulfate, and ammonium. For the purpose of precursor demonstrations, elemental carbon and crustal PM<sub>2.5</sub> can be ignored (since they are primary species). One basic way of developing a concentration-based analysis for a particular precursor is to calculate the portion of the total PM<sub>2.5</sub> mass measured at the relevant location that is associated with the precursor. The EPA's default recommendation for "assigning" the measured secondary PM<sub>2.5</sub> species to their respective precursors is shown in Table 1 below:

PM <sub>2.5</sub> Recommended Assignment to		Comment
Precursor	PM <sub>2.5</sub> Species	
NO <sub>x</sub>	Nitrate ion + portion of	Include all measured nitrate ion plus
	ammonium associated with	the ammonium that is in the form of
	nitrate	ammonium nitrate (do not include
		the ammonium attached to sulfate).
SO <sub>2</sub>	Sulfate ion	All measured sulfate ion.
NH <sub>3</sub>	Ammonium + nitrate ion	Include all measured ammonium
		(including ammonium attached to
		sulfate and nitrate), and nitrate ion.
VOC	SOA	Estimate the secondary component
		of OM. This can be further
		disaggregated into the impact on
		SOA from anthropogenic VOC
		sources.

Table 1. Default Recommended Assignment of PM<sub>2.5</sub> Precursors to PM<sub>2.5</sub> Species

Further explanation of the recommended assignments outlined in Table 1 is provided as follows:

• **NO**<sub>x</sub>- the default recommendation assigns measured nitrate to NO<sub>x</sub> as well as the portion of ammonium that is attached to nitrate in the form of ammonium nitrate. When considering the impact of NO<sub>x</sub> on PM<sub>2.5</sub>, NO<sub>x</sub> directly influences the formation of ammonium nitrate. However, nitrate ion cannot exist in the atmosphere as a particle without being neutralized by NH<sub>3</sub> (it would exist as a gas in the form of nitric acid). Therefore, the ammonium portion of ammonium

nitrate should also be counted when evaluating whether  $NO_{x}$  contributes to  $PM_{2.5}\ mass.$ 

- **SO**<sub>2</sub>- The default recommendation assigns measured sulfate to SO<sub>2</sub>. Note that the ammonium attached to sulfate (mostly in the form of ammonium sulfate) is not counted toward the SO<sub>2</sub> impact on PM<sub>2.5</sub> mass because sulfate can exist in the atmosphere as a particle in the form of sulfuric acid even if it is not neutralized by NH<sub>3</sub>.
- NH<sub>3</sub>- The default recommendation assigns all measured ammonium to NH<sub>3</sub> as well as the entire nitrate ion mass. This is for the same reason that part of ammonium is assigned to NO<sub>x</sub>. Ammonium nitrate cannot exist in the atmosphere as a particle without being neutralized by NH<sub>3</sub>. Therefore, if no NH<sub>3</sub> were present, nitrate would exist only as a gas (in the form of nitric acid). As a result, all of the mass of ammonium nitrate should also be counted towards ammonia's impact on PM<sub>2.5</sub> mass. <sup>28</sup>
- **VOC** The default recommendation assigns measured SOA to VOC. The most conservative assumption is to assume that all of the measured organic aerosol mass is SOA.<sup>29</sup> However, SOA is only a portion of measured organic mass and is not directly measured. Therefore, in some cases, the SOA portion can be estimated through data analysis techniques (Cabada, 2004; Saylor, 2006; Lewandowski, 2008; and Rutter, 2014). In some areas, a high percentage of SOA originates from biogenic sources (especially in the summer). Therefore, if SOA is estimated as a percentage of total organic mass, the SOA concentration can be further refined by estimating the portion of SOA that is a result of anthropogenic VOC emissions.<sup>30</sup>

The default recommendations above are the simplest and most straightforward assignment of precursors to species. However, other methods may be used to estimate alternative PM<sub>2.5</sub> concentration apportionment. For example, the PM<sub>2.5</sub> attainment demonstration modeling guidance recommends the use of the "sulfate, adjusted nitrate, derived water, inferred carbonaceous material balance approach" (SANDWICH) (Frank, 2006) to adjust measured PM<sub>2.5</sub> species data to match better the total PM<sub>2.5</sub>

 $<sup>^{28}</sup>$  If an air agency submits precursor demonstrations for both ammonia and NO<sub>x</sub>, the nitrate component should be counted towards the contribution of both precursors to ambient PM<sub>2.5</sub> levels. This is appropriate since particulate ammonium nitrate formation is dependent on having both nitric acid (from NO<sub>x</sub>) and ammonia available.

<sup>&</sup>lt;sup>29</sup> The measured organic carbon should be multiplied by an appropriate factor (typically 1.4 to 1.8) to convert from organic carbon to organic mass (which includes additional mass attached to the carbon).

<sup>&</sup>lt;sup>30</sup> Due to the difficulty in calculating SOA and the contribution of VOC to ambient PM<sub>2.5</sub> data, air quality modeling may be the most straightforward way to determine the VOC contributions (see section 5).

mass, which is measured on FRM filters. The FRM mass, which is compared to the NAAQS to determine attainment/nonattainment, suffers from various artifacts, which can affect the concentration of some PM<sub>2.5</sub> species collected on Teflon filters. For example, organic mass experiences both positive and negative artifacts, and nitrate mass is generally lower (negative artifact) on FRM filters compared to species measurements, due to temperature and humidity influences. In addition, the SANDWICH technique estimates particle bound water mass, which is attached to both sulfate and nitrate particles. The water mass should be counted in assessing a contribution to PM<sub>2.5</sub> because it is collected on the filter and counted as measured PM mass that is part of total PM<sub>2.5</sub>. In addition to SANDWICH, there may be other technically credible adjustments that can be applied to measured species data, depending on the nature of the species, the area of the country, and the season in which the measurement occurs. Although prior guidance recommends these methods, all adjustments to ambient data should be discussed with the EPA Regional office and carefully documented and explained.

#### 3.1.6 Evaluating Concentration Based Analysis Results

The estimated impact on PM<sub>2.5</sub> mass from a specific precursor should be compared to the recommended "contribution" thresholds for the annual and/or 24-hour NAAQS that were identified in section 2.2.

#### 3.1.7 Additional Information

In addition to ambient PM<sub>2.5</sub> species data, other information can be used to support the concentration-based analyses. Emissions inventory data (i.e., such as data from the National Emissions Inventory<sup>31</sup> or from the inventory developed for the nonattainment area plan by the state or local air agency) can help support claims that a precursor does not contribute significantly to PM<sub>2.5</sub> concentrations in the nonattainment area, particularly when emissions of the precursor are small. Other considerations in the demonstration can be the size of the nonattainment area, the population of the nonattainment area, geographical considerations (such as an isolated mountain valley area), meteorological considerations, etc. The default recommendation is to compare the measured ambient  $PM_{2.5}$  species data to the relevant air quality "contribution" threshold. However, there are other techniques that can be used to attempt to further account for the impact of sources in the nonattainment area on ambient data concentrations. Analyses to support the disaggregation of ambient data into the local nonattainment area impact should be as detailed as possible, focused on the precursor(s) of interest in the demonstration, and discussed with the appropriate EPA Regional office. Note also that air quality modeling is the most technically credible way

<sup>&</sup>lt;sup>31</sup> NEI data can be found at: <u>https://www.epa.gov/air-emissions-inventories/national-emissions-inventory-nei.</u>

to calculate the concentration of  $PM_{2.5}$  mass due to emissions sources from within the nonattainment area. *See* section 3.2 below for more details.

## 3.2 Air Quality Modeling

Air quality modeling can also be used to quantify the impact of precursors on PM<sub>2.5</sub> concentrations in a nonattainment area. In general, air quality modeling is resource intensive, but it is the most direct method to capture the non-linear and complicated associations between PM<sub>2.5</sub> precursor emissions and PM<sub>2.5</sub> concentrations. For example, in the ambient data analysis section above, we delineated many caveats and assumptions that need to be considered when estimating the impact of precursor emissions on measurements of specific  $PM_{2.5}$  species. Many of those assumptions are not necessary when evaluating air quality modeling outputs (although there are different considerations and assumptions that are involved). A photochemical grid model takes into account the complicated chemical interactions among precursors and tracks the individual species concentrations, including species like SOA,<sup>32</sup> which cannot be directly quantified from measurements. Photochemical modeling also allows a potentially more precise accounting of impacts from precursor emissions in the nonattainment area. In addition, since air quality modeling is both a statutory and regulatory requirement for Moderate and Serious PM<sub>2.5</sub> attainment demonstrations,<sup>33</sup> most nonattainment areas will have photochemical air quality modeling available to support their modeled attainment demonstration.

Air agencies have several choices to analyze modeled air quality impacts of precursor emissions on PM<sub>2.5</sub> as part of a concentration-based analysis. The simplest approach would be to perform brute force "zero-out" model runs, which involves at least two model runs: one "baseline" run with all emissions, and one with anthropogenic emissions of the precursor of interest removed from the nonattainment area in the original baseline simulation (Cohan et al., 2005). The difference between these simulations provides an estimate of the air quality change due to the precursor emissions.

<sup>&</sup>lt;sup>32</sup> Photochemical modeling of SOA is generally more uncertain than the other PM<sub>2.5</sub> components. SOA formation is not yet fully understood mechanistically and, therefore, cannot yet be reliably modeled. Because we lack reliable tools for distinguishing between primary and secondary organic aerosol in the ambient air and have even less confidence that models can reliably simulate SOA formation, it is difficult to validate a modeled conclusion that VOC precursor emissions have an insignificant contribution to PM<sub>2.5</sub>. Therefore, especially in the case of VOC as a precursor, additional evidence should be submitted to help validate modeling results. Additional information could include ambient data analyses, special study data and research, and detailed emissions information (*e.g.*, VOC speciation data showing that the makeup of the nonattainment area VOC emissions are not likely to form SOA).

<sup>&</sup>lt;sup>33</sup> See CAA section 189(a)(1)(B), CAA section 189(b)(1)(A), 40 CFR 51.1009(a)(4) and 40 CFR 51.1010(a)(5).

An alternative approach to isolating precursor impacts in photochemical grid models is "photochemical source apportionment." Some photochemical models have been developed with a photochemical source apportionment capability, which tracks emissions from specific sources or groups of sources and/or source regions through chemical transformation, transport, and deposition processes to estimate the apportionment of predicted PM<sub>2.5</sub> species concentrations (Kwok et al., 2015; Kwok et al., 2013). Source apportionment (ENVIRON, 2016; Kwok et al., 2015; Kwok et al., 2013; Wang et al., 2009) has been implemented in modeling systems such as the Comprehensive Air Quality Model with Extensions (CAMx) (ENVIRON, 2016) and the Community Multiscale Air Quality (CMAQ) (Byun and Schere, 2006).

#### 3.2.1 Evaluating Modeling Results

The calculated impact of the precursor on total  $PM_{2.5}$  concentrations should be compared to the "contribution" thresholds for annual and 24-hour  $PM_{2.5}$  identified in section 2.2. See section 5 for more details on the choice of models, model setup, and post-processing of model results.

# 4.0 Sensitivity Based Analysis

The PM<sub>2.5</sub> SIP Requirements Rule also allows for an optional "sensitivity-based" analysis for attainment plan demonstrations.<sup>34</sup> This modeling analysis examines the sensitivity of ambient PM<sub>2.5</sub> concentrations in the nonattainment area to decreases in precursor emissions in the area. This type of optional analysis is only necessary if the concentration-based analysis described above fails to demonstrate that a precursor does not contribute significantly to PM<sub>2.5</sub> concentrations in the nonattainment area. By performing a sensitivity analysis, it may still be possible for an air agency to demonstrate adequately that a precursor contribution is insignificant. Where decreases in emissions of the precursor result in insignificant air quality impacts (*i.e.*, the area is "not sensitive" to decreases), such a small degree of impact can be considered to not "contribute" to  $PM_{2.5}$  concentrations for the purposes of determining whether control requirements should apply. Accordingly, the EPA expects that it will approve a precursor demonstration if it can adequately be shown that the area is not sensitive to precursor emissions reductions. Note that the sensitivity analysis described in this section is only applicable to evaluating emissions reductions as part of the attainment plan part of the SIP. A similar but distinct sensitivity analysis is applicable to NNSR precursor demonstrations, but addresses sensitivity to precursor emissions *increases* rather than decreases (see section 6 for more details on NNSR precursor demonstrations).

A sensitivity-based analysis demonstrates the degree to which PM<sub>2.5</sub> concentrations in the nonattainment area are sensitive to decreases of one or more precursors. Changes in PM<sub>2.5</sub> concentrations at a particular location often will not be linear with respect to

<sup>&</sup>lt;sup>34</sup> See 40 CFR 51.1006(a)(1)(ii) and 40 CFR 51.1006(a)(2)(ii).

changes in  $PM_{2.5}$  precursor emissions. As previously discussed, several  $PM_{2.5}$  components are secondarily formed in the atmosphere as the result of chemical reactions between various  $PM_{2.5}$  precursors. In some nonattainment areas, one precursor may be abundant while a second precursor, with which it primarily reacts, may be less abundant. In such cases, a modeled sensitivity analysis may find that  $PM_{2.5}$  concentrations in the area are relatively insensitive to emissions reductions of the more abundant precursor.

## 4.1 Modeling for Sensitivity Demonstrations

Precursor demonstrations analyze the relationship between precursor emissions and the formation of secondary PM<sub>2.5</sub> components. Air quality models are the most appropriate tool to be able to predict the impact of precursor emissions reductions on PM<sub>2.5</sub> concentrations. Since PM<sub>2.5</sub> precursors form secondary PM<sub>2.5</sub> through chemical reactions, a chemical transport model (CTM) is best able to examine the sensitivity of precursor emissions to secondary PM<sub>2.5</sub> concentrations. See section 5 for more details on CTMs.

As part of performing a sensitivity analysis, there are two additional questions that need to be addressed:

- 1) What amount of emissions reduction should be examined as part of a sensitivity analysis?
- 2) What air quality concentration threshold should be used to determine if the modeled air quality change from the precursor is insignificant?

#### 4.1.1 Emissions Reductions for Sensitivity Analyses

When deciding on the appropriate emissions reduction to model in a sensitivity analysis, it is important to consider the nature of the question being asked. In this case, the CAA and the PM<sub>2.5</sub> SIP Requirements Rule allow a demonstration to show that emissions of a precursor in the area do not contribute significantly to PM<sub>2.5</sub> levels that exceed the standard in the area.<sup>35</sup> Given the emissions makeup and resultant interactions between precursors in the area, the pertinent question is whether PM<sub>2.5</sub> concentrations in the nonattainment area are "insensitive" to certain amounts of emissions reductions of the precursor. This question should not be confused with whether there are known available emissions reductions of a certain size within the nonattainment area. For example, an air agency may identify only a very small percentage precursor reduction from available controls. However, modeling the sensitivity of the area to that very small percentage reduction and then comparing it to EPA's recommended thresholds does not effectively answer whether the area is sensitive to the precursor. The analysis should use a percentage emissions reduction (or a series of different percentage

<sup>&</sup>lt;sup>35</sup> See CAA section 189(e) and 40 CFR 51.1006(a).

reductions model runs) that is large enough to provide a robust answer (given nonlinearities due to complex secondary PM<sub>2.5</sub> chemistry).

The EPA recommends modeling a range of percentage emissions reductions for all sensitivity analyses. For attainment plan analyses of existing emissions sources, a fixed tonnage reduction of a precursor would not be appropriate since the number of tons of precursors in each nonattainment area may vary by orders of magnitude. Therefore, a percentage reduction is appropriate for this type of analysis because it allows for consistency between nonattainment areas and takes into consideration the amount of existing emissions of the particular precursor in each area.

The definition of the range of percentage emissions reductions to model should consider two basic factors:

- 1) The reduction should be large enough to test the interaction and non-linearity of the secondary PM<sub>2.5</sub> components, such as those considered in the published literature.
- 2) The reduction should not be so large that it alters the chemistry in such a way that gives an unrealistic PM<sub>2.5</sub> concentration response, especially given emissions reductions that could possibly occur within the 6-10 year timeframe of Moderate and Serious area attainment demonstrations.

The percentage reduction should not be solely based on an analysis of potential emissions reductions over the next 6-10 year period. This approach could lead to claims of very small emissions reductions, which may not be large enough to truly test whether the area is sensitive to precursor emissions reductions. Therefore, the EPA is recommending a range of percentage precursor emissions reductions that is applicable to all sensitivity demonstrations.

Based on the information available at this time, the EPA recommends application of multiple percentage emissions reductions sensitivities, which span what has typically been seen in the published literature.<sup>36</sup> The EPA recommends a range of 30-70 percent reductions in precursor emissions in the nonattainment area to test the PM<sub>2.5</sub> concentration sensitivity of an area. Multiple model runs can be conducted which test the PM<sub>2.5</sub> sensitivity within the recommended range. For example, model runs of 30 percent, 50 percent, and 70 percent precursor reductions would test the entire

<sup>&</sup>lt;sup>36</sup> The EPA examined examples in the published literature of general sensitivity modeling studies that look at the impact of across-the-board percentage reductions in precursor emissions on secondary pollutants (including PM<sub>2.5</sub>, PM<sub>10</sub>, and ozone) (Vieno, 2016; Megaritis, 2013; Harrison, 2013; Derwent, 2014; Liu, 2010; Pun, 2001). The majority of studies have used across-the-board percentage precursor emissions reductions of between 30 and 60 percent, with the most common reduction percentages being 30 and 50 percent.

sensitivity range to see whether the contribution threshold is exceeded within the range of reductions. Air agencies can perform multiple model runs to test various sensitivity levels and provide a range of impacts. However, modeling the *highest end* of the percent reduction range as the initial model run will potentially limit the resources involved in the analysis. If the modeled PM<sub>2.5</sub> concentration change at the highest end of the percent reduction range is below the recommended threshold, then additional lower percentage model sensitivity runs will likely not be needed. If, however, the modeled concentration change is above the threshold, then additional lower percentage sensitivity model runs would help identify the point where the threshold is exceeded. For the reasons stated above, in most cases, the EPA recommends that air agencies do not use percent reductions of less than 30 percent for sensitivity analyses.

Review of recent projections of expected emission changes suggests that EPA's recommended range is reasonable. For example, the EPA compiled the estimated state level percent change in precursor emissions between 2011 and 2017 from the Cross-State Air Pollution Rule Update rulemaking documentation (USEPA, 2016a). This represents an emissions change, which occurred over a 6-year period, which is the same amount of time allowed for a Moderate PM<sub>2.5</sub> area to attain the NAAQS. Table 2 shows a summary of the emissions analysis.

Table 2. Nationwide State Level<sup>37</sup> Total Percent Change<sup>38</sup> in Anthropogenic<sup>39</sup> PM<sub>2.5</sub> Precursors Between 2011 and 2017

PM <sub>2.5</sub> Precursor	Median emissions change (%)	Range of emissions changes (%)
NOx	-31.8%	-7.7% to -39.9%
SO <sub>2</sub>	-63.6%	-15.2% to -89.0%
VOC	-18.8%	57.5 % to -26.9%
NH <sub>3</sub>	0.8%	6.1% to -9.3%

The percent change in emissions in Table 2 show a wide variation by precursor. In general, the largest reductions were seen in  $SO_2$  emissions (median value of -64 percent), with NO<sub>x</sub> having the second largest reductions (median value of -32 percent). VOC had a larger range of changes (including some increases) and more than half of the states had estimated increases in NH<sub>3</sub> over the example 6-year period. The emissions data show that at least half of the states achieve more than a 30-percent reduction in NO<sub>x</sub> and SO<sub>2</sub> in the 6-year period.

<sup>&</sup>lt;sup>37</sup> The percent change in precursor emissions was calculated for each of the lower 48 states. The 2011 data are historical emissions, derived primarily from the National Emissions Inventory. The 2017 emissions were projected from the 2011 data.

<sup>&</sup>lt;sup>38</sup> Negative percent changes reflect a de*crease* in emissions. Positive percent changes reflect an *increase* in emissions.

<sup>&</sup>lt;sup>39</sup> Emissions totals do not include biogenic (NO<sub>x</sub> or VOC) emissions or fires.

In addition, it can be seen in Table 2 that certain PM<sub>2.5</sub> precursors (*e.g.*, SO<sub>2</sub>) have been reduced by as much as 60-90 percent over the 2011-2017 period. This does not indicate an additional 60 plus percentage reduction in SO<sub>2</sub> (or any other precursor) will occur in any future 6 or 10-year period. However, depending on the circumstances in the area, it may be appropriate to consider emissions sensitivities that are much larger than a 30 percent reduction (e.g, up to 70 percent, as referenced above). This is especially true in nonattainment areas which can expect large additional emissions reductions of certain precursors from on-the-books controls and in areas that are dominated by one or a few stationary sources or categories of sources that are largely uncontrolled.

Consistent with the PM<sub>2.5</sub> SIP Requirements Rule, the EPA may in some cases require air agencies to evaluate available emissions controls in support of a precursor demonstration that relies on a sensitivity analysis.<sup>40</sup> It is particularly important for states to evaluate available controls where the recommended contribution threshold – that is, the threshold used for identifying an impact that is "insignificant" – is close to being exceeded at the low end of the recommended sensitivity range (e.g., 30 percent). In these cases, the EPA may determine that to sufficiently evaluate whether the area is sensitive to reductions, the state must determine the potential precursor emission reductions achievable through the implementation of available and reasonable controls for a Moderate area (or best controls for a Serious area). For example, an area that determines it is close to exceeding the contribution threshold with a 30-percent precursor emissions reduction may need to evaluate the impact (*i.e.*, the percent reduction in the precursor) of the application of reasonably available controls of the relevant precursor. An evaluation of potential controls is less likely to be needed for areas that do not exceed the contribution threshold at a higher modeled percent reduction (e.g., 50-70 percent). The air agency should consult the appropriate EPA Regional office to determine whether an emissions control analysis is needed to support a particular precursor demonstration.

In summary, for a comprehensive sensitivity-based analysis, the EPA recommends modeling reductions of 30-70 percent of all existing anthropogenic emissions of the precursor (including stationary, area, and mobile sources) in the nonattainment area. For a major stationary source sensitivity-based analysis, the EPA recommends modeling reductions of 30-70 percent of anthropogenic emissions of the precursor from existing major stationary sources in the nonattainment area. In addition, the EPA may in some cases require air agencies to evaluate available emissions controls in support of a precursor demonstration.

<sup>&</sup>lt;sup>40</sup> See 40 CFR 51.1009(a)(2) and 51.1010(a)(2).

#### 4.1.2 Evaluating Sensitivity Modeling Results

As noted previously, the EPA recommends comparing the estimated impacts of precursor emissions on PM<sub>2.5</sub> mass from sensitivity modeling to the contribution thresholds for the annual average and 24-hour NAAQS, as appropriate, identified in section 2.2.<sup>41</sup> The EPA generally expects that if modeling demonstrates that reductions in the 30-70 percent range produce an air quality impact below these thresholds, then it would approve such a demonstration as adequate to show that the precursor is insignificant. However, the higher the modeled percentage reduction, the stronger the demonstration. Therefore, modeling the high end of the range is encouraged. The EPA recommends submittal of supporting information for all sensitivity demonstrations, especially for demonstrations that can only pass the recommended threshold(s) at the low end of the range.

# 5.0 Attainment Plan Precursor Demonstrations

Quantifying secondary pollutant formation requires simulating chemical reactions and thermodynamic gas-particle partitioning in a realistic chemical and physical environment. Chemical transport models treat atmospheric chemical and physical processes such as 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).

A variety of Lagrangian and Eulerian modeling systems exist that could potentially be used to estimate impacts on secondarily-formed PM<sub>2.5</sub>. These modeling systems represent varying levels of complexity in the treatment of chemistry and the chemical and physical environment in which precursors exist. 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 are advantageous by providing a spatially and temporally dynamic realistic chemical and physical environment for plume growth and chemical transformation (Baker and Kelly, 2014; Zhou et al., 2012). Publicly available and documented Eulerian photochemical grid models such as CMAQ (Byun and Schere, 2006) and CAMx (Environ, 2016) 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). These models have been used extensively to

<sup>&</sup>lt;sup>41</sup> Note that when calculating the PM<sub>2.5</sub> impact of the precursor sensitivity, all components of modeled PM<sub>2.5</sub> mass should be added together to get the total PM<sub>2.5</sub> impact from the individual precursor emissions (see section 3.1.4).

support SIPs and to 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).

## 5.1 Modeling for Attainment Plan Precursor Demonstrations

In general, attainment plan precursor demonstration modeling should follow the recommendations in the PM<sub>2.5</sub> photochemical modeling guidance for attainment demonstrations [*Modeling Guidance for Demonstrating Air Quality Goals for Ozone, PM<sub>2.5</sub>, and Regional Haze* (USEPA, 2018c)]. As noted above, since air quality modeling is a required element of PM<sub>2.5</sub> attainment demonstrations<sup>42</sup>, most air agencies will already have a photochemical grid modeling platform available for precursor demonstrations. Where a grid modeling platform is available for an attainment demonstration, the process of setting up and running the model will generally be the same for a precursor demonstration. If a photochemical modeling platform is not available, the air agency should consult with the appropriate EPA Regional office to discuss options. Possible alternative options include the use of a simplified box model, regional or national photochemical grid modeling that may separately be available, or other conservative techniques for estimating the impact of precursor emissions on PM<sub>2.5</sub> concentrations in the particular area.

### 5.1.1 Air Quality Modeling Process

Typically, the air quality modeling process starts with the development of base year emissions and meteorology for input to an air quality run to evaluate model performance. The photochemical PM<sub>2.5</sub> modeling guidance describes the process for evaluating model performance and performing diagnostic analyses. After evaluating the model and making any necessary input changes or adjustments, the model is run for a future year, which corresponds to the appropriate attainment year for the area. The air quality model outputs are then used to apply the modeled attainment test to support an attainment demonstration.

At the beginning of the modeling process, the EPA recommends a modeling protocol be developed to support the modeling exercise. A modeling protocol is intended to communicate the scope of the analysis and generally includes the types of analysis performed, the specific steps taken in each type of analysis, the rationale for the choice of modeling system, names of organizations participating in preparing and implementing the protocol, and a complete list of model configuration options. The 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,

<sup>&</sup>lt;sup>42</sup> See 40 CFR 51.1011(a)(2) and 51.1011(b)(2) and CAA section 189(a)(1)(B) and 189(b)(1)(A).

describing procedures for using the model to demonstrate whether regulatory levels are met, and producing documentation to be submitted for review and approval.

If a modeling protocol is already available in support of an attainment demonstration, then it may not be necessary to develop a separate protocol to document a precursor demonstration. In that case, the details of the modeling and analyses to support a precursor demonstration can be incorporated into the existing structure of the modeling protocol. If a modeling protocol is not otherwise available, the EPA recommends developing a separate protocol that outlines the elements of the precursor demonstration. A modeling protocol 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
  - Identify how modeling and other analyses will be archived and documented
  - Identify 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
  - Identify relevant ambient data and provide relevant model performance in the modeling domain with a focus on the nonattainment area
  - List evaluation procedures
  - Identify possible diagnostic testing that could be used to improve model performance
- 4. Model Outputs
  - Describe the process for calculating precursor impacts to annual average and/or 24-hour average PM<sub>2.5</sub> concentrations in the nonattainment area.

The existing attainment demonstration modeling guidance provides recommendations on all of the protocol elements above (USEPA, 2018c). This includes selecting air quality models, meteorological modeling, episode selection, the size of the modeling domain, the grid size and number of vertical layers, and model performance. Precursor demonstrations for attainment plans should generally follow the recommendations in the attainment demonstration modeling guidance.

#### 5.1.2 Modeling Approaches

The simplest sensitivity modeling approach (brute force change to emissions) would be to simulate two sets of conditions, one with all emissions and one with an across-theboard anthropogenic emissions reduction (or zero precursor emissions in the case of a "zero-out" model run). The difference between these simulations provides an estimate of the air quality change related to the change in emissions from the precursor. Additionally, some photochemical models have been instrumented with source apportionment, which tracks emissions from specific sources, source sectors, and/or source regions through chemical transformation, transport, and deposition processes to estimate the apportionment of predicted PM<sub>2.5</sub> species concentrations (Kwok et al., 2015; Kwok et al., 2013). Source apportionment has been used to calculate the contribution from multiple states on model predicted ozone and PM<sub>2.5</sub> as part of several transport related rulemakings (USEPA, 2011; USEPA, 2016b). Air agencies can choose the most efficient modeling technique for their particular situation and should discuss the options with the appropriate EPA Regional office.

#### 5.2 Base Year and Future Year Model Assessments

Modeled attainment demonstrations typically include modeling for a base year (used to evaluate model performance), and modeling using future year emissions to simulate the impact of emissions changes (both emission reduction programs and emissions growth) on future air quality concentrations. Attainment demonstrations (and impracticability demonstrations) use the future year modeled air quality concentrations to determine if attainment is likely to be reached by the nonattainment area attainment deadline.

Where air agencies have both base year and future year modeling in support of an attainment demonstration or an impracticability demonstration, precursor demonstration modeling to demonstrate that precursor emissions do not contribute significantly to PM<sub>2.5</sub> concentrations in the nonattainment area could be done in either a base year or a future year. The base year modeling has less uncertainty compared to the future year since model performance is known for the base year and the modeling does not depend on projections of emissions to a future year. In addition, some control requirements (*e.g.*, RACT) may apply before the maximum statutory future year attainment date. However, there may be situations, such as with the NNSR precursor demonstration (see section 6), where it could be more appropriate to model future conditions that provide a more representative sensitivity analysis based on the period of time when a new source will begin to operate.

In most cases, the modeled base year is the best representation of current conditions. Note, however, that the modeled base year is not necessarily the same as modeling a "current" year. In some cases, the base year used for modeling purposes may be several years or more in the past. Therefore, future year baseline modeling may in some cases be more appropriate for attainment plan-modeled precursor demonstrations. Given the multitude of considerations, air agencies should consult the appropriate EPA Regional office to determine the appropriate analysis year(s). In addition, air agencies should provide an explanation of how the choice of analysis year(s) and associated assumptions are appropriate for the particular precursor demonstration.

#### 5.3 Calculating the Modeled Impact from Precursors

The modeled precursor impact on PM<sub>2.5</sub> levels can be calculated as either the absolute modeled concentration change or as the relative concentration change, based on the percent modeled change in PM<sub>2.5</sub> species, applied to ambient data. The photochemical modeling guidance (USEPA, 2018c) recommends performing a "relative" attainment test for modeled attainment demonstrations. The recommended test uses model estimates in a "relative" rather than "absolute" sense to estimate future year design values. The fractional changes in air pollutant concentrations between the model future year and model base year are calculated for all valid monitor locations. These ratios are called relative response factors (RRF). Future PM<sub>2.5</sub> design values are estimated at existing monitoring sites by multiplying the modeled RRFs for each monitor by the monitorspecific base year design value. The resulting estimates of future concentrations are then compared to the NAAQS. If the model is over-or-under-predicting PM species concentrations, the absolute modeled response to emissions precursor changes may be biased (high or low). However, the relative attainment test has the benefit of anchoring the projected PM<sub>2.5</sub> concentrations to measured ambient data, which helps mitigate modeled over-or under-predictions, relative to the level of the NAAQS.

In contrast to an attainment demonstration, precursor demonstrations do not examine changes in emissions between a base year and a future year. Instead, the calculation of changes in PM<sub>2.5</sub> concentrations occur between a modeled case with all emissions and a modeled case with reduced precursor emissions.

Even though it may be appropriate to calculate absolute modeled PM<sub>2.5</sub> concentration changes, there are advantages to calculating relative concentration changes, using the relative attainment test procedures for the modeled attainment test in the modeling guidance. The relative attainment test procedure involves applying adjustments to the ambient data to reconstruct the measured species components so that they add up to the measured FRM mass. Data analyses (Frank, 2006) have noted that the FRM monitors do not measure the same components and do not retain all of the PM<sub>2.5</sub> that is measured by routine speciation samplers and, therefore, cannot be directly compared

to speciation measurements from the Chemical Speciation Network (CSN).<sup>43</sup> It is possible to reconstruct PM<sub>2.5</sub> species so that they more closely match the composition of mass retained by the FRM. This adjustment can be applied to the modeled change in PM<sub>2.5</sub> species components. This will result in calculated PM<sub>2.5</sub> species mass, which is anchored to the measured mass, and more closely reflects the species concentrations that are retained on the FRM filters, including an estimate of particle bound water. See the photochemical modeling guidance (USEPA, 2018c; Frank, 2006) for more details on the recommended calculations.

The EPA provides a software package called the Software for the Modeled Attainment Test (SMAT) (USEPA 2018d), which provides default ambient data and performs the relative attainment test calculations. Assuming that the precursor impacts are calculated using base year modeling, a single SMAT run is needed to calculate precursor impacts. SMAT can be run with the base case concentrations as the "base year" and the zero-out/source apportionment (see page 26) or sensitivity model run (see page 27) case(s) as the "future year" (even though the model run does not actually represent a future year).<sup>44</sup> The "future year" PM<sub>2.5</sub> concentration values are subtracted from the base year values to get the total PM<sub>2.5</sub> contribution from the precursor. The precursor impact is then compared to the threshold(s) identified in section 2.2. If the precursor impacts are calculated using future year modeling, two SMAT runs are needed to calculate precursor impacts. The first SMAT run will calculate future year base case PM<sub>2.5</sub> concentrations using the base case and future year model outputs. The second SMAT run will calculate future year PM<sub>2.5</sub> concentrations from the zero-out/source apportionment or sensitivity model run(s). The two future year PM<sub>2.5</sub> concentration values are subtracted from each other to get the total PM<sub>2.5</sub> impact from the precursor. The precursor impact is then compared to the threshold(s) identified in section 2.2.

When calculating modeled precursor impacts to PM<sub>2.5</sub>, it is important to consider model performance. This is especially true in cases where air agencies choose to use absolute model results. If the model over-predicts PM<sub>2.5</sub> species concentrations, the absolute modeled concentration changes may be biased high. Similarly, if the model under-predicts PM<sub>2.5</sub> species concentration changes may be biased high. Similarly, if the model under-predicts PM<sub>2.5</sub> species concentration changes may be biased low. Therefore, model under-predictions are a particular concern (especially

<sup>&</sup>lt;sup>43</sup> The information in this section applies to the most common samplers in the CSN. Some networks use alternative special purpose samplers to collect both PM<sub>2.5</sub> and PM<sub>2.5</sub> speciation data. The characteristics of the sampler and the analytical procedures used to produce chemical speciation data should be considered in determining which, if any adjustments are appropriate to make the data useful for comparison to FRM data.

<sup>&</sup>lt;sup>44</sup> In a typical attainment demonstration, base year model outputs and future year model outputs are used to calculate RRFs. Therefore, the SMAT attainment test software graphical user interface uses the terms "base year" and "future year" when referring to the input files needed to calculate RRFs. The text here is referring to the SMAT software terms "base year" and "future year", even though in this case the year is the same in both model runs used to calculate RRFs.

when considering absolute modeled impacts) since this could lead to modeled precursor impacts that may be biased low.

#### 5.3.1 Estimating the Annual PM<sub>2.5</sub> Impact from Precursors

The first step for estimating annual  $PM_{2.5}$  impacts from a precursor is to estimate the annual average  $PM_{2.5}$  at each monitor location (the grid cell where the monitor is located) for the baseline scenario. Second, calculate the annual average  $PM_{2.5}$  at each monitor for the zero-out/source apportionment or sensitivity scenario. Calculate the difference between the zero-out/source apportionment or sensitivity scenario annual average  $PM_{2.5}$  and baseline scenario annual average  $PM_{2.5}$  for each monitor location. This difference is the impact from the  $PM_{2.5}$  precursor. Based on the recommendation in section 2.4, the impacts are calculated at monitor locations. When using the relative attainment test, the default recommendation is to average the concentrations at the nine (9) surrounding grid cells (a 3 x 3 matrix of grid cells, with the monitor in the center grid cell).<sup>45</sup>

#### 5.3.2 Estimating the Daily PM<sub>2.5</sub> Impact from Precursors

The first step for estimating 24-hour PM<sub>2.5</sub> impacts from a precursor is to estimate the 24-hour average PM<sub>2.5</sub> mass at each monitor location (the grid cell where the monitor is located) for the baseline scenario. Second, calculate the 24-hour average PM<sub>2.5</sub> at each monitor for the zero-out/source apportionment or sensitivity scenario. Calculate the difference between the zero-out/source apportionment or sensitivity scenario 24-hr average PM<sub>2.5</sub> and baseline scenario 24-hour average PM<sub>2.5</sub> for each day for each monitor location. This difference is the contribution from the PM<sub>2.5</sub> precursor. Based on the recommendation in section 2.4, the contributions are calculated at monitor locations. When using the relative attainment test, the default recommendation is to use the single grid cell where the monitor is located to represent the location of the monitor.

When calculating absolute daily impacts, the highest 24-hour average  $PM_{2.5}$  impact from the modeled time period should be compared to the daily  $PM_{2.5}$  "contribution" threshold at each monitor location. If the highest daily average secondarily-formed  $PM_{2.5}$  impact is greater than the level of the threshold, then a 2<sup>nd</sup> tier analysis may be appropriate to further examine the precursor impacts on the high modeled and/or observed  $PM_{2.5}$  days. Air agencies should consult with the appropriate EPA Regional office to discuss the details of the calculations.

Application of the relative attainment test (using SMAT) for the 24-hour NAAQS already takes into consideration the high measured PM<sub>2.5</sub> days. Therefore, no further (2<sup>nd</sup> tier)

<sup>&</sup>lt;sup>45</sup> See the photochemical modeling guidance section 4.2.2 for more details (USEPA, 2018c).

analysis is necessary to calculate the impact on exceedance days. The SMAT 24-hr air quality impact is calculated on high measured PM<sub>2.5</sub> days in the area.

# 6.0 Nonattainment New Source Review (NNSR) Precursor Demonstration

The PM<sub>2.5</sub> SIP Requirements Rule identifies a specific type of precursor demonstration that air agencies may use to demonstrate that sources of a particular precursor do not need to be controlled with respect to that precursor under the NNSR program for a particular PM<sub>2.5</sub> nonattainment area.<sup>46</sup> As detailed in the PM<sub>2.5</sub> SIP Requirements Rule, the NNSR precursor demonstration is based on the premise that the sensitivity of a particular nonattainment area to precursor emissions from future new major stationary sources and major modifications is best indicated by an emissions *increase* test. The sensitivity of an area to precursor increases may be different from the sensitivity of that same area to decreases (*e.g.*, where there are low emissions of the precursor from only a few sources). Therefore, for NNSR, the rule allows an air agency to undertake a sensitivity-based test in order to demonstrate that *increases* in emissions of a particular precursor would not contribute significantly to PM<sub>2.5</sub> levels that exceed the standard, and that sources of such precursor may in some cases be exempted from PM<sub>2.5</sub> controls for that precursor(s) under the NNSR permitting requirements.

Note that the NNSR precursor demonstration is optional and an air agency may satisfactorily demonstrate that a precursor is insignificant for all other control requirements other than NNSR, using the analyses previously described in this guidance or other appropriate analyses, without analyzing whether the precursor contributes significantly to PM<sub>2.5</sub> levels for the purposes of NNSR. In such cases, the nonattainment planning requirements would not apply to existing sources of that precursor, but the NNSR requirements would apply in the event that a new major stationary source or major modification in that area triggers NNSR permitting. Such an approach may be efficient for air agencies who do not want to expend the resources necessary to complete an NNSR precursor demonstration because they expect few (or no) new or modified major stationary sources of the precursor in question.

The NNSR precursor demonstration differs from the other two demonstrations (comprehensive and major stationary source precursor demonstrations), which are attainment plan tests, in that the latter two demonstrations examine air quality changes resulting from emissions reductions from existing sources. An attainment demonstration deals with existing emissions sources and how emissions reductions from those sources can help a nonattainment area reach attainment of the NAAQS. In contrast, the NNSR program addresses the management of major stationary source growth (new major stationary sources and major modifications) in the nonattainment area. Thus, by its nature, NNSR deals with *increases* of emissions in the nonattainment area. Even in an area that currently has no existing major stationary sources, PM<sub>2.5</sub>

<sup>&</sup>lt;sup>46</sup> See 40 CFR 51.1006(a)(3).

precursors from *new* major stationary source growth occurring in the nonattainment area could still contribute significantly to PM<sub>2.5</sub> levels in the area. Therefore, the PM<sub>2.5</sub> SIP Requirements Rule mandates that, if performed, NNSR precursor demonstrations be based on a sensitivity analysis which examines potential increases of emissions in the nonattainment area.<sup>47</sup>

Similar to the questions described in section 4.1, in performing a sensitivity analysis for NNSR, there are several questions that need to be addressed:

- 1) What amount of emissions increase should be examined as part of the NNSR sensitivity analysis?
- 2) What location(s) should be used to model the precursor emissions increases resulting from potential major stationary source growth?
- 3) What air quality concentration threshold should be used to determine if the modeled air quality change from the precursor is insignificant?

The EPA recognizes that there may be a number of factors inherent to a particular nonattainment area that could influence the potential emissions increase from new major stationary sources and major modifications. The following section addresses these factors and sets forth guidance for air agencies to consider in completing the NNSR precursor demonstration.

#### 6.1 NNSR Demonstrations

The purpose of the NNSR precursor demonstration is to determine if the nonattainment area is sensitive to PM<sub>2.5</sub> precursor emissions increases that may occur in a particular area from new major stationary sources and/or major stationary source modifications. It would be appropriate for the air agency to base estimates of any potential emissions increases in part on the types and size of new major stationary sources that are most likely to locate within the nonattainment area and/or existing sources most likely to undergo a major modification. To help determine the size and types of potential sources, the EPA also recommends an examination of recent (*e.g.*, the last 5 years) major stationary source permits in the region. In order to gather enough information on recently permitted emissions sources, it may be necessary to examine a broad region encompassing the nonattainment area. For example, an air agency may want to examine permits issued within the entire Northeast, Southeast, or Midwest region. Gathering information concerning permitted major stationary sources that have located elsewhere (magnitude of emissions, stack parameters, etc.) can help inform the process and make the modeling of precursor emissions more realistic.<sup>48</sup>

<sup>&</sup>lt;sup>47</sup> See 40 CFR 51.1005(a)(3)(i).

<sup>&</sup>lt;sup>48</sup> This recommendation is not meant to direct or limit the information that an air agency can use to develop appropriate model inputs for an NNSR precursor demonstration. Available information on the nature (*i.e.*,. type, size, location) of existing (and potential) major stationary

The identified range of emissions from recently permitted major stationary sources may vary widely among PM<sub>2.5</sub> precursors. SO<sub>2</sub>, NO<sub>x</sub> and VOC are PM<sub>2.5</sub> precursors that are also regulated as pollutants associated with other NAAQS (while NH3 is not nationally regulated under any other NAAQS). All new major stationary sources and major modifications of SO<sub>2</sub>, NO<sub>x</sub> and VOC must already meet Best Available Control Technology (BACT) level controls (or Lowest Achievable Emissions Rate controls if they are located in nonattainment areas) and all other NSR program requirements. The treatment of SO<sub>2</sub>, NO<sub>x</sub> and VOC under the NSR program for other NAAQS pollutants (besides PM<sub>2.5</sub>) thus serves to limit the potential increase of PM<sub>2.5</sub> precursor emissions from new sources, even absent controls as a PM<sub>2.5</sub> precursor. Therefore, how the particular precursor is treated as a result of regulation pursuant to other NAAQS is an important consideration when determining the potential emissions increases that should be modeled for a PM<sub>2.5</sub> NNSR precursor demonstration.

Other important considerations for determining the amount of emissions increase that should be analyzed in the NNSR precursor demonstration include but are not limited to: the size of the nonattainment area; the size, location, number, and types of existing major stationary sources (from which major modifications could occur); and current and future land use and zoning.

Upon the EPA's approval of an NNSR precursor demonstration, the air agency would not need to apply the PM<sub>2.5</sub> control requirements to new major stationary sources and major modifications with respect to that precursor under the NNSR program for PM<sub>2.5</sub> (for the current SIP). Therefore, the NNSR demonstration should include a conservative representation of potential emissions increases from new and modified major stationary sources. For example, the modeled size of sources (in tons per year of emissions) and the number and location of sources should be adequately conservative to analyze more than what is merely "likely" to occur in the area. The goal of the NNSR demonstration is not simply to determine the PM<sub>2.5</sub> air quality impact of likely new sources. Instead, it is to examine whether the nonattainment area is sensitive to increases of precursor emissions and whether the resulting PM<sub>2.5</sub> air quality change that could result from potential major stationary source growth would represent a significant contribution to PM<sub>2.5</sub> levels that exceed the NAAQS in a PM<sub>2.5</sub> nonattainment area. It is, however, important to consider the potential size and number of new sources of PM<sub>2.5</sub> precursors that may possibly locate in the nonattainment area (using conservative assumptions) when planning the analysis.

sources will vary considerably from area to area. Each air agency should consider the facts and circumstances most relevant to their situation.

#### 6.2 Modeling for NNSR Demonstrations

The fundamental approach for analyzing changes in emissions pursuant to the NNSR precursor demonstration involves the use of a photochemical model to project the air quality changes associated with potential emissions increases from hypothetical new major stationary sources and/or major modifications. In most cases, it will not be sufficient to model potential emissions increases from existing major stationary sources in the area. Some nonattainment areas may only have one or, in some cases, no existing major stationary sources. Moreover, it is important to examine the area's sensitivity to emissions increases from potential source locations across the entire nonattainment area because a new source may locate in any part of the nonattainment area (notwithstanding relevant land use and/or zoning restrictions). New and/or modified sources could contribute significantly to existing monitored locations within the nonattainment area or cause new exceedances of the standard in other parts of the nonattainment area. Therefore, as discussed in section 2.4, in most cases it will be necessary to model a number of hypothetical new sources, placed in various locations across the nonattainment area. EPA expects the air agency to analyze the air quality sensitivity of multiple locations of potential new sources that may locate anywhere within the nonattainment area. A reasonable number of sources (depending on the size of the nonattainment area) should be modeled in different parts of the area to ensure that the spatial variability of chemistry response to additional precursor emissions is well represented in the demonstration. (Section 6.3 provides additional considerations for the location of potential major source growth.) The location of existing major stationary sources and the stack parameters of those sources can be used to help design the NNSR modeling demonstration. The existing major stationary source information can be the starting point of the analysis, with additional hypothetical new sources (that may or may not resemble existing sources) placed in other parts of the area, as necessary.

The EPA also recommends modeling multiple hypothetical sources with emission rates and stack release characteristics typical of existing sources in the area or region. The overall approach for hypothetical source impact assessment would be generally similar to the analysis documented in *"Estimating ozone and secondary PM<sub>2.5</sub> impacts from hypothetical single source emissions in the central and eastern United States"* (Baker, 2016). Choices made for these hypothetical sources should be done in consultation with the appropriate EPA Regional office.

Due to the unique sensitivity levels of nonattainment areas to air quality impacts from individual PM<sub>2.5</sub> precursors, the EPA is not making default recommendations on the size and number of hypothetical new and/or existing sources to model in an NNSR demonstration. The details of the analysis, including a modeling protocol, should be discussed in advance with the appropriate EPA Regional office.

#### 6.2.1 Types of Models

Quantifying secondary pollutant formation requires simulating chemical reactions and thermodynamic gas-particle partitioning in a realistic chemical and physical environment. Therefore, in most cases, the EPA believes it will be necessary to employ a CTM for NNSR precursor demonstrations. CTMs treat atmospheric, chemical, and physical processes such as deposition and transport. In some limited cases, a simplified box model<sup>49</sup> that employs chemistry may be sufficient. Below, we describe additional details for the purposes of estimating the magnitude of secondarily-formed PM<sub>2.5</sub> from PM<sub>2.5</sub> precursor emissions associated from major stationary source growth.

#### 6.2.2 Modeling for Major Stationary Sources

As previously described in section 5.0, a variety of modeling systems exist that could potentially be used to estimate stationary source impacts from new and/or modified major stationary sources on secondarily-formed pollution such as PM<sub>2.5</sub>. These modeling systems represent varying levels of complexity in the treatment of plume chemistry and the chemical and physical environment in which the plume exists. It is important that any modeling system be appropriately applied for assessing the effects of major stationary sources on secondarily-formed pollutants such as PM<sub>2.5</sub> for the purposes of a precursor demonstration (USEPA, 2005).

Puff or dispersion (Lagrangian) modeling systems that have been used to assess single source impacts in North America include CALPUFF, HYSPLIT, FLEXPART, SCIPUFF, and SCICHEM. Some Lagrangian models treat in-plume gas and particulate chemistry. These models require time and space varying oxidant concentrations and, in the case of PM<sub>2.5</sub>, also neutralizing agents (such as NH<sub>3</sub>) as important secondary impacts happen when plume edges start to interact with the surrounding chemical environment (Baker and Kelly, 2014; ENVIRON, 2012). These oxidant and neutralizing agents are not routinely measured, but can be generated with a three dimensional photochemical transport model and subsequently input to a Lagrangian modeling system.

Because a NNSR demonstration adds hypothetical point sources, it is, therefore, possible to use a Lagrangian model to support an NNSR precursor demonstration. However, since it is likely that multiple hypothetical sources will need to be modeled and the Lagrangian model requires realistic background oxidant information (which can be supplied from a photochemical model), it will be easier in most cases to use a photochemical grid model for the demonstration. *See* section 5 for more details on photochemical grid models.

It is important that modeling systems used for these assessments be fit for this purpose and evaluated for skill in replicating meteorology and atmospheric chemical and

<sup>&</sup>lt;sup>49</sup> A box model is a simplistic single cell model that can represent photochemistry in a small isolated area.

physical processes that result in secondary pollutant formation and deposition. A candidate model for use in estimating the effects of precursors emitted from potential major stationary sources on secondarily-formed PM<sub>2.5</sub> for the purposes of an NNSR precursor demonstration should meet the general criteria for an "alternative model" outlined in 40 CFR part 51, Appendix W, Section 3.2 (USEPA, 2017). Whether an air agency chooses to use a photochemical grid model such as CAMx or CMAQ, or a plume model such as SCICHEM, they should consult the appropriate EPA Regional office to determine the appropriate model and modeling approach for an NNSR precursor demonstration.

#### 6.2.3 Modeling Approaches

The simplest modeling approach to calculate impacts in a photochemical grid model for an NNSR precursor demonstration is to model a brute force change in emissions by simulating two sets of conditions: one with all existing emissions, and one that includes an increase in emissions of the precursor that could result from major stationary source growth (new major stationary sources and major modifications) (Baker and Kelly, 2014; Bergin et al., 2008; Kelly et al., 2015; Zhou et al., 2012). The difference between these simulations provides an estimate of the air quality change related to the increase in emissions from the precursor. Additionally, some photochemical grid models have been instrumented with source apportionment, which tracks emissions from specific sources, source sectors, and/or source regions through chemical transformation, transport and deposition processes to estimate an impact to predicted air quality (Kwok et al., 2015; Kwok et al., 2013). Source apportionment has been used to differentiate the impact from single sources on model predicted ozone and PM<sub>2.5</sub> (Baker and Foley, 2011; Baker and Kelly, 2014; Baker et al., 2016).

Alternatively, the Direct Decoupled Method (DDM) source sensitivity technique 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; Cohan et al., 2005; Cohan et al., 2006; Kelly et al., 2015).

Since an NNSR precursor demonstration may require modeling multiple sources in multiple locations, an advanced technique such as source apportionment may save resources compared to numerous brute force photochemical grid model runs. Air agencies can choose the most efficient modeling technique for their particular situation; discussing the options in advance with the appropriate EPA Regional office is strongly advised.

#### 6.2.4 Horizontal Grid Resolution

NNSR precursor demonstrations for nonattainment areas should be conducted at horizontal grid resolutions between ~1 kilometer (km) up to ~12 km. Photochemical grid model application with grid cells up to 12 km has been shown to estimate similar urban area changes in air quality due to changes in emissions from a specific source on

secondary pollutants when estimated with finer grid resolution (Cohan et al., 2006). In instances where the air agency is considering modeling sources either at coarser resolutions or at resolutions finer than 1 km, consultation with the appropriate EPA Regional office is advised.

Even though single source emissions are averaged 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 impact of single sources on secondarily-formed pollutants, photochemical grid models could be used with a variety of approaches to estimate these impacts (see section 6.2.3, above). In some instances, where the source and key receptors are in very close proximity, the source and receptor may be located in the same photochemical grid model cell. Since physical and chemical processes represent a volume average, this may not adequately represent the gradients of pollution possible between the source and receptor when they are located in such proximity. The preferred approach to better represent the spatial gradient in source-receptor relationships when they are in close proximity is to use smaller sized grid cells. In such cases, grid resolution should be defined such that the source and receptor are no longer in the same grid cell. Ideally, there should also be several grid cells between the source and receptor to resolve best near-source pollution gradients.

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. Sub-grid plume treatment extensions in photochemical models typically solve for in-plume chemistry and use a set of physical and chemical criteria for a determination of when puff mass is merged back into the host model grid. A notable limitation of sub-grid plume treatments is that these implementations do not have more refined information related to meteorology or terrain than the host grid cell. In addition to tracking puffs at sub-grid scale, the host modeling systems must be able to track and output surface layer sub-grid puff concentrations, "sub-grid plume sampling," to best represent receptor concentrations that are in close proximity to the source (Baker et al., 2014). Another important reason sub-grid plume sampling is necessary is that 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 subgrid plume information or just 3-dimensional model output would miss some of the source's impacts on air quality, which means that accounting for both is necessary either with sub-grid sampling or options that integrate puffs within a grid cell with grid cell concentrations. Sub-grid plume treatments in photochemical grid models do not track grid resolved source impacts separately from other sources in the model simulation. When either sub-grid treatment is applied for an NNSR precursor demonstration, source apportionment or source sensitivity is necessary to track the grid

resolved source impact in addition to sub-grid plume treatment to fully capture source impact.

## 6.3 Location and Source Characteristics of Potential Major Stationary Source Growth

As discussed in section 2.4 above, the EPA believes that the analysis should evaluate the projected air quality change from potential future major stationary sources in all parts of the nonattainment area. Air agencies should consult with the appropriate EPA Regional office to determine the appropriate number, and location, of potential major stationary sources in an NNSR precursor demonstration. Enough locations should be included in the demonstration such that new sources are placed in a variety of chemical regimes to provide full coverage over the nonattainment area. The journal article "Estimating ozone and secondary PM<sub>2.5</sub> impacts from hypothetical single source emissions in the central and eastern United States" (Baker, 2016) provides examples of different types of hypothetical sources, modeled to examine secondary PM<sub>2.5</sub> impacts. This article examined the PM<sub>2.5</sub> concentration impacts from several different size sources with different stack parameters. For example, hypothetical sources were modeled in different areas across the country using stack parameters that represented both elevated sources and near ground level sources. The techniques applied in that study may be useful for designing future major stationary sources for sensitivity modeling in NNSR precursor demonstrations. In addition, the air agency may demonstrate that certain locations are clearly unsuitable for major stationary source growth (e.g., agricultural, residential and resort areas) so that they can be eliminated as potential growth sites for the modeling analysis.

#### 6.4 Base Year and Future Year Model Assessments

Modeled attainment demonstrations typically include modeling for a base year (used to evaluate model performance), and future year emissions are used to simulate the impact of emissions changes (due to emission reduction programs or any emissions growth) on future air quality concentrations. Attainment demonstrations (and impracticability demonstrations) use the future year modeled air quality concentrations to determine if attainment is likely to be reached by the applicable attainment deadline. Where air agencies have both base year and future year modeling in support of an attainment demonstration or an impracticability demonstration, modeling emissions increases to support an NNSR precursor demonstration could be done in either a base year or a future year. A demonstration based on future year modeling may be appropriate because air agencies should evaluate emissions controls in the context of achieving needed air quality improvements in the attainment year. On the other hand, air agencies should account for the fact that new major stationary sources could locate in the nonattainment area at any time between the nonattainment designation date and the date when the area is eventually redesignated to attainment. Since NNSR provisions are effective immediately after the area is designated as nonattainment,

there is some basis for using base year modeling for an NNSR precursor demonstration. However, in some situations, particularly where no new major stationary source permit applications have yet been filed and any new major stationary sources therefore would not be in operation for a number of years, air agencies may find that future year modeling may more accurately reflect atmospheric conditions for secondary PM<sub>2.5</sub> formation when precursor emissions increases from potential major stationary source growth may occur. Given the multitude of considerations, air agencies should consult the appropriate EPA Regional office to determine the appropriate analysis year.

#### 6.5 Calculating the Modeled Impact from Precursors

The modeled precursor impacts on PM<sub>2.5</sub> concentrations can be calculated either as the absolute modeled concentration changes or as relative concentration changes, based on the percent modeled change in PM<sub>2.5</sub> species, applied to ambient data. The photochemical modeling guidance recommends performing a "relative" attainment test for modeled attainment demonstrations. However, modeling for PSD analyses of single stationary sources typically uses absolute model results (USEPA, 2017 and USEPA, 2014). Since the modeled emissions and stack parameters from existing major stationary sources are well characterized and known, the use of absolute concentration change estimates from those sources in a photochemical model is, in most cases, appropriate. Adjusting the single source impacts up or down based on overall modeled concentrations of species (using the relative attainment test procedures) may, in some cases, inappropriately adjust the absolute modeled concentration change. Therefore, the EPA recommends using absolute model outputs to calculate major stationary source impacts for NNSR precursor demonstrations. However, there may be some cases where relative impacts for an NNSR precursor demonstration may be appropriate. Air agencies should consult with the appropriate EPA Regional office to determine the most appropriate post-processing procedures for the particular demonstration.

#### 6.5.1 Estimating the Annual PM<sub>2.5</sub> Impact from Precursors

The first step for estimating annual  $PM_{2.5}$  impacts from a precursor is to estimate the annual average  $PM_{2.5}$  at each receptor in the nonattainment area (if using a grid model, each grid cell is a receptor) for the baseline scenario. The second step is to calculate the annual average  $PM_{2.5}$  at each receptor for the sensitivity scenario. The final step is to calculate the difference between the sensitivity scenario annual average  $PM_{2.5}$  and baseline scenario annual average  $PM_{2.5}$  for each receptor. This difference yields the impact from the  $PM_{2.5}$  precursor. Based on the recommendation in section 2.4, the impacts are calculated for all locations (grid cells) within the nonattainment area and should be compared to the thresholds recommended in section 2.2.

#### 6.5.2 Estimating the Daily PM<sub>2.5</sub> Impact from Precursors

The first step for estimating 24-hour  $PM_{2.5}$  impacts from a precursor is to estimate the 24-hour average  $PM_{2.5}$  at each receptor in the nonattainment area (if using a grid model,

each grid cell is a receptor) for the baseline scenario. The second step is to calculate the 24-hour average PM<sub>2.5</sub> at each receptor for the sensitivity scenario. The final step is to calculate the difference between the sensitivity scenario 24-hour average PM<sub>2.5</sub> and baseline scenario 24-hour average PM<sub>2.5</sub> for each day for each receptor. This difference yields the impact from the PM<sub>2.5</sub> precursor. Based on the recommendation in section 2.4, the contributions are calculated for all locations (grid cells) within the nonattainment area and should be compared to the thresholds recommended in section 2.2.

When calculating absolute daily impacts, the highest 24-hour average  $PM_{2.5}$  impact from the modeled time period should be compared to the daily  $PM_{2.5}$  threshold at each grid cell. If the highest daily average secondarily-formed  $PM_{2.5}$  contribution is greater than the level of the threshold, then a 2<sup>nd</sup> tier analysis may be appropriate to further examine the precursor impacts on the highest modeled  $PM_{2.5}$  days. Air agencies should consult with the appropriate EPA Regional office to discuss the details of the calculations.

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