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Interagency Workgroup on Air Quality Modeling Phase 3 Summary Report: Long Range Transport and Air Quality Related Values

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Executive Summary

The Interagency Workgroup on Air Quality Modeling (IWAQM) was originally formed in 1991 to provide a focus for development of technically sound regional air quality models for regulatory assessments of pollutant source impacts on Federal Class I areas. The IWAQM process largely concluded in 1998 with the publication of the Interagency Workgroup on Air Quality Modeling (IWAQM) Phase 2 Summary Report and Recommendations for Modeling Long Range Transport Impacts (EPA-454/R-98-019) (U.S. Environmental Protection Agency, 1998). The IWAQM Phase 2 process provided a series of recommendations concerning the application of the CALPUFF model for use in long range transport (LRT) modeling and informed the promulgation of that model for such regulatory purposes in 2003. The IWAQM process was reinitiated in June 2013 to inform EPA's commitment to update Appendix W to address chemically reactive pollutants in near field and long range transport applications (U.S. Environmental Protection Agency, 2012b). This report provides information and recommendations from the "Phase 3" effort focused on long-range transport of primary and secondary pollutants. The idea of applying photochemical grid models for these purposes is explored in more detail in response to a growing community interest in using these types of models for estimating single source secondary pollutant impacts over long distances.

This document describes chemical and physical processes important to the formation of ground-level O_3, PM2.5, visibility, and deposition in the context of modeled long range transport assessments for permit review programs. Chemical transport models that characterize these processes include both Lagrangian which typically only have a single source included in the model and photochemical grid models which include some representation of all anthropogenic, biogenic, and geogenic sources. Modeling systems appropriate for the purposes of estimating long-range transported single source secondary impacts are described and recommendations are made with respect to the use of certain types of modeling systems for this type of application. Model evaluation is important to ensure that a particular system is fit for the purpose of estimating long-range single source secondary impacts. One aspect of this type of evaluation for long-range transport assessments would be demonstrating model skill in meteorological processes important for long distant transport by replicating appropriate mesoscale tracer release experiments. In addition to establishing whether a modeling system is generally appropriate for this purpose, project specific evaluations that compare model estimated meteorology and chemical estimates with measurements near the project source and key receptors is also an important model evaluation component.

Regulatory context for estimating long-range transport of visibility and deposition is provided to present the range of purposes for single source impact assessments. In the case of visibility, single source impact assessment approaches are compared within the Regional Haze Rule context, Prevention of Significant Deterioration, and National Environmental Policy Act to better illustrate the similarities in these demonstrations and note where differences should be expected.

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1 BACKGROUND: IWAQM Phase 3 process overview

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

The IWAQM process was reinitiated in June 2013 to inform EPA’s commitment to update Appendix W to address chemically reactive pollutants in near field and long range transport applications (U.S. Environmental Protection Agency, 2012b). Comments received from the 10th Modeling Conference (March 2012) from stakeholders support this interagency collaborative effort to provide additional guidance for modeling single source impacts on secondarily formed pollutants in the near-field and for long range transport. Stakeholder comments also support the idea of this collaborative effort working in parallel with stakeholders to further model development and evaluation.

This “Phase 3” effort includes the establishment of 2 separate working groups, one focused on long-range transport of primary and secondary pollutants and the other on near-field single source impacts of secondary pollutants. While many of the objectives are similar for each of these groups, the focus and regulatory end-points are different for each.

It is expected the “Phase 3” effort will continue with future efforts related to reviewing and responding to comments given on the 2015 proposed changes to Appendix W related to single source impact assessments for air quality related values. IWAQM3 long-range transport team members include Rick Gilliam (US EPA), Kirk Baker (US EPA), Michael Feldman (US EPA), Gail Tonnesen (US EPA), Chris Owen (US EPA), Bret Anderson (USFS), Tim Allen (US FWS), John Notar (NPS), John Vimont (NPS), and Craig Nicholls (BLM). Additional participation was provided by Erik Snyder (US EPA), Rebecca Matichuk (US EPA), and Robert Elleman (US EPA).

2 REGULATORY MOTIVATION

Sections 165, 169A, and 169B of the Clean Air Act sets visibility goals for Class I areas. The 1999 Regional Haze Rule expands on Section 169 of the Clean Air Act and “Phase I” of the Visibility Protection Program. The Regional Haze Rule (RHR) has multiple provisions that may be supported by air quality modeling. The reasonable progress and BART determination components of the RHR and modeling requirements for the first planning period and future planning periods are shown in Table 1. Additional sections contain requirements of other programs including Prevention of Significant Deterioration (PSD) and National Environmental Policy Act (NEPA) for visibility modeling.

Table 1. Modeling requirements for multisource and single source assessments to support various regulatory programs.

Program	**Multisource Assessment Requirement**	**Single Source Assessment Requirement**
Regional Haze Rule Reasonable Progress	Yes	No
Regional Haze Rule BART	No	Yes (initial planning cycle only)
PSD	No	Yes
NEPA	Yes (method 2)	Yes (method 1)

2.1 Regional Haze Rule Visibility Impairment Modeling: Reasonable Progress Goals (RPG)

Modeling may be used to assess Reasonable Progress by projecting future year visibility impairment at Class I areas due to all emissions sources. Projected visibility is compared to the Uniform Rate of Progress, which is a linear interpolation between recent air quality measurements and the 2064 “natural” visibility goal for each Class I area (U.S. Environmental Protection Agency, 2005b). Single source modeling is not a requirement in setting reasonable progress goals. However, single source modeling can be used to evaluate visibility impacts or benefits from emissions sources or emissions controls to inform decisions on emission reduction measures that may be necessary to meet long-term strategy requirements toward meeting the goal of natural visibility conditions and thus supporting a demonstration of the reasonableness of the reasonable progress goal.

A modeling system that treats emissions from all known anthropogenic and biogenic emissions sources with realistic chemical and physical transformations should be utilized to estimate future visibility conditions at a Class I area. The most appropriate tool that contains these qualities is a photochemical grid model. Commonly applied photochemical grid models for estimating visibility include the Comprehensive Air-Quality Model with Extensions (CAMx) and the Community Multiscale Air Quality Model (CMAQ). EPA has issued SIP modeling guidance for Regional Haze (U.S. Environmental Protection Agency, 2014b) in which an approach for assessing future year visibility impacts with photochemical grid models has been established and applied by States for their initial RH SIP demonstrations for 2018. This same type of photochemical model based assessment will need to be done for upcoming SIP demonstrations for subsequent planning periods (e.g. 2028, 2038, etc.) to determine if Class I areas will be on the glidepath to “natural” conditions.

The estimates of “natural” conditions are critically important for the estimation of the uniform rate of progress. However, any future updates to the calculation of “natural” conditions will not substantively change the nature of the air quality model based assessments of projected visibility impairment. However, changes to the metrics (e.g. 20% worst days) used for demonstrating progress will provide for more influential changes to projected visibility improvements.

2.2 Regional Haze Rule Visibility Impairment Modeling: BART program

Dispersion modeling was recommended by US EPA to support decisions about which BART eligible sources “cause or contribute” to visibility impairment and may need enforceable emissions limits and/or emissions controls (U.S. Environmental Protection Agency, 2005b). If a BART eligible source “contributes” to visibility impairment then additional modeling was done to assess the improvement in visibility due to source control measures. BART-eligible sources meet specific criteria for source category, date of operation or existence, and potential to emit (see 70 FR 39158–39161; July 6, 2005). BART is a program that only applies to the 1st regional haze planning period (the planning period ending 2018).

Single-source air quality modeling for BART assessments was typically done using the CALPUFF modeling system and daily maximum emission rates. However, it is important to note that other Lagrangian models or photochemical grid modeling systems can be used to isolate the primary and secondary impacts of single sources and thus be used for single source visibility assessments (Baker and Foley, 2011; Baker and Kelly, 2014; ENVIRON, 2012a, c; Zhou et al., 2012). Photochemical grid models have been used to support regulatory single source visibility impact assessments (U.S. Environmental Protection Agency, 2014a).

The daily visibility metric for each Class I area is expressed as the change in deciviews compared to natural visibility conditions (U.S. Environmental Protection Agency, 1998). Natural visibility conditions are found in Appendix B of EPA’s Guidance for Estimating Natural Visibility Conditions under the Regional Haze Rule (U.S. Environmental Protection Agency, 2003). The daily average visibility degradation beyond natural conditions expressed in deciviews is kept for each Class I area and ranked over the length of the modeling simulation. A threshold expressed in deciviews was commonly employed to determine whether a BART-eligible source “contributes” or “causes” visibility impairment as suggested in U.S. EPA guidance (U.S. Environmental Protection Agency, 2005b). BART assessments consider an estimate of maximum impacts over all modeled days, not the 20% best or 20% worst days which are considered for the reasonable progress assessment.

The air quality impacts of BART controls are sometimes estimated in aggregate rather than on a source-by-source basis. A cumulative “BART alternative” or “Better than BART” analysis can also be completed to examine the visibility benefits of alternative state and/or Federal controls programs that may provide more reasonable progress benefits compared to BART (U.S. Environmental Protection Agency, 2012a). Most “Better than BART” analyses to date have used photochemical modeling to examine the regional visibility benefits of NO_X, SO_2, and primary PM2.5 emissions reductions from BART controls and BART alternatives. These “Better than BART” analyses have focused on changes in visibility due to emissions changes on the 20% best and 20% worst visibility days.

2.3 Differences between single source assessments for BART and RPG

Fundamental differences in required approaches for evaluating source impacts for the purposes of BART determinations and RPG along with inherent differences in the models used for these purposes make directly comparing results for specific sources impossible. Single-source air quality modeling for BART assessments was typically done using the CALPUFF modeling system (69 FR 25,193-194), using maximum emission rates (24-hr maximum emission rates during the baseline period) and consideration of the maximum visibility impact from the source. On the other hand, due to the need to quantify the future year visibility impairment from all types of emissions sources on the 20% best and 20% worst days, reasonable progress assessments require the use of photochemical grid models. Photochemical grid models include all emissions sources and have realistic representation of formation, transport, and removal processes of particulate matter less than 2.5 microns that causes visibility degradation. Similarly, single source modeling for the purpose of evaluating visibility impacts or benefits from emissions sources or emissions controls for reasonable progress and long-term strategy development may utilize photochemical grid models to estimate potential visibility benefits from controls on future year visibility conditions.

Modeling for the purpose of establishing a reasonable progress goal (RPG) differs from the single source BART determination modeling for a variety of reasons. BART determinations are intended to provide information about current year impacts from a single facility at Class I areas to supplement other relevant emissions control information. Since BART controls need to be assessed against "worst case" emissions from specific sources, these model assessments are done using maximum 24-hr average emissions rates. The 8th highest model estimate of facility impacts at Class I areas from each year modeled are averaged and compared to that Class I area's natural conditions to provide an estimate of a "worst case" scenario (70 FR 39124). The highest modeled impacts are not typically compared directly to visibility thresholds, recognizing some uncertainty exists in the modeling system and abnormal meteorology may result in an unusually high source contribution. In contrast, RPG assessments and single-source assessments for the purposes of reasonable progress and long-term strategy development use actual emission rates to provide a realistic estimate of current and future year visibility impacts on the 20% best and 20% worst days at a Class I area.

Given differences in emissions and modeled impacts for these different assessment approaches, visibility impacts will be lower using the RPG approach compared to a BART assessment. BART determinations are current year "worst case" single source impact scenarios and RPG assessments are intended to provide realistic projections of future visibility. RPG necessitates using actual emissions rather than maximum 24-hour average emissions. In addition, RPG assessments average impacts over the 20% worst days rather that selecting the 8th highest facility impact in a given year. RPG impacts are examined relative to the projected future year 20% worst days visibility estimate, while BART impacts are maximum source impacts compared to background natural conditions irrespective of the relationship to the 20% worst days.

Finally, single source impacts estimated for RPG and BART will be different due to fundamental differences between photochemical grid models and puff dispersion models such as CALPUFF. Photochemical grid models include all emissions sources and provide a dynamic and realistic chemical and physical environment to estimate source emission impacts. The CALPUFF model uses fixed uniform concentrations of important oxidants such as ozone and neutralizing agents such as ammonia and does not perform key thermodynamic transformations that strongly influence atmospheric residence time and thus transport (Karamchandani et al., 2009; Karamchandani et al., 2008). CALPUFF's representation of these important chemical species and PM2.5 chemistry will result in different estimated source impacts than a photochemical grid model even if the exact same source emissions and release characteristics are used in both modeling systems. Additionally, Lagrangian puff models such as CALPUFF allow the project source full access to oxidants (e.g. ozone) and neutralizing agents (e.g. ammonia) while the same source in a photochemical model competes for oxidants and neutralizing agents which may result in different and possibly lower impacts.

In sum, the differences in the types of models, the inputs to the models, and how the models and model results are used means that the results from a BART determination or similar modeling using CALPUFF cannot be directly compared to estimated impacts of emissions controls from a single source on a reasonable progress goal. If recommended procedures change for either BART determination impact assessments or reasonable progress goal impact assessments the comparability between approaches would also change. Photochemical grid models could be applied to estimate single source impacts and post-processed in a manner consistent with requirements for a BART-like assessment but Lagrangian puff models are not ideal for reasonable progress demonstrations since they typically characterize one or a small group of sources.

2.4 Prevention of Significant Deterioration

Pursuant to 40 CFR part 51.166 and 52.21, subsections (k)(1)(i) and (k)(1)(ii), new or modified sources emitting in significant amounts (see 40 CFR part 51.166 and 52.21, subsection (b)(23)(i)) are required to demonstrate that the source under review does not cause or contribute to a violation of any applicable national ambient air quality standards ((k)(1)(i)) or maximum allowable increases over a baseline concentration ((k)(1)(ii)). Additionally, 40 CFR parts 52.27, subsection (d)(1), requires that the permit reviewing authority must provide to all affected FLM's written notification for any permit application which may affect visibility in any Federal Class I area. Notification must include a proposed source's anticipated impact on visibility on any Federal Class I area. The requirements of PSD potentially require the use of LRT models for both the maximum allowable increases (increments) and for air quality related values (AQRV's) including visibility. Unique to this is the authorities under which each of these elements of air quality analyses is administered. The relevant permitting authority administers the NAAQS and increments component of the air quality analysis, while the Federal Land Manager is responsible for recommending models and analytical procedures for the air quality related values analysis (see 40 CFR part 51, Appendix W, subsection 6.1(b)).

Single source impacts are typically compared to significant impact levels (SILs) and increments. For the purposes of long range transport it is expected based on an analysis of multiple hypothetical plants that O_3 and secondary PM2.5 impacts would typically be below any significance threshold beyond 50 km (U.S. Environmental Protection Agency, 2015a). Analysis for primarily emitted pollutants indicates that in most situations significance thresholds are not exceeded beyond 50 km (U.S. Environmental Protection Agency, 2015b). Long-range transport assessments may be necessary in certain limited situations for PSD increment. In these situations, a screening approach could be used that relies upon the near-field application of the appropriate screening and/or preferred model to determine the significance of ambient impact at or about 50 km from the new of modifying source. If this initial screening indicates there may be significant ambient impacts at that distance, then further screening is necessary.

Where a long range transport assessment is still needed for primary pollutant impacts a Lagrangian (e.g. CALPUFF without chemistry) or photochemical grid modeling system (e.g. CAMx, CMAQ) could be used to estimate those impacts. Typically, a Lagrangian model is the type of model appropriate to use for these screening assessments; however, applicants should reach agreed upon approaches (models and modeling parameters) on a case-by-case basis in consultation with the appropriate reviewing authority, Regional Office, and the affected Federal Land Manager(s) (FLM(s)). If a cumulative increment analysis is necessary, for these limited situations, the selection and use of an alternative model shall occur in agreement with the appropriate reviewing authority (paragraph 3.0(b)) and approval by the EPA Regional Office based on the requirements of section 3.2.2(e).

PSD analyses are also completed for NEPA air quality assessments using dispersion models or photochemical grid models. The typical PSD assessment description includes the following:

> The PSD demonstrations are for information and comparison purposes only and do not constitute a regulatory PSD increment consumption analysis. This PSD comparison analysis is used as an indicator of the relative change of air quality, which is a useful metric for analyzing and comparing air quality impacts. The comparison is made to allowable PSD increments for Class I and Class II areas for project-specific and cumulative impacts.

2.4.1 Visibility

Visibility impairment due to single sources may be assessed for the purposes of satisfying requirements for other programs such as PSD. PSD ensures the preservation of certain levels of air quality related values (AQRVs), including visibility, at designated Class I areas. Model assessments for AQRVs follow the Federal Land Managers' Air Quality Related Values Work Group (FLAG) Phase I Report (revised 2010) (U.S. Department of the Interior, 2010). Visibility in important natural areas (e.g., Federal Class I areas) is protected under a number of provisions of the Clean Air Act, including Sections 169A and 169B (addressing impacts primarily from existing sources) and Section 165 (new source review).

Visibility regulations (40 CFR 51.300–309) require States to mitigate current and prevent future visibility impairment in any of the 156 mandatory Federal Class I areas where visibility is considered an important attribute. In 1999, EPA issued revisions to the regulations to address visibility impairment in the form of regional haze, which is caused by numerous, diverse sources (e.g., stationary, mobile, and area sources) located across a broad region (40CFR 51.308–309). Section 169A of the Act requires states to develop SIPs containing long-term strategies for remedying existing and preventing future visibility impairment in the 156 mandatory Class I Federal areas, where visibility is considered an important attribute. In order to develop long-term strategies to address regional haze, many States will need to conduct regional-scale modeling of fine particulate concentrations and associated visibility impairment.

The FLAG visibility modeling recommendations are divided into two distinct sections to address different requirements for 1) near field modeling where plumes or layers are compared against a viewing background and 2) distant/multi-source modeling for plumes and aggregations of plumes that affect the general appearance of a scene. The recommendations separately address visibility assessments for sources proposing to locate relatively near and at farther distances from these areas (U.S. Department of the Interior, 2010).

2.4.2 Deposition

FLAG (2010) recommends that applicable sources assess impacts of nitrogen and sulfur deposition at Class I areas. This guidance recognizes the importance of establishing critical deposition loading values ("critical loads") for each specific Class I area, as these critical loads are completely dependent on local atmospheric, aquatic and terrestrial conditions and chemistry. Critical load thresholds are essentially a level of atmospheric pollutant deposition below which negative ecosystem effects are not likely to occur. FLAG (2010) does not include any critical load levels for specific Class I areas and refers to site-specific critical load information on FLM websites for each area of concern. However, this guidance does recommend the use of deposition analysis thresholds (DATs) developed by the National Park Service and the Fish and Wildlife Service. The DATs represent screening level values for nitrogen and sulfur deposition. If the DAT is exceeded then the modeling results are considered significant and further AQRV analysis is required. If a source exceeds the DAT level then a comparison to Class I specific critical load values is necessary (U.S. Department of the Interior, 2011). Project source annual total sulfur deposition and annual total nitrogen deposition are added to Class I area specific measured or estimated total sulfur and total nitrogen deposition to determine whether the Class I area specific screening level or critical load value would be exceeded.

2.5 National Environmental Policy Act – Visibility Assessments

NEPA air quality impact analyses assess potential air quality impacts that could occur from development within the project area and from other documented regional emissions sources within a defined study area. Visibility impairment due to project-specific sources and groups of sources are quantified and compared to applicable state and federal standards and thresholds for AQRV impacts (e.g., visibility) (U.S. Department of Agriculture et al., 2011). Two methodologies are typically used to process model results and evaluate visibility impacts.

The first methodology follows recommendations in the Federal Land Managers' Air Quality Related Values Work Group (FLAG) Phase I Report – Revised 2010 (U.S. Department of the Interior, 2010). This method assesses project-specific visibility impacts at Class I and sensitive Class II areas by determining the incremental changes in light extinction relative to estimated natural background conditions and comparing the incremental changes to visibility thresholds. The visibility evaluation metric used in this analysis is the Haze Index, which is measured in deciview (dv) and used in EPA's Regional Haze Rule. The change in visibility impacts of the proposed development is obtained by calculating the differences between the Haze Index with added project concentrations and the Haze Index based solely on background concentrations. Estimated visibility degradation at the Class I and sensitive Class II areas is presented in terms of the number of days that exceed a threshold percent change in extinction, or deciview (dv), relative to natural background conditions. The maximum and 98th percentile incremental changes in Haze Index (Δdv) at any receptor that intersects with the area of interest are compared to 0.5 dv and 1.0 dv thresholds. A source whose 98th percentile value of the haze index is greater than 0.5 deciview (dv) (approximately a 5% change in light extinction) is considered to contribute to regional haze visibility impairment. Similarly, a source that exceeds 1.0 dv (approximately a 10% change in light extinction) causes visibility impairment and corresponds to a change in visibility impairment that is just perceptible to the human eye.

The second methodology examines the cumulative (all sources) visibility impacts at Class I and sensitive Class II areas (Silva and McCoy, 2012). The cumulative visibility assessments use the estimates of actual emissions that could occur from the proposed development and all sources within a defined study area. This approach consists of five steps, as follows:

Step 1: Calculate the average baseline visibility for each Class I and sensitive Class II area based on five years of monitoring data for the 20 percent best and 20 percent worst days.

Step 2: Estimate site-specific relative response factors (RRFs) for each visibility component (as specified in the new IMPROVE equation) based on the future-year and base-year modeling results. Note that the RRF is defined as the ratio of the future-year to base-year simulated concentration in the vicinity of a monitoring site. The “future year” may simply be a scenario including the new project source(s).

Step 3: Apply the RRFs to the monitoring data to estimate future-year concentrations corresponding to the 20 percent best and 20 percent worst visibility days.

Step 4: Use the concentration estimates from Step 3 to calculate future-year visibility for the best and worst days.

Step 5: Using the information from Step 4, calculate the future-year mean visibility for the 20 percent best and worst days.

Steps 2 through 5 are applied for model scenarios with and without the proposed project emissions, and then differences in visibility between the model scenarios are calculated and used to quantify the change in cumulative visibility resulting from project-specific emissions. The cumulative multisource (method 2) visibility assessments (Silva and McCoy, 2012) are similar to the multi-source RPG assessments for Regional Haze except that the future year is typically the maximum emission year projected for the proposed project, which in most cases is much closer to the baseline period than a projected future year for reasonable progress goals or 2064 natural conditions.

2.6 National Environmental Policy Act – Sulfur and Nitrogen Deposition Assessments

Wet and dry fluxes of sulfur- and nitrogen-containing species are processed to estimate total annual sulfur and nitrogen deposition values at each Class I and sensitive Class II area. The maximum annual sulfur and nitrogen deposition values from any grid cell that intersects the area of interest are used to represent deposition for that area, in addition to the average annual deposition values of all grid cells that intersect a Class I area and identified grid cells for a sensitive Class II receptor area. Maximum and average predicted sulfur and nitrogen deposition impacts are estimated separately for each area and together across all areas. Nitrogen deposition impacts are calculated by taking the sum of the nitrogen contained in the fluxes of all nitrogen species modeled by the air quality model. If a photochemical grid model is used this includes reactive gaseous nitrate species, organic nitrates, particulate nitrate formed from primary emissions plus secondarily formed particulate nitrate, gaseous nitric acid, gaseous ammonia, and particulate ammonium. Sulfur deposition calculations are sulfur dioxide and particulate sulfate ion from primary emissions plus secondarily formed sulfate.

2.7 National Environmental Policy Act – Acid Neutralizing Capacity

Total annual sulfur and nitrogen deposition impacts from the project source is also used to assess the change in water chemistry associated with atmospheric deposition from project activities and cumulative sources for each of the sensitive lakes. This analysis assesses the change in the acid neutralizing capacity (ANC) for sensitive water bodies, or a threshold for a soil or lichen indicator. Estimates of potential changes in ANC follow the procedure developed by the USFS Rocky Mountain Region (USFS, 2000). Region 2 of the U.S. Forest Service identifies water bodies with background ANC values less than 25 uel/l as being extremely sensitive to additional deposition. However, impacts to sensitive biota can occur below 100 ueq/L. The predicted changes in ANC are compared to threshold specified by the USFS, which include a 10 percent change in ANC for lakes with background ANC values greater than 25 micro equivalents per liter [μeq/L], and no more than a 1 μeq/L change in ANC for lakes with background ANC values equal to or less than 25 μeq/L (U.S. Department of Agriculture, 1985).

3 MODEL SELECTION

This section describes the types of air quality impacts that need to be assessed and the tools that are best suited for this purpose. For a variety of regulatory programs secondary pollutant impacts such as O_3 and PM2.5 need to be assessed at various spatial scales (near-source and long-range transport). It is important that modeling systems used for these assessments be fit for this purpose and be evaluated for skill in replicating meteorology and atmospheric chemical and physical processes that result in secondary pollutants, visibility degradation, and deposition.

3.1 Secondary Pollutant Formation: O_3 and PM2.5

PM and O_3 are closely related to each other in that they share common sources of emissions and are formed in the atmosphere from chemical reactions with similar precursors (U.S. Environmental Protection Agency, 2005a). Air pollutants formed through chemical reactions in the atmosphere are referenced as secondary pollutants. For example, ground-level ozone (O_3) is predominantly a secondary pollutant formed through photochemical reactions driven by emissions of nitrogen oxides (NO_x) and volatile organic compounds (VOCs). Ozone formation is a complicated nonlinear process that typically requires favorable meteorological conditions in addition to VOC and NO_x emissions (Seinfeld and Pandis, 2012). Warm temperatures, clear skies (abundant levels of solar radiation), and stagnant air masses (low wind speeds) increase ozone formation potential (Seinfeld and Pandis, 2012).

In the case of particulate matter with aerodynamic diameter less than 2.5 µm ($PM_{2.5}$ or fine PM), $PM_{2.5}$ can be either primary (i.e. emitted directly from sources) or secondary in nature. The fraction of $PM_{2.5}$ which is primary versus secondary varies by location and season. In the United States, $PM_{2.5}$ is dominated by a variety of chemical species: ammonium sulfate, ammonium nitrate, organic carbon (OC) mass, elemental carbon (EC), and other soil compounds and oxidized metals. $PM_{2.5}$ elemental (black) carbon and soil dust are both directly emitted into the atmosphere from primary sources. Organic carbon particulate is directly emitted from primary sources but also has a secondary component formed by atmospheric reactions of VOC emissions. $PM_{2.5}$ sulfate, nitrate, and ammonium ions are predominantly the result of chemical reactions of the oxidized products of sulfur dioxide (SO_2) and NO_x emissions and direct ammonia (NH_3) emissions (Seinfeld and Pandis, 2012).

3.2 Visibility and Deposition

In most areas of the country, light scattering by PM2.5 is the most significant component of visibility impairment (U.S. Department of the Interior, 2010). The key components of PM2.5 contributing to visibility impairment include sulfates, nitrates, organic carbon, elemental carbon, and crustal material (U.S. Department of the Interior, 2010). Stream acidification is accompanied by decreasing pH levels, increasing aluminum concentrations, and decreasing acid-neutralizing capacity (ANC). As ANC decreases, macroinvertebrate communities begin to decline, followed by fish species richness reductions, and eventually lethal and sub-lethal effects on brook trout populations and marked declines in aquatic insect families. At the same time, as sulfuric acid is deposited from the atmosphere onto the landscape, molecules separate into positively charged hydrogen ions and a negatively charged sulfate molecule. In order to maintain an ionic balance, an equivalent amount of positively charged base cations adhere to the negatively charged sulfates and move into the soil water solution, acidifying the remaining soil and fundamentally altering soil processes. The reduced availability of these base cations in the soils (specifically, calcium, magnesium and potassium) hinders the capacity for sensitive soils to recover from acidic deposition and compromises the health and continued growth of the plants dependent on these nutrients. Additionally, when soils become sufficiently acidic, aluminum may become mobile, eventually entering plant roots more easily than other bases and displacing other nutrients during uptake, resulting in a nutrient deficiency. This deficiency is compounded by the toxic effect of aluminum on fine roots, further reducing the potential uptake of nutrients and water by plants. More information about acidification effects associated with deposition are available elsewhere (U.S. Department of the Interior, 2010).

3.3 Air Quality Models for Secondary Pollutants

Chemical transformations can play an important role in defining the concentrations and properties of certain air pollutants. Models that take into account chemical reactions and physical processes of various pollutants are needed for determining the current state of air quality, as well as predicting and projecting the future evolution of these issues (U.S. Environmental Protection Agency, 2005a). The chemical and physical processes discussed above are interrelated in a complex system. It is often not possible to predict the response of a certain pollutant to emissions reductions without the aid of models. Models can simultaneously account for these various chemical reactions and physical processes or the chemical coupling of multiple pollutants. A regulatory need exists to model secondary pollutants such as O_3 and PM and appropriately estimating secondary PM necessitates realistic estimates of O_3 and O_3 precursors.

Chemical transport models treat atmospheric chemical and physical processes such as deposition and motion. There are two types of chemical transport models which are differentiated based on a fixed frame of reference (Eulerian grid based) or a frame of reference that moves with parcels of air between the source and receptor point (Lagrangian) (McMurry et al., 2004). Photochemical grid models are three-dimensional grid-based models that treat chemical and physical processes in each grid cell and use Eulerian diffusion and transport processes move chemical species to other grid cells (McMurry et al., 2004). These types of models are appropriate for assessment of near-field and regional scale impacts from specific sources (Baker and Foley, 2011; Baker and Kelly, 2014; Bergin et al., 2008; Zhou et al., 2012) or all sources (Chen et al., 2014; Russell, 2008; Tesche et al., 2006). Photochemical transport models have been used extensively to support State Implementation Plans and 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).

3.3.1 Lagrangian models

Quantifying secondary pollutant formation requires simulating chemical reactions and thermodynamic partitioning in a realistic chemical and physical environment. Some Lagrangian models treat in-plume gas and particulate chemistry. These models require as input background fields of time and space varying oxidant concentrations, and in the case of PM2.5 also neutralizing agents such as ammonia, because important secondary impacts happen when plume edges start to interact with the surrounding chemical environment (Baker and Kelly, 2014; ENVIRON, 2012c). These oxidant and neutralizing agents are not routinely measured, but can be generated with a three dimensional photochemical transport model. Photochemical models simulate a more realistic chemical and physical environment for plume growth and chemical transformation (Baker and Kelly, 2014; Zhou et al., 2012), but simulations may sometimes be more resource intensive than Lagrangian or dispersion models.

3.3.2 Photochemical grid models

Publically available and documented Eulerian photochemical grid models such as the Comprehensive Air Quality Model with Extensions (CAMx) (ENVIRON, 2014) and the Community Multiscale Air Quality (CMAQ) (Byun and Schere, 2006) model treat emissions, chemical transformation, transport, and deposition using time and space variant meteorology. These modeling systems include primarily emitted species and secondarily formed pollutants such as ozone and PM2.5 (Chen et al., 2014; Civerolo et al., 2010; Russell, 2008; Tesche et al., 2006). Even though single source emissions are injected into a grid volume, photochemical transport models have been shown to adequately capture single source impacts when compared with downwind in-plume measurements (Baker and Kelly, 2014; Zhou et al., 2012). Where set up appropriately for the purposes of assessing the contribution of single sources to primary and secondarily formed pollutants, photochemical grid models could be used with a variety of approaches to estimate these impacts. These approaches generally fall into the category of source sensitivity (how air quality changes due to changes in emissions) and source apportionment (how emissions contribute to air quality levels under modeled atmospheric conditions).

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

Some photochemical models have been instrumented with source apportionment, which tracks emissions from specific sources through chemical transformation, transport, and deposition processes to estimate a contribution to predicted air quality at downwind receptors (Kwok et al., 2015; Kwok et al., 2013). Source apportionment has been used to differentiate the contribution from single sources on model predicted ozone and PM2.5 (Baker and Foley, 2011; Baker and Kelly, 2014). DDM has also been used to estimate O_3 and PM2.5 impacts from specific sources (Baker and Kelly, 2014; Bergin et al., 2008; Kelly et al., 2015) as well as the simpler brute-force sensitivity approach (Baker and Kelly, 2014; Bergin et al., 2008; Kelly et al., 2015; Zhou et al., 2012). Limited comparison of single source impacts between models (Baker et al., 2013) and approaches to identify single source impacts (Baker and Kelly, 2014; Baker et al., 2013) show generally similar downwind spatial gradients and impacts.

3.4 Recommendations

Photochemical transport models are suitable for estimating visibility and deposition since important physical and chemical processes related to the formation and transport of PM are realistically treated. Source sensitivity and apportionment techniques implemented in photochemical grid models have evolved sufficiently and provide the opportunity for estimating potential visibility and deposition impacts from one or a small group of emission sources. Photochemical grid models using meteorology output from prognostic meteorological models have demonstrated skill in estimating source-receptor relationships in the near-field (Baker and Kelly, 2014; ENVIRON, 2012c) and over long distances (ENVIRON, 2012b). In order to provide the user community flexibility in estimating single source secondary pollutant impacts and given the emphasis on the use of photochemical transport models for these purposes, Appendix W should no longer contain language that requires the use of a Lagrangian puff model (CALPUFF). A candidate model for use in estimating single source impacts on secondarily formed pollutants such as ozone and PM2.5 for the purposes of PSD and NSR programs should meet the general criteria for an “alternative model” outlined in 40 CFR 51.112 and 40 CFR part 51 (U.S. Environmental Protection Agency, 2005a). The acceptability of a particular model and approach for that model application is an EPA Regional Office responsibility that could include consultation with EPA Headquarters if appropriate. The use of models incorporating complex chemical mechanisms should be considered on a case-by-case basis with proper demonstration of applicability (U.S. Environmental Protection Agency, 2005a). It is important that the application of the wide range of modeling systems be appropriately applied for the purposes of assessing the impacts of sources on secondarily formed pollutants, such as ozone and $PM_{2.5}$. Use of photochemical grid models for AQRV analysis requirements, while not subject to specific EPA model approval requirements outlined in 40 CFR 51.166(l)(2) and 40 CFR 52.21(l)(2), should be justified for each application and concurrence sought with the affected FLM(s).

4 MODEL EVALUATION

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

Visibility and deposition are estimated at receptors placed inside Class I areas. This means it is important that a long range transport modeling system be able to capture these types of source-receptor relationships. In addition, since visibility is largely PM2.5 and deposition a combination of primary emitted and secondarily formed pollutants, it is important that a modeling system be able to capture single source primary and secondary impacts. Both of these components are important for generating confidence that a modeling system is theoretically fit for this purpose. Comparing model estimates against regional tracer experiments is one way to generate confidence that a modeling system can replicate long-range transport between a source and downwind receptors. Near-source in-plume measurements are useful to develop confidence that a modeling system captures secondarily formed pollutants from specific sources. These types of assessments are typically only done occasionally when a modeling system has notably changed from previous testing or has never been evaluated for this purpose. This type of assessment is discussed in more detail in section 4.1.

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

4.1 Long Range Transport Models – Fit for Purpose Evaluations

The typical regulatory application of an LRT modeling system is for Prevention of Significant Deterioration of Air Quality (PSD) Class I air quality related values (AQRVs) (visibility, deposition, etc.). When employed for these purposes, it is customary to only model discrete receptors defined within the boundaries of national parks and wilderness areas (federal mandatory Class I areas with specially protected air quality related values) and compare modeled concentrations against short-term averaging periods with few exceedance periods. Given the need to capture impacts at specific locations and times, some emphasis is needed on the evaluation of the spatial and temporal metrics. This implies a fundamentally different evaluation philosophy than typically used for dispersion models such as AERMOD that are applied within 50 kilometers, which is noted in the Guideline on Air Quality Models (EPA, 2005) with the statement "the models are reasonably reliable in estimating the magnitude of the highest concentrations occurring sometime, somewhere within an area." Based on this principle, the evaluation of near-source primary pollutant dispersion models focus on a model's ability to replicate the highest end of the concentration distribution, regardless of temporal or spatial pairing. Since model skill in replicating transport in time and space is important for ARQV analysis, model evaluation should place a similar level of emphasis upon a model's ability to simulate spatial and temporal pairing.

It is important that modeling tools used for single source long-range transport impacts assessments demonstrate skill in adequately replicating source-receptor relationships that are not in close proximity. For source-receptor distances greater than 50 km, regional scale models may be applied for the assessment of visibility impacts due to one or a small group of sources. Skill in estimating source-receptor relationships on this scale can be illustrated by evaluating modeling systems against regional scale inert tracer release experiments. These field study releases of inert tracers with downwind receptors typically arranged in arcs or distributed over a given area are designed for assessing model skill in long-range transport (Hegarty et al., 2013). The regional tracer release experiments with designs most relevant for evaluating long range transport modeling systems include the 1980 Great Plains Mesoscale Tracer Field Experiment, the 1983 Cross-Appalachian Tracer Experiment (CAPTEX), the 1987 Across North American Tracer Experiment (ANATEX), and 1994 European Tracer Experiment (ETEX) (ENVIRON, 2012b; Hegarty et al., 2013). Photochemical grid models have been shown to demonstrate similar skill to Lagrangian models for pollutant transport when compared to measurements made from multiple mesoscale field experiments (ENVIRON, 2012b).

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

4.2 Long Range Transport Models – Meteorology Evaluation

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

Development of the requisite meteorological databases necessary for use of photochemical transport models should conform to recommendations outlined in Guidance on the Use of Models and Other Analyses for Demonstrating Attainment of Air Quality Goals for Ozone, PM2.5, and Regional Haze (EPA-454/B-07-002) (U.S. Environmental Protection Agency, 2007). Demonstration of the adequacy of prognostic or diagnostic meteorological fields can be established through appropriate diagnostic and statistical performance evaluations consistent with recommendations provided in the appropriate model guidance (U.S. Environmental Protection Agency, 2007).

4.3 Long Range Transport Models – Chemistry Evaluation

An operational evaluation is used to assess how accurately the model predicts observed concentrations. Therefore, an operational evaluation can provide a benchmark for model performance and identify model limitations and uncertainties that require diagnostic evaluation for further model development/improvement. An operational evaluation for PM2.5 is similar to that for ozone. Some important differences are that PM2.5 consists of many components and is typically measured with a 24-hour averaging time. The individual components of PM2.5 should be evaluated individually. In fact, it is more important to evaluate the components of PM2.5 than to evaluate total PM2.5 itself. Apparent "good performance" for total PM2.5 does not indicate whether modeled PM2.5 is predicted for "the right reasons" (the proper mix of components). If performance of the major components is good, then performance for total PM2.5 should also be good. Databases that contain ambient O_3, PM2.5, and key precursors are noted in section 4.4. Section 4.4 is not intended to provide an exhaustive review of all ambient databases but provide an initial set of data that could be used for this purpose.

Regardless of the modeling system (e.g. photochemical transport or Lagrangian puff model) used to estimate secondary impacts of ozone and/or PM2.5, model estimates should be compared to observation data to generate confidence that the modeling system is representative of the local and regional air quality. For ozone related projects, model estimates of ozone should be compared with observations in both time and space. For PM2.5, model estimates of speciated PM2.5 components (such as sulfate ion, nitrate ion, etc) should be matched in time and space with observation data in the model domain. Model performance metrics comparing observations and predictions are often used to summarize model performance. These metrics include mean bias, mean error, fractional bias, fractional error, and correlation coefficient (Simon et al., 2012). There are no specific levels of any model performance metric that indicate “acceptable” model performance. Model performance metrics should be compared with similar contemporary applications to assess how well the model performs (Simon et al., 2012).

Accepted performance standards for speciated and total PM2.5 and ozone for photochemical models used in attainment demonstrations may not be applicable for single source assessments. Since the emissions and release parameters for the project source are well known, a direct connection between general photochemical model performance and the ability of the modeling system to characterize the impacts of the project source would be difficult to make. It is important that any potential approaches for photochemical model performance for the purposes of single source assessments for PSD and NSR use an approach that would be universally applicable to any single source modeling system, which includes the Lagrangian models described above.

4.4 Model performance evaluation data sources

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

AQS: The Air Quality System (AQS) is not an air quality monitoring network. However it is a repository of ambient air pollution data and related meteorological data collected by EPA, state, local and tribal air pollution control agencies from tens of thousands of monitors. AQS contains all the routine hourly gaseous pollutant data collected from State and Local Air Monitoring Stations (SLAMS) and National Air Monitoring Stations (NAMS) sites. SLAMS is a dynamic network of monitors for state and local directed monitoring objectives (e.g., control strategy development). A subset of the SLAMS network, the NAMS has an emphasis on urban and multi-source areas (i.e, areas of maximum concentrations and high population density). The AQS database includes criteria pollutant data (SO2, NO2, O3, and PM2.5) and speciation data of particulate matter (SO4, NO3, NH4, EC, and OC), and meteorological data. The data are measured and reported on an hourly or daily average basis. An overview of the AQS can be found at http://www.epa.gov/ttn/airs/airsaqs/index.htm.

IMPROVE: The Interagency Monitoring of PROtected Visual Environments (IMPROVE) network began in 1985 as a cooperative visibility monitoring effort between EPA, federal land management agencies, and state air agencies (IMPROVE, 2000). Data are collected at Class I areas across the United States mostly at National Parks, National Wilderness Areas, and other protected pristine areas. Currently, there are approximately 160 IMPROVE rural/remote sites that have complete annual PM2.5 mass and/or PM2.5 species data. The website to obtain IMPROVE documentation and/or data is http://vista.cira.colostate.edu/improve/.

STN: The Speciation Trends Network (STN) began operation in 1999 to provide nationally consistent speciated PM2.5 data for the assessment of trends at representative sites in urban areas in the U.S. The

STN was established by regulation and is a companion network to the mass-based Federal Reference Method (FRM) network implemented in support of the PM2.5 NAAQS. As part of a routine monitoring program, the STN quantifies mass concentrations and PM2.5 constituents, including numerous trace elements, ions (sulfate, nitrate, sodium, potassium, ammonium), elemental carbon, and organic carbon. In addition, there are approximately 181 supplemental speciation sites which are part of the STN network and are SLAMS sites. The STN data at trends sites are collected 1 in every 3 days, whereas supplemental sites collect data either 1 in every 3 days or 1 in every 6 days. Comprehensive information on the STN and related speciation monitoring can be found at http://www.epa.gov/ttn/amtic/specgen.html and http://www.epa.gov/aqspubl1/select.html.

CASTNet: Established in 1987, the Clean Air Status and Trends Network (CASTNet) is a dry deposition monitoring network where data are collected and reported as weekly average data (U.S. EPA, 2002b). Relevant CASTNet data includes weekly samples of inorganic PM2.5 species and ground-level ozone. More information can be obtained through the CASTNet website at http://www.epa.gov/castnet/.

SEARCH: The South Eastern Aerosol Research and CHaracterization (SEARCH) monitoring network was established in 1998 and is a coordinated effort between the public and private sector to characterize the chemical and physical composition as well as the geographical distribution and long-term trends of PM2.5 in the Southeastern U.S. SEARCH data are collected and reported on an hourly/daily basis. Background information regarding standard measurement techniques/protocols and data retrieval can be found at http://www.atmospheric-research.com/studies/SEARCH/index.html.

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

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