

6.0 Models for Ozone, Particulate Matter, Carbon Monoxide, Nitrogen Dioxide, and Lead

6.1 Discussion

a. This section identifies modeling approaches or models appropriate for addressing ozone (O_3)¹, carbon monoxide (CO), nitrogen dioxide (NO_2), particulates (PM-2.5^a and PM-10), and lead. These pollutants are often associated with emissions from numerous sources. Generally, mobile sources contribute significantly to emissions of these pollutants or their precursors. For cases where it is of interest to estimate concentrations of CO or NO_2 near a single or small group of stationary sources, refer to Section 4. (Modeling approaches for SO_2 are discussed in Section 4.)

b. Several of the pollutants mentioned in the preceding paragraph are closely related to each other in that they share common sources of emissions and/or are subject to chemical transformations of similar precursors.^{39, 40} For example, strategies designed to reduce ozone could have an effect on the secondary component of PM-2.5 and vice versa. Thus, it makes sense to use models which take into account the chemical coupling between O_3 and PM-2.5, when feasible. This should promote consistency among methods used to evaluate strategies for reducing different pollutants as well as consistency among the strategies themselves. Regulatory requirements for the different pollutants are likely to be due at different times. Thus, the following paragraphs identify appropriate modeling approaches for pollutants individually.

c. The NAAQS for ozone was revised on July 18, 1997 and is now based on an 8-hour averaging period. Models for ozone are needed primarily to guide choice of strategies to correct an observed ozone problem in an area not attaining the NAAQS for ozone. Use of photochemical grid models is the recommended means for identifying strategies needed to correct high ozone concentrations in such areas. Such models need to consider emissions of volatile organic compounds (VOC), nitrogen oxides (NO_x) and carbon monoxide (CO), as well as means for generating meteorological data governing transport and dispersion of ozone and its precursors. Other approaches, such as Lagrangian or observational models may be used to guide choice of appropriate strategies to consider with a photochemical grid model. These other approaches may be sufficient to address ozone in an area where observed concentrations are near the NAAQS or only slightly above it. Such a decision needs to be made on a case-by-case basis in concert with the Regional Office.

d. A control agency with jurisdiction over one or more areas with significant ozone problems should review available ambient air quality data to assess whether the problem is likely to be significantly impacted by

regional transport.⁴¹ Choice of a modeling approach depends on the outcome of this review. In cases where transport is considered significant, use of a nested regional model may be the preferred approach. If the observed problem is believed to be primarily of local origin, use of a model with a single horizontal grid resolution and geographical coverage that is less than that of a regional model may suffice.

e. The fine particulate matter NAAQS, promulgated on July 18, 1997, includes particles with an aerodynamic diameter nominally less than or equal to 2.5 micrometers (PM-2.5). Models for PM-2.5 are needed to assess adequacy of a proposed strategy for meeting annual and/or 24-hour NAAQS for PM-2.5. PM-2.5 is a mixture consisting of several diverse components. Because chemical/physical properties and origins of each component differ, it may be appropriate to use either a single model capable of addressing several of the important components or to model primary and secondary components using different models. Effects of a control strategy on PM-2.5 is estimated from the sum of the effects on the components composing PM-2.5. Model users may refer to guidance⁴² for further details concerning appropriate modeling approaches.

f. A control agency with jurisdiction over one or more areas with PM-2.5 problems should review available ambient air quality data to assess which components of PM-2.5 are likely to be major contributors to the problem. If it is determined that regional transport of secondary particulates, such as sulfates or nitrates, is likely to contribute significantly to the problem, use of a regional model may be the preferred approach. Otherwise, coverage may be limited to a domain that is urban scale or less. Special care should be taken to select appropriate geographical coverage for a modeling application.⁴²

g. The NAAQS for PM-10 was promulgated in July 1987. A SIP development guide⁴³ is available to assist in PM-10 analyses and control strategy development. EPA promulgated regulations for PSD increments measured as PM-10 in a notice published on June 3, 1993. As an aid to assessing the impact on ambient air quality of particulate matter generated from prescribed burning activities, a reference⁴⁴ is available.

h. Models for assessing the impacts of particulate matter may involve dispersion models or receptor models, or a combination (depending on the circumstances). Receptor models focus on the behavior of the ambient environment at the point of impact as opposed to source-oriented dispersion models, which focus on the transport, diffusion, and transformation that begin at the source and continue to the receptor site. Receptor models attempt to identify and apportion sources by relating known sample compositions at receptors to measured or inferred compositions of source emissions. When complete and accurate emission inventories or meteorological characterization are unavailable, or unknown pollutant sources exist, receptor modeling may be necessary.

i. Models for assessing the impact of CO emissions are needed for a number of different purposes. Examples include evaluating effects of point sources, congested intersections and highways, as well as the cumulative effect of numerous sources of CO in an urban area.

j. Models for assessing the impact of sources on ambient NO_2 concentrations are primarily needed to meet new source review requirements, such as addressing the effect of a proposed source on PSD increments for annual concentrations of NO_2 . Impact of an individual source on ambient NO_2 depends, in part, on the chemical environment into which the source's plume is to be emitted. There are several approaches for estimating effects of an individual source on ambient NO_2 . One approach is through use of a plume-in-grid algorithm imbedded within a photochemical grid model. However, because of the rigor and complexity involved, and because this approach may not be capable of defining sub-grid concentration gradients, the plume-in-grid approach may be impractical for estimating effects on an annual PSD increment. A second approach is to develop site specific conversion factors based on measurements. If it is not possible to develop site specific conversion factors and use of the plume-in-grid algorithm is also not feasible, other screening procedures may be considered.

k. In January 1999 (40 CFR part 58, Appendix D), EPA gave notice that concern about ambient lead impacts was being shifted away from roadways and toward a focus on stationary point sources. EPA has also issued guidance on siting ambient monitors in the vicinity of such sources.⁴⁵ For lead, the SIP should contain an air quality analysis to determine the maximum quarterly lead concentration resulting from major lead point sources, such as smelters, gasoline additive plants, etc. General guidance for lead SIP development is also available.⁴⁶

6.2 Recommendations

6.2.1 Models for Ozone

a. *Choice of Models for Multi-source Applications.* Simulation of ozone formation and transport is a highly complex and resource intensive exercise. Control agencies with jurisdiction over areas with ozone problems are encouraged to use photochemical grid models, such as the Models-3/Community Multi-scale Air Quality (CMAQ) modeling system⁴⁷, to evaluate the relationship between precursor species and ozone. Judgement on the suitability of a model for a given application should consider factors that include use of the model in an attainment test, development of emissions and meteorological inputs to the model and choice of episodes to model.⁴¹ Similar models for the 8-hour NAAQS and for the 1-hour NAAQS are appropriate.

b. *Choice of Models to Complement Photochemical Grid Models.* As previously noted, observational models, Lagrangian models, or the Empirical Kinetics Modeling Approach (EKMA)^{48, 49} may be used to help guide choice of strategies to simulate with a photochemical grid model and to corroborate results obtained with a grid model. Receptor models have also been used

¹ Modeling for attainment demonstrations for O_3 and PM-2.5 should be conducted in time to meet required SIP submission dates as provided for in the respective implementation rules. Information on implementation of the 8-hr O_3 and PM-2.5 standards is available at: <http://www.epa.gov/ttn/naqs/>.