Identifying Control Strategies to Meet NAAQS for $PM_{2.5}$

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Overview

Guidance for demonstrating attainment of the $PM_{2.5}$ NAAQS is currently being prepared by the EPA. As with ozone, the guidance for $PM_{2.5}$ will likely consist of two parts: (1) how to use results of modeling and other analyses and (2) how to generate the results used to demonstrate attainment or reasonable progress. Because causes of high $PM_{2.5}$ and poor regional visibility have the potential for being diverse, the guidance will likely be flexible. Choices will likely be heavily influenced by use of available data to develop a qualitative, conceptual description of an area's problem early in the State Implementation Plan (SIP) development process.

The federal Clean Air Act (CAA) places most of the responsibility on the states to prevent air pollution and to control air pollution at its source. In order for a state to conduct certain air quality programs, the state must adopt a plan and obtain approval of the plan from the EPA. Federal approval provides for some consistency in different state programs and ensures that a state program complies with the requirements of the CAA and EPA rules. The vehicle for demonstrating compliance with the CAA and EPA rules is the SIP. SIPs contain rules and facility-specific requirements that address control of PM and PM precursors. SIPs also delineate areas in the state where the air does not meet the standards set by EPA (nonattainment areas) and outlines what the state is doing to address these problems.

There are many **existing modeling tools** for the development of source-receptor relationships for PM concentrations. Models are essentially of two types: source models and receptor models. **Source models** are based on fundamental or empirical representations of the relevant physical-chemical atmospheric processes. These models predict ambient concentrations of PM knowing the characteristics of the sources, their emission rates of PM and precursor gases, and the meteorology. Three-dimensional Eulerian air quality models with a PM module are typically used for attainment demonstrations. These models can be grouped into two categories: episodic models that have a detailed treatment of atmospheric chemistry but are generally limited to simulations of 5 to 10 days because of high computational costs and long-term (or annual) models that use a simplified treatment of atmospheric chemistry and thus can be applied to a longer time period. **Receptor models** are based on statistical analyses of ambient PM data and on PM emission characterization (in some cases). These models provide empirical relationships between ambient data at the receptors and PM emissions (and/or PM precursor emissions) by source category. Receptor models can be grouped into three categories: those that apportion primary PM using source information, those that apportion primary PM without using source information, and those that apportion both primary (directly emitted) and secondary (formed from gas-phase precursors) PM. Receptor models that apportion secondary PM are currently under development (see Seigneur et al., 1997).

Summarized on the next page.

Overview

- Guidance for demonstrating attainment of the $PM_{2.5}$ NAAQS is needed:
  - How do I design an analysis to identify effective $PM_{2.5}$ control strategies?
  - How do I use results of modeling and other analyses?
  - How do I generate the results used to demonstrate attainment or reasonable progress?
- Modeling tools exist for the development of source-receptor relationships:
  - Source models are based on fundamental or empirical representations of the relevant physical-chemical atmospheric processes.
  - Receptor models are based on statistical analyses of ambient PM data and on PM emission characterization.

Model Applications and Evaluation

- Develop a conceptual description of an area's nonattainment problem
- Develop a modeling and analysis protocol
  - Choose an appropriate air quality modeling system
  - Select which episodes to model
  - Select a modeling domain and horizontal and vertical resolution
- Produce meteorological and air quality inputs
- Produce emissions inputs
- Run the model(s)
- Evaluate model performance and perform diagnostic tests

Multiple iterations are usually required to refine model inputs and to improve model performance. Data analysis is an important part of all modeling steps

Developing a Conceptual Description

- Speciated PM and PM mass data are used with meteorological information to qualitatively describe an area's nonattainment problem.
- Before modeling is performed, the conceptual description is needed to help
  - Choose the PM components to focus the modeled strategy upon
  - Define how to perform the modeling (e.g., regional vs. urban modeling, spatial detail required, etc.)
- The following tools are useful in assessing the air quality data to develop the conceptual description:
  - Chemical mass balance model (CMB)
  - Multivariate models
  - Gradient analyses
  - Spatial and temporal analyses of PM composition (e.g., high vs. low concentration days)

Developing a Modeling and Analysis Protocol

- Air quality models are essential tools for the development of attainment demonstration plans for areas with severe nonattainment problems.
- The models and databases are used to characterize the contributions of emission sources for recent periods and to estimate concentrations in the future under hypothetical emission reduction scenarios.
- Air quality models need to reliably estimate 24-hr and annual average PM concentrations for primary and secondary particles and to reliably characterize the attribution of the PM in the region to sources.
- Receptor models, such as the CMB model, estimate the attribution for the major categories of primary PM emission sources.

Selecting Air Quality Models to Use in the Demonstration (1 of 2)

- Guidance will likely provide flexibility in choosing air quality model(s) to use to support the attainment demonstration.
- The choice of models will depend on the conceptual description of the problem.
  - If secondary PM is important, use a detailed dispersion model.
  - If sulfate is important, use a model that has detailed cloud processes.
  - If nitrate and sulfate are important, use a model with the best gas-particle partitioning.
- For example, if the PM data suggest that sulfates are a major component, a regional photochemical model that treats formation of secondary PM (sulfate, nitrate, ammonium, organic carbon) will be needed. If the problem is mostly primary PM, urban-scale inert modeling (without chemistry) may suffice.

Selecting Air Quality Models to Use in the Demonstration (2 of 2)

- The following analyses are useful in assessing the air quality data to select appropriate model(s):
  - Review measured PM mass and composition.
  - Assess variability of PM mass and composition among sites.
  - Assess variability of the PM mass and composition at a given site.
  - Analyses of data on exceedances days are important for episodic modeling, but all days are included in annual average modeling.

Analysis needs may differ for episodic (i.e., 24-hr $PM_{2.5}$ violations) versus annual average $PM_{2.5}$ issues.

Key Attributes of $PM_{2.5}$ that Affect Modeling Approach

- PM is a mixture. Some components of the mixture can be independent of others; others are interdependent.
- Some components of PM may vary over small distances while others may not.
- Secondary components are usually a much larger fraction of $PM_{2.5}$ than of PM_{10}.
- Secondary PM components are related to processes also occurring in ozone formation.
- The modeled attainment demonstrations for PM should relate to the definition of the NAAQS (i.e., both 24-hr and annual).
- Modeling for different times of year may be needed to address air quality goals for PM.
- Meteorological conditions and emissions (e.g., soil moisture, crop cycles, biogenic emission cycles, etc.) are likely to differ significantly by season.

Example Episodic PM Models

PM Model	Air Quality Model	Meteorological Model
California Institute of Technology (CIT)	CIT	Diagnostic
Denver Air Quality Model (DAQM)	Regional acid Deposition Model (RADM)	Meteorological Mesoscale model version 4 (MM4)
Gas, Aerosol, Transport and Radiation model (GATOR)	GATOR	Mesoscale Meteorological and Tracer Dispersion model (MMTD)
Regional Particulate Model (RPM)	RADM	MM4
SARMAP Air Quality Model with aerosols (SAQM-AERO)	SAQM	Meteorological Mesoscale model version 5 (MM5)
Urban Airshed Model Version IV with aerosols (UAM-AERO)	UAM-IV	Diagnostic or prognostic
UAM Version IV with aerosol module based on the Aerosol Inorganic Model (UAM-AIM)	UAM-IV	Diagnostic or prognostic
Models-3/Community multi-scale air quality (CMAQ)	CMAQ Chemistry transport modeling system	MM5

Air quality models that include a detailed treatment of chemistry tend to be limited in their application to five to ten days of simulation because of the computational costs.

Adapted from Seigneur et al., 1997.

Example Long-term PM Models

PM Model	Air Quality Model	Meteorological Model
Regulatory modeling System for Aerosols and Deposition (REMSAD)	UAM-V	Diagnostic or MM5
Urban Airshed Model Version IV with linearized chemistry (UAM-LC)	UAM-LC	Diagnostic or prognostic
Visibility and Haze in the Western Atmosphere model (VISHWA)	ADOM	NGM and RAMS

- Air quality models that use a simplified treatment of atmospheric chemistry can be applied to longer time periods without prohibitive computational costs. However, the ability to simulate long time periods is generally obtained at the expense of some accuracy since the treatment of chemistry is less accurate in these long-term models.
- Other air quality models that can be used to predict long-term and average concentrations and source attribution include some receptor models and the Speciated Rollback model (SPROLL). The SPROLL model is a simple empirical model relating observed components of ambient PM concentrations to gaseous and particulate emissions.

Adapted from Seigneur et al., 1997.

Example Receptor Models

Receptor Model	Uses Source Profiles?
Chemical Mass Balance (CMB)	Yes
Artificial Neural Networks (Backpropogation)	Yes
Artificial Neural Networks (Kohonen)	No
Principal Components Analysis (PCA)	No
Target Transformation Factor Analysis (TTFA)	No
UNMIX	No
Positive Matrix Factorization (PMF)	No
Multi-linear Engine (ME)	No
Empirical Orthogonal Function Analysis (EOF)	No

- CMB and other receptor models can usually only separate four to six categories of PM emissions with acceptable accuracy. This is a major limitation in practice.
- These models also do not estimate future year conditions with different emissions.

Adapted from Seigneur et al., 1997.

Choosing Episodes to Model

- Goals of selecting modeling episodes to support the attainment demonstration include
  - Providing a suitable variety of days to model, including days with different PM chemical compositions.
  - Covering prototypical meteorological scenarios in which exceedances are observed.
  - Selecting a balance of high and low concentration days to model for applications related to the annual NAAQS.
- Proper episode selection is needed to
  - Ensure a strategy is robust (i.e., works well under a variety of meteorological conditions).
  - Choose a representative mix of conditions for applications relating to the annual NAAQS.
  - Serve as a resource-saving device, so that it is not necessary to model every exceedance day with a resource-intensive model.
- The following analyses are useful in assessing the air quality data to select appropriate episodes:
  - Assess whether a different mix of pollutant signatures are observed under different prototypical meteorological conditions.
  - Assess meteorological conditions using CART or cluster analysis.
  - Assess whether cases with seemingly similar meteorological conditions can be further subdivided based on the chemical composition of PM.

Selecting Model Domain and Grid Size (1 of 2)

- The choice of domain and grid cell size determines the geographical extent of the area modeled and the spatial detail inherent in the model prediction.
  - Choice of model domain size and spatial detail of modeling depends, in part, on which measured species of PM appear most important in the nonattainment area.
  - The larger the domain and the smaller the grid cells are, the greater the resources are required.
  - Generally, primary PM can be modeled for urban-scale domains, but the primary PM usually requires greater spatial detail than secondary PM.
  - Modeling secondary PM requires larger, regional domains but does not need as much spatial detail as modeling primary PM.

Selecting Model Domain and Grid Size (2 of 2)

- The following analyses are useful in assessing the air quality data to select appropriate model domain and grid cell size:
  - Review mix of PM components (i.e., sulfate, nitrate, primary and secondary organic carbon, elemental carbon, crustal material) on days selected for modeling.
  - Choose domain and grid size depending upon the tentative strategy selected (on basis of monitored data and inventory).
  - Meteorology needs to be considered. The model domain needs to be specified so as to contain material that is recirculated over multiple days in the region. This can be assessed with surface and upper air trajectory analysis.

Generating Meteorological and Air Quality Inputs for an Air Quality Model (1 of 2)

- Meteorological and air quality data are used in an air quality model to simulate transport from source to receptor, as well as the transport of pollution from outside the modeled area.
  - The necessary data can be generated in several ways including objective interpolation of observations, diagnostic wind models, and dynamic prognostic meteorological models with four dimensional data assimilation (FDDA).
  - Observations or diagnostic wind models may suffice for a small domain; dynamic models with FDDA are needed for regional domains.
- Appropriate model inputs are required because the inputs
  - Affect the relative importance of different source categories
  - Affect mixing of emissions and, therefore, the chemistry of secondary PM
  - Affect deposition of PM
  - Can affect emissions
  - Affect model performance and evaluation

Generating Meteorological and Air Quality Inputs for an Air Quality Model (2 of 2)

- The following analyses are useful in assessing the air quality data to generate appropriate model inputs:
  - Review speciated air quality data and spatial patterns.
  - Assess relative importance of primary and secondary components of PM.
  - Assess upwind/downwind gradients of secondary PM.
  - Assess dominance of primary components and gradients of secondary components.

Generating Emissions Inputs to an Air Quality Model

- The amount of PM and gaseous precursors of PM (including SO_2, ammonia, NO_x, VOC, and CO) emitted within the domain as a function of time and location should be generated. The PM emissions must be size-resolved and chemically speciated.
  - Emissions are critical to PM model performance.
  - Emissions are the central focus of control strategy analysis.
- The following analyses using air quality data are useful in evaluating and refining emissions inputs:
  - Compare ambient air quality and emissions estimates to aid in quality assurance of the emissions (emission inventory evaluation).
  - Use CMB model and ambient data to evaluate source profiles and emissions estimates.
  - Compare weekend/weekday species mixes (both primary PM emissions and PM precursors) as a means for checking assumed emission-related activity patterns.

Evaluating Model Performance Using Diagnostic Tests (1 of 2)

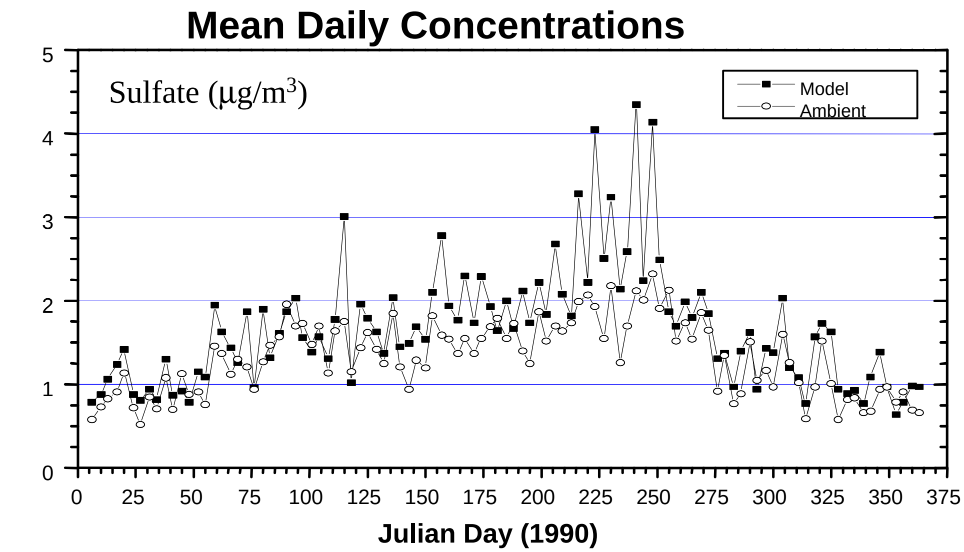
- As model results are available, perform an evaluation of how well the model is able to reproduce observed conditions.
  - Model predictions for key gaseous compounds (ozone, NO_x, SO_2, NH_3, HNO_3, VOC, and CO) and the principal chemical constituents of PM must be compared with observed concentrations for the shortest possible averaging times.
  - Since the modeled attainment test (discussed as the next topic area) focuses on major components of PM, performance tests will focus on the ability to predict observed concentrations of sulfate, nitrate, organic compounds (primary and secondary), elemental carbon and other, inorganic primary PM.
  - Diagnostic tests address the sensitivity of model predictions to changes in inputs; this is done as a preliminary step to help understand model performance problems and also to help select general control strategies.
  - Model performance evaluation is needed to establish credibility of a particular model application.

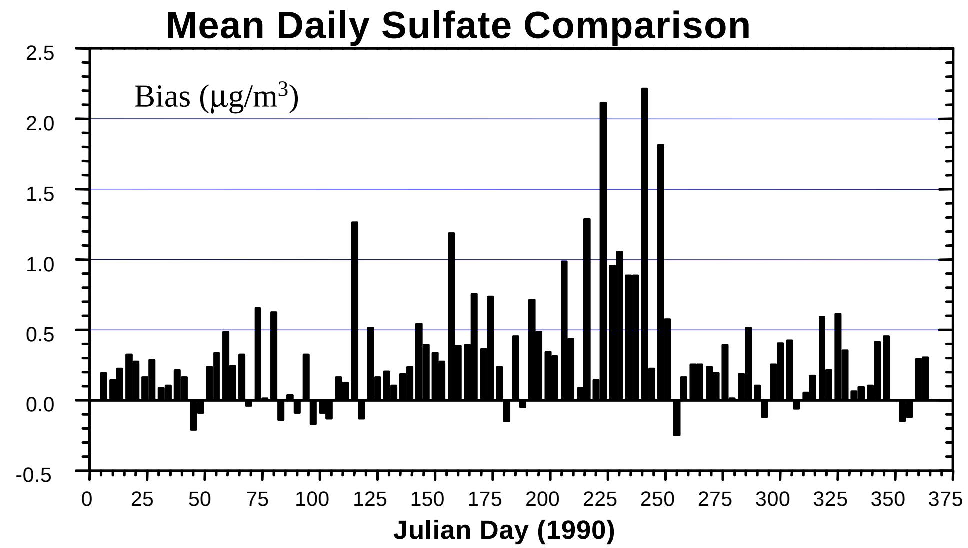
Evaluating Model Performance Using Diagnostic Tests (2 of 2)

- The following analyses using air quality data are useful in evaluating model performance:
  - Air quality observations, particularly speciated data, serve as the basis for the evaluation.
  - Spatial and temporal analyses of the air quality data including time series plots and spatial plots of concentrations.
  - Weekend/weekday comparisons could test the accuracy of a model’s response to differing emissions.
  - Speciated data may ultimately be useful in “indicator species” approaches to estimate whether a model’s response to a control strategy is likely to be accurate; data analysis would entail computing ratios of the indicator species.
  - Investigate possible tracer species to help establish priorities for controlling certain types of sources.

Example Model Performance Evaluation (1 of 2)

- Mean daily variation in sulfate predictions and observations in this example show that the model predictions were greater than the ambient observations during most of the year.
- The largest over-predictions occurred on Julian days 200-250 (mid- to late summer).
- There are some occurrences when the model under-predicts.
- The tendency for over-prediction is most easily seen in the bias display.

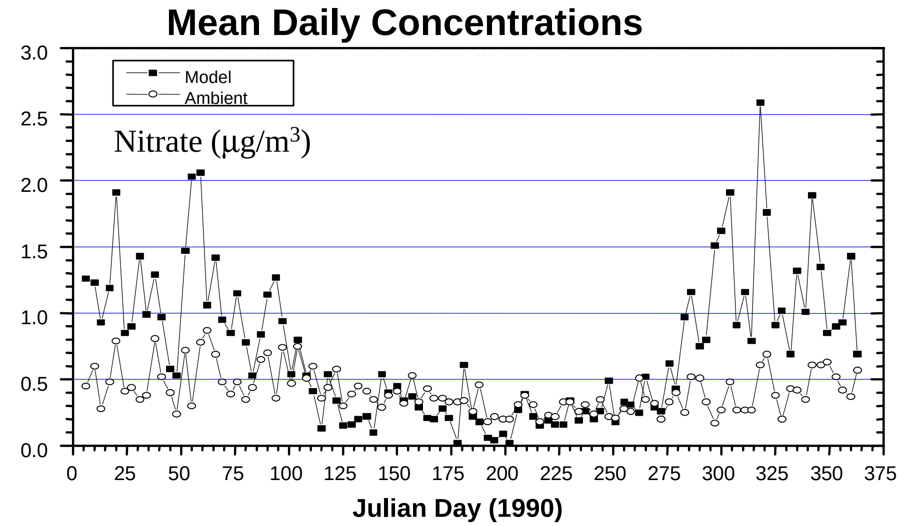


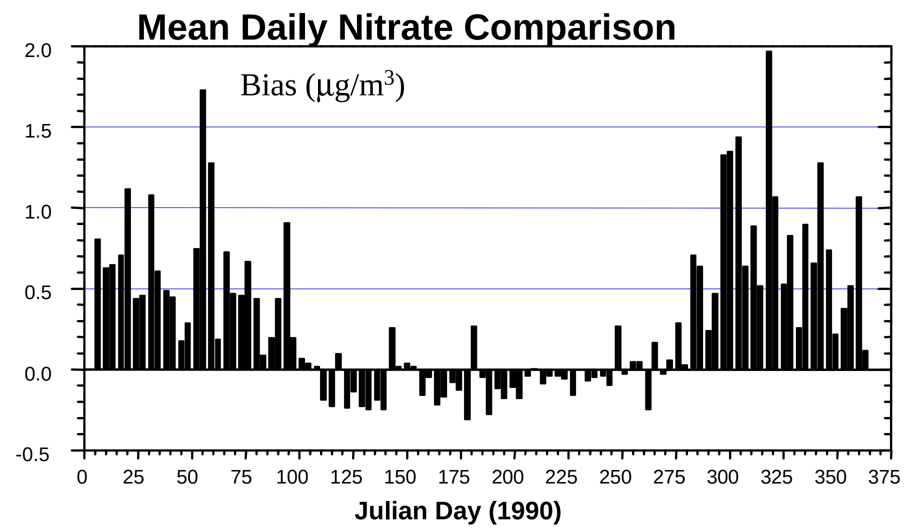


Adapted from Wayland, 1999.

Example Model Performance Evaluation (2 of 2)

- Mean daily variation in nitrate predictions and observations in this example show two distinct groups:
  - the model over-predicts in the winter and early spring and mid to late fall;
  - the model under-predicts ambient nitrate during Julian days 100-275.





Adapted from Wayland, 1999.

Applying a Modeled Attainment Test (1 of 2)

- The attainment test divides the $PM_{2.5}$ design value at each monitor site into five major components using monitored (observed) data: mass associated with sulfate, nitrate, organic carbon, elemental carbon, and inorganic primary PM.
  - Current and future emissions are simulated with a model, and results are used to develop rollback factors for each of the monitored components of the design value.
  - Each measured component of the design value is multiplied by the component-specific rollback factor to estimate a future concentration for each component.
  - Future component concentrations are added to obtain a future predicted $PM_{2.5}$ mass concentration, which is compared to 15.0 $\mu g/m^3$ (annual NAAQS) or 65 $\mu g/m^3$ (24-hr NAAQS) to see if attainment is likely.

Applying a Modeled Attainment Test (2 of 2)

- The following analyses using air quality data are useful in assessing attainment:
  - Monitored mass and $PM_{2.5}$ speciated data are used directly in the modeled attainment test. The test's credibility increases as more speciated measurements are available at more monitoring sites.
  - Analyses to quality assure measured data and to reduce "unexplained" portions of measured $PM_{2.5}$ data will also increase the credibility of the modeled attainment test.
  - The modeled attainment test addresses total mass associated with each major component; this requires making assumptions about cations, such as those associated with sulfate and nitrate (NH_4^+, HNH_3^+, Na^+, Ca^+, K^+ or H^+). Data analysis of ammonium vs. sulfate concentrations, for example, would permit this to be done with more confidence.
  - To estimate potential uncertainties in the modeled attainment test, comparisons of speciated data at collocated monitors using Federal Reference Method (FRM) procedures and other speciated analyses should be performed. These comparisons will allow the analysts and modelers to better understand potential interferences (such as volatilization losses) with the FRM and to test compatibility between speciated measurements using different methods and FRM mass measurements.

Using Weight of Evidence to Demonstrate Attainment

- Weight of evidence uses analyses performed on monitored data to see if conclusions corroborate or refute conclusions drawn in the modeled attainment test. Results of these analyses are weighed together with the outcome of the attainment test to estimate whether attainment is likely.
  - These tests are used as a means of acknowledging uncertainty associated with model predictions.
  - The tests are likely applied most often when the attainment test is almost, but not quite, passed.
  - The tests enable states to take full advantage of all information when assessing if attainment is likely.
- The following analyses using air quality and emissions data are applicable in weight of evidence tests:
  - Perform trend analyses of measured components and PM mass
  - Compare past reductions vs. future projections in emission trends
  - Use receptor models to see if strategy seems to be addressing the right source categories
  - Assess model uncertainty by looking at such things as differences among measurement techniques, size of unexplained mass, and variability of measured composition at mass concentrations approaching the monitor-specific $PM_{2.5}$ design values.

What to Include in a $PM_{2.5}$ Attainment Demonstration

- Always include results of a modeled attainment test applied at monitoring sites.
- Sometimes include an additional “screening test” applied at flagged locations without monitors.
- Possibly include supplementary analyses in a weight of evidence determination to assess whether attainment is likely if the modeled attainment and screening tests are passed or close to being passed.

Summary

- Guidance for demonstrating attainment of the $PM_{2.5}$ NAAQS is currently being prepared by the EPA. The guidance will likely consist of two parts: (1) how to use results of modeling and other analyses and (2) how to generate the results used to demonstrate attainment or reasonable progress.
- This work book section contains an overview of model applications and evaluations including ideas for using ambient air quality data throughout the assessment of attainment. Example PM models and performance evaluations are also discussed.

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