

United States  
Environmental Protection  
Agency

Office of Air Quality  
Planning and Standards  
Research Triangle Park, NC 27711

EPA-450/4-92-011a  
June 1992

Air

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# **GUIDELINE FOR REGULATORY APPLICATION OF THE URBAN AIRSHED MODEL FOR AREAWIDE CARBON MONOXIDE**

## **VOLUME I: TECHNICAL REPORT**



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MONOXIDE

VOLUME I: TECHNICAL REPORT

U.S. Environmental Protection Agency  
Office of Air Quality Planning and Standards  
Technical Support Division  
Research Triangle Park, NC 27711

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This report has been funded by the United States Environmental Protection Agency (EPA) under contract 68D00124 to Systems Applications International (SAI). Thomas N. Braverman served as the EPA work assignment manager. Any mention of trade names or commercial products is not intended to constitute endorsement or recommendation for use.

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## **ABBREVIATIONS**

<b>AIRS</b>	<b>Aerometric Information Retrieval System</b>
<b>CAAA</b>	<b>Clean Air Act Amendments</b>
<b>CARB</b>	<b>California Air Resources Board</b>
<b>CMSA</b>	<b>Consolidated Metropolitan Statistical Area</b>
<b>CO</b>	<b>Carbon Monoxide</b>
<b>DWM</b>	<b>Diagnostic Wind Model (UAM preprocessor program)</b>
<b>EPA</b>	<b>U.S. Environmental Protection Agency</b>
<b>EPS</b>	<b>Emissions Preprocessor System for the UAM</b>
<b>FIP</b>	<b>Federal Implementation Plan</b>
<b>LAV</b>	<b>Link Attribute Value</b>
<b>MSA</b>	<b>Metropolitan Statistical Area</b>
<b>NAAQS</b>	<b>National Ambient Air Quality Standard(s)</b>
<b>NTIS</b>	<b>National Technical Information Service</b>
<b>NWS</b>	<b>National Weather Service</b>
<b>OAQPS</b>	<b>EPA Office of Air Quality Planning and Standards</b>
<b>OMS</b>	<b>EPA Office of Mobile Sources</b>
<b>ORD</b>	<b>EPA Office of Research and Development</b>
<b>RWC</b>	<b>Residential Wood Combustion</b>
<b>SAI</b>	<b>Systems Applications International</b>
<b>SCRAM BBS</b>	<b>EPA Support Center for Regulatory Air Models Bulletin Board System</b>
<b>SIP</b>	<b>State Implementation Plan</b>
<b>TAZ</b>	<b>Transportation Analysis Zones</b>
<b>TCM</b>	<b>Transportation Control Measures</b>

<b>UAM</b>	<b>Urban Airshed Model</b>
<b>USGS</b>	<b>United States Geologic Survey</b>
<b>VMT</b>	<b>Vehicle Miles Traveled</b>

## **ACKNOWLEDGMENTS**

Much of the format, style, and, where applicable, content of this guidance document was borrowed from the EPA guidance document titled "Guideline for Regulatory Application of the Urban Airshed Model." The principal authors of that document were Mr. Dennis C. Doll (U.S. Environmental Protection Agency (EPA), Office of Air Quality Planning and Standards (OAQPS)), Dr. Richard D. Scheffe (EPA, OAQPS), Dr. Edwin L. Meyer (EPA, OAQPS), and Mr. Shao-Hang Chu (EPA, OAQPS).

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## **CHAPTER 1**

### **INTRODUCTION**

Under the Clean Air Act Amendments of 1990, over 40 urban areas are classified as nonattainment with respect to the 8-hour National Ambient Air Quality Standard (NAAQS) for carbon monoxide (CO). Of these urban areas, those whose 8-hour average design value exceeds 12.7 ppm are recommended to use an urban areawide model to address attainment of the CO NAAQS of 9.0 ppm in the revision of their State Implementation Plan (SIP). SIP revisions demonstrating attainment of the CO NAAQS are required by the Clean Air Act Amendments of 1990. The Urban Airshed Model (UAM) has been identified as an effective tool for evaluating emission control requirements needed to attain and maintain the CO NAAQS.

The purpose of this document is to provide guidance in the procedures used to apply the UAM for CO SIP attainment demonstrations and to ensure national consistency in model applications.

Methodologies and procedures used in the preparation of UAM inputs and applications to carbon monoxide regulatory issues are addressed in this report. This document also describes recommendations for the preparation of all input files needed to exercise the UAM. The technical explanation and rationale for the development of UAM inputs are discussed in Appendix C.

The UAM source code is maintained and distributed by the Source Receptor Analysis Branch, Technical Support Division, of the EPA Office of Air Quality Planning and Standards (OAQPS). Users will be informed of modifications or enhancements to the UAM through the Support Center for Regulatory Air Models Bulletin Board System (SCRAM BBS). Additionally,

the UAM source code, user's guide, and test case data base are available from the National Technical Information Service (NTIS)(703-737-4600).

Steps needed to conduct an urban-scale modeling study consist of the following:

1. Establish a protocol for the modeling study in which candidate modeling episodes are identified.
2. Compile air quality, meteorological, and emissions data to develop UAM input files for each meteorological episode to be used in the attainment demonstration model simulations.
3. Execute the model for each meteorological episode.
4. Conduct diagnostic analyses on each meteorological episode simulation. The principal purpose of diagnostic analyses is to ensure that the model properly characterizes physical phenomena (e.g., wind fields, spatial and temporal emission patterns) instrumental in leading to observed CO concentrations. The visible product is enhanced model performance (i.e., better spatial and temporal agreement with observed data). Diagnostic model simulations are intended to uncover potential model input data gaps that, when corrected, may lead to improved model performance.
5. Exercise the model for each meteorological episode and use a series of performance measures to determine overall model performance in replicating observed CO concentrations and patterns.
6. For each meteorological episode, estimate emissions and air quality for the projected attainment year required under the CAAA. Perform model simulations

for each episode to determine whether the CO NAAQS can be met in the attainment year.

7. If the model simulations for the attainment year do not show attainment for each modeled episode, develop additional emission control measures on selected source categories.
8. Perform model simulations for the emission control measures to demonstrate attainment of the CO NAAQS for each meteorological episode. If the control measures do not show attainment, repeat steps 7 and 8 as an iterative process until attainment is shown for each modeled episode.

This report is divided into six sections. Section 1 provides background information about air quality problems related to high CO concentrations and describes the philosophies underlying UAM areawide CO applications. Section 2 describes the modeling protocol and development processes. Section 3 discusses domain and data base issues. Section 4 discusses data quality assurance and model diagnostic analysis. Section 5 discusses model performance evaluation and Section 6 describes the methodology to be followed in attainment demonstration.

### **1.1 Background**

High 8-hour CO concentrations in urban areas often result from periods of high emissions (the afternoon and evening mobile traffic peak) coinciding with adverse meteorological conditions (low wind speeds and poor vertical dispersion). Under such conditions, concentrations can increase rapidly near heavy traffic areas. The greatest problem in achieving ambient 8-hour CO standards in an urban area is controlling the neighborhood-scale buildup and persistence (over 8 hours or more) of elevated CO concentrations. Under meteorological conditions conducive to high concentrations, CO emissions become trapped in a shallow, stable surface layer caused by the radiational cooling of the air next to the ground. When winds are light and variable, this high-concentration air mass may extend over a large portion of an

urbanized area depending upon topography and emission distribution and can remain relatively stationary or meander during nighttime hours, with the result that one or several areas may experience high CO concentrations throughout the night and early morning hours. Maximum 8-hour average CO concentrations result from the combined effect of microscale and neighborhood-scale processes. For some urban areas, sites on the downwind edge of high emission density regions can experience extended periods of high concentrations even if wind speeds are moderate.

Carbon monoxide emissions result from incomplete combustion of fossil fuels which include residential wood combustion and industrial emissions. However, motor vehicle exhaust accounts for most of the CO emissions in urban areas. To reduce motor vehicle emissions injected into the atmosphere, either the emission rates of individual vehicles must be reduced or traffic conditions (volumes, speeds, stops and idling periods) must be modified. To estimate the effects of these control measures, both microscale and neighborhood-scale modeling must be conducted. Areas with significant stationary sources as determined under Section 187c (Laxton, 1991a) should perform modeling following the techniques cited in the Guideline on Air Quality Models (Revised) (EPA, 1986).

Previous UAM modeling studies of CO have been performed in Phoenix (Haney, 1988; Causley et al., 1991) and Denver (Anderson et al., 1977; Rogers, 1986). In the studies conducted in Denver, only neighborhood-scale modeling was performed. In later studies, neighborhood-scale and microscale processes were modeled separately, and the results of each were added to estimate the total concentrations at selected roadway intersections to assess attainment. This approach allowed use of the UAM to describe the accumulation of emissions over several hours and kilometers within a three-dimensional modeling grid, as well as the separate estimation of roadway impacts within a few hundred meters of the roadway intersection. The combined model results were then used to evaluate the effectiveness of control measures. Procedures for determining the roadway intersection concentration for CO SIP applications are addressed in the guidance document Guideline for Modeling Carbon from Roadway Intersections (EPA, 1992a).



## 1.2 Application of the UAM

Conditions that often are conducive to high areawide 8-hour CO concentrations (low wind speeds, stable conditions) are the same conditions for which the steady-state assumption inherent in Gaussian formulated models is invalid. The steady-state assumption results in the accumulation of large errors due to the inability of the Gaussian models to gradually build carbon monoxide concentrations from hour to hour. The grid cell and time step modeling approach of the UAM is more appropriate for CO modeling because it is capable of handling low wind speeds and stable conditions by allowing concentrations to accumulate over time.

A number of past studies involving the UAM relied on intensive and expensive monitoring studies to provide information to adequately prepare model inputs. Recent studies have shown that routine meteorological and air quality observations are adequate for UAM SIP applications. This set of procedures (known as PLANR, or Procedures for Low-cost Airshed applications to Nonattainment Regions) was applied to determine its feasibility in future SIP efforts (Morris et al., 1990). Although the PLANR methodology was initially confined to ozone nonattainment problems, the same general methodology can be applied equally well to carbon monoxide nonattainment areas. The method relies on the ability of the UAM to accurately predict hourly concentrations within a certain distance and time using routine data gathered from the monitoring station measuring the highest carbon monoxide values. Although the PLANR method may prove to be applicable to most CO nonattainment areas, some areas with complex terrain and/or meteorology may still require more intensive data for successful application of the UAM.

## CHAPTER 2

### MODELING PROTOCOL

The UAM modeling domain may encompass multiple geopolitical boundaries (counties, cities, and states) with a potentially large regulated community. Therefore, the development of a modeling protocol is recommended to (1) promote technical credibility, (2) encourage the participation of all interested parties, (3) provide for consensus building among all interested parties concerning modeling issues, and (4) provide documentation for technical decisions made in applying the model as well as the procedures followed in reaching these decisions.

The protocol should detail and formalize procedures for conducting all phases of the modeling study, such as (1) describing the background and objectives of the study, (2) creating a schedule and organizational structure for the study, (3) developing the input data, (4) conducting diagnostic and model performance evaluations, (5) interpreting modeling results, (6) describing procedures for using the UAM and roadway intersection models to demonstrate whether proposed strategies are sufficient to attain the CO NAAQS, and (7) producing documentation and data analyses that must be submitted for EPA regional office review and approval.

All issues concerning the modeling study must be thoroughly addressed during the protocol development. Thus, modifications to the protocol as the study progresses should not be needed unless unforeseen procedural and/or technical issues are encountered. All parties involved in the study should agree to protocol modifications through the modeling policy oversight committee, if applicable (see below). It is especially important that the state/local agencies and EPA regional office(s) overseeing the study concur on protocol modifications.

## **2.1 Protocol Development Process**

The state agency responsible for developing the CO State Implementation Plan (SIP) is usually the lead agency responsible for developing the modeling protocol. For domains encompassing parts of more than one state, the responsible state agencies need to develop the modeling protocol jointly. Since the protocol should describe the modeling policy and technical objectives of the study, input will be required from various EPA and state/local personnel dealing with regulatory policy issues and from others with modeling expertise. In some cases a modeling policy oversight and technical committee will need to be organized to address these issues. The composition and responsibilities of the committee should be defined in the modeling protocol.

Responsibilities of the modeling policy oversight committee will be, at a minimum, to set the objectives of the study, set the schedule, determine resource needs, and implement any modifications to the protocol as the modeling study proceeds. The committee should include representatives from the appropriate EPA regional office(s), state/local agencies, the regulated community, and public interest groups. It is important that appropriate policy-oriented personnel be identified for membership on the committee.

Responsibilities of the technical committee will be, at a minimum, to develop the protocol's technical specifications concerning emission inventories, meteorological data, air quality data, data quality assurance, emission control strategies, model diagnostic analyses, model performance evaluation procedures, and interpretation of model results. The technical committee should include appropriate technically oriented members from the EPA regional office(s), state/local agencies, the regulated community, and public interest groups.

The modeling protocol must be submitted to the appropriate EPA regional modeling contact for review and approval. The EPA regional modeling contact should be a member of the policy oversight and/or technical committee so that rapid review and approval of the protocol is assured.

### **Recommendations**

A protocol document is recommended for each UAM application used for a CO attainment demonstration. This protocol should describe the methods and procedures to be used for conducting the CO modeling study.

Additionally, it is suggested that both a policy oversight committee and a technical committee be established to develop the modeling protocol. The composition and responsibilities of the committees should be defined in the protocol.

The modeling protocol and any modifications to it should be agreed upon by all parties involved in the study through the policy oversight committee. It is especially important that the state/local agency participants and EPA regional office(s) overseeing the modeling study concur on any protocol modifications. Protocol modifications should be documented for subsequent public review.

The modeling protocol must be submitted to the appropriate EPA regional modeling contact for review and approval.

## **2.2 Contents of Protocol Document**

### **Recommendations**

It is recommended that the applicable components listed in Table 2-1 be included in the protocol document for each attainment demonstration modeling study. A description of each component is presented in Appendix A.

TABLE 2-1

**EXAMPLE TABLE OF CONTENTS FOR PROTOCOL DOCUMENT**

1. UAM Modeling Study Design
  - Background and Objectives
  - Schedules
  - Deliverables
  - Management Structure/Technical Committees
  - Participating Organizations
  - Relationship to Planning/Strategy Groups
2. Domain and Data Base Issues
  - Data Bases:
    - Air quality
    - Meteorology
  - Base Meteorological Episode Selection
  - Modeling Domain
  - Horizontal Grid Resolution
  - Number of Vertical Layers
  - Emission Inventory
  - Specification of Initial and Boundary Conditions
  - Wind Field Specification
  - Inversion Depth
  - Sources of Other Input Data
3. Quality Assurance and Diagnostic Analyses
  - Quality Assurance Tests of Input Components
  - Diagnostic Tests of Base Case Simulation
  - Test Results/Input Modifications
4. Model Performance Evaluation
  - Performance Evaluation Tests
5. Roadway Intersection Modeling
  - Selection Methodology for Intersections Modeled
  - Modeling Methodology
6. Attainment Demonstrations
  - Identification of Attainment-Year Mandated Control Measures
  - Methodologies for Generating Control Strategy Emission Inventories
  - Procedures for Attainment Demonstration
7. Submittal Procedures
  - Data Analysis Review
  - Documentation Review and Approval

## CHAPTER 3

### DOMAIN AND DATA BASE ISSUES

Described in this chapter are the following topics: episode selection, domain selection, meteorological inputs, air quality data, and emissions inventories. Choices made in each topic area are often interrelated. Accordingly, decisions concerning a particular topic area probably will be based on consideration of several areas. In several topic areas, recommendations are made concerning minimum requirements for data availability and modeling resolution. To reduce uncertainties in modeling inputs and outputs, users are encouraged to exceed these minimum recommendations whenever possible.

#### 3.1 Overview of Model Inputs

This section provides an overview of the 13 input files required to exercise the Urban Airshed Model (UAM). Table 3-1 presents a list of these input files and indicates the amount of effort required to create each one. A more complete reference for the UAM is contained in the UAM User's Manual (EPA, 1990).

Of the 13 input files, two are considered "universal" in that they do not vary from one simulation to another. The first file, CHEMPARAM, run in the unreactive mode for carbon monoxide modeling, contains the list of species to be modeled. Other unreactive species may be simulated for little additional cost if the emission inventory data are available. The other input file, SIMCONTROL, contains parameters controlling the UAM simulation. In general, the date and time will vary for different meteorological episodes but not for the same episode.

TABLE 3-1. Overview of the 13 Urban Airshed Model input files.

Input File	Description	Typical Preparation Procedure	Relative Level of Effort
<b>AIRQUALITY</b>	Contains CO initial concentrations. Only the first hour of the simulation is needed.	1/R Interpolation of the monitor data. Assumed to be vertically constant through the mixed layer. Values above the DIFFBREAK are set to the concentrations at the top of the modeling region	minimal
<b>BOUNDARY</b>	Contains species concentrations along the boundary of the modeling domain.	Generally assumed to be spatially and temporally constant as a first approximation. Modeling domain should be large enough to minimize upwind transport situations. Use ambient data if there are stations near the boundary.	minimal
<b>TOPCONC</b>	Species concentrations at the top of the modeling region.	Generally assumed to be spatially and temporally constant. If special sampling data are available, data should be used.	minimal
<b>EMISSIONS</b>	Ground-level emissions of mobile and stationary sources.	Emissions inventory of total CO is prepared through survey and engineering analysis. Emissions must be spatially and temporally allocated.	large
<b>PTSOURCE</b>	Elevated emissions.	Same as for ground-level emissions. Requires information on stack parameters (exit temperature, velocity). Should be day-specific, if available. In some locations this may be entirely skipped if no significant point sources of CO exist.	minimal
<b>WIND</b>	3-dimensional gridded wind fields.	Prepared using Diagnostic Wind Model and surface and upper air data. Data are usually sparse. May need to rely on conceptual model of wind field based on previous studies.	moderate

TABLE 3-1. Concluded.

Input File	Description	Typical Preparation Procedure	Relative Level of Effort
DIFFBREAK	Height of the top of the ground-level inversion.	Use recommended method discussed in Section 3. Most uncertain piece of data required by UAM. Recommend sensitivity test by repeating simulations while varying DIFFBREAK height. Use of tethersondes, acoustic sounders, tower data, etc., if available, is preferred.	moderate (if data available)
TEMPERATUR	2-dimensional gridded surface temperature fields.	Prepared using surface temperature data collected at NWS and air quality monitoring networks	moderate
TERRAIN	Surface roughness and deposition factors.	Based on land use information. Deposition factors and surface roughness values have been developed for urban-scale model applications.	moderate
REGIONTOP	Height of the modeling region.	Generally assumed to be temporally and spatially constant. Usually set to a value greater than the maximum DIFFBREAK height.	minimal
METSCALARS	Contains miscellaneous meteorological scalars such as water concentration, exposure class, temperature gradients, and atmospheric pressure.	Water concentrations are based on relative humidity data, temperature gradients from Weather Service data, exposure class is based on cloud cover and solar zenith angle.	moderate
CHEMPARAM	Contains information on species to be modeled.	Does not vary with UAM applications.	minimal
SIMCONTROL	Controls the UAM simulation period.	Most parameters do not vary between simulations.	minimal



Of the other 11 UAM input files, the most time-consuming and resource-intensive to create is the low-level carbon monoxide emission file, EMISSIONS. This file is usually prepared concurrently with the preparation of the meteorological and air quality files. State/local agency participants using the UAM for areawide CO modeling should concentrate their efforts on the emissions inventory development, especially the mobile source component, preparation of the 3-dimensional wind fields, ground-level inversion height, and specification of thickness of model layers.

### **3.2 Episode Selection**

This subsection describes the criteria to be considered in selecting carbon monoxide (CO) meteorological episodes appropriate for modeling. The modeling protocol should include a complete discussion regarding episode selection. A trained meteorologist familiar with local and regional weather patterns should be consulted in the episode selection process. The following approach is recommended for selecting episodes for use in modeling:

1. Use the most recent years (1988 to present) of CO monitoring data as the period from which to select candidate modeling episodes.
2. Select as candidate modeling episodes the three highest non-overlapping 8-hour CO episodes from each year as determined by the highest monitored concentration per episode.
3. Examine the meteorological conditions for each candidate modeling episode.
4. Determine the different types of meteorological regimes for the candidate episodes. Conditions resulting in dissimilar source-receptor configurations should be the prime consideration in distinguishing different meteorological regimes. In areas dominated

by mobile source CO emissions and stagnation conditions, there may be only one meteorological regime. In areas with major point sources of CO and/or significant wood-burning CO emissions in addition to mobile source CO emissions, there may be multiple meteorological regimes because of dissimilar source-receptor configurations.

5. Rank each candidate episode within each meteorological regime according to the magnitude of the peak 8-hour CO concentration.
6. Model a minimum of one episode for each meteorological regime. Select the episode(s) for modeling from among the three highest ranked episodes from each meteorological regime. In general, the highest ranked episode within the meteorological regime should be selected for modeling. However, there may be circumstances in which the second or third ranked episode is more appropriate for modeling, e.g. (1) the air quality and meteorological data base is much better than that of the first ranked episode, (2) the second or third ranked episode is from a later year that includes controls that were not in effect in the year of the highest ranked episode; consequently, the use of the second or third ranked episode would be more conservative, and (3) the CO pattern for the highest ranked episode is distinctly different from all other candidate episodes (i.e., weekend instead of weekday).

States may want to consider a procedure other than the one outlined in Steps 1-6 for selecting modeling episodes. Any such procedure should be described in the modeling protocol and approved by the appropriate EPA Regional Office.

#### Recommendations

The modeling protocol should include a complete discussion of the choice of modeling episodes. It is recommended that episodes selected for modeling be from the four most recent years, 1988 to present. A trained meteorologist should assist in determining the different types of meteorological regimes under which 8-hour exceedances occur during

the four-year period. At a minimum, one episode for each meteorological regime should be modeled.

### **3.3 Selection of Modeling Domain and Resolution**

#### **3.3.1 Domain definition**

The size and location of the modeling domain define the data requirements for the modeling. Definition of the modeling domain (both horizontal and vertical dimensions and duration of simulation) depends upon the meteorology of the particular episode to be modeled. Criteria that play an important role in determining the modeling domain include:

- Stagnation period and duration of elevated CO levels
- Location of major current and future emission sources
- Wind flow pattern
- Size of recirculation pattern
- Available aerometric data
- Preassumed emission inventory region

Generally, the domain should be set as large as feasible in order to reduce the dependence of predictions on uncertain boundary concentrations and to provide flexibility in simulating different meteorological episodes. It is generally much easier to subsequently reduce the size of a modeled area than it is to subsequently increase it.

#### **Recommendations**

It is recommended that the domain be set large enough to encompass all major current and future emission sources, and reduce the dependence of predictions on uncertain boundary concentrations.

### **3.3.2 Horizontal grid cell size**

The horizontal dimension of each model grid square is based upon (1) the sensitivity of predicted concentrations to horizontal grid size, (2) the resolution of observed meteorological and air quality data and/or estimated emissions data, and (3) limitations imposed by other considerations such as a required minimum domain size. Air parcel trajectories can be performed using wind observations taken on each day of the candidate carbon monoxide episodes to determine the horizontal limits of the modeling domain.

Relatively high horizontal grid cell resolution should be used in UAM carbon monoxide modeling applications. It is recommended that at a minimum the horizontal resolution should be no greater than 2 x 2 km. Model applications with finer grid resolution lead to slightly higher peak values because artificial dilution is kept to a minimum. Larger (or coarser) horizontal grid resolutions (> 2 km) are not recommended because (1) artificial dilution will result for point emissions sources, and (2) loss of spatial resolution will result in less effective evaluation of control strategy effectiveness.

#### **Recommendations**

It is recommended that, at a minimum, horizontal grid cell resolution should be no greater than 2 x 2 km. Smaller grid cell sizes are encouraged because they allow more accurate gridding of area and mobile sources. Additionally, point sources are better characterized by smaller grid cell sizes.

### **3.3.3 Number of vertical layers**

In most UAM CO applications, nearly all CO emissions are confined to the near surface; as a result, model applications will need at a minimum two vertical layers: a lower layer extending from the surface to the diffusion break, and an upper layer extending from the diffusion break to the top of the model domain. However, in some cases additional model layers may be warranted. At a minimum, these situations would include (1) multi-day elevated CO events in which carryover from the previous day's emissions suspended aloft is believed to play

a significant role; (2) episodes where vertical wind shear is significant, resulting in differential transport of CO emissions within each model layer; (3) episodes where elevated point source emissions are significant, resulting in emissions being suspended aloft under stable nighttime conditions and not mixing downward until the surface-based inversion is fully eroded; and (4) episodes where the vertical CO concentration profile changes rapidly below the diffusion break.

To accurately describe the vertical structure, it is recommended that data be collected describing both the vertical temperature and CO concentration profile. The number of vertical layers below the inversion base should characterize the vertical CO concentration profile. The modeling protocol document should include a complete discussion regarding the basis for choosing the number of vertical layers.

#### Recommendations

Based on previous UAM CO applications, it is recommended that a minimum of two vertical model layers be used in the modeling study. However, additional layers may be warranted in cases where meteorology or emission source type justifies the use of additional layers. The modeling protocol document should discuss the basis for choosing the number of vertical layers. It is recommended that 20 m be used as the minimum depth of the vertical layers below the diffusion break and 20 m for the vertical layers above the diffusion break.

#### 3.3.4 Time span

The time span of the UAM simulations should be at least 18 hours. Longer time spans may be required to examine episodes where carryover from earlier emissions is believed to play a role in producing high carbon monoxide concentrations. For example, an 8-hour exceedance ending in mid morning may include substantial contributions from the previous evening. These emissions must be modeled to properly treat future changes in daily emissions. If an episode is selected that shows persistent recirculation of materials or lengthy stagnation, longer simulation periods may have to be defined.

A primary reason for extending the simulation period is to reduce the influence of the

initial conditions on the predicted carbon monoxide concentration. The starting time of the simulation should be during the mid-afternoon hours when ambient concentrations are still low, just prior to the development of the ground-level inversion. The ending time usually extends into the mid-morning hours.

### Recommendations

Simulations should extend for at least 18 hours. Longer time spans may be preferable when one day's exceedance can be traced to emissions from the previous day.

## **3.4 Preparation of Meteorological Inputs**

The availability of meteorological data varies widely among prospective modeling domains. Also, a variety of techniques are available for developing wind fields, temperature fields, and mixing heights. Although high resolution and confidence for all meteorological data are desirable, time and resource constraints force a compromise between desirable and acceptable methods. Historically, measured meteorological data have been spatially and temporally interpolated for most UAM applications. More recently, diagnostic and prognostic meteorological modeling techniques have been explored as possible means to develop input fields (particularly wind fields) for air quality models. Procedures for preparation of the meteorological inputs are presented in this section. As shown in Table 3-1, with the exception of the EMISSIONS file, the WIND file is the most resource-intensive file to prepare.

### **3.4.1 Surface roughness and deposition (TERRAIN)**

The TERRAIN file contains (1) surface roughness lengths and (2) deposition factors. The surface roughness lengths are used in computation of vertical exchange coefficients. Both the roughness lengths and deposition factors are used in computing deposition of gaseous species.

Because deposition of CO is negligible for most CO UAM applications, detailed representation of surface characteristics is not crucial. The magnitudes of vertical exchange coefficients are unimportant, given that maximum CO concentrations occur at the surface under very stable conditions when mixing between UAM layers is minimal. It may be sufficient to assume values of surface roughness and deposition factors typical of urban land use over an entire CO modeling domain. Appendix C details a methodology for developing surface roughness and deposition factors.

### Recommendations

Previous applications have found that using surface roughness and deposition factors typical of "urban" land use over the entire CO modeling domain is sufficient because deposition of CO is slight.

It is recommended that, unless important urban versus rural land use areas are contained within the modeling domain, a surface roughness length of 0.5 m and a deposition factor of 0.3 be used.

#### **3.4.2 Diffusion break (DIFFBREAK)**

In UAM terminology, the diffusion break (DIFFBREAK) is the height at which the upper and lower layers are divided. The value of DIFFBREAK affects the way many of the other parameters are used by the UAM.

Predictions from the UAM have been shown to be fairly sensitive to the diffusion break field. Therefore, the temporal variations in the diffusion break field over the UAM domain should be described as realistically as possible. The UAM modeling system contains a methodology for deriving the diffusion break based on surface temperatures, vertical sounding measurements of temperature, and cloud cover (EPA, 1990). Appendix C contains a technical discussion of important considerations for determining the diffusion break for CO applications. However, because of the diversity of techniques and data bases that may be available on a case-by-case basis, a specific procedure for deriving the diffusion break field cannot be recommended in all cases.

### Recommendations

It is recommended that, at a minimum, the techniques described in the UAM User's Guide and/or Appendix C be used in establishing the diffusion break field in the domain.

The choice of upper-air stations to be used in the diffusion break calculations should be based on prevailing wind fields and location of the upper-air stations relative to the UAM domain. If there are no upper-air stations within the domain, stations outside the domain may need to be used. An experienced meteorologist should be consulted on the selection of upper-air stations for use in determining the diffusion break.

The techniques for generating the diffusion break field should be described in the Appendix C protocol document. Techniques other than that described in the UAM User's Guide or should be documented and justified.

Because the assignment of DIFFBREAK in CO UAM applications is relatively uncertain, it is recommended that the sensitivity of CO predictions to DIFFBREAK assumptions be assessed by repeating the UAM simulations with DIFFBREAK values (1) decreased by 50 percent; and (2) increased by 100 percent.

#### **3.4.3 Top of the modeling domain (REGIONTOP)**

A spatially and temporally constant top of the modeling region (REGIONTOP) is recommended for virtually all UAM applications. Most 8-hour CO violations of the National Ambient Air Quality Standards (NAAQS) occur during nighttime hours following the evening traffic rush. Thus, it is recommended that for most CO applications (nighttime) the REGIONTOP be set at 200 m. However, this value may be low when: (1) episodes extend over several days, (2) high CO events are not associated with strong surface-based inversions, or (3) elevated point source CO contributions are significant. In these cases the REGIONTOP should be specified above the highest DIFFBREAK height by at least the depth of one upper-layer cell.

### Recommendations

For most CO applications (nighttime) set the REGIONTOP to 200 m.



#### 3.4.4 Winds (WINDS)

Methodologies to construct wind fields for UAM applications have historically fallen into three categories:

1. Objective analyses that interpolate observed surface and aloft data throughout the modeling domain
2. Diagnostic wind models in which physical constraints are used in conjunction with objective analyses to determine the wind field
3. Prognostic models based on numerical solution of the governing equations for mass, momentum, energy, and moisture conservation along with numerical solutions for thermodynamic processes

Objective analysis. These procedures generally involve straightforward interpolative techniques. They have the advantage of being relatively simple and inexpensive to use. The primary disadvantages are that these analyses contain limited physical concepts, and results are highly dependent upon the temporal and spatial resolution of the observed values. Thus, in domains containing sparse observational data or complex topography, results may be unsatisfactory.

Diagnostic wind models. These models improve mass consistency for the flow fields. This may be addressed through parameterizations for terrain blocking effects and upslope and downslope flows, as in the UAM Diagnostic Wind Model (EPA, 1990). Diagnostic models generally require minimal computer resources and can produce a three-dimensional wind field; however, they need representative observational data to generate features such as land and sea breezes. Appendix C contains a detailed technical discussion of the use of the DWM for CO model applications.

Prognostic models. These models simulate relevant atmospheric physical processes while requiring minimal observational data. Prognostic models require specification of the synoptic-scale flow. Reliability of these approaches is usually enhanced if sufficient observations are available to "nudge" solutions closer to observations. Since these models can simulate temperature fields in addition to the wind field, it is possible to determine stabilities and inversion depth, thus eliminating the need to generate these from sparse observational data. Another significant advantage is that interdependencies of various meteorological inputs with one another are considered in prognostic models. A major disadvantage is the extensive computational resources needed to run a prognostic model. Additionally, the availability of evaluated models and expertise needed to apply them for general application with grid models is limited.

Selection of a specific technique for generating the domain wind field depends largely on (1) the spatial and temporal resolution of surface and upper-air observations, (2) available modeling expertise in applying alternative meteorological models, and (3) available computer resources. However, some guidelines on preferences for generating the wind fields are as follows.

The development of a wind field for each modeling episode depends upon ground-level and elevated wind observation data. It is preferred that a surface-based monitoring network report wind speed and direction as hourly averages because an hour is the time period commensurate with most UAM concentration output analyses. The surface monitoring network should be broad and dense so that diagnostic models can depict major features of the wind field. Data representing vertical profiles of wind speed and direction are required in order to establish upper-level wind fields. Preferably, data should provide adequate spatial (horizontal) and temporal resolution. Results of UAM applications are often criticized because of inadequate meteorological data, and lack of sufficient meteorological data often prevents definitive diagnostic analyses. Thus, the need for adequate meteorological data cannot be overstated. Appendix C contains a detailed technical discussion about the data needs for the DWM for CO applications.

Time and/or resource constraints may preclude consideration of new meteorological monitoring stations. Thus, it is likely that the base case to be used in the attainment demonstration will be from a historical episode for which model performance has been deemed acceptable.

### Recommendations

It is recommended that the DWM be used to generate the UAM gridded wind fields. As discussed in Appendix C, the DWM modeling domain should encompass terrain features outside the UAM modeling domain which may affect the DWM representation of the flow field. The use of other techniques for deriving the wind field, such as prognostic wind models or other objective techniques, may be employed on a case-by-case basis, subject to approval from the appropriate EPA regional office.

Meteorological data routinely available for a UAM modeling demonstration usually consist of National Weather Service (NWS) hourly surface and upper-air observations (for winds aloft). If these data are the only data available for use in a modeling demonstration, they may have to suffice. However, the NWS data consist of observations made over very short periods rather than hourly averaged values. An assumption that wind velocity measured over a very short period persists unaltered over an hour may lead to an overestimate of transport. Therefore, whenever possible, hourly averaged meteorological data (e.g., from an intensive field study) should be used. Additional meteorological data may be available from other sources in the domain (e.g., an on-site meteorological monitoring program at an industrial facility). These data may be used to supplement the NWS data, provided the data have been adequately quality assured. Additionally, the EPA guideline entitled On-Site Meteorological Program Guidance for Regulatory Modeling Application (EPA, 1987) should be consulted to assess whether the supplementary data reflect proper siting of meteorological instruments and appropriate data reduction procedures.

In planning a special field study to provide a more spatially and temporally dense meteorological data base, the number of surface meteorological monitoring stations should be sufficient to describe the predominant wind flow features within the modeling domain. An experienced meteorologist familiar with local climatic patterns should be consulted concerning the location and suitability of the surface meteorological stations. Vertical sounders or profilers are highly encouraged in a special field study to resolve winds aloft and vertical temperature gradients. Any special field study and monitoring program should be planned in consultation with the appropriate EPA regional office before implementing the study.

### **3.5 Preparation of Air Quality Inputs**

Ambient air quality data are generally used to specify initial- and boundary-condition concentrations. In the UAM, these functions are performed by the Air Quality, Top Concentration and Boundary Condition files. In addition, air quality data are needed to diagnose problems in setting up model applications and assessing model performance for the meteorological episodes being considered in the attainment demonstration. A lean air quality data base may introduce significant uncertainties in characterizing model performance. This section discusses the procedures for preparing air quality inputs needed by the UAM.

#### **3.5.1 Air quality (AIRQUALITY)**

The air quality (AIRQUALITY) file specifies the initial pollutant concentrations to be modeled by the UAM. The concentrations are specified for the full three-dimensional grid.

A routine monitoring data base usually does not, by itself, make a complete, three-dimensional specification of initial conditions possible. For instance, spatial coverage provided by monitoring stations is generally incomplete, with most stations located within urban centers and therefore strongly influenced by local emissions sources. Monitors located in rural areas, which can give an indication of appropriate local background concentrations, are rare. As a rule, only surface measurements are available, so no direct indicator of the vertical distribution of carbon monoxide will be available. The problem, therefore, is to specify the three-dimensional concentration field from a very sparse data set. A detailed technical discussion is presented in Appendix C for developing initial conditions from a sparse data set.

#### **Recommendations**

At the inflow boundaries, air quality data at the surface and aloft should be used whenever available to specify the initial boundary conditions.

For values near the surrounding perimeter of the model domain, default values as shown

in Table 3-2 may be used where necessary. Selection of these values should be based on how pristine the surrounding areas are considered to be. For example, if the area near the boundary can be classified as rural, then the low CO value should be used; if that area is better classified as suburban, then the middle value should be used.

To diminish dependence on arbitrary specification of initial conditions, a simulation should begin prior to the buildup of high carbon monoxide concentrations.

### **3.5.2 Top concentration (TOPCONC)**

The recommended method for setting the top concentrations in cells above the DIFFBREAK is to set them equal to the observed concentration at the top of the region. When top concentration is not known, the concentration should be no higher than the middle concentration level of Table 3-2. If measurements are available indicating higher concentrations exist at the top of the region, they can be used, but the user should verify that they are representative of more than just a local value before using them for the entire grid.

In the absence of upper air concentration data, the values in TOPCONC would be the low values from Table 3-2 for a relatively remote area. If there is evidence that considerable recirculation of carbon monoxide pollutants may occur, these values should be raised to the mid-level values. The mid-level values should also be used if the region is surrounded by other urban/suburban areas that would elevate the background pollutant concentrations.

### **Recommendations**

It is recommended that the concentration at the top of the region be used to set concentrations in cells above the DIFFBREAK. If no data are available for upper air concentrations, values should be set by referring to Table 3-2, considering the level of urbanization and the importance of recirculation.

### **3.5.3 Boundary conditions (BOUNDARY)**

The BOUNDARY file contains both the definition of the physical boundaries of the

TABLE 3-2. Recommended background concentrations for carbon monoxide (Killus et al., 1982).

Value	Area Classification	Concentration (ppm)
Low	Rural	0.1
Middle	Suburban	0.2
High	Urban	0.5

region to be modeled and the concentrations along each of the lateral boundaries. When there are no available data near the lateral boundaries of the region, specification of the boundary concentrations can be difficult.

Two approaches for specifying boundary conditions for UAM simulations are as follows: (1) use objective/interpolation techniques with a sufficient amount of measured data (i.e., data from an intensive field program) and (2) use default background values and expand the upwind modeling domain to mitigate uncertainties due to paucity of measurements.

Ideally, the preferred technique would be based on an intensive field program. However, this approach is seldom feasible for historical episodes. Presented next are recommendations for implementing each technique just identified for deriving boundary conditions, including discussion of the advantages and disadvantages of each technique. A detailed technical discussion for developing boundary conditions for a sparse data set is presented in Appendix C.

Use of measured data. All sources of air quality data for a particular modeling domain should be evaluated for applicability in establishing boundary conditions. Unfortunately, most ongoing monitoring programs have been designed (understandably so) with a receptor-based orientation. While available monitoring data are useful for evaluating model performance, they usually are not adequate for establishing boundary concentrations.

Use of default values - Some urban areas may lack adequate data suitable for establishing boundary conditions. Section 3.3 on domain selection and Chapter 4 on diagnostic analyses recommend constructing domains large enough to minimize the sensitivity of inner core and downwind concentrations to assumed boundary conditions.

Boundary-condition concentrations are influenced by large- and small-scale weather patterns and emissions distributions that are unique to each modeling domain. Thus, case-specific attributes should be used in estimating these concentrations whenever feasible. For example, boundary concentrations of regions where residential wood combustion is significant

are likely to be higher during very cold conditions than during periods of more mild temperatures.

#### Recommendations

To develop boundary conditions, it is recommended that one or more monitoring stations be sited upwind of the central urban area along prevailing wind trajectories that give rise to carbon monoxide exceedances.

At the inflow boundaries, air quality data at the surface and aloft should be used whenever available to specify the boundary conditions.

Those having to use default values should plan to perform diagnostic/sensitivity simulations (see Chapter 4) to evaluate the sensitivity of domain-interior model predictions to the boundary conditions.

Table 3-2 lists the recommended default boundary values depending on the area classification. When using default values, the boundary of the domain should extend as far upwind as practicable.

### **3.6 Performance Evaluation Data**

Ambient carbon monoxide measurements are needed to diagnose problems in setting up model applications and assessing model performance for the meteorological episodes being considered in the attainment demonstration. A lean air quality data base may introduce significant uncertainties in characterizing model performance. The Technical Committee should agree on the adequacy of the existing data for assessing model performance.

#### Recommendations

For lean data bases the Technical Committee should scrutinize in detail the adequacy of the data base to ensure that model performance that appears to be acceptable has not actually resulted from compensating errors in the data bases. Additional diagnostic analyses may be necessary for lean data bases from historical episodes.



### 3.7 Emission Inventory

The credibility of UAM applications is directly tied to formulating the best possible emission inputs. Model performance may hinge on how well emissions are estimated. Also, in the attainment demonstration, modeling results are used to determine emission scenarios that lead to improved air quality levels consistent with the NAAQS. A faulty emission inventory could lead to erroneous conclusions about the extent of needed controls.

Carbon monoxide emissions in most regions are primarily from motor vehicles. However, in some regions emissions from residential wood combustion may contribute significantly to the total carbon monoxide emissions. Stationary sources are composed of either point sources, which are sizeable stationary emission sources at specific locations, or area sources, which are emissions from stationary and non-roadway mobile sources that are too small and/or too numerous to be included in the point source inventory (e.g., wood stoves). For most, but not all, areas of the country, the peak CO season is the wintertime months. Therefore, the focus of CO emission inventory development is the on-road vehicle emissions for wintertime CO episodic conditions. However, discussion will begin with an overview of information sources that are available to explain the development of stationary and area source CO emission inventories suitable for use with UAM.

Much of the information required to assemble CO modeling inventories will have already been assembled for the base year inventory, which is required for all CO nonattainment areas under the Clean Air Act Amendments of 1990 (CAAA). Specific information on base year inventory requirements is contained in Emission Inventory Requirements for Carbon Monoxide State Implementation Plans (EPA, 1991b). The base year inventory for the CO SIP submittals due November 1992 will be from the 1990 base year. Other documents (EPA, 1991c; EPA, 1988; Laxton, 1991b) describe the development of emission inventories from raw data, and specifically address questions regarding the methodology to spatially and temporally resolve CO emission estimates contained in the base year inventory so that they can be used with the UAM.

For use in regulatory applications of the UAM, the base year modeling inventory will have to undergo several adjustments. First, the inventory needs to be adjusted to be consistent with meteorological conditions during each selected episode (i.e., "base year day-specific emissions"). Second, the resulting "base year day-specific emissions" should be adjusted to reflect control programs and activity levels prevailing during the year(s) of selected episodes. For example, if a selected episode occurred in 1988, the "base year day-specific emissions" would be further adjusted to reflect controls and activity levels prevailing in 1988. This latter adjustment is needed to provide an estimate of emissions most suitable for evaluating performance of the UAM.

As noted in Chapter 1, once the UAM's performance has been evaluated and the model has been determined to perform satisfactorily, it is used to derive control strategies to attain the NAAQS. This requires another adjustment to the "base year day-specific emissions" that entails use of growth factors, ongoing control programs and retirement rates for obsolete sources of emissions to project "base year day-specific emissions" to the years by which the CAAA specify that the NAAQS must be attained. The resulting attainment year modeling inventory is used as a starting point from which to construct a control strategy inventory, which is obtained by superimposing additional control measures on sources of emissions in the attainment year modeling inventory.

In summary, a base year modeling inventory is first adjusted to evaluate UAM performance. The base year modeling inventory is then readjusted to reflect emissions most likely to occur at the time the CAAA require attainment of the NAAQS.

Two emission files drive the UAM--a file of emissions that are injected into the first, surface-based vertical layer, and a file of elevated point source emissions that are injected into vertical layers above ground level. The UAM Emissions Preprocessing System (EPS) (EPA, 1992b) reads county-level area- and point-source files and performs three major functions: (1) area sources and point sources are allocated to grid cells; (2) temporal profiles are assigned to source categories; and (3) point sources with effective plume heights greater than a prescribed

cutoff level are assigned to the elevated point source file, and the remaining point sources are assigned to the surface-layer emissions file.

Emission inventories are developed for stationary area, stationary point, and off-road emission inventories that are appropriate for the UAM. The following issues arise in developing emission input data: (1) use of surrogate factors to grid area sources, (2) treatment of mobile sources, (3) episodic adjustment of inventories to day-specific modeling inputs, and (4) consistency with national inventories.

### **3.7.1 Use of surrogate factors to spatially grid area sources**

Area source emission data, including motor vehicle emission data, are often supplied on a county basis. Spatial allocation of county-level emission estimates to grid cells is performed for each identified area source category and requires use of surrogate distribution factors such as population distribution, land use, and road type. The UAM EPS (EPA, 1992b) contains a program that uses gridded surrogate factors to allocate county-level emissions data to the grid cell size of the modeling domain.

#### **Recommendations**

It is recommended that the emission inventory guidance document (EPA, 1991c) be consulted for alternative surrogate factor choices and sources of information for assimilating surrogate data. The EPA is currently developing a utility to provide gridded surrogate data. States will be notified of the availability of gridded surrogate data through the EPA regional offices.

### **3.7.2 Development of mobile source inventories**

Under the requirements of the CAAA, all CO nonattainment areas are required to develop base year inventories of mobile sources. These represent base year emission levels for a typical operating day during the designated peak CO season. As part of the development of a base year inventory, estimates of VMT must be developed from traffic ground counts

consistent with the existing Highway Performance Monitoring System (HPMS). Projections of vehicle miles traveled (VMT) growth must be developed for moderate CO nonattainment areas through historically based extrapolation techniques if better methods are not locally available. Non-exempt serious areas must use a transportation demand model to project VMT growth (EPA, 1991a). These VMT estimates will serve as the basis of the modeling inventory. Guidance for making projections is detailed in Procedures for Preparing Emissions Projections (EPA, 1991f).

The mobile source CO emission are complex and difficult to prepare because they are strongly affected by the ambient temperature and motor vehicle speed. There are two primary ways to prepare a mobile source inventory. One relies upon county-wide estimates of VMT, which are multiplied by a "composite" emission factor (expressed as grams pollutant emitted per mile of travel). The emission factor is referred to as "composite" in that it is a weighted average value that is representative of the average vehicle operated under average conditions (Ireson et al., 1991). The other method relies upon the output of transportation models. These models can provide roadway link-specific estimates of distance, traffic volumes, and speed, and estimates of trip ends for specific transportation analysis zones (TAZ), which are combined with "composite" emission factors to arrive at regional mobile source emission inventories. Examples of commonly used travel demand models are the Urban Transportation Planning System (UTPS), which is maintained by the U.S. Department of Transportation, and commercial travel demand modeling software packages such as TRANPLAN (UAG, 1990) and MINUTP (Comsis Corp., 1991). These models have traditionally been used in regional transportation planning offices as planning tools for roadway expansions, highway development, land use, etc. However, the information provided by travel demand models, coupled with EPA's MOBILE model (EPA, 1991d), can be used to produce better estimates of mobile source emissions rather than estimates based on county-wide VMT estimates.

### Recommendations

Use of output from a transportation demand model is the preferred approach for estimating vehicle activity levels and emission factors because this method allows

resolution of variations in speed and vehicle miles traveled (VMT) among different grids over hourly time slices. The transportation demand model approach is the most appropriate for addressing the inner urban core of modeling domains. Peripheral, less dense traffic areas can be treated by disaggregating county-level estimates of VMT. Care should be taken not to double count mobile source emissions as part of both the transportation demand model approach and county level disaggregation approach (EPA, 1992b). Exceptions to these recommendations should be considered by the Technical Committee on a case-by-case basis. Justification for more extensive use of disaggregating county-level emissions should be sought in discussions with the appropriate EPA regional office.

Appendix C contains a detailed technical discussion of procedures specific to the use of EPA's latest MOBILE model to develop emission factors for area-wide CO modeling.

### 3.7.3 Episode-specific adjustments

Both motor vehicle and residential wood combustion emissions are sensitive to ambient temperature. Thus, it is important for modeling inventories to reflect episode-specific ambient temperature. In addition, known episode-specific events such as changes in process operations for point sources affect emissions rates and should be reflected in the episode modeling inventory.

#### Recommendations

Mobile-source emissions should be adjusted for episode-specific temperatures. Emission factors for deriving episode-specific mobile-source emissions should use the latest MOBILE model. Use of models other than the latest EPA MOBILE model should be reviewed by the Technical Committee on a case-by-case basis, and is subject to approval by the EPA regional office.

If available, episode-specific operating rates for point sources are preferable for estimating temporal point-source emissions. Procedures for temporally adjusting point and area sources are also provided in the emission inventory guidance document.

#### 3.7.4 Consistency with national inventories

Comparisons should be made between the modeling inventory and the 1990 SIP and RFP tracking emission inventories reported in the EPA Aerometric Information Retrieval System (AIRS). Although these inventories will not be identical, such a check can be considered part of the quality assurance process. Major inconsistencies should be noted and documented.

#### Recommendations

For an acceptable attainment demonstration, documentation should be provided that shows that the modeling emission inventory is consistent with the emission inventory being reported in AIRS in accordance with applicable guidance and regulations.



## CHAPTER 4

### DATA QUALITY ASSURANCE AND MODEL DIAGNOSTIC ANALYSES

This chapter provides general guidance for quality assurance testing of component data input fields and diagnostic testing of base case episodes. These analyses are designed to establish and improve reliability of the input data and proper functioning of the model.

Although the UAM has been evaluated on a number of historical data bases, measures of model behavior with respect to observed data are necessary for new applications. Model developers and users perform diagnostic tests to uncover potential input data gaps that, when corrected, may lead to improved treatment of model processes. Regulators need some indication that the model captures the key features of the base meteorological episodes being applied in the model simulations in order to have confidence in the model's ability to predict future carbon monoxide (1) after applying projected growth and planned emission controls, and (2) after applying alternative emission control strategies.

Important prerequisites for a model performance evaluation (see Chapter 5) are (1) quality assurance testing of model inputs and (2) diagnostic testing of the base meteorological episode simulation to ensure that the model is functioning properly and that apparently accurate model results are being obtained for the right reasons. For example, quality assurance testing of input data helps to ensure that apparently good model results have not resulted from compensating errors in input data.

An excellent compilation of model performance evaluation techniques, including diagnostic tests and related issues, is contained in Tesche et al. (1990). Although the Tesche study was developed for photochemical modeling, much of what is presented is applicable to



area-wide CO modeling. The study by Tesche also serves as the basis for the model performance evaluation described in Chapter 5 of the work reported here. Various graphical and numerical measures described in the following paragraphs are treated in detail in Tesche et al. (1990). Two graphical displays used for both quality assurance and diagnostic testing are mapping and time-series plots.

Mapping is a two- or three-dimensional spatial display of values illustrated with various contouring and tiling methods. These displays may depict political boundaries and monitoring site locations as well. Mapping capability is a multipurpose tool applicable for all forms of gridded data, such as future-year emission control strategy results and most input data fields (e.g., gridded wind fields, temperatures, and emission densities). Point- source locations may also be depicted to ensure that they are properly located. Spatial displays of predicted and observed carbon monoxide patterns are particularly useful as part of a model performance evaluation.

Time-series plots display hourly and eight-hourly measured and predicted carbon monoxide values for specific locations such as monitoring sites. Time-series plots provide an overview of the temporal performance of the model predictions. Comparison of time-series plots across multiple monitoring sites provides an indication of spatial response. These plots may provide insights to carbon monoxide prediction patterns and also to data base inconsistencies requiring further investigation.

The following sections describe steps recommended for conducting diagnostic testing of each base case meteorological episode simulation.

#### **4.1 Step 1: Quality Assurance Testing of Component Fields**

Starting with initial, quality-assured data, input data are developed for use in various UAM preprocessors. The first stage of diagnostic testing should focus on assessing the accuracy of major UAM input fields produced by the UAM preprocessors. Generally, the testing is

qualitative in nature and based on comparing visual displays of preprocessor outputs with patterns exhibited by the observed data. Prior to conducting a base case meteorological episode simulation, individual air quality, meteorological, and emissions fields should be reviewed for consistency and obvious omission errors. Both spatial and temporal characteristics of the data should be evaluated. These checks may be only cursory, but errors uncovered by this component testing might be extremely difficult to diagnose later in the modeling process, when errors could arise from any subset of the data inputs. Examples of component testing include the following:

**Air Quality:** Check for correct order of magnitude, especially when using background values

**Emissions:** Plot various source types by grid cell and review major source locations with local emissions patterns; check major highway routes; generally, look for obvious omission errors; plot CO by grid cell and cross-check with source distribution for logical patterns, such as high motor vehicle emissions near the urban core

**Meteorology:** Plot surface and elevated wind vectors and compare with monitoring stations and weather maps for consistent patterns; compare diffusion break heights with sounding data; check temperature fields

In quality assurance testing of component input fields, the emphasis is on capturing large errors before performing model simulations.

### Recommendations

It is recommended that quality assurance testing of the air quality, emissions, and meteorological data input files be conducted before proceeding to diagnostic testing of the base case meteorological episodes. At a minimum, emissions data should be quality assured by looking at emission distribution maps and known source locations and emission strengths.

## 4.2 Step 2: Diagnostic Testing of the Base Case Meteorological Episodes

After confidence in the accuracy of UAM input fields has been achieved, the UAM should be exercised for each base case meteorological episode. The initial run is termed a diagnostic simulation because review of initial base case simulations may uncover additional input errors requiring correction before an acceptable set of base case inputs can be derived. During this stage of the process, emphasis is placed on assessing the model's ability to correctly depict area-wide distribution and the timing of observed carbon monoxide maxima. Accordingly, visual methods such as mapping and time-series plotting, using measured data as reference marks, may be used to assess model behavior.

### Recommendations

To aid in interpreting simulation results, it is recommended that predicted and observed carbon monoxide concentration maps be constructed for each base meteorological episode simulation. Concentration maps present spatial information on the structure of the carbon monoxide cloud. Maps at 1-hour intervals should be constructed over the modeling period.

Consideration should also be given to constructing a map that depicts the highest predicted 1-hour and 8-hour maximum carbon monoxide value for each grid cell. Examples of various mapping techniques are described in Tesche et al. (1990).

It is also recommended that the method used to predict concentrations used in time-series plots be consistent with the method for deriving predicted concentrations for the model performance evaluation described in Chapter 5. Time-series of both 1- and 8-hour average periods should be constructed.

Other methods for deriving predicted concentrations for time-series comparisons may be judged appropriate by the Technical Committee; some suggestions are contained in Chapter 5. These methods should be described in the Modeling Protocol.

#### 4.3 **Step 3: Additional Base Meteorological Episode Sensitivity Testing**

In addition to running the base meteorological episode diagnostic simulation, other episode diagnostic simulations that perturb levels of emissions, initial and boundary conditions, and meteorological inputs may provide valuable information for identifying critical input areas and ensuring proper domain and episode selection. The following simulations, which are equivalent to sensitivity tests on major model inputs, illustrate the utility of this exercise.

1. **Zero emissions.** To indicate levels of sensitivity to emissions, all emissions are set to zero and the resulting predicted concentrations are compared with the base meteorological episode predictions that include emissions. A lack of substantial sensitivity may indicate a need to reexamine the selection of episodes or domains. Variations can be performed by zeroing out emission subsets, such as mobile-source emissions, and individual source categories.
2. **Zero boundary concentrations.** Inflow concentrations at the lateral boundaries and top of the modeling domain are reduced to zero or low background levels. Sensitivity of concentrations in the inner core and downwind portions of the modeling domain provide a measure of the boundary conditions' influence. This simulation provides assurance that the upwind extent of the domain is adequate.
3. **Zero initial concentrations.** Initial concentrations for all grid cells are reduced to zero or low background levels. Sensitivity of concentrations within the modeling domain provides a measure of the initial conditions' influence. Changes of less than a few percent indicate that the initial conditions are not dominating concentration estimates with the domain.

- \ 4. Diffusion break and wind speed variations. Much uncertainty is associated with the diffusion break and wind speeds, and simulated concentrations are often sensitive to these inputs. Simulations that test the sensitivity of model estimates to variations in wind speed and/or diffusion break provide bounds on some of the uncertainty resulting from these parameters. Large sensitivity values may suggest that future model applications will need improvement in the meteorological data bases.

Certain numerical measures, which are recommended in the discussion of model performance evaluation in Chapter 5, are also useful diagnostic tools. For example, consistent underpredictions usually produce numerical values greater than zero using these measures (see Appendix B). This phenomenon could be due to various factors, such as overstatement of wind speeds or diffusion break heights, or underestimation of emissions or the number of vertical layers. Modelers are encouraged to use numerical as well as graphical techniques in the diagnostic process.

The diagnostic analyses described in this chapter are considered to be a starting point for a specific modeling study. Diagnostic tests discussed in Tesche et al. (1990) should be considered whenever possible.

#### Recommendations

Diagnostic testing of the model should begin with quality assurance testing on input data files (Section 4.1). Diagnostic testing of each base meteorological episode should follow (Section 4.2). Additional diagnostic sensitivity tests for the base episode should also be considered (Section 4.3), including using zero emissions and/or zero boundary conditions, zero initial conditions, and varying diffusion break and wind speed estimates.

Agreement should be obtained among members of the Technical Committee concerning input field modifications arising from the quality assurance testing. These modifications should be based on scientific or physical reasoning and not just on what will improve model performance. All changes to the data that result from the diagnostic testing should be documented and justified.

In addition, all diagnostic steps should be documented to avoid misinterpretation of model performance results. After confidence is gained that the simulation is based on reasonable interpretations of observed data, and model concentration fields generally behave both spatially and temporally with known carbon monoxide distribution, a performance evaluation based on numerical measures is conducted for each base meteorological episode (see Chapter 5).

## CHAPTER 5

### MODEL PERFORMANCE EVALUATION

The purpose of the UAM application is to simulate a historical CO episode in order to estimate the area-wide contribution to concentrations measured at neighborhood-scale monitors. Once the model has adequately simulated observed CO magnitudes and spatial and temporal patterns for a historical day, greater confidence can be placed in its ability to provide reliable estimates of concentrations under the same meteorological conditions for a variety of emission scenarios. Thus UAM applications can serve as predictors of future concentrations and assist in the formulation of control strategies for attaining CO air quality standards.

Comparison of model predictions with observed values may lead to uncertainty, especially if samplings are from locations not representative of area-wide concentrations. Furthermore, the UAM output represents a volumetric ( typically,  $8 \times 10^7 \text{ m}^3$  ) concentration, whereas air quality data represent point locations that may or may not represent the same volume. Because of these uncertainties, specification of rigid rejection/acceptance criteria has not been generally supported by model developers or decision makers participating in previous modeling efforts. Instead, performance measures based on past modeling applications are thought to provide a reasonable benchmark for acceptable model performance.

Poor performance may necessitate (1) delaying model applications until further diagnostic testing and quality assurance checks are reflected in the input data base, or (2) selecting another meteorological episode for modeling. Cases where good model performance is shown should also be reviewed because compensating errors can induce spurious agreement among observed and predicted values.

## 5.1 Performance Measures

This section describes recommended graphical and statistical performance measures for carbon monoxide predictions.

The measures used in the performance evaluation should include both qualitative (e.g., graphical) and quantitative (e.g., statistical) analyses. Statistical measures may provide a meaningful test of model performance for dense monitoring networks, such as those for special field studies. However, for some routine monitoring networks where coverage may be sparse, statistical measures may provide a distorted view of model performance, especially for paired values.

Tesche et al. (1990) provides detailed descriptions of graphical and statistical measures available for assessing model performance. Although these methods were formulated primarily for photochemical grid models, most of the model performance measures are applicable to area-wide carbon monoxide modeling. The Technical Committee should consult the Tesche study when formulating model performance evaluation methods, and may want to use it for developing additional performance evaluation procedures other than those recommended in this guidance document.

### 5.1.1 Graphical performance procedures

Graphical displays can provide important information on qualitative relationships between predicted and observed concentrations. At a minimum, the following graphical displays should be developed for each meteorological episode: time-series plots and ground-level isopleths.

Time-series plots. The time-series plot, developed for each monitoring station in the modeling domain, depicts the hourly predicted and observed concentrations for the simulation period. The time series reveals the model's ability to reproduce the peak prediction, the



presence of any significant bias within the diurnal cycle, and a comparison of the timing of the predicted and observed maxima.

Ground-level isopleths or tile maps. Ground-level isopleths or tile maps display the spatial distribution of predicted concentrations at a selected hour. Isopleths of predicted maxima may also be constructed. The isopleths provide information on the magnitude and location of predicted carbon monoxide concentration. Superimposing observed hourly or daily maximum concentrations on the predicted isopleths reveals information on the spatial alignment of predicted and observed concentrations.

#### Recommendations

At a minimum, the following graphical displays are recommended in the evaluation of each meteorological episode:

Time-series plots of predicted\* and observed hourly carbon monoxide values should be constructed for each simulation period for each monitoring station where data are available.

Ground-level isopleths or tile maps of the spatial distribution of predicted concentrations should be constructed for selected hours. Also, ground-level isopleths or tile maps of the carbon monoxide maxima should be constructed. The corresponding observed concentrations should be superimposed on the predicted concentration isopleths to analyze spatial patterns and carbon monoxide magnitudes.

Additional graphical displays such as scatterplots of predictions and observations may also be used to assess model performance. The graphical displays to be used in the model performance evaluation should be described in the modeling protocol.

#### **5.1.2 Statistical performance measures**

Statistical measures provide a useful measure of model performance for spatially dense monitoring networks; however, for routine urban area CO monitoring networks, the typically

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\*For this purpose, the predicted value is the weighted average of the predictions from the four grid cells nearest to the monitoring station. The four-cell weighted average is derived from bilinear interpolation as described in EPA (1991e).

sparse coverage may result in a statistically distorted view of model performance. However, on the basis of UAM applications in past area-wide CO modeling, it is recommended that the following three statistical criteria be applied to all neighborhood-scale monitors (and, if applicable, roadway intersection monitors showing persistently high CO values during low traffic volumes):

### Recommendations

It is recommended that, at a minimum the following three formulations be applied as measures for model performance evaluation.

1. Unpaired (time or space) highest 8-hour prediction accuracy. This measure quantifies the difference between the highest observed 8-hour value and the highest predicted 8-hour value over all hours and monitoring locations.
2. Average absolute error in 8-hour peak prediction accuracy paired (time and space) values greater than 5.0 ppm. This measure quantifies the difference between the highest observed 8-hour value and the highest predicted 8-hour value at the time and location of each observed maximum.
3. Average absolute error in the predicted time of the 8-hour peak concentration, paired by station values greater than 5.0 ppm. This measure quantifies the difference between the highest observed 8-hour value and the highest predicted 8-hour value at the location of each observed maximum within a window of time.

Additional statistical measures may also be applied. Other available measures are listed in the Guideline for Regulatory Application of the Urban Airshed Model (EPA, 1991e).

## **5.2 Assessment of Model Performance**

As noted, both graphical and statistical performance measures should be used for the performance evaluation. However, statistical measures should be used with caution when interpreting results derived from sparse monitoring networks. The Technical Committee should consider the monitoring network design in interpreting statistical measures.

Although only a limited number of UAM area-wide CO modeling evaluations have been conducted, the following statistical performance measures should be achievable for SIP applications:

- Unpaired (time or space) highest 8-hour prediction accuracy:  $\pm$  30-35 percent
- Average absolute error in 8-hour peak prediction accuracy for paired values (time and space)  $> 5.0$  ppm: 25-30 percent
- Average absolute error in the predicted time of the 8-hour peak concentration, paired by station  $> 5.0$  ppm: 2 hours

In general, performance results that fall within these ranges would be acceptable. However, caution is urged in using these ranges as the sole basis for determining the acceptability of model performance. These ranges were derived from limited past model performance evaluations with varying densities of air quality and meteorological monitoring networks and corresponding variations in the quality and quantity of aerometric model input data. In some cases, they reflect use of earlier versions of the UAM. Thus, these ranges should be used in conjunction with the graphical procedures to assess overall model performance.

If statistical results are worse than the above ranges and graphical analyses also indicate poor model performance, users should consider choosing an alternative meteorological episode for modeling. Performance evaluations should be done on other candidate episodes to identify those that might result in better model performance.

If statistical results are worse than the above ranges for any of the three statistics, but graphical analyses generally indicate acceptable model performance, simulation results used for attainment demonstration should be applied with caution. Users may consider conducting

performance evaluations on other candidate episodes to identify any that might yield improved model performance.

When performance is less than expected, the assumptions and data used as model inputs should be assessed, and probable causes of poor performance should be examined before the model is applied to attainment demonstrations. If performance is poorer than expected using the existing aerometric data as model input and the existing data base is considered inadequate, the responsible regulatory agency should consider an enhanced monitoring program to improve the aerometric data base for future attainment demonstration modeling studies.

Decisions regarding the acceptability of using a modeling episode with poor performance should be reviewed and approved by the EPA regional office. Supporting documentation should include a discussion as to why performance was poorer than expected, and the potential adverse effects of poor model performance on control strategy evaluations.

#### Recommendations

It is recommended that the model performance for each meteorological episode be assessed as follows:

1. The graphical performance procedures specified in Section 5.1.1 should be conducted for each meteorological episode. To assess model performance, the Technical Committee should review the time-series plots and ground-level isopleth plots.
2. The statistical performance measures specified in Section 5.1.2 should also be derived and evaluated for each meteorological episode. When interpreting these measures, the monitoring network density and design should be considered. Caution is urged when interpreting the statistical measures for a sparse monitoring network.

It is recommended that the statistical performance measures be compared with the following ranges:

- Unpaired highest 8-hour prediction accuracy:  $\pm 30$ -35 percent
- Average absolute error in 8-hour peak prediction accuracy for paired (time and space) values > 5.0 ppm: 25-30 percent
- Average absolute error in the predicted time of the 8-hour peak concentration, paired by stations > 5.0 ppm: 2 hours

If all of these statistical measures are within the ranges shown, and the graphical performance procedures also are interpreted to yield acceptable results, then the model is judged to be performing acceptably.

If any of the statistical measures are worse than the above ranges, or the graphical procedures are interpreted to yield unacceptable performance, users should consider choosing an alternative highly ranked meteorological episode for the attainment demonstration. Performance evaluations should be conducted on a prospective alternative episode to determine whether it yields improved model performance.

## CHAPTER 6

### ATTAINMENT DEMONSTRATION

The primary purpose for conducting area-wide and roadway intersection modeling is to demonstrate the effectiveness of control strategies in attaining the National Ambient Air Quality Standard (NAAQS) for CO. Such demonstration of effectiveness consists of four parts:

1. Development of attainment-year base case emission inventories;
2. Development of future-year emission control strategies;
3. Performing attainment year model simulations to assess control strategies;
4. Use of modeling results in the attainment demonstration.

#### **6.1 Developing Attainment Year Base Case Emission Inventories**

Base year inventories and initial and boundary concentrations must be projected to the future attainment year. The future modeling year is a function of the attainment dates required in the CAAA of 1990. Projections of base year inventories reflect the net effect of existing required controls and growth projections for all source types.

The methodology for creating future year emission inventories is contained in Procedures for the Preparation of Emission Projections (EPA, 1991f), which covers development of emission projections for stationary and mobile sources. When transportation model outputs are used to develop the mobile source portion of the inventory through the use of a mobile source emission

model (e.g., TRFCONV, Causley, 1992), questions of which base inventory to use for developing vehicle emissions growth estimates must be resolved. Appendix C provides a technical discussion of procedures for developing vehicle emissions growth estimates.

Projection to future year boundary and initial concentrations is usually accomplished by applying factors that are the ratio of the future year emission totals to the base year totals. An exception to this occurs when low values have been specified for all boundary conditions. These conditions would not be expected to become even cleaner, so they would remain the same. Before applying the factors, a background value that is assumed to be unaffected by the emission controls being considered is subtracted. Then the factor is applied to the remaining values and the background is added back on. If the concentration is already at or below the background value, it is left unchanged. The background values used are normally the mid-level concentrations of 0.2 ppm. In a few cases, there might be some question about whether the boundary conditions should be scaled. For example, if the boundary concentrations are affected by an upwind urban area, will control measures similar to those being applied in the current simulation be in effect in the upwind area? If so, should the current simulation reflect the change due to local emission controls or changes due to all controls? If upwind controls will be in effect, boundary concentrations should be reduced to reflect control changes; simulation results should reflect all changes, not only local ones.

#### Recommendations

It is recommended that the EPA guidance document entitled Procedures for Preparing Emissions Projections EPA (1991f) be consulted for developing attainment-year inventories. The guidance document provides procedures for projecting point-source, area-source, mobile-source, and addresses projections of spatial and temporal, changes between the base year inventory and the attainment-year inventory.

### **6.2 Developing Future Year Emission Control Strategies**

Numerous future year emission control strategies can be developed and simulated using the area-wide model and the roadway intersection model. Eventually, a modeling analysis must

be submitted for approval for a SIP demonstration. The effectiveness of a given set of control measures in reducing CO is an important factor in selecting the final strategy.

Prior studies have used a number of control measures to ascertain an effective control strategy for attainment. Because of the low reactivity of CO in the wintertime, there is a near linear relationship between domain-wide predicted changes in CO emissions and the domain-wide predicted changes in CO concentrations for future year simulations. However, depending upon the control strategy employed, highly nonlinear changes may occur within each model grid cell. For example, control strategies which employ the use of such transportation control measures (TCM's) as a parking management program (PMP) will reduce CO emissions locally and within and near a model grid cell, but will have much less effect elsewhere in the modeling domain.

Prior studies have typically used a progression of control strategy scenarios in the modeling to ascertain an effective strategy for attainment. A suggested logical progression is the following:

1. Simulate the CAAA and other mandated control measures for the attainment year to determine if these measures are sufficient to demonstrate attainment.
2. If mandated controls are insufficient to demonstrate attainment, then the approximate emission-reduction targets may be estimated by the use of linear rollback.
3. Once an approximate target range is ascertained in steps 1 and 2, simulate control strategies that reflect source-specific or source-category-specific control measures that realize the approximate emission reductions identified as sufficient to reduce maximum 8-hour CO concentration to 9.0 ppm or less.
4. Adjust the strategy chosen in step 3 until it is sufficient to demonstrate attainment of the CO NAAQS, as described in Section 6.4.



### **Recommendations**

Find the emission reduction target needed to establish attainment by using linear rollback of emissions. Using this as an estimate, the level of emission reductions needed for control strategies can be assessed. Adjustments to the strategy should continue until it is sufficient to demonstrate attainment. An outline of procedures for deriving control strategies for evaluation in the attainment demonstration must be specified in the model protocol.

## **6.3 Performing Attainment-Year Simulations to Assess Various Control Strategies**

Many graphical display and numerical procedures are available for illustrating the effects of alternative emission control strategies on predicted concentrations of carbon monoxide. For example, the emission levels in the control strategies are often compared with the attainment-year base emissions. Also of interest are comparisons with the inventory derived for purposes of model performance evaluations and corresponding base-case UAM results. Difference maps are extremely useful for illustrating changes in the daily 8-hour maximum carbon monoxide predictions throughout the modeling domain.

### **Recommendations**

The primary focus of the carbon monoxide attainment demonstration is on the maximum 8-hour concentration predicted at each location in the modeling domain. However, in some cases the scope of the attainment demonstration should be broader to assess the effects on the subdomain and temporal impacts.

## **6.4 Using Modeling Results in the Attainment Demonstration**

To demonstrate attainment of the carbon monoxide NAAQS, the combined results from the areawide and roadway intersection modeling should show no predicted 8-hour maximum carbon monoxide concentrations greater than 9.0 ppm anywhere in the modeling domain for the episode modeled. Procedures for combining the area wide and roadway intersection modeling are given in EPA (1992c). Alternative methods for demonstrating attainment must be approved by the appropriate EPA regional office on a case-by-case basis.

The attainment test described in the preceding paragraph is consistent with the flexibility allowed in the choice of episode day (see Section 3.2) and reflects concerns over the difficulty of accurately estimating emissions inputs to the model.

#### Recommendations

To demonstrate attainment of the carbon monoxide NAAQS, the combined results of areawide and roadway intersection modeling should show no predicted 8-hour maximum carbon monoxide concentrations greater than 9.0 ppm anywhere in the modeling domain for the episode modeled.

States may opt to conduct more comprehensive statistical testing of the modeling results for the attainment demonstration. Any alternative methods for attainment demonstration must be approved by the appropriate EPA regional office on a case-by-case basis. Any optional methods should be agreed upon during the development of the modeling protocol.

### **6.5 Exceptions to Guidance Document**

It is not possible in a general guidance document like this to anticipate all contingencies associated with developing an attainment demonstration study. The modeling policy oversight and technical committees responsible for a specific modeling study may propose an alternative modeling approach provided that (1) the modeling protocol requires consensus on the proposed alternative approach within the Technical Committee, and (2) justification for the proposed approach is documented. Application of any alternative grid modeling approach must first receive concurrence in writing from the responsible EPA regional office(s).



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**TECHNICAL REPORT DATA**  
(Please read Instructions on the reverse before completing)

1. REPORT NO. EPA-450/4-92-011a		2.	3. RECIPIENT'S ACCESSION NO.	
4. TITLE AND SUBTITLE Guideline for Regulatory Application of the Urban Airshed Model for Areawide Carbon Monoxide Volume I: Technical Report			5. REPORT DATE June 1992	
			6. PERFORMING ORGANIZATION CODE	
7. AUTHOR(S) Edward L. Carr, Julie L. Fieber and Robert C. Kessler			8. PERFORMING ORGANIZATION REPORT N	
9. PERFORMING ORGANIZATION NAME AND ADDRESS Systems Applications International San Rafael, California 94903			10. PROGRAM ELEMENT NO.	
			11. CONTRACT/GRANT NO.	
12. SPONSORING AGENCY NAME AND ADDRESS Office of Air Quality Planning and Standards U.S. Environmental Protection Agency Research Triangle Park, N.C. 27711			13. TYPE OF REPORT AND PERIOD COVERE	
			14. SPONSORING AGENCY CODE	
15. SUPPLEMENTARY NOTES				
16. ABSTRACT State Implementation Plan (SIP) revisions demonstrating attainment of the Carbon Monoxide (CO) National Ambient Air Quality Standards (NAAQS) are required under the Clean Air Act Amendments of 1990. Urban areawide modeling and intersection modeling are recommended to address attainment of the CO NAAQS. The Urban Airshed Model (UAM) has been identified as an effective urban areawide model for evaluating emission control requirements needed to attain the CO NAAQS. The purpose of this document is to provide guidance in the procedures used to apply the UAM for CO SIP attainment demonstrations.				
17. KEY WORDS AND DOCUMENT ANALYSIS				
a. DESCRIPTORS		b. IDENTIFIERS/OPEN ENDED TERMS		c. COSATI Field/Group
Atmospheric Dispersion Models Carbon Monoxide (CO) State Implementation Plan (SIP) Clean Air Act Amendments Urban Areawide Modeling				
18. DISTRIBUTION STATEMENT		19. SECURITY CLASS (This Report)		21. NO. OF PAGES 65
		20. SECURITY CLASS (This page)		22. PRICE