Chapter 5

Regional modeling of air pollution transport in the southwestern United States

Marek Uliaasz, Roger A. Stocker and Roger A. Pielke
Department of Atmospheric Sciences, Colorado State University, Fort Collins, CO 80523, USA

Abstract

Numerical simulations of air pollution transport in the southwestern United States have been performed for the entire year of 1992 with the aid of the CSU Regional Atmospheric Modeling System (RAMS) and a Lagrangian particle dispersion (LPD) model. This chapter presents the design of these simulations, some examples of simulated meteorological fields and influence functions, validation of the RAMS wind fields and dispersion simulations, and, finally, a comparison with simpler modeling approaches. The validation of dispersion simulations using a tracer of opportunity (methylchloroform) demonstrates that our modeling approach can correctly reproduce the regional transport of pollutants between the Los Angeles Basin and the Grand Canyon region.

Key words
atmospheric dispersion, long range transport, Lagrangian particle model, mesoscale models, receptor modeling, visibility

1 Introduction

The reduction of visibility in the Grand Canyon and other national parks and wilderness areas in the southwestern United States has been the subject of several studies conducted over the last 15 years. The results from these studies are summarized in a recent report released by the National Research Council (NRC, 1993). Visibility protection requires the assessment of contributions from various emission sources to visibility-reducing pollutants in the Grand Canyon and other receptor areas of interest. Potential anthropogenic sources include both local power plants located along the Colorado River as well as distant urban areas. Transport of pollutants in
this region have been examined using a variety of relatively simple models including backward trajectory analysis (e.g., Green and Gebhart, 1994). These models can simulate years of pollution transport. However, they do not include any mesoscale features, which can be important for atmospheric dispersion in the extremely complex terrain of the southwestern United States. On the other hand, several 3-D meteorological numerical simulations have also been conducted within the past few years relating to visibility and air pollution transport in this region. They were performed on a regional scale (e.g., Yamada et al., 1989; Poulos and Pielke, 1994; Stauffer and Seaman, 1994), or on the local scale (e.g., Yamada, 1992; Enger and Koracin, 1995). Nevertheless, all these simulations were limited to short term case studies involving only a few days of simulation. Recent advances in computer technology and developments in mesoscale modeling, including grid nesting, have made it possible to perform a long term air pollution transport study on the regional scale with the aid of mesoscale meteorological models.

This chapter describes a long term numerical study for the southwestern United States conducted at Colorado State University. The Regional Atmospheric Modeling System (RAMS) and the Lagrangian Particle Dispersion (LPD) model were used to perform daily meteorological and dispersion simulations for the entire year of 1992 as a part of the Measurement of Haze and Visibility Experiment (MOHAVE). All simulations were run on IBM RISC-6000/550 workstations dedicated to the project. The design of a one-year numerical study required a careful compromise between model accuracy and computer efficiency. Configuration of the models used in this study is discussed with emphasis on selection of modeling domain, difficulties of processing a large volume of data, and the problem of model resolution. After presenting some examples of simulated meteorological fields and influence functions, a validation of our modeling approach is discussed. The simulations of transport from the Los Angeles Basin to the Grand Canyon region were validated with the aid of a tracer of opportunity.

2 Numerical models

2.1 Regional Atmospheric Modeling System

RAMS is a primitive equation, prognostic modeling system which has evolved from the mesoscale model developed by Pielke (1974) and the cloud-scale model of Tripoli and Cotton (1982) and Cotton et al. (1982). It is among the more widely used prognostic mesoscale codes. RAMS is a highly modular modeling system with a variety of potential applications from large eddy simulations to real-time forecasts of large scale weather patterns. A user can select different options from a namelist framework in order to create a model configuration which is the best suited for a particular application.

An overview of RAMS features and its recent meteorological applications can be found in Pielke et al. (1992) and Nicholls et al. (1995). Applications to air quality problems are reviewed in Pielke et al. (1991) and Lyons et al. (1993a). Recent applica-
tions of RAMS in this area include modeling impacts of mesoscale vertical motions on dispersion in coastal areas (Lyons et al., 1995b) and providing meteorological input to photochemical grid models for the Lake Michigan Ozone Study (Eastman et al., 1995; Lyon et al., 1995b). Some issues related to operational applications of RAMS are discussed in the next chapter of this book (Lyons, 1996).

2.2 Lagrangian Particle Dispersion Model

The Lagrangian Particle Dispersion (LPD) model was originally developed on a personal computer as a part of a Mesoscale Dispersion Modeling System (MDMS) in the late 1980s at Warsaw University of Technology, Poland (Uliasz, 1990a; Uliasz, 1993). Later, it was used in several applications on Unix workstations at Colorado State University. Gradually, the LPD model has evolved into a family of particle models designed with different features and levels of sophistication (Uliasz, 1994). These particle models can use output from different meteorological modeling systems (the mesoscale model MESO from MDMS (Uliasz, 1993), CSU RAMS with nested grids, Uppsala University mesoscale model (Enger, 1990), and the LES model (Sorbjan, 1995)). One can also configure the LPD model as a subroutine to be called from a meteorological model.

The LPD model was validated using data from the Øresund experiment tracer performed over a land-water-land area (Uliasz, 1990b). Applications include mesoscale and regional transport of air pollutants in different areas with a complex terrain: a coastal zone of the Baltic Sea in Poland (Uliasz, 1990b), Sudety Mountains and the Black Triangle in Central Europe (Uliasz, 1994), and the eastern and southwestern United States (Uliasz, 1993; Uliasz, 1994). The model has also been used as a tool for visualization and analysis of output created by mesoscale and LES models.

3 Design of simulations

3.1 Modeling domain

The prime area of interest for this modeling study is the Colorado Plateau in the southwestern United States including Grand Canyon National Park. Figure 1 presents the assumed modeling domain covered by two nested grids. The coarse grid #1 with horizontal spacing $\Delta x = 60$ km extends from 125W longitude on the west to east of the Rocky Mountains on the east, and from northern Mexico in the south to southern Canada in the north. Large areas are included to the north and west of the area of interest in order to more fully resolve synoptic features upwind of this region. The purpose of the finer grid #2 with $\Delta x = 12$ km was to resolve some of the mesoscale features important to determining both local and regional transport in the area while keeping the simulations from being prohibitively expensive with respect to computer resources. The grid #2 covers most of the emission sources and receptors discussed further in the paper (Figure 2).
Figure 1: Modeling domain for MOHAVE simulations: RAMS grids #1 and #2, and dispersion domain (LPD).

Figure 4 shows an extremely complex terrain topography within the grid #2 while Figure 3 presents a west east cross-section of terrain elevation at $y = -500$ km and its representation by model grids #1 and 2. An attempt was made to apply spectral analysis of terrain height in order to determine the horizontal grid spacing necessary to resolve dominant terrain features in the numerical model (Young and Pielke, 1983). This preliminary analysis was limited to only one cross-section of terrain topography ($y = -500$ km). Terrain heights extracted from a 30" data base were first smoothed by running averages with windows of 10 or 100 km and then these smoothed values were subtracted from the original values. These steps are demonstrated in Figure 3 for a smoothing window of 10 km. A dramatic difference in terrain features between mountainous terrain in the central part of the modeling domain and the Great Plains in its eastern part is clearly visible. Spectra of terrain height (Figure 5) relate a terrain
Figure 2: Receptors and emission sources in MOHAVE simulations. Receptors: MEAD - Meadview, SPMO - Spirit Mountain, LOME - Long Mesa, HOPO - Hopi Point, MEVE - Mesa Verde, urban emission sources: LA - Los Angeles, SD - San Diego, SF - San Francisco, PH - Phoenix, LV - Las Vegas, SL - Salt Lake City; and other sites: EDAF - Edwards AFB, MPP - Mohave Power Plant.

height variance to different horizontal wavelengths. It is evident that terrain changes below 10 km are still important and should be represented in the model.

A numerical model cannot resolve any features with a scale below $2\Delta x$ and an acceptable representation may be expected for the scale of $4\Delta x$. This means that our simulations with the horizontal grid spacing $\Delta x = 12$ km can resolve only relatively large terrain features above a 48 km scale. This compromise was dictated not by the model physics, but by time and computer constraints and was necessary in order to perform meteorological simulations for the entire year. Implications of this compromise will be discussed further in the paper.

Mountain ridges in the considered area show a strong south-north directionality. To obtain a better spectral representation of terrain height, the spectra should be
Figure 3: West east cross-sections of terrain height ($y=-500$ km): a) derived from the $30^\circ$ data base, b) smoothed by 10 km running average, c) difference between (a) and (b), d) represented by the model grids #1 and #2.
Figure 4: Terrain topography within the RAMS grid #2

Figure 5: Examples of terrain height spectra calculated for the cross-section $y=-500$ km using 100 km (left axis) and 10 km (right axis) running average.
duration of each particle simulation was limited by the disk space available for meteorological files and anticipated output from the LPD model.

The third step involves processing stored particle distributions to calculate concentrations or influence functions in the form of 3D fields or time series at specified locations. All calculations are made with the aid of a simple uniform kernel with constant bandwidths typically equal to half of the assumed grid spacing. A review of methods to calculate concentration in Lagrangian particle models is given with some examples in Uliasz (1994). No pollution mass is assigned to particles in the LPD model because chemical transformation or removal processes are not simulated. Therefore, emission rates for different sources can be prescribed during the concentration calculation. Since particles are tagged with emission sources, it is possible to perform these calculations separately for selected sources or any combinations of sources. This allows one to study different emission scenarios and contributions of different sources into the concentration at a given receptor.

4 Examples of results from RAMS simulations

Examples of simulated meteorological fields presented here for 30 April 1992 were selected to illustrate the development of mesoscale circulations under different synoptic conditions. The daily weather maps from National Climatic Data Center suggest weak synoptic forcing for the southwestern United States on 29 April as indicated by weak gradients of surface pressure and the evidence of a cold core high over the region. However, the next day, the synoptic forcing was getting stronger due to the influence of a long-wave trough impacting the region. Therefore, the RAMS results from 12 GMT on April 30 and 00 GMT on May 1 demonstrate two types of circulations related to weak and strong synoptic forcing. These two times correspond to early morning on April 30 (0500 MST) and to afternoon on the same day (1700 MST) in Mountain Standard Time. Figures 6-9 compare selected meteorological fields from the RAMS grid #2 at these two times. Plan x-y views are taken at the lowest model level of 48 m to show the development and strength of the surface mesoscale circulations in the region. Vertical x-z cross-sections are centered on the Mohave Power Project (MPP). The terrain associated with the grid #2 was presented in Figure 4.

Vertical velocity field in the morning of April 30 shows that the most dominant mesoscale feature in this domain is the downslope winds that develop around the Sierra Nevada Mountains in California (Figure 6a). The maximum values of the velocities in this region are 0.75 \( ms^{-1} \). A secondary maximum can be observed to the south of the Sierra Nevadas in the San Bernardino Mountains to the east of Los Angeles. These areas of stronger mesoscale circulations have been observed to be important as a venting mechanism during the daytime hours for the Los Angeles Basin and San Joaquin Valley which produce large volume of polluted air. As indicated by the streamline plot for this time (Figure 7a), the off-shore sea breeze circulation has been established along the coast of California. This circulation is quite common in this region and is responsible for coastal stratus and fog formation. The downslope winds associated with the strong vertical velocities along the Sierra Nevada Mountains
Table 1: RAMS configuration for MOHAVE simulations

<table>
<thead>
<tr>
<th>MODEL CHARACTERISTIC</th>
<th>OPTION/VALUE CHOSEN</th>
</tr>
</thead>
<tbody>
<tr>
<td>model version</td>
<td>3a</td>
</tr>
<tr>
<td>basic equations</td>
<td></td>
</tr>
<tr>
<td>w-momentum eqn.</td>
<td>nonhydrostatic</td>
</tr>
<tr>
<td>continuity eqn.</td>
<td>anelastic</td>
</tr>
<tr>
<td>numerics</td>
<td></td>
</tr>
<tr>
<td>time differencing</td>
<td>hybrid</td>
</tr>
<tr>
<td>time step</td>
<td>80 s long, 40 s short</td>
</tr>
<tr>
<td>horizontal coordinates</td>
<td>polar-stereographic</td>
</tr>
<tr>
<td>vertical coordinate</td>
<td>terrain following</td>
</tr>
<tr>
<td>grid structure</td>
<td>Arakawa C grid</td>
</tr>
<tr>
<td>nested grids</td>
<td>#1 #2</td>
</tr>
<tr>
<td>grid dimensions</td>
<td>62 × 62 × 30</td>
</tr>
<tr>
<td></td>
<td>87 × 62 × 30</td>
</tr>
<tr>
<td>horizontal spacing</td>
<td>60 km</td>
</tr>
<tr>
<td>vertical spacing</td>
<td>12 km</td>
</tr>
<tr>
<td></td>
<td>Δz =50 m at surface,</td>
</tr>
<tr>
<td></td>
<td>1.2 stretch factor, 20 km top</td>
</tr>
<tr>
<td>physical parameterizations</td>
<td></td>
</tr>
<tr>
<td>radiation</td>
<td>shortwave - Mahrer/Pielke</td>
</tr>
<tr>
<td>moist processes</td>
<td>longwave - Chen/Cotton</td>
</tr>
<tr>
<td></td>
<td>passive water vapor only,</td>
</tr>
<tr>
<td></td>
<td>no condensation or CU parameterization</td>
</tr>
<tr>
<td>horizontal diffusion</td>
<td>deformation tensor</td>
</tr>
<tr>
<td>vertical diffusion</td>
<td>Mellor-Yarnada level 2.5</td>
</tr>
<tr>
<td>surface layer</td>
<td>Louis scheme</td>
</tr>
<tr>
<td>soil model</td>
<td>Tremback-Kessler scheme</td>
</tr>
<tr>
<td>boundary conditions</td>
<td></td>
</tr>
<tr>
<td>lateral boundaries</td>
<td>Klemp/Wilhelmsn</td>
</tr>
<tr>
<td>upper boundary</td>
<td>wall on top</td>
</tr>
<tr>
<td>bottom boundary</td>
<td>30°terrain, 10’land cover, 1° SST data,</td>
</tr>
<tr>
<td></td>
<td>1°km USGS vegetation</td>
</tr>
<tr>
<td>initialization</td>
<td></td>
</tr>
<tr>
<td>method</td>
<td>variable initialization</td>
</tr>
<tr>
<td>input data</td>
<td>2.5° NMC tropospheric analysis</td>
</tr>
<tr>
<td></td>
<td>standard NWS surface and sounding data</td>
</tr>
</tbody>
</table>
The major problem encountered in running dispersion simulations for the entire year was the volume of output produced and stored every 20 minutes by RAMS (nearly 1Gb for one day). Therefore, our dispersion simulations involved three steps:
1. processing RAMS output
2. particle simulations with the LPD model;
3. processing particle distributions: concentration or influence function calculations.

This procedure may be recommended for any dispersion simulations covering periods of time longer than a typical case study when output from a 3D meteorological model is used.

The purpose of the first step is to reduce the volume of RAMS output by extracting only those fields which are necessary to run dispersion calculations and by reducing the size of the modeling domain. This step also allows one to link the LPD model to different meteorological modeling systems which may require a change of coordinate system. The LPD model needs the following meteorological fields: wind velocity components $u$, $v$, $w$, potential temperature, $\theta$, turbulent kinetic energy, TKE, and mixing length, $l$. Some of the input fields ($u$, TKE, and $l$) may be diagnostically recalculated in the LPD model if they are missing in the meteorological output. Wind velocity variances and Lagrangian time scales are always calculated by the LPD model using the modified Mellor-Yamada level 2.5 or level 2 closure schemes. In the discussed simulations, $u$ and $v$ velocity components, potential temperature, TKE and, additionally, temperature and specific humidity were extracted from the RAMS output. We needed the last two fields in some dispersion simulations where particles were used to estimate mean temperature, mean and maximum humidity and time spent within clouds between sources and receptors. These extracted meteorological fields were also distributed to other research teams running their own dispersion and chemistry models. The domain of extracted meteorological fields used in dispersion simulations is shown in Figure 1.

The extracted RAMS output was organized into 7 to 12 day sequences and used to run particle simulations forward in time (source-oriented mode) and backward in time (receptor-oriented mode). Particles were released continuously from each source or receptor with a rate up to 240 particles per hour. Each particle had assigned the following attributes: $x$, $y$, $z$ coordinates, time of release, source/receptor identification number, and particle status. In special simulations, additional attributes were used (e.g., values of selected meteorological fields at particle location). Particles older than a prescribed age (5 days) or particles transported outside the modeling domain were removed from the calculations. The modeling domain assumed for particle simulations should be large enough to minimize a problem with particles which could return back to the modeling domain following a recirculating flow. The output from the LPD model, including required particle attributes (usually limited to the first five attributes), was stored every hour. The particle simulation for each new sequence of meteorological files was initiated with a "restart" option, i.e., by reading the particle attributes from the last output written in the previous particle simulation. The
calculated for several cross-sections and then averaged, or the 2-D spectral analysis should be applied (Steyn and Ayotte, 1985).

3.2 Configuration of RAMS

The main RAMS options and characteristics selected for the study are listed in Table 1. This particular configuration was designed as a compromise between a good description of mesoscale transport phenomena in complex terrain of the southwestern United States and computer efficiency required to perform simulations over the entire year.

Initial conditions for the simulations were obtained from the National Meteorological Center (NMC) gridded 2.5° global tropospheric analysis files which are available twice daily at 00 GMT and 12 GMT. These data were supplemented with standard National Weather Service (NWS) surface and rawinsonde network data. Four-dimensional data assimilation (4DDA) was applied over the entire domain by nudging model equations at each grid element towards the gridded observation fields.

The choice of the vertical diffusion parameterization is obviously important in an atmospheric dispersion modeling study. The Mellor-Yamada level 2.5 scheme based on the prognostic equation for turbulent kinetic energy (TKE) was used. The parameterization of moist processes in our simulations was selected simply in the interest of computer economy. It allowed only for the conversion of water vapor to liquid water in an oversaturated state but no precipitation.

The simulations were run on two nested grids described in the previous section in sets of three day segments where the model was integrated continuously. The full year had to be discretized into three day segments in order to limit the growth of phase speed and amplitude errors inherent in finite difference modeling. Each three day segment was reinitialized from its corresponding meteorological fields. These three day segments were then linked together to produce the full year of simulation. Output from simulations was stored every 20 minutes. This frequency of meteorological output was determined in several sensitivity tests as necessary for dispersion simulations.

3.3 Configuration of LPD model

The simplified version of the LPD model based on a fully random walking scheme with neglected horizontal diffusion was selected for this study. Several tests using output from different meteorological simulations have proved that this level of simplification is acceptable in mesoscale applications (Uliasz, 1994). This model version can be an order of magnitude faster than the Markov chain particle models since a longer time step is used to move particles and a lower number of meteorological variables must be interpolated to a position of each particle at each time step. The computer efficiency of this particle model allows us to design a variety of dispersion simulations in both the source- and receptor-oriented mode. All simulations were limited to a passive (conservative) tracer. Particles were tracked only for five days.
Figure 6: Vertical velocity fields at x-y plane (z=48 m) on April 30: a) 0500 MST, b) 1700 MST (contours from -0.5 to 0.1 by 0.1 m s^{-1}).
Figure 7: Same as in Figure 6 but for streamlines.
Figure 8: $u$-velocity field in $xz$ cross-section on April 30: a) 0500 MST (contours: from -4 to 28 by 2 m s$^{-1}$), b) 1700 MST (contours: from 2 to 36 by 2 m s$^{-1}$).
can be seen as the divergence line in the northwest quadrant. One particular local circulation of note around the Nevada Arizona border is the southerly wind flow along the southern tip of Nevada. This circulation is very important in determining pollution transport from the Mohave Power Project (MPP) and is caused by the channeling of synoptic scale air and the development of mesoscale circulations in the valley region around MPP.

The Grand Canyon National Park region shows little evidence of circulations associated with this geological feature with southerly flow dominating the northern Arizona region. The lack of significant circulations around this area can be explained by the model’s insufficient resolution. However, the complexity of the flow patterns over this grid do demonstrate a significant amount of variability. Flow features in the area around MPP (Figure 8a) suggest downslope winds off the higher terrain features to the east with the strongest winds associated with this mesoscale flow feature being on the order of 4 m/s$^{-1}$. This downslope to the east of the Valley is opposite to the synoptic flow seen at higher levels. Little turbulence is present in the very shallow atmospheric boundary layer during the early morning hours (Figure 9a).

The synoptic forcing for the afternoon of April 30 has been strengthened due the influence of a long wave trough. It is evident from the uniform flow patterns presented in Figure 7b that the mesoscale structure seen in the early morning example has been replaced by strong synoptic activity. This late afternoon time period shows uniform flow from the southwest associated with the approach of a surface cold front. Figure 6b shows the associated vertical velocities with the windward side of the mountain ranges producing upslope conditions and the lee side showing downslope due to the shading effect of the mountains during the late afternoon. Some smaller scale circulations can be seen in southern Nevada mountains around Las Vegas. A small scale circulation can also be seen in northern Arizona associated with differential heating off of the Kaibab Plateau to the north of Grand Canyon National Park. The cross-section of the $u$ velocity component for this time suggests that the synoptic scale is the dominant forcing (Figure 8b). The TKE field does indicate some differences over the region (Figure 9b). The coastal areas with the onshore flow are producing only a shallow boundary layer while a more fully developed boundary layer with a depth of between 1.5 and 2 km can be found in the more inland areas.

5 Examples of results from dispersion simulations

In this section, we present some examples of our results from receptor-oriented dispersion simulations performed for the summer intensive period. The receptor-oriented approach in dispersion modeling is discussed in more detail in Uliaasz, (1994). Particles are released from a receptor and they are traced backward in time. The influence function derived from particle distributions characterizes dispersion conditions in the atmosphere from the point of view of the considered receptor. It is calculated for a given averaging time for the concentration at the receptor and provides information on potential contributions from any emission sources within the modeling domain to this concentration.
Figure 9: Turbulent kinetic energy in xz cross-section on April 30: a) 0500 MST (contours: from 0 to 1.6 by 0.1 m²s⁻²), b) 1700 MST (contours: from 0 to 2.2 by 0.1 m²s⁻²).
Figure 10: Examples of influence function calculations for Hopi Point (left) and Mesa Verde (right) for the 24 hour sampling period (August 20, 1992) and the layer 0-500 m. Top: contours of influence functions ($\log(\cdot) = -11$, -10.5, -10, ... s m$^{-3}$). Middle: contours of mean travel time (6, 12, 24, 48, 72 hours). Bottom: contours of impact frequency (5, 25, 50, 75, 95 %).
Figure 11: The same as in Figure 10 but for the two month period (July-August 1992).
Figure 12: Vertical XZ cross sections of influence functions for Hopi Point (left) and Mesa Verde (right) receptors calculated for the 24 hour period (August 20, 1992). Top: Y=-300 km, middle: Y=-200 km, bottom: Y=-100 km (contour values as in Figure 10).

Figures 10-12 demonstrate examples of the influence functions determined for two receptors: Hopi Point (HOPO) in Grand Canyon National Park and Mesa Verde National Park (MEVE). It should be pointed out that the influence functions are, in general, 3-D time dependent fields, so some assumptions must be made to present them graphically. The influence functions shown here are integrated over the time of the simulations. Therefore, they show the potential impact of sources with emission rates fixed in time. A value of the influence functions at a given point multiplied by the emission rate from the point source in this location directly provides the contribution from this source to the concentration at the receptor. It is easy to include a variable emission rate for a given source if required. The influence functions plotted at horizontal plane (Figures 10 and 11) are averaged vertically within the layer from 0 to 500 m, so they only represent the impact of emission sources located within this layer. The transport patterns for higher emission sources, e.g., power plant chimneys with a significant plume rise, may be somewhat different. XZ cross-sections of the influence function presented in Figure 12 illustrate complexity of dispersion conditions in the atmosphere.

Figures 10 and 12 shows the influence functions for the 24 hour averaging period of 20 August 1992. This was selected as a day with a typical summer southwest transport pattern when the Los Angeles area affects the Grand Canyon. The transport
path for the Mesa Verde receptor located about 500 km eastward is quite different on this day. It is influenced by air coming from the north and northwest as well as from the southwest. The area covered by the Mesa Verde influence function is split into separate parts which indicate that the transport takes place above the 500 m layer. Figure 11 demonstrates the influence functions for the same two receptors but calculated for the two month averaging period: July-August 1992. These plots also show significant differences in transport patterns between the different receptors.

In addition to the influence functions, distributions of mean travel time and impact frequency are presented. They provide information about the origin and aging time of pollution arriving at the receptor as well as how often the receptor is impacted by air originating from a given source area during the analyzed sampling period. These plots also suggest that influence functions may be interpreted as an extension of the popular backward in time trajectory approach. However, instead of a single trajectory, the influence functions provide spatially distributed information since they are derived for a certain averaging period for concentrations at the receptor. The influence functions are also calculated from particle distributions with a certain resolution (grid spacing for the presented examples: $\Delta x = \Delta y = 50$ km, $\Delta z = 500$ m). Finally, the main difference is that our approach takes into account the effect of mixing processes in the atmosphere. More examples of the influence functions calculated in the MOHAVE project and other applications are presented by Uliasz (1994).

6 Validation of simulated wind fields

The meteorological fields simulated by RAMS were compared to profile measurements from several rawinsonde sites which were not used in model initialization. In this section, a comparison of simulated and observed wind roses for the summer intensive period of the MOHAVE field study (July 10 - September 5 1992) will be discussed for two selected sites: Edwards AFB (Air Force Base) and the Mohave Power Project (Figure 2). The summer intensive period was chosen over the winter intensive period due to the occurrence of transport patterns from the Los Angeles Basin to the Grand Canyon area. Additionally, the lack of the strong synoptic features in the summer leads to a stronger influence from mesoscale circulations in pollution dispersion. The selected sites characterize well the RAMS performance and its limitations in the configuration set up for the daily simulations. The first location, EDAF, is dominated by large scale synoptic flow with relatively little complex terrain to produce mesoscale circulations while the second site, MPP, is located within a narrow valley of the Colorado River with channeled flow below 1 km.

Figure 13 shows the observed and simulated wind rose distributions at MPP and EDAF at two heights. In the case of the MPP site, the first height, 863 m, represents flow within the Colorado River valley, whereas the second height, 2891 m, represents flow at the top of the planetary boundary layer during the late afternoon sounding and above the boundary layer for the morning sounding. Data from both the 00 GMT and 12 GMT soundings are included in this wind rose analysis. This comparison clearly points out limitations of the RAMS resolution in reproducing flow features
Figure 13: Simulated and observed wind rises at Mohave Power Project (MPP) and Edwards AFB (EDAF) at heights 863 and 2891 m for the summer intensive period.
in the narrow canyon regions which are prevalent in the southwestern United States. Observations suggest that the dominant wind direction during the summer intensive period is from the south below the canyon top. This channeling is only moderately demonstrated by the RAMS simulation windrose where the dominant direction is from the southwest. The southwest flow seen in the RAMS results represents the dominant direction for the synoptic flow during the summer months over the southwest United States. The wind rises at the higher elevation demonstrate that observations and model results more closely resemble each other. This is typical of all sites which were used in this analysis and is due to the increasing influence of synoptic flow with height and the lessening influence of complex terrain features which were not well represented within RAMS.

The same plots for the EDAF site show a much better RAMS performance. This site is important because it gives an indication of how well RAMS reproduces transport patterns between California and the Colorado Plateau. This is the dominant transport path over this region during the summer months. RAMS reproduces wind distributions at this site quite well with the dominant transport being from the west at 863 m and from the southwest at 2891 m. This suggests that RAMS does a good job of simulating the large scale flow patterns during the summer months. The validation of the RAMS meteorological fields is discussed further by Stocker et al. (1994).

It is important to understand that the comparisons of winds modeled on a numerical grid to point observations are not sufficient for evaluating how well a model reproduces a transport flow pattern. Grid values for this model represent an average wind direction and speed over a 12 × 12 km grid cell, whereas observed winds may not be representative for the flow patterns in such a large area, especially in a complex terrain. This fact was clearly demonstrated by observational studies where wind was measured on a mesoscale grid in northeast Colorado. Hanna and Chang (1992) found that even for hourly averaged winds, the root mean squared difference (RMSD) of 10 km separated stations was 0.7 \( m \cdot s^{-1} \) with a correlation of 0.47. Even at 312 m separation stations, the RMSD was 0.4 \( m \cdot s^{-1} \). This leads to the question of which wind is most useful in reproducing actual pollution transport in a region. This question cannot be answered by meteorological analysis alone but needs to be answered by comparing dispersion model results with observed concentrations of an inert tracer.

7 Validation of dispersion simulations using a tracer of opportunity

During both the summer and winter intensive periods of the MOHAVE field study, tracers were released from the Mohave Power Project and several other locations. Unfortunately, data from these tracer experiments are still not available. Therefore, a preliminary validation of our dispersion simulations was performed using a tracer of opportunity: methylchloroform (CH\(_3\)CCL\(_3\)). Hourly concentrations of methylchlor-
Methylchloroform and other halocarbons were measured at three locations in the Grand Canyon area: Spirit Mountain (SPMO), Meadview (MEAD) and Long Mesa (LOME).

Methylchloroform is entirely anthropogenic and is released primarily in the metal fabrication, electronics and aerospace industries. Most emission sources of methylchloroform are concentrated in the Los Angeles area. White et al. (1990) examined methylchloroform data at SPMO, MEAD, and Cajon Pass on the edge of the Los Angeles Basin during June-August 1985-1987. They found that summertime concentrations at SPMO and MEAD show strong weekly cycles with the lowest values typically from late Sunday to Tuesday and lag similar cycles observed in the Los Angeles Basin by 1 to 2 days. This observed pattern is caused by a nearly complete shutdown of methylchloroform emission during weekends. These findings imply that methylchloroform may be used as an endemic tracer of the Los Angeles area. Contributions from other urban areas, e.g., San Francisco, Phoenix, and Las Vegas are expected to be much lower. Therefore, several studies of long range transport in southwestern United States have used methylchloroform as a tracer of opportunity (Miller et al., 1990; Pryor and Hoffer, 1992; Pryor et al., 1995).

Our validation study was performed for a period of six months from May to October 1992 during which air pollution transport from the Los Angeles Basin to the Grand Canyon area was frequently expected. Particle simulations were carried out backward in time for three receptors with methylchloroform observations and the corresponding influence functions were calculated in one hour sampling intervals. No attempt was made to estimate emission rate of methylchloroform from the Los Angeles area or other potential sources. A contribution from a given source was calculated in terms of concentration normalized by emission rate. A complete shutdown of emission during weekends was assumed. Each source was approximated by a 50 × 50 × 0.5 km box.

Figure 14 presents observed methylchloroform concentration above background by hour of the day and day of the week during the analyzed six month period. The background concentration was estimated using the 25th percentile concentration (Pryor et al., 1995). The regular weekly cycles with the lowest values on Tuesdays are evident in the observed data. The amplitude of these cycles is the highest for the SPMO receptor which is the closest one to the Los Angeles Basin and is significantly less for the MEAD and LOME receptors located farther east. The model results are presented as normalized concentrations from the Los Angeles source multiplied by a factor of 0.25 × 10^{12} to be comparable with the magnitude of the observed values. The simulated Los Angeles contribution with the emission shut down during weekends reproduce the weekly cycles of the observed data quite well. A very similar reproduction of the weekly cycles (except lower concentration values) was obtained from the simulation where the emission was further limited to working hours (8am-5pm) only. For reference, the Los Angeles contribution simulated for the constant emission is also presented. It is interesting to note that the effect of zero emission during Saturdays and Sundays is evident for a large part of the week. This suggests that the transport time between Los Angeles and the considered receptors is much longer than two days due to the effect of mesoscale circulations.
Figure 14: Methylchloroform concentrations above background by hour of the day and day of the week at three receptors during May-October, 1992: observed values (thick line), simulated contribution from the Los Angeles Basin without weekend emission (thin line) and with weekend emission (dash line).

Figure 15: Time series of the observed methylchloroform concentration at SPMO (thick line) and time series of corresponding percentiles (thin line).
In order to directly compare the observed and simulated methylchloroform episodes, the time series of one hour values were smoothed using a 24 hour running average. Next, frequency distributions were calculated for each time series for the 6 month period and, finally, the concentration values in time series were replaced by their corresponding percentiles with values varied between 0 and 1. Figure 15 illustrates this procedure by comparing the methylchloroform concentration time series observed at SPMO with its corresponding percentile time series. It should be pointed out that this procedure enhances the appearance of the concentration episodes. The observed time series contain a few periods with missing values.

The analysis is performed under the assumption that the Los Angeles Basin is the only significant source of methylchloroform. Since neither the release rate of methylchloroform nor its exact location is known, it would not be reasonable to expect that any model can reproduce values of the observed data. Therefore, it is more interesting to examine whether the model can reproduce the timing of episodes of elevated methylchloroform concentration. Figure 16 presents comparison of the observed concentrations and the simulated contribution from the Los Angeles source. Most of the observed methylchloroform episodes are well reproduced by the model at all three receptors although the model performance is less accurate at MEAD. The model does not simulate a background concentration which is always present in the observations.

Correlation coefficients between the observed and simulated percentiles of concentration at all three receptors for each month and for the entire period are presented in Figure 17. This figure also shows the results from additional simulations (RAMS-1 and ATAD) which will be discussed later. The correlation coefficients are evidently lower for MEAD than for the two other receptors which is probably due to the fact that MEAD is located in the more complicated terrain at the mouth of the Grand Canyon. Several sensitivity tests were performed for the Los Angeles area using emission boxes with different horizontal sizes and different heights. It was difficult to clearly interpret the effect of horizontal changes of the emission area. However, the best results (in terms of correlation with observations) were obtained for the box with the height 500 m, while results for the 2 km box were much worse.

The correlation coefficient is not the best measure to characterize agreement between model predictions and observations. As demonstrated in Figure 16 there are several small time lags between simulated and observed methylchloroform episodes which contribute to a low correlation. An interesting alternative to compare model results with observations is offered by spectral analysis (e.g., Sirois et al. (1995)). Coherence derived from a cospectrum calculated for two time series varies between 0 and 1 and may be interpreted as a correlation between these time series expressed as a function of frequency or wavelength. The coherence between the simulated and observed time series of methylchloroform concentration varies significantly with wavelength (time scale) but have similar features for each receptor site (Figure 18). All cospectra show that simulated time series are to some extent coherent with the observed ones for the time scale longer than about three days. For the shorter time scale, the cospectra become very noisy. The maximum coherence (between 0.6 and
Figure 16: Time series of percentiles of the observed methylchloroform concentration (thick grey line) and simulated Los Angeles contribution (thin line) for three receptors.
Figure 17: Correlation between methylchloroform concentration observed at three receptors (Spirit Mountain, Meadview, Long Mesa) and concentrations simulated by RAMS/LPD system (RAMS - using both grids, RAMS-1 - using the coarse grid only) and ATAD model.
0.8) appears at time scales between 150 and 180 hours at SPMO and MEAD. This corresponds to the weekly cycles presented in Figure 14. For LOME this maximum is not so well marked and is shifted to longer time scales. There is also another maximum in all three coherence spectra corresponding to a time scale of about four days. It should be noted that the maximum value of coherence for MEAD is lower than that of the two other sites.

Figure 19 presents coherence spectra calculated for the concentration time series at two receptor sites: SPMO and MEAD. The coherence between simulated time series is much higher than between the observed values. It indicates that the model does not take into account some features, like local topography, which distinguish MEAD from SPMO. A higher model resolution is required to correctly simulate concentration affecting MEAD than is necessary for the other receptor sites.

In the above analysis, the Los Angeles Basin was treated as the only significant source of methylchloroform. In order to examine the validity of this assumption, potential contributions from five other urban areas were determined (Figure 20). Due to transport patterns, some of these areas, e.g., Phoenix, may have high potential contributions to concentrations at the receptors. However, concentration predictions for these sources show no correlation with observations. On the other hand, the predicted contribution from San Francisco shows a positive correlation with measurements, but the potential impact of this source is an order of magnitude lower than the contribution from Los Angeles. Due to lack of transport patterns from the north there was practically no impact from the Salt Lake City area. Therefore, one can assume with a good approximation that methylchloroform can be used during the analyzed period as an endemic tracer for the Los Angeles Basin. However, it should be noted that the potential contribution from Las Vegas shows some correlation with the observations at MEAD. Because of its proximity to the receptors of interest, the role of this source area should be more carefully examined with the aid of higher resolution modeling. It is also interesting to see that the model can distinguish between contributions from closely located source areas like Los Angeles and San Diego.

It should be pointed out that in order to improve the simulation of regional transport in complex terrain a better model resolution is required not only in the vicinity of receptors. An adequate model resolution in the source area may be equally or even more important as demonstrated by a numerical study of Poulos and Pielke (1994) for the case of the Los Angeles Basin.

To further investigate the problem of model resolution, additional particle simulations (RAMS-1) were performed in the same manner as the dispersion simulations discussed above except that meteorological fields from the coarse RAMS grid #1 only were used by the LPD model. One can expect that these meteorological fields include much less mesoscale motion than the fields from the finer grid #2. The correlation coefficients in Figure 17 indicate that the model performance is better at SPMO and MEAD when meteorological fields from both RAMS grids are used. At the same time, there is no improvement of the model performance at LOME, the most distant receptor along the transport path from Los Angeles. It is important to realize that the grid #1 does not really represent an independent coarse resolution simulation since there
Figure 18: Cospectra of the observed methylchloroform concentrations and simulated Los Angeles contribution for three receptors.

Figure 19: Cospectra of the methylchloroform concentrations at SPMO and MEAD: observed (solid line) and simulated (dash line).
Figure 20: Simulated potential contributions (impact) to concentrations at the SPMO and MEAD receptors during six months (May-October 1992) from different urban source areas and correlations with the observed methylchloroform concentrations.
is a two-way interaction between nested grids in RAMS. Nevertheless, concentration plots in Figure 21 demonstrate an evident and important difference between these two sets of particle simulations. The coarse grid particle simulations provide much higher concentration values in comparison to the simulations where input from both nested grids was used. Mesoscale motions simulated on the finer grid # 2 cause much more intensive dispersion of the tracer.

The above finding has important implications for mesoscale and regional air quality studies. Models without sufficient resolution to adequately represent mesoscale motions will overestimate the impact from distant sources and at the same time underestimate the impact from local sources at a given receptor.

8 Comparison with simpler modeling approaches

It is interesting to compare our modeling approach with simpler modeling techniques as applied to the same area in the southwestern United States (Uliasz et al., 1994). Two simple modeling approaches will be briefly discussed:

- ATAD (Atmospheric Transport and Diffusion) model (Heffter, 1980)

- dispersion models driven by meteorological fields from National Weather Service (NGM) (Nested Grid) model

The ATAD model is a tool commonly used by National Park Service (NPS) for a trajectory analysis. In this model, a 2-D wind field \((u,v)\) is interpolated from rawinsonde and pibal data. The wind field is averaged within a transport layer determined from a temperature inversion height. Forward or backward in time part, trajectories are calculated with particles released typically every 6 hours. No diffusion parameterization is used in the NPS applications. The ATAD model is easy to handle and can be run on a PC. The computations are so fast that a multi-year analysis is easy to perform. However, there are some serious weaknesses of this modeling approach when applied to the regional transport in complex terrain. This model does not include any explicit effects of complex terrain, or effect of stagnation or recirculation (the transport layer depth is always between 300 and 3000 m). The 2D wind fields are interpolated from a coarse rawinsonde network and vertical motions are not taken into account.

Several research groups have utilized wind fields from the NGM model to run their dispersion or chemistry models, e.g., (Schichtel and Husar, 1994; Venkatram et al., 1994). The NGM model is a hydrostatic primitive equation hemispheric model used operationally by National Weather Service. Availability of archived NGM output is very attractive since it allows one to perform a multi-year transport study when combined with a rather simple dispersion model. However, these meteorological fields have low time and space resolution: \(\Delta z \approx 80\) km (archived with \(2\Delta z\) spacing), vertical grid spacing: \(\Delta z \approx 150\) m close to the surface. Therefore, the representation of terrain topography is very crude.

The ATAD model was used to simulate the Los Angeles Basin contribution to methylchloroform concentration observed at SPMO, MEAD and LOME during the
Figure 21: Concentration of passive tracer at SPMO during three month period (July-August) as simulated for the Los Angeles source by two version of RAMS/LPD simulations and ATAD model (concentrations presented at the same scale).

Figure 22: Examples of influence functions for Hopi Point calculated August 20 1992 (left) and July-August 1992 (right) using ATAD model (contour values: the same as in Figures 10 and 11).
three month period (July-September 1992). Correlation coefficients shown in Figure 17 indicate that this modeling approach has some skills in reproducing the observed episodes but generally its performance is worse in comparison to results from the RAMS-LPD simulations. In some cases, the correlations are negative. Figure 21 demonstrates that the concentrations simulated by ATAD are higher than those predicted by the RAMS-LPD simulations which take into account more mesoscale motions. Finally, the influence functions were derived from ATAD trajectories for the Hopi Point receptor (Figure 22) for the 24 hour and two month sampling periods corresponding to the influence functions presented in Figures 10 and 11. The transport patterns predicted by ATAD differ significantly from those obtained in the RAMS simulations. It is also clearly visible that ATAD can reasonably reproduce long range transport patterns in these areas only where sufficient observational data are available. As one could expect the most dramatic differences between RAMS and ATAD simulations appear in predicting transport paths along the Pacific coast where the observational data needed by ATAD are sparse. It should be pointed out that all results for the ATAD model are quite approximate since the influence functions were derived from standard backward trajectories provided by NPS. Only four trajectories per day were calculated.

For the same 3 month period the LPD model was run with the aid of NGM meteorological fields instead of RAMS output. The correlation coefficients between simulated contributions from Los Angeles and observed methylene chloride were always negative (Uliasz et al., 1994). These findings agreed with results obtained using another dispersion model driven by NGM output (Schichtel and Husr, 1994). It seems that the NGM model is not able to reproduce summer monsoonal flow in southern California due to a lack of sufficient initialization data in this area and coarse resolution. It is interesting that the same NMC analysis data were used to initialize the RAMS simulations which were much more successful due to a better resolution and physics. This problem with the NGM fields in the southwestern United States has been recognized and RAMS wind fields from our daily simulations have been also used by other research groups instead of the NGM fields.

The presented comparison shows that RAMS combined with the LPD model is superior to the other simpler modeling approaches in application to regional transport in complex terrain. Even with the relatively coarse resolution the RAMS is able to resolve some mesoscale atmospheric circulations while wind fields in the NGM and ATAD approaches represent only synoptic scale flow. However, the RAMS modeling is also the most expensive tool, especially, in the case of a long term study. In addition, the RAMS or similar sophisticated models cannot be used as a "black box". They demand more knowledge and qualifications from the user.

9 Summary and conclusions

This chapter demonstrates the feasibility of a long term regional air pollution study using CSU RAMS and the Lagrangian particle dispersion model. The simulations performed over the entire year of 1992 required careful design and processing a large
volume of data. The study was completed on IBM RISC-6000/550 workstations dedicated to this project. However, it should be pointed out that modern personal computers based on the Pentium processor offer even higher speed of numerical computations at a much lower price than our workstations. Therefore, this type of intensive numerical study is becoming accessible to an even wider community of modelers.

The RAMS/LPD simulations for the entire year of 1992 resulted in the creation of a unique database containing:

- original RAMS outputs;
- meteorological fields extracted for dispersion calculations;
- particle distributions simulated backward in time for selected receptors;
- influence functions derived from the particle simulations.

Forward in time particle dispersion simulations were mostly limited to the winter and summer intensive periods of the MOHAVE field study. This database offers interesting possibilities for air quality, visibility and climatological studies for the southwestern United States.

Despite necessary compromises in the design of our simulations, the results from validation of the RAMS/LPD modeling with the aid of both meteorological and methylchloroform observations are encouraging. We are able to correctly reproduce the regional scale transport between the Los Angeles Basin and the Grand Canyon region. Performance of the RAMS/LPD modeling is evidently better than the performance of simpler modeling approaches applied to the same region.

However, it is also obvious that the numerical resolution of RAMS in the daily simulations was not sufficient to resolve all important mesoscale circulations related to complex terrain features. One can expect major improvements of the simulation results from increasing resolution of RAMS by setting up additional nested grids. It was demonstrated that the higher resolution of a meteorological simulation results in longer travel times and higher dilution of pollutant plumes from distant emission sources. This finding has important implications for the source apportionment when distant and local emission sources are taken into account.

Further research should include higher resolution RAMS and dispersion simulations for selected case studies and their comparison to the already completed daily simulations. Both high resolution and daily simulations should be used to validate models with the aid of tracer data when available. This is especially important in order to evaluate the RAMS/LPD performance in simulation of air pollution transport from local point emission sources in complex terrain. Simpler modeling approaches like the ATAD model, due to their simplicity and efficiency, are still useful tools for the performance of a multi-year analysis of long range transport. We recommend a comparison of ATAD results against the RAMS/LPD results for the entire year to examine ATAD's applicability and limitations. One can expect that the ATAD model may be successful in regional scale transport modeling to investigate general source areas assuming that sufficient observational data are available and sufficiently long averaging times are considered. However, this model is not suitable for shorter range
transport, nor for quantitative source apportionment where mesoscale circulations are more important.

Acknowledgments. Thanks are due to Dr. Walter Lyons who thoroughly reviewed the paper and provided many valuable comments. ATAD trajectories were calculated by Kristi Gebhart, National Park Service. Funding for this research was partially provided by the National Park Service through Interagency agreement #0475-4-8003 with the National Oceanic and Atmospheric Administration through agreement #CM0200 DOC-NOAA to the Cooperative Institute for Research in the Atmosphere (Project #5-31796).

References


