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Comparison of Average Transport and Dispersion Among a Gaussian, a Two-Dimensional, and a Three-Dimensional Model

Lawrence Livermore National Laboratory

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ABSTRACT

The simplifying atmospheric transport and dispersion assumption used by MACCS2, the Nuclear Regulatory Commission's code for predicting off-site consequences, is tested by comparison to ADAPT/ LODI, a state-of-the-art, three-dimensional advection-dispersion code. Also included in the comparison is the Nuclear Regulatory Commission's code for rapid emergency response, RASCAL, and a newer related code with upgraded dispersion and deposition modules, RATCHET. Meteorological data for the test were provided by the Department of Energy's Atmospheric Radiation Measurement Program Southern Great Plains site in central Oklahoma and Kansas, a site with a unique and comprehensive set of mesoscale meteorological data. Each model was run in its normal manner to produce the annual average integrated exposure and deposition for a series of rings at 16.1, 32.2, 80.5, and 160.9 km (10, 20, 50, and 100 miles) from a hypothetical release, and the integrated exposure and deposition for arc-sectors at the same set of distances and the 16 compass directions. Nearly all the annual average ring exposures and depositions and the great majority of the arc-sector values for MACCS2, RASCAL, and RATCHET were within a factor of two of the corresponding ADAPT/ LODI values.

CONTENTS

ABSTRACT . . . iii

FIGURES . . . vii

TABLES . . . viii

APPENDICES . . . ix

EXECUTIVE SUMMARY . . . xi

FOREWORD . . . xv

ACKNOWLEDGMENTS . . . xvii

ACRONYMS . . . xix

1. BACKGROUND . . . 1

2. SELECTION OF THE STUDY SITE . . . 3

3. MODELS . . . 5
- 3.1 MACCS2 . . . 5
  - 3.1.1 Meteorological Representation . . . 5
  - 3.1.2 Atmospheric Transport and Dispersion . . . 8
  - 3.1.3 Deposition . . . 9
- 3.2 RASCAL and RATCHET . . . 9
  - 3.2.1 Meteorological Representation . . . 10
  - 3.2.2 Atmospheric Transport . . . 12
  - 3.2.3 Atmospheric Dispersion . . . 12
  - 3.2.4 Dry Deposition . . . 13
  - 3.2.5 Wet Deposition . . . 13
- 3.3 NARAC Models - ADAPT and LODI . . . 14
  - 3.3.1 ADAPT . . . 15
  - 3.3.2 LODI . . . 16
    - 3.3.2.1 Dry Deposition . . . 17
    - 3.3.2.2 Wet Deposition . . . 17

4. METEOROLOGICAL DATA . . . 19
- 4.1 ARM Site . . . 19
- 4.2 Surface Data . . . 20

4.2.1 ARM SMOS Sites 20
4.2.2 Oklahoma Mesonet 20
4.3 Upper Air Data 20
4.3.1 Sondes 21
4.3.2 Radar Wind Profiler/ Radio Acoustic Sounding System 23
4.3.3 NOAA Profiler Network 23
4.3.4 Atmospheric Emitted Radiance Interferometer 24

5. METEOROLOGICAL DATA PROCESSING 25
5.1 Pasquill-Gifford (P-G) Stability Category 25
5.2 Mixing Height 25
5.3 Low-Level Nocturnal Jet 26
5.4 MACCS2 Input Meteorology File 27
5.5 RASCAL/ RATCHET Input Meteorology Files 28
5.6 ADAPT/ LODI Input Files 29

6. DATA QUALITY ISSUES 33
6.1 SMOS Data 33
6.2 NPN and 915 MHz RWP Data 33

7. SOURCE TERM 39

8. SIMULATION PROCEDURE 41
8.1 MACCS2 41
8.2 RASCAL/ RATCHET 41
8.3 ADAPT/ LODI 42
8.3.1 Grids 42
8.3.2 Solution Steps 43
8.4 Computer Time Requirements 45
8.4.1 MACCS2 45
8.4.2 RASCAL/ RATCHET 46
8.4.3 ADAPT/ LODI 46

9. WIND CHARACTERISTICS OF THE ARM SGP SITE 47

10. RESULTS 53
10.1 Arc Averages 53
10.2 Arc-Sector Averages 55
10.3 Two-Dimensional Exposure and Deposition 62
10.4 Summary of Results 72

11. REFERENCES 73

FIGURES

Figure 1. Location of Surface Meteorological Sites 21
Figure 2. Location of ARM Upper Air Observations 22
Figure 3. Cumulative Number of Hours with Mixing Heights less than a Given Height 26
Figure 4. Example of a Nocturnal Jet 27
Figure 5. Central Facility Sonde Launched at 5:29 am CST on January 31, 2000. 34
Figure 6. 915 MHz RWP Wind Profile for the Central Facility at 10:00 pm CST on March 18, 2000 35
Figure 7. Central Facility Sonde Launched at 5:33 am CST on November 15, 2000 36
Figure 8. 915 MHz RWP Wind Profile for Beaumont at 11:00 am CST on May 14, 2000 37
Figure 9. Topography of the ARM SGP Site 43
Figure 10. Wind Rose for the ARM Central Facility at Lamont, OK 47
Figure 11. Surface Wind Rose for the ARM Central Facility for Winter, 2000 48
Figure 12. Surface Wind Rose for the ARM Central Facility for Spring, 2000 48
Figure 13. Surface Wind Rose for the ARM Central Facility for Summer, 2000 48
Figure 14. Surface Wind Rose for the ARM Central Facility for Autumn, 2000 48
Figure 15. Surface Wind Rose for the Elk Falls, KA Site 49
Figure 16. Surface Wind Rose for the Ashton, KA Site 49
Figure 17. Surface Wind Rose for the Byron, OK Site 49
Figure 18. Surface Wind Rose for the Ringwood, OK Site 49
Figure 19. Surface Wind Rose for the Meeker, OK Site 49
Figure 20. Wind Rose from 915 MHz Profiler at 87 m Height at Lamont, OK 50
Figure 21. Wind Rose from 915 MHz Profiler at 87 m Height at Beaumont, KA 50
Figure 22. Wind Rose from 915 MHz Profiler at 87 m Height at Medicine Lodge, KA 50
Figure 23. Wind Rose from 915 MHz Profiler at 87 m Height at Meeker, OK 50
Figure 24. Wind Rose from 915 MHz Remote Wind Profiler (RWP) at 495 m height at Lamont, OK 51
Figure 25. Wind Rose from NOAA Wind Profiler (NWP) at 500 m Height at Lamont, OK 51
Figure 26. Arc-Sector Exposure for Non-Depositing Species on 16.9-km (10-mile) Arc 56
Figure 27. Arc-Sector Exposure for Non-Depositing Species on 32.2-km (20-mile) Arc 56
Figure 28. Arc-Sector Exposure for Non-Depositing Species on 80.5-km (50-mile) Arc 57
Figure 29. Arc-Sector Exposure for Non-Depositing Species on 160.9-km (100-mile) Arc 57
Figure 30. Arc-Sector Exposure for Depositing Species on 16.1-km (10-mile) Arc 58

Figure 31. Arc-Sector Exposure for Depositing Species on 32.2-km (20-mile) Arc 58
Figure 32. Arc-Sector Exposure for Depositing Species on 80.5-km (50-mile) Arc 59
Figure 33. Arc-Sector Exposure for Depositing Species on 160.9-km (100-mile) Arc . . . 59
Figure 34. Arc-Sector Deposition on 16.1-km (10-mile) Arc 60
Figure 35. Arc-Sector Deposition on 32.2-km (20-mile) Arc 60
Figure 36. Arc-Sector Deposition on 80.5-km (50-mile) Arc 61
Figure 37. Arc-Sector Deposition on 160.9-km (100-mile) Arc 61
Figure 38. Normalized Exposure for Non-Depositing Material on the 16.1-km (10-mile) Arc. 63
Figure 39. Normalized Exposure for Non-Depositing Material on the 32.2-km (20-mile) Arc. 63
Figure 40. Normalized Exposure for Non-Depositing Material on the 80.5-km (50-mile) Arc. 64
Figure 41. Normalized Exposure for Non-Depositing Material on the 160.9-km (100-mile) Arc. 64
Figure 42. Normalized Exposure for Depositing Material on the 16.1-km (10-mile) Arc. 65
Figure 43. Normalized Exposure for Depositing Material on the 32.2-km (20-mile) Arc. 65
Figure 44. Normalized Exposure for Depositing Material on the 80.5-km (50-mile) Arc. 66
Figure 45. Normalized Exposure for Depositing Material on the 160.9-km (100-mile) Arc. 66
Figure 46. Normalized Deposition on the 16.9-km (10-mile) Arc. 67
Figure 47. Normalized Deposition on the 32.2-km (20-mile) Arc. 67
Figure 48. Normalized Deposition on the 80.5-km (50-mile) Arc. 68
Figure 49. Normalized Deposition on the 160.9-km (100-mile) Arc. 68
Figure 50. Annual Average Exposure for Non-Depositing Species 69
Figure 51. Annual Average Exposure for Depositing Species 70
Figure 52. Annual Deposition 71

TABLES

Table 1. Description of Weather Bins Used in MACCS2 7
Table 2. RASCAL and RATCHET Precipitation Rates 11
Table 3. RASCAL Washout Coefficients (s^{-1}) 13
Table 4. RATCHET Wet Deposition Model Parameters 14
Table 5. Number of Sondes at Each Site 23
Table 6. Number of Hours in Each Stability Category for MACCS2 Site 28
Table 7. Seasonal Average Mixing Heights 28
Table 8. Number of Hours in Each Stability Category for RASCAL Sites 29
Table 9. Number of Hours vs Number of Valid Surface Observations 29

Table 10. Number of Hours vs. Number of Upper Air Profiles 31
Table 11. Hours with Valid Data for Profiler and Sonde Sites 31
Table 12. Source Term Specification 39
Table 13. Meteorology Grid Vertical Levels and Corresponding Central Facility Altitudes 42
Table 14. Non-Depositing Species Arc Average Exposure 53
Table 15. Depositing Species Arc Average Exposure 54
Table 16. Arc Average Deposition 54

APPENDICES

APPENDIX A - CONTENTS OF DATA CD 77

EXECUTIVE SUMMARY

The Nuclear Regulatory Commission's code for predicting off-site consequences and probabilistic risk assessments, MACCS2, uses a straight-line Gaussian model for atmospheric transport and dispersion that has been criticized as overly simplistic. Because of an increased interest in level-3 probabilistic risk analyses, testing of the simplifying transport and dispersion assumption is performed here using comparison of MACCS2 to ADAPT/ LODI, a state-of-the-art, three-dimensional advection-dispersion code. Also included in the comparison is the Nuclear Regulatory Commission's code for rapid emergency response, RASCAL3.0, and RATCHET, a newer related code with upgraded dispersion and deposition modules.

The site chosen for the test was the Department of Energy's Atmospheric Radiation Measurement Program Southern Great Plains site in central Oklahoma and Kansas, which was selected primarily on the basis of the available atmospheric data. The data set consisted of hourly average measurements of wind, temperature, and turbulence both at the surface and aloft, and hourly precipitation during the entire year 2000. This is the only site we know of that has multiple upper air wind and temperature measurements within a 322-km (200-mile) square area over a period longer than one year, and it allowed us to perform the comparison without using any pseudo observations from forecast or prediction models. We would have preferred a site with greater topographical and diurnal heterogeneity, but with frequent low-level nocturnal jets and occasional severe storms there was sufficient variability.

Each model was run in its normal mode by personnel familiar with it, and each used its typical set of meteorological observations. MACCS2 used only the surface observations (winds at 10 m, and surface precipitation) at one site, the Central Facility. RASCAL and RATCHET used surface data at the Central Facility and at five additional sites. ADAPT/ LODI used the entire three-dimensional data set consisting of 100 surface sites and fifteen upper air sites (ten remote wind profiler and five sonde sites). ADAPT is an advanced data assimilation model designed to convert such large and diverse sets of observations into gridded three-dimensional wind and turbulence fields that agree with the observations and are mass-consistent; these gridded meteorological data allow LODI to accurately calculate atmospheric transport and dispersion for individual releases.

MACCS2 used its binning procedure to select a representative set of 610 release start times and associated weights from the 8760 hourly observations. A hypothetical point source was defined that released 10^{16} Bq each of a depositing and non-depositing material uniformly over a period of 30 minutes at a height of 50 m with a buoyant heat flux of 10^{6} W. RASCAL, RATCHET, and LODI calculated individual exposure (air concentration at the surface integrated over the passage of the plume) and deposition (total material deposited on the ground by wet and dry deposition during plume passage) spatial distributions for each of these releases and averaged them using the associated weights to produce an annual average for comparison with MACCS2.

Two comparison metrics were used. The first metric consisted of the average exposure and deposition in four circular rings around the source at distances between 14.4 and 16.1, 30.6 and 32.2, 78.7 and 80.5, and 159.3 and 160.9 km (9 and 10, 19 and 20, 49 and 50, and 99 and 100 miles). The second metric considered the average exposure and deposition in arc-sectors using the same four distances for the arcs and the 16 compass sectors from N clockwise around to NNW, a total of 64 values for each exposure (depositing and non-depositing material) and deposition (for depositing material). Similar comparisons were performed with RASCAL and RATCHET but only for the inner three rings because RASCAL and RATCHET only followed the plume for 80.5 km (50 miles).

MACCS2's ring average values ranged from a minimum of 0.64 to a maximum of 1.58 times the corresponding LODI ring average with higher ratios occurring for the 16.1-km (10-mile) ring and lower for the 80.5- and 160.9-km (50- and 100-mile) rings. All these ratios are well within a factor of two. The arc-sector exposures and depositions for MACCS2 were also usually within a factor of two of the corresponding value for LODI. Of the 192 exposures and depositions (4 arcs, 16 sectors, 2 exposures and 1 deposition), only nine were more than twice as large (all in the 16.1-km arc) and twelve were less than half as large (four in the 80.5-km and eight in the 160.9-km arc), and these were usually in sectors where the exposure or deposition was smaller. Differences greater than a factor of three occurred only twice. Overall, the arc average and the great majority of the arc-sector average exposures and depositions were within a factor of two when comparing MACCS2 to LODI.

RASCAL calculated exposures and depositions consistently larger than LODI (ratio range for rings from 1.12 to 1.65) while RATCHET calculated values smaller than LODI (ratio range for rings from 0.48 to 0.88). Still, nearly all these values are within a factor of two of LODI. The larger ratios for RASCAL and the smaller ratios for RATCHET must be due to the dispersion and deposition modules since those are the only differences between the models. The arc-sector exposures and depositions for RASCAL and RATCHET often differ from LODI by more than a factor of two, but this is partly related to the fact that RASCAL tends to consistently produce higher and RATCHET lower values than LODI. RASCAL has 33 of 144 exposures and depositions (3 arcs, 16 sectors, 2 exposures and 1 deposition) more than twice as large as LODI, and none less than half as large. Ten of these are more than three times as large as LODI. RATCHET has three of 144 exposures and depositions more than twice as large as LODI and 33 less than half as large. Of these 33, ten are less than one-third as large as LODI. Differences between RASCAL/ RATCHET and LODI may be due to different parameterizations of dispersion and deposition, to different representations of transport, or to both.

FOREWORD

The comparisons presented in this report are among three different models that can be used for determining how radioactive material that could be released following a postulated incident at an NRC-licensed facility could move through and spread within the atmosphere. This process of moving and spreading is called atmospheric transport and dispersion (ATD). Some materials are gaseous in nature, while others are in the form of small particles, which can fall out onto the ground, a process called deposition. This comparison was undertaken because the simple models have been criticized as being too-simple, which could lead to inaccurate estimates of risk. Since weather is a key factor in the transport and dispersion of radioactive material, the results that were compared were averages over hundreds of weather trials. A weather trial is a set of sequential (timewise) weather observations used to move and spread a plume of material from the place of release to the place where it exits the region of interest.

ATD models are referred to as one-dimensional, two-dimensional, or three-dimensional. The difficulty in defining these terms for ATD models is that, for all three, dispersion actually takes place in all three dimensions. The differences among the models occur in the estimation of the transport. A one-dimensional model assumes that a plume moves downwind along a straight line at the speed of the wind. As the plume moves downwind, it broadens (in the crosswind direction) and grows taller (in the vertical direction). A two-dimensional model allows the plume to bend and change direction. Again, the plume broadens and grows taller as it moves downwind. A three-dimensional model is the most complex. It allows individual particles (making up the plume) to move in any direction. With the three-dimensional model, the plume can split into two plumes as it encounters a hill, a canyon, or another complex wind pattern.

The models are:
(1) the one-dimensional, straight-line Gaussian model that the NRC uses for cost/ benefit calculations, for emergency planning, and for estimating off-site consequences for a Probabilistic Risk Assessment (PRA). The code is MACCS2, the MELCOR Accident Consequence Code System, Version 2. Sandia National Laboratories ran this code.

(2) two two-dimensional models with slightly different representations of dispersion and of deposition. The first code is RASCAL, Radiological Assessment System for Consequence Analysis, which is used today in NRC's Incident Response Center for response to radiological emergencies. The second code is RATCHET, Regional Atmospheric Transport Code for Hanford Emission Tracking, which was developed for use in the Hanford Environmental Dose Reconstruction Project. Development of RATCHET emphasized upgrading the methods in RASCAL for calculating dispersion and deposition. Pacific Northwest National Laboratory ran these codes.

(3) a three-dimensional model that employs two codes, one that was used in this case to estimate the wind field in three dimensions based on thousands of data points and another that was used to estimate the gaseous and particulate material transport. The wind-field code was ADAPT (Atmospheric Data Assimilation and Paramerterization Techniques) and the dispersion and deposition code was LODI (Lagrangian Operational Dispersion Integrator). Lawrence Livermore National Laboratory ran these codes.

The results from ADAPT/ LODI calculations were used as a benchmark for the simpler (1-D and 2-D) codes. It would have been preferable to compare the simpler codes with measured values, but such measurements do not exist over the distance of interest to the NRC.

The location selected for this comparison, the Department of Energy's Atmospheric Radiation Measurement Southern Great Plains site (ARM SGP), was chosen to provide the most realistic test of the models' capabilities. No other site in the United States provides the regularly-collected measurements at the surface and above the surface at more than one location within 160.9 km (100 mi) necessary to allow this comparison to be based solely on measured weather data.

Each model was run by users familiar with its operation, using each code in its normal manner and relying on its typical set of observations of the weather. Comparisons were made for 4 different distances from the site of the assumed released (3 for RASCAL and RATCHET) and for 16 different directions, representing compass directions. Good agreement was found among all the models tested, considering the purposes of the various codes. The averages over one-mile wide rings at the four distances were within a factor of two for both the MACCS2 and the RASCAL/ RATCHET results compared with the LODI/ ADAPT results.

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ACRONYMS

ADAPT	Atmospheric Data Assimilation and Parameterization Techniques
AERI	Atmospheric Emitted Radiance Interferometer
ARM	Atmospheric Radiation Measurement
ATD	Atmospheric Transport and Dispersion
DOE	Department of Energy
GMT	Greenwich Meridian Time
LLNL	Lawrence Livermore National Laboratory
LODI	Lagrangian Operational Dispersion Integrator
LST	Local Standard Time
MACCS2	MELCOR Accident Consequence Code System, Version 2
MSL	Mean Sea Level
NARAC	National Atmospheric Release Advisory Center
netCDF	Network Common Data Format
NOAA	National Oceanic and Atmospheric Administration
NPN	NOAA Profiler Network
NRC	Nuclear Regulatory Commission
PRA	Probabilistic Risk Analyses
RASCAL	Radiological Assessment System for Consequence Analysis
RASS	Radio Acoustic Sounding System
RATCHET	Regional Atmospheric Transport Code for Hanford Emission Tracking

RWP	Radar Wind Profiler
SGP	U.S. Southern Great Plains Site
UTC	Coordinated Universal Time

1. BACKGROUND

The Nuclear Regulatory Commission's (NRC's) code for predicting off-site consequences, MACCS2 (Chanin, et al. 1998) (MELCOR Accident Consequence Code System, Version 2), uses a simplified model for atmospheric transport and dispersion (ATD), that is, a straight-line Gaussian model. The MACCS2 calculations are used by the NRC for planning purposes, for cost-benefit analyses, and in level-3 probabilistic risk analyses (PRAs). The MACCS2 ATD model has been criticized as being overly simplistic, even for its purposes. The justification for its use has been that only average or expected values of metrics of interest are needed for the NRC's purposes and that a simplified model, by averaging metrics of interest obtained using numerous weather sequences one-by-one, compensates for the loss of structure in the meteorology that occurs away from the point of release. The simple model has been retained because of the desire to have short running times on personal computers covering the entire path through the environment, including the food and water pathway, and covering essentially a lifetime of exposure to a contaminated environment.

The assumption about the adequacy of averaging metrics of interest over numerous weather sequences has never been tested for the NRC's purposes. Because of increased interest in level-3 PRA, testing of this assumption is performed here using comparison of MACCS2 , the simplified model, to LODI (Nasstrom, et al. 2000) (Lagrangian Operational Dispersion Integrator), a state-of-the-art, three-dimensional advection-dispersion code that uses a Lagrangian stochastic, Monte Carlo method. LODI is coupled to ADAPT (Sugiyama and Chan 1998) (Atmospheric Data Assimilation and Parameterization Technique), which provides time-varying, three dimensional fields of mean winds, turbulence, pressure, temperature, and precipitation based on, in this case, observed meteorology.

RASCAL3.0 (Sjoreen, et al. 2001) (Radiological Assessment System for Consequence Analysis, Version 3.0) is used by the NRC for emergency response applications which require rapid response. RASCAL3.0 contains ATD components that are intermediate in complexity between MACCS2 and ADAPT/ LODI. It employs time-varying, two-dimensional meteorological fields of wind, stability, and precipitation based on surface-level meteorological observations as input to a Lagrangian trajectory transport model and a Gaussian puff dispersion model. The dispersion portions of RASCAL3.0 are similar to those of MACCS2, while the transport portions are significantly different. NRC is considering upgrading RASCAL3.0 by replacing the dispersion portions of the code with dispersion modules from the RATCHET code (Ramsdell, et al. 1994). RASCAL3.0 and RATCHET were developed from the same precursor code. In this study, RATCHET refers to a developmental version of RASCAL that incorporates dispersion and deposition modules from the original RATCHET code. The RATCHET dispersion and deposition modules are more modern than those in RASCAL. A comparison of RASCAL and RATCHET to ADAPT/ LODI has been included.

The objective of this study is to determine if the average ATD results from these codes are sufficiently close that more complex models are not required for the NRC purposes of planning, cost-benefit, and PRA or different enough that one or both of the NRC codes should be modified to provide more rigorous ATD. The decision will be made by the NRC using results of this study and other factors, most notably run time and input requirements.

It would be best if MACCS2 and RASCAL/ RATCHET results could be compared with measurements over the long distances and types of terrain of interest to the NRC. However, such measurements do not exist, so the less desirable comparison with a state-of-the-art code was chosen to provide input into the decision on the adequacy of MACCS2 ATD. The comparison was also an opportunity to gain additional baseline information on the performance of the RASCAL/ RATCHET code. Comparisons of LODI/ ADAPT results with intentional and unintentional releases can be found in Foster, et al. (2000). These comparisons, although over shorter ranges than those of interest to the NRC, demonstrate that LODI/ ADAPT is sufficiently accurate for the purposes of this study.

2. SELECTION OF THE STUDY SITE

Quite a few locations were considered as possible sites for this study. These included currently operating nuclear power plants, several DOE laboratory sites, and a few other locations. The following criteria were considered in making a final selection:

- a data set with sufficient observations to characterize the horizontal wind field as a three-dimensional function of height and position from the source out at least 160.9 km (100 miles),
- topography that would interact with the large-scale flow producing local modification of wind speed and direction, and
- a site with changes in surface properties that could affect the local flow, such as a coastal site with a land-sea breeze.

As we considered the possible sites, we could identify only one that satisfied the first criterion, the Department of Energy (DOE) Atmospheric Radiation Measurement (ARM) Southern Great Plains (SGP) site in Oklahoma and Kansas. No other site provided regular upper air data at more than one location within 160.9 km (100 miles) of the source. To use a different site would have required use of a regional model to determine the flow fields, and we wanted to base this study solely on observations. The topography of Oklahoma and Kansas is relatively smooth and has minimal effect on the wind field, and the surface is fairly uniform and therefore produces relatively little local thermal forcing. However, wind fields in Oklahoma and Kansas are frequently affected by low-level nocturnal jets and occasional severe storms. Therefore, the last two criteria were only partially satisfied, but there was sufficient variability for the purpose of this study. At the outset we realized that if the differences between MACCS2 and ADAPT/ LODI were large at the ARM site, they would be large everywhere, and the transport and dispersion module in MACCS2 would likely require replacement. But if the differences were small, the adequacy of MACCS2's atmospheric transport and dispersion module might still be unresolved for some special locations.

3. MODELS

3.1 MACCS2

The MELCOR Accident Consequence Code System Version 2 (MACCS2) (Chanin et al. 1998) was developed at Sandia National Laboratories for the NRC. Its primary use is in performing consequence analyses in support of level-3 probabilistic risk assessments (PRAs). It is also used by the NRC for planning purposes and cost-benefit analyses.

MACCS2 is the latest in a series of NRC-sponsored codes for estimating off-site consequences following a release of radioactive material into the environment. The first code in the series was CRAC (Calculation of Reactor Accident Consequences), which was developed for the Reactor Safety Study (WASH-1400, 1975). The first version of MACCS was released to the public in 1987. A subsequent version was used in the benchmark PRA study reported in NUREG-1150.

MACCS2 is a versatile code, with most of its parameters being under user control to facilitate the performance of sensitivity and uncertainty analyses. The principal phenomena considered by MACCS2 are atmospheric transport and dispersion (ATD), short- and long-term mitigative actions, exposure pathways and doses, deterministic and stochastic health effects, and economic costs. Of these capabilities, only the ATD processes are considered in the present study.

The atmospheric models in MACCS2 are relatively simple. Released material is assumed to travel downwind in a straight line. The concentration profiles in the cross-wind and vertical dimensions are approximated as being Gaussian. The Gaussian plume model was chosen for MACCS2 because it requires minimal computational effort and allows large numbers of realizations to be calculated. These realizations represent uncertainty in weather data at the time of a hypothetical accident and uncertainty in other input parameters to represent degree of belief. Large numbers of realizations (hundreds) are generally needed to perform PRA and sensitivity studies.

3.1.1 Meteorological Representation

The normal calculation mode for MACCS2 is to sample from hourly weather data for one year and to calculate ATD using a Gaussian model in each of 16 directions. Each direction corresponds to a 22.5 degree-wide sector that is centered on a standard compass point. Each weather sequence is weighted by its probability of occurrence. The weather sequences are normally chosen, and have been chosen for this study, to emphasize sampling of sequences believed to be important to the prediction of early health effects in an exposed population. This emphasizes selection of weather sequences in which it rains while the plume remains within about 32.2 km (20 miles) from the point of release.

MACCS2 was used to select the weather sequences that were used in this study. A total of 610 sequences was chosen using the standard weather binning approach. This approach bins each of the 8760 hours of data in an annual weather file into 36 bins, as shown in Table 1. The last two columns of the table represent the values for the ARM SGP site.

The columns in Table 1 show for each weather bin the included stability class or classes, the wind speed range, and the range of distances traveled by the plume when rain of a prescribed intensity occurs. It also shows the overall number of weather sequences in the bin and the number of weather sequences selected from the bin in this study. The algorithm used to determine the number of sequences selected from each bin is the larger of two quantities: 12 or 5% of the number of sequences in the bin. In 13 cases, the number of weather sequences in the bin is fewer than 12. In these cases, all of the sequences in the bin are selected. Selection of sequences from a bin where not all sequences are chosen is performed by a sequential Monte-Carlo process.

The probability associated with a weather trial is calculated within MACCS2 using the following algorithm. First, the probability that a weather trial falls into a particular bin, P_B, is proportional to the number of trials that are assigned to that bin,

$$P_B = N_B / N,$$

where N_B is the number of weather trials in bin B and N is the total number of weather trials for the year (8760 in a 365-day year). The probability for a weather trial from bin B is then expressed as

$$P_T = P_B / N_{SB},$$

where P_T is the probability associated with weather trial T and N_{SB} is the number of weather trials sampled from bin B (given in the last column of Table 1). Thus, the sum of the probabilities of the weather trials selected from bin B is P_B. Values for the probabilities for each weather trial were determined from the MACCS2 output and were used in the averaging process for all the results presented in this report.

The standard practice of allowing wind rotation was used for the MACCS2 results, which essentially expands the number of weather trials by a factor of 16. This practice was not adopted by the other codes. For each weather trial, a set of calculations is performed to account for the fact that the wind could have been blowing in any of the 16 compass directions. Each of the 16 results for wind rotation is weighted by the

Table 1. Description of Weather Bins Used in MACCS2

Bin No.	Stability Class	Wind Speed Range (m/s)	Rain		Number of Weather Sequences in Bin	Number of Weather Sequences Selected
			Distance (km)	Intensity (mm/hr)		
1	A/ B	0 – 3	< 32	0	312	16
2	A/ B	> 3	< 32	0	194	12
3	C/ D	0 – 1	< 32	0	13	12
4	C/ D	1 – 2	< 32	0	100	12
5	C/ D	2 – 3	< 32	0	361	18
6	C/ D	3 – 5	< 32	0	1077	54
7	C/ D	5 – 7	< 32	0	2202	110
8	C/ D	> 7	< 32	0	2370	119
9	E	0 – 1	< 32	0	6	6
10	E	1 – 2	< 32	0	69	12
11	E	2 – 3	< 32	0	177	12
12	E	> 3	< 32	0	998	50
13	F	0 – 1	< 32	0	29	12
14	F	1 – 2	< 32	0	67	12
15	F	2 – 3	< 32	0	52	12
16	F	> 3	< 32	0	3	3
17	all	all	0 – 3	0 – 2	331	17
18	all	all	3 – 6	0 – 2	8	8
19	all	all	6 – 11	0 – 2	31	12
20	all	all	11 – 21	0 – 2	108	12
21	all	all	21 – 32	0 – 2	118	12
22	all	all	0 – 3	2 – 4	39	12
23	all	all	3 – 6	2 – 4	1	1
24	all	all	6 – 11	2 – 4	1	1
25	all	all	11 – 21	2 – 4	5	5
26	all	all	21 – 32	2 – 4	9	9
27	all	all	0 – 3	4 – 6	27	12
28	all	all	3 – 6	4 – 6	0	0
29	all	all	6 – 11	4 – 6	3	3
30	all	all	11 – 21	4 – 6	5	5
31	all	all	21 – 32	4 – 6	7	7
32	all	all	0 – 3	> 6	27	12
33	all	all	3 – 6	> 6	0	0
34	all	all	6 – 11	> 6	1	1
35	all	all	11 – 21	> 6	4	4
36	all	all	21 – 32	> 6	5	5
Total					**8760**	**610**

probability of the wind blowing in the specified direction. The probabilities associated with the possible wind directions are constructed for each weather bin and are proportional to the number of trials in the bin in which the wind blows in the specified direction. This probability is given by

$$P_{BR} = N_{BR} \, / \, N_B ,$$

where P_{BR} is the probability of a sample in bin B having wind direction R and N_{BR} is the number of weather trials in bin B with wind direction R. The final probability for weather trial T with wind rotation R used in the MACCS2 code is simply the product of the two probabilities, as follows:

$$P_{TR} = P_{BR} \cdot P_T ,$$

where P_{TR} is the probability of weather trial T with wind direction R.

MACCS2 uses single-point weather data. Thus, it approximates weather data as spatially uniform. The weather data file contains the following information: Julian day of the year, hour of the day, wind direction, stability class, and precipitation rate. It also contains seasonal mixing heights (discussed in subsection 5.2). While MACCS2 does not model spatial variation in wind conditions, it does model time dependence. Once a plume is formed, its direction is not allowed to change; however, the wind speed, stability class, and precipitation rate can change hour-by-hour.

3.1.2 Atmospheric Transport and Dispersion

The plume is assumed to move downwind at the prescribed wind speed adjusted for plume centerline elevation. The plume broadens by dispersion due to atmospheric turbulence as it is transported downwind. MACCS2 allows dispersion to be treated either by means of a lookup table or as a power-law function of distance. For this work, the standard Tadmor and Gur lookup tables (Tadmor and Gur 1969, Dobbins 1979) were used to determine cross-wind and vertical dispersion as a function of downwind distance and stability class.

Vertical dispersion is assumed to occur only within the mixing layer. MACCS2 uses four mixing heights to represent the four seasons of the year. These mixing heights represent seasonal averages of the daily maximum values of the mixing heights. Calculation of the mixing heights used in this study is discussed in section 5. The MACCS2 Gaussian plume model treats the ground surface and a surface at the mixing height as planes of reflective symmetry.

3.1.3 Deposition

Dry deposition is treated in MACCS2 by means of a deposition velocity. Aerosols can be distributed among 10 aerosol bins, each with its own deposition velocity. For this study, a single aerosol bin was used and the deposition velocity was chosen to be 0.01 m/ s. The MACCS2 model calculates deposition rate as the product of deposition velocity and aerosol concentration in the air at ground level.

The model for wet deposition (washout) in MACCS2 accounts for the effect of rain intensity. The model has the following form (Brenk and Vogt 1981):

$$\Lambda = \exp(-C_1 \cdot \Delta t \cdot I^{C_2}),$$

where Λ is the fraction of aerosol that remains in the atmosphere (dimensionless), C_1 is the linear washout coefficient (s^{-1}), Δt is the duration of rainfall (s), I is the rain intensity (mm/ hr), and C_2 is the nonlinear washout coefficient (dimensionless). The values of C_1 and C_2 used in this study are $7 \cdot 10^{-5}$ and 0.75, respectively.

3.2 RASCAL and RATCHET

RASCAL (Sjoreen, et al. 2001) is an NRC radiological assessment tool for use in emergency response applications. It consists of modules that estimate accident source terms for nuclear power plants and other nuclear fuel cycle facilities; transport, dispersion, and deposition of radionuclides; and doses. It also includes a meteorological preprocessor that prepares meteorological data for use by the atmospheric transport modules. For this study, the meteorological preprocessor module and one of the atmospheric transport modules were used to estimate time-integrated air concentrations of depositing and non-depositing species and surface deposition of the depositing species for comparison with estimates made by MACCS2 and ADAPT/ LODI. These two modules are referred to as RASCAL, although they were run outside the usual RASCAL framework to efficiently accomplish the required calculations. Minor modifications were made in the codes to accumulate time-integrated concentrations for the full period of plume passage for each release rather than for 15-min intervals and to run from the time of release until the plume left the model domain rather than for a specified period of time. These coding changes did not alter the atmospheric transport, dispersion, or deposition calculations.

The atmospheric models in RASCAL are between MACCS2 and ADAPT/ LODI in complexity. They include a more complete representation of temporal and spatial changes in meteorological conditions than MACCS2, but they do not include the full three-dimensional representation of the atmosphere included in ADAPT/ LODI.

RASCAL is a Lagrangian trajectory Gaussian-puff dispersion model derived from the MESORAD model (Sherpelz, et al. 1986, Ramsdell, et al. 1988). Development of RASCAL emphasized addition of radioactive decay and dose calculations. Another code, RATCHET, (Ramsdell, et al. 1994) was developed from MESORAD for use in the Hanford Environmental Dose Reconstruction Project (Shipler, et al. 1996). The development of RATCHET emphasized upgrading methods for calculating dispersion and deposition. The NRC is considering using RATCHET's dispersion and deposition methodology in RASCAL's atmospheric models. In this study, RATCHET refers to a developmental version of the RASCAL atmospheric model that incorporates dispersion and deposition algorithms from the original version of RATCHET. The developmental model includes the methods of treating atmospheric transport that are included in the existing version of RASCAL.

3.2.1 Meteorological Representation

ARM SGP meteorological data for the model comparison were obtained from Lawrence Livermore National Laboratory, LLNL. The following paragraphs briefly describe the processing of the meteorological data for use by RASCAL and RATCHET, which both use the same meteorological input. A separate meteorological file containing hourly data was received for each of six meteorological stations. These files were combined into a single file containing records with data for all stations for each hour. In creating this file, the original data were copied as received, except for precipitation data. The original files contained temperature and precipitation rates, this information was used to estimate precipitation form and intensity, for example light rain or moderate snow, which is the input needed for RASCAL and RATCHET.

The meteorological preprocessor program converted the hourly data from the meteorological stations into the spatially and temporally varying meteorological fields used by RASCAL and RATCHET (Sjoreen, et al. 2001). The wind field is derived by interpolation of available surface wind data. Fields for atmospheric stability and precipitation type and rate are generated using reported values for the closest observation to each node. Finally, the mixing height field is generated in two steps. In the first step, an initial field is prepared using values calculated from surface observations at the available stations. Then a low pass, spatial filter is used to smooth the initial field.

Surface wind data, initially recorded as wind direction and speed are converted to Cartesian components of the transport vector. A wind field is generated for each of these components using $1/r^2$ weighted interpolation, where r is the distance between the node on the Cartesian grid and the meteorological observation location. Winds at the release height, which are used for transport calculations, are estimated from the surface layer winds using boundary layer wind speed profiles that are a function of atmospheric stability and surface roughness. A uniform surface roughness of 0.2 m was used for this study. The RASCAL meteorological processor has a relatively simple routine to adjust wind field for the effects of topography in stable atmospheric conditions; however, that routine was not used in this study.

There are two atmospheric stability fields. One consists of Pasquill-Gifford stability classes (Pasquill 1961, Gifford 1961, Turner 1964), and the other consists of the inverse Monin-Obukhov length (Monin and Obukhov 1954). The Monin-Obukhov length is estimated from the Pasquill-Gifford stability class using a graphical relationship between Monin-Obukhov length, stability class, and surface roughness derived by Golder (1972).

Mixing height is calculated for each meteorological observation using relationships derived by Zilitinkevich (1972). Calculated mixing heights, which are a function of wind speed, stability, surface roughness, and latitude, are constrained to a minimum of 50 m and a maximum of 2000 m. When mixing heights have been calculated for all of the observations, a mixing height field is generated as indicated above.

RASCAL and RATCHET accept three precipitation conditions – no precipitation, rain, and snow. Every hour, the precipitation grid is updated using the hourly observations. Each node on the grid is assigned the precipitation, or lack thereof, from the closest meteorological station. If the closest station doesn't have a current observation, the precipitation from the closest station with a current observation is used. If there are no stations with current observations, persistence is assumed and the last precipitation grid is used. No interpolation or smoothing is performed on the precipitation data.

Rain, which includes any form of liquid precipitation, may have an intensity of light, moderate, or heavy. Similarly the intensity of snow, which includes all forms of frozen precipitation, may be light, moderate, or heavy. Precipitation intensity determines the precipitation rate as listed in Table 2. The rates for moderate and heavy precipitation are set to the same value, but could be made different. In most parts of the country, heavy precipitation is sufficiently infrequent that setting precipitation rates equal has little effect on the climatological dispersion estimates.

Table 2. RASCAL and RATCHET Precipitation Rates (mm hr^{-1})

Intensity	Rain	Snow
Light	0.6	0.3
Moderate	3.8	1.7
Heavy	3.8	1.7

3.2.2 Atmospheric Transport

RASCAL and RATCHET use the same method for calculation of atmospheric transport. In both codes, the plume is represented by a series of puffs released at 5-minute intervals. Each puff contains the activity released during a 5-minute period. The height of release is the sum of the actual release height and final plume rise. A modification, made to RASCAL's plume rise calculation for use in this model comparison, was to add the option of calculating plume rise from the heat of release based on equations of Briggs (1984). Puff movement is controlled by the wind at the release height with the movement vector updated every 5 minutes using winds interpolated to the puff's current position from the wind fields (Sjoreen, et al. 2001).

3.2.3 Atmospheric Dispersion

RASCAL's atmospheric dispersion calculations use methods developed in the 1950s and 1960s (Sjoreen, et al. 2001). The dispersion parameters are a function of distance traveled and atmospheric stability using numerical approximations to the Pasquill-Gifford dispersion curves similar to those in numerous NRC computer codes, e.g., PAVAN (Bander 1982) and XOQDOQ (Sagendorf 1982).

Dispersion in RATCHET represents advances in the science during the 1970s and 1980s (Ramsdell, et al. 1994), and the technique used is outlined here. RATCHET's dispersion parameters are calculated from travel time and measures of the atmospheric turbulence. During the first hour following release, the horizontal dispersion parameter is proportional to the product of a measure of the horizontal component of turbulence in the wind and time since release. After the first hour, the rate of increase in the horizontal dispersion parameter is a function only of travel time until an upper limit of 10^5 m is reached.

The vertical dispersion parameter is calculated as the product of a measure of the vertical component of turbulence and a function that accounts for decreasing effectiveness of turbulence in dispersing the puffs at long travel time. For neutral and unstable atmospheric conditions (Pasquill-Gifford stability classes A through D), the function is equal to 1.0. For stable conditions (Pasquill-Gifford stability classes E through G), the function decreases the rate of growth of the vertical dispersion parameter from being proportional to time to the first power near the release point to being proportional to the square root of travel time after the first few minutes.

If material is released within the mixing layer, the vertical dispersion coefficient is limited by the top of the mixing layer. The coefficient will resume growth if the mixing height increases. However, the vertical dispersion parameter is not allowed to decrease if the mixing height decreases.

Calculation of the dispersion parameters requires estimates of turbulence parameters. These parameters are estimated as they are required using the available meteorological data and atmospheric boundary layer relationships (Hanna, et al. 1982; Panofsky, et al. 1977). In no case is either of the turbulence parameters permitted to decrease below 0.01 m/ s.

3.2.4 Dry Deposition

In RASCAL, deposition is calculated using a source depletion model with a constant dry deposition velocity of 0.01 m/ s and wet deposition is calculated using a simple washout model with constant washout coefficients. These methods are described in detail in Sjoreen, et al. (2001). The washout coefficients used in RASCAL are listed in Table 3.

Table 3. RASCAL Washout Coefficients (s^{-1}).

Intensity	Rain	Snow
Light	2.2×10^{-4}	1.0×10^{-4}
Moderate	6.1×10^{-4}	3.3×10^{-4}
Heavy	1.1×10^{-3}	6.4×10^{-4}

The deposition calculations in RATCHET are described in Ramsdell, et al. (1994). Dry deposition is still calculated using a deposition velocity; however, the dry deposition velocity is no longer constant. It is a function of characteristics of the material, surface roughness, and atmospheric conditions. Consequently, the dry deposition velocity is a function of both position and time. The model used to calculated dry deposition velocity in RATCHET is based on an analogy with electrical systems (Seinfeld 1986). The analogy assumes that deposition velocity is inversely proportional to the sum of three resistance components – an aerodynamic resistance, a surface-layer resistance, and a transfer resistance. The aerodynamic and surface-layer resistances are functions of wind speed, stability and surface roughness. The transfer resistance is a function of the characteristics of the depositing material and the surface type. In RATCHET, transfer resistance is used as a means of placing a lower limit on the total resistance, or, in other terms, placing an upper limit on dry deposition velocities. Assuming transfer resistances of 10 s/ m for reactive gases and 100 s/ m for fine particles ($\lesssim$ 10 microns) yield dry deposition velocities that are consistent with experimentally determined deposition velocities.

3.2.5 Wet Deposition

There are two wet deposition parameterizations in RATCHET, one for particles and another for gases. The gas scavenging parameterization uses a source-depletion model similar to the model used for dry deposition. The wet deposition velocity for scavenging gases by rain is a function of a solubility coefficient, which is related to the

Henry's Law constant for the gas, and precipitation rate to the ¾ power (Slinn 1984). The wet deposition velocity for scavenging of non-reactive gases (e.g., CH_3I) by rain is about three orders of magnitude lower than for reactive gases (e.g., I_2). Snow is not a particularly good scavenger of gases. For temperatures above -3°C, wet deposition velocities for snow are estimated using the water equivalent precipitation rate. For temperatures below -3°C, the snow surface is frozen and the wet deposition of gases is low; therefore, RATCHET sets the wet deposition velocity to zero.

Particles are collected by precipitation as it falls through the puffs. We assume that rain or snow falls through the entire vertical extent of the puff, and we calculate wet deposition of particles with a washout model where the washout coefficient is a function of precipitation type and rate as given in Table 4.

Table 4. RATCHET Wet Deposition Model Parameters.

	Reactive Gas Wet Deposition Velocity (m/ s)	Particle Washout Coefficient (1/ s)
Light Rain	1.7×10^{-4}	2.7×10^{-4}
Moderate Rain	1.1×10^{-3}	1.1×10^{-3}
Light Snow	8.4×10^{-5}	1.5×10^{-5}
Moderate Snow	4.8×10^{-4}	8.5×10^{-5}

3.3 NARAC Models - ADAPT and LODI

A key component of this study is utilization of a state-of-the-art atmospheric transport and dispersion model, driven by observed meteorological data, to provide the exposure (concentration of a material in near-surface air integrated over plume passage) and deposition (total amount of a material deposited on the ground during plume passage) for each of the sample cases. The weighted average of these accurate individual case results then represents a standard for judging the appropriateness of simpler models.

The National Atmospheric Release Advisory Center (NARAC) at Lawrence Livermore National Laboratory (LLNL) is a national support and resource center for planning, real-time assessment, emergency response, and detailed studies of incidents involving the spread of hazardous material accidentally or intentionally released into the atmosphere. Within its emergency response system, NARAC provides a suite of multi-scale (local-, regional-, continental- and global-scale) atmospheric flow and dispersion models. The numerical methods used by these models have been verified using exact mathematical solutions, and model results have been evaluated using field experiments (Foster, et al. 2000). These evaluations provide confidence in the accuracy of the NARAC models.

The NARAC emergency response modeling system consists of a coupled suite of meteorological and dispersion models. The data assimilation model, ADAPT, constructs fields of mean winds, pressure, precipitation, temperature, and turbulence, using a variety of interpolation methods and atmospheric parameterizations. Non-divergent wind fields are produced by an adjustment procedure based on the variational principle and a finite-element discretization. The dispersion model, LODI, solves the 3-D advection-dispersion equation using a Lagrangian stochastic, Monte Carlo method. LODI includes methods for simulating the processes of mean wind advection, turbulent diffusion, radioactive decay and production, bio-agent degradation, first-order chemical reactions, wet deposition, gravitational settling, dry deposition, and buoyant/ momentum plume rise. The models are coupled to NARAC databases providing topography, geographical data, real-time meteorological observational data, and global and mesoscale forecast model predictions. In this study we use ADAPT to convert the observed meteorological data into 3-D gridded fields of wind and turbulence parameters and LODI to calculate the release, transport, dispersion, and wet and dry deposition of representative pollutants and the corresponding exposures at the surface.

The NARAC models ADAPT and LODI have great flexibility and numerous options that were not necessary for this study. The following discussion focuses primarily on the models as used in this study. For a full discussion of ADAPT/ LODI capabilities see the references.

3.3.1 ADAPT

ADAPT is an atmospheric data assimilation model that builds three-dimensional gridded meteorological fields (Sugiyama and Chan 1998). It provides a selection of approaches to process input meteorological data provided in this study by observations at a set of stations. The model incorporates a number of interpolation and extrapolation techniques, including both direct and iterative solvers, and atmospheric parameterizations. We used ADAPT's capabilities to coherently blend the surface data with the upper air soundings on a uniformly spaced, four km resolution, horizontal grid, and to mass-consistently calculate the three dimensional wind fields and turbulence parameters which then were used to drive NARAC's dispersion model, LODI .

ADAPT produces non-divergent (mass-consistent) winds by minimal adjustment of input fields derived from observational data. This adjustment provides not only the horizontal winds but the vertical component as well. The algorithm is based on a variational formulation and a finite-element spatial discretization, which uses a grid-point representation of the wind fields (in contrast to the flux-based staggered grid representation often used in finite-difference approaches) and provides a rigorous, flexible treatment of boundary conditions. Two iterative solvers, the incomplete Cholesky conjugate gradient and the diagonally scaled conjugate gradient, provide an efficient numerical solution of the Poisson equation derived from the variational principle.

The output meteorological fields are highly dependent on the density and distribution of measurements, the complexity of terrain, and the proper parameterization of atmospheric structure to represent physical processes not directly modeled. ADAPT does not add unverified structure to the output. The mass-consistent wind algorithm minimally adjusts the winds to add stability dependent steerage around topographical features; structures such as re-circulations not supplied by the initial observations are usually not generated by such a procedure.

ADAPT's data assimilation procedures ingest and blend data from a variety of sources. There are two broad classes of meteorological data - observational data and gridded fields. The former are measurements, forecast soundings, or user generated pseudo-observations for one to many vertical levels at a single station location (latitude and longitude location) and time. Gridded fields are analyses or forecasts either acquired from external sources or generated by other models. In this study we used only observational data.

ADAPT divides observational data into three categories - surface, tower, and upper air. Surface data consist of measurements at a single near-ground height. Tower data contain measurements at a single elevated height or at multiple levels, the lowest of which is at or near the surface. Upper air soundings provide multi-level data with the lowest levels in the planetary boundary layer (that portion of the atmosphere from the surface to the geostrophic wind level). Here we categorized all data as either surface or upper air.

ADAPT output files provide the three-dimensional wind components, u (zonal or east-west wind), v (meridional or north-south wind), and w (vertical wind), and turbulence parameters, all of which vary in the three spatial dimensions − east-west, x; north-south, y; and height, z. The files also provide planetary boundary layer height, Monin-Obukov length, and surface friction velocity, all of which were assumed spatially uniform in this study.

3.3.2 LODI

LODI is an atmospheric dispersion model that uses a Lagrangian stochastic, Monte Carlo method which calculates possible trajectories of fluid “particles” in a turbulent flow to solve the 3-D advection dispersion equation (Nasstrom et al. 2000, Ermak and

Nasstrom 2000). Particles are marked at the source with an appropriate amount of contaminant mass based upon prescribed emission rates and geometry. A large number of independent trajectories are calculated by moving particles in response to the various processes represented within the simulation, and the mean contaminant air concentration is estimated from the spatial distribution of the particles at a particular time. LODI uses a coordinate system with a continuous terrain representation at the lower boundary.

In general, the two most important processes are advection by the mean wind and dispersion by turbulent motion. To calculate mean wind advection, 3-D gridded mean wind fields from ADAPT were input into LODI. Turbulent dispersion was modeled via random diffusive movements using atmospheric eddy diffusivity (K) parameterizations. Wet and dry deposition were also simulated.

In this study the source was modeled as a continuous point release with buoyancy and momentum, and the integrated exposure and combined wet and dry deposition were output.

3.3.2.1 Dry Deposition

Dry deposition is parameterized in terms of a deposition velocity at a reference height (1-1.5 m in this study over land). The dry deposition flux onto the surface is then given by the product of this deposition velocity and the concentration at the reference height. The deposition velocity is composed of two independent velocities: the "non-settling deposition velocity", and the gravitational settling velocity. The non-settling deposition velocity is usually calculated in terms of a resistance model. However, for this study it was set to 0.01 m/ s to match the assumption in MACCS2; the settling velocity was set to 0.

3.3.2.2 Wet Deposition

To minimize differences in the models by parameterizations other than transport and dispersion, wet deposition was calculated using a scavenging rate with the same coefficients as MACCS2. The rate of depletion of mass, m, from a LODI particle occurs at a rate

$$\frac{dm}{dt} = m(t)e^{-\Lambda t}$$

where t is time and Λ is the scavenging coefficient which is given by

$$\Lambda = ap^{b}$$

where *p* is the rain rate in mm/ hr and the coefficients a and b are set to $7 \cdot 10^{-5}$ s^{-1} and 0.75, respectively, the same values used by MACCS2 in this study.

4. METEOROLOGICAL DATA

The usefulness of the comparison of MACCS2 or RASCAL/ RATCHET with ADAPT/ LODI is only as good as the ADAPT/ LODI meteorology for the chosen site; therefore, the preparation of the meteorology files will be discussed in detail. The location of this study is the DOE ARM Southern Great Plains site in Oklahoma and Kansas. This site provides an extensive regional data set, with data from the ARM Program as well as the Oklahoma Mesonet and National Oceanic and Atmospheric Administration (NOAA) Profiler Network (NPN), covering a period of over 10 years. We selected the year 2000 for this project because we knew from previous experience that this year had a complete data set with no extended periods of missing data.

4.1 ARM Site

The ARM Program is a multi-laboratory, interagency program created in 1989 with funding from the U.S. Department of Energy as part of its effort to resolve scientific uncertainties about global climate change with a specific focus on improving the performance of general circulation models used for climate research and prediction. The ARM Program established and operates field research sites in several climatically significant locations where scientists collect and analyze data obtained over extended periods of time from large arrays of instruments to study the effects and interactions of sunlight, radiant energy, and clouds on temperatures, weather, and climate.

The U.S. Southern Great Plains (SGP) site was the first field measurement site established by the ARM Program. It was chosen for several reasons including its relatively homogenous geography and easy accessibility, wide variability of climate cloud type and surface flux properties, and large seasonal variation in temperature and specific humidity. The SGP site consists of *in situ* and remote-sensing instrument clusters arrayed across approximately 143,000 square kilometers (55,000 square miles) in north-central Oklahoma and south-central Kansas. The heart of the SGP site is the heavily instrumented Central Facility located on 0.647 km^2 (160 acres) of cattle pasture and wheat fields southeast of Lamont, Oklahoma. The instruments at the Central Facility and throughout the site automatically collect data on surface and atmospheric properties, routinely providing data to the ARM Archive and Data Center. The Data Center acquires additional data from other sources, such as National Weather Service satellites and surface data.

With our focus on atmospheric transport and dispersion, we selected data from the ARM archive that provide vertical profiles of wind and temperature, and surface wind, temperature, precipitation, and stability. The selected data were then tailored to meet the specific needs of each model. MACCS2 required only hourly surface wind, stability, and precipitation data at the Central Facility. RASCAL/ RATCHET used hourly surface wind, stability, precipitation, and temperature data from the Central Facility and the five other ARM surface sites closest to the Central Facility. ADAPT/ LODI used all the hourly surface wind, temperature and precipitation data and all the vertical profiles of wind and temperature described later to construct three-dimensional flow fields and turbulent diffusion coefficients.

4.2 Surface Data

4.2.1 ARM SMOS Sites

The Surface Meteorological Observation System (SMOS) mostly uses conventional *in situ* sensors to obtain 1-minute and 30-minute averages of surface wind speed, wind direction, air temperature, relative humidity, barometric pressure, and precipitation at the central facility and many of the extended facilities. Detailed information on these observations is available on the ARM Web site (http:/ / www.arm.gov). The locations of these sites are shown by the ×'s in Figure 1. The winds are measured at 10 m and the rest of the parameters at 2 m. From the archived ARM Network Common Data Format (netCDF) data files we extracted the 30-minute data and produced hourly average values for wind speed and direction, temperature, pressure, vapor pressure, precipitation, and standard deviation of the wind direction at each of the 15 ARM sites. This data set provided all the data needed by MACCS2 and RASCAL/ RATCHET.

4.2.2 Oklahoma Mesonet

The Oklahoma Mesonet is network of environmental monitoring stations designed and implemented by scientists at the University of Oklahoma and at Oklahoma State University. In 2000 it consisted of 114 automated stations covering the state of Oklahoma. At each site, the environment is measured by a set of instruments located on or near a 10 m tower. Detailed information on these observations is available on the Oklahoma Mesonet web site (http:/ / www.mesonet.org). The ARM data archive netCDF files contain five-minute averages of the observations for all these sites. We extracted the wind speed and direction, temperature, pressure, precipitation, solar radiation, and standard deviation of the wind direction at each of the 83 Oklahoma Mesonet sites within the SGP boundaries as shown by the +'s in Figure 1. From the five-minute average data we produced hourly average observations, and these data plus the 15 ARM SMOS sites provided the surface data input for ADAPT.

4.3 Upper Air Data

At the ARM SGP site there are several different measurement platforms that provide profiles of above-surface winds. These data sets include measurements from balloon sondes at five sites, 915 MHz radar wind profiler (RWP) and Radio Acoustic Sounding

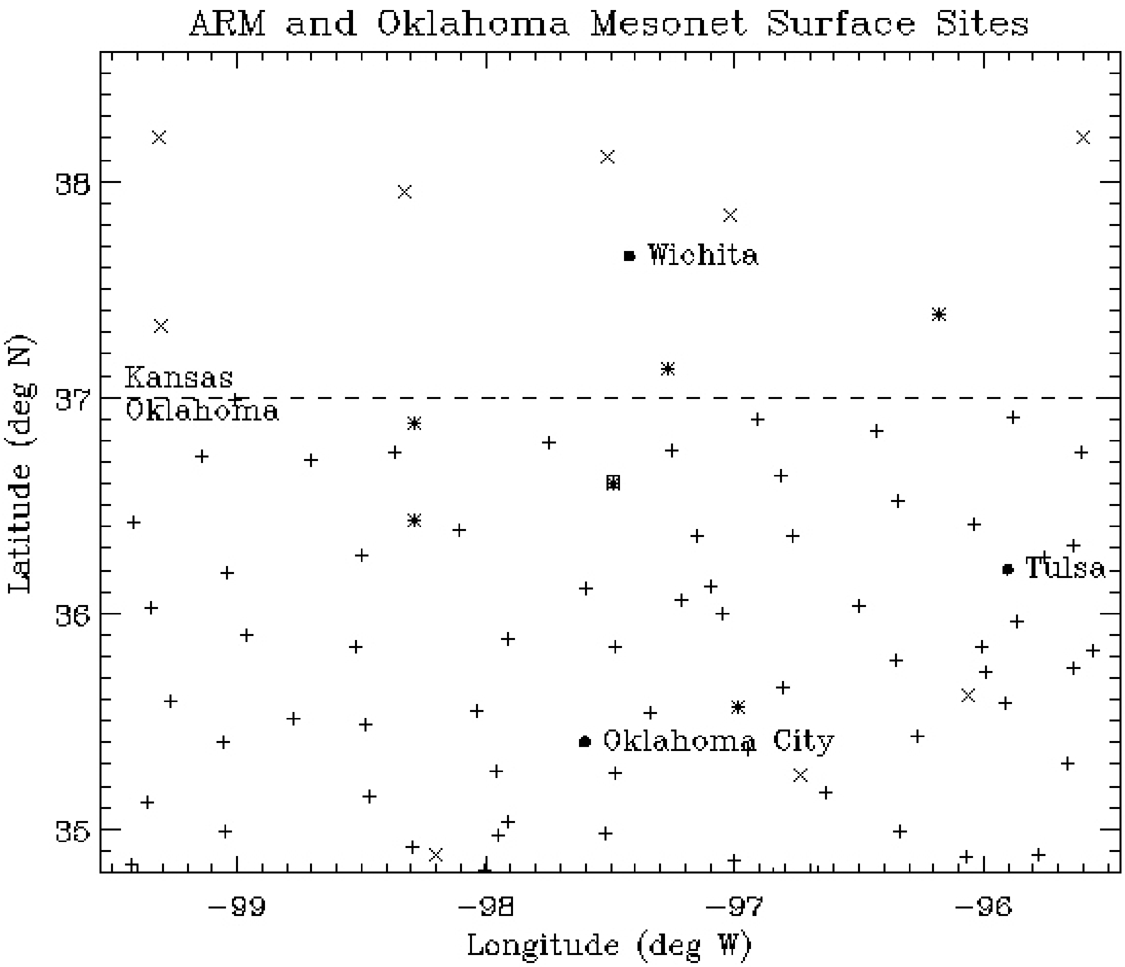


Figure 1. Location of Surface Meteorological Sites. + indicates Oklahoma Mesonet sites, ⊠ the Central Facility, ∗ the ARM SMOS sites used by RASCAL/ RATCHET, and × the other ARM SMOS sites.

System (RASS) at four sites, and the NOAA Profiler Network (a 404 MHz RWP/ RASS system) at seven sites in the ARM Southern Great Plains area. In addition, Atmospheric Emitted Radiance Interferometer (AERI) vertical temperature profiles at the same five sites as the sondes were used to help determine boundary layer heights. The locations of these sites are given in Figure 2. Detailed information on these observations is available on the ARM web site (http:/ / www.arm.gov).

4.3.1 Sondes

Balloon sondes are launched throughout the year at the Central Facility and during Intensive Operational Periods (IOP) at the other four sites. The routine sondes at the Central Facility are launched every 6 hours Monday through Friday. During IOP's

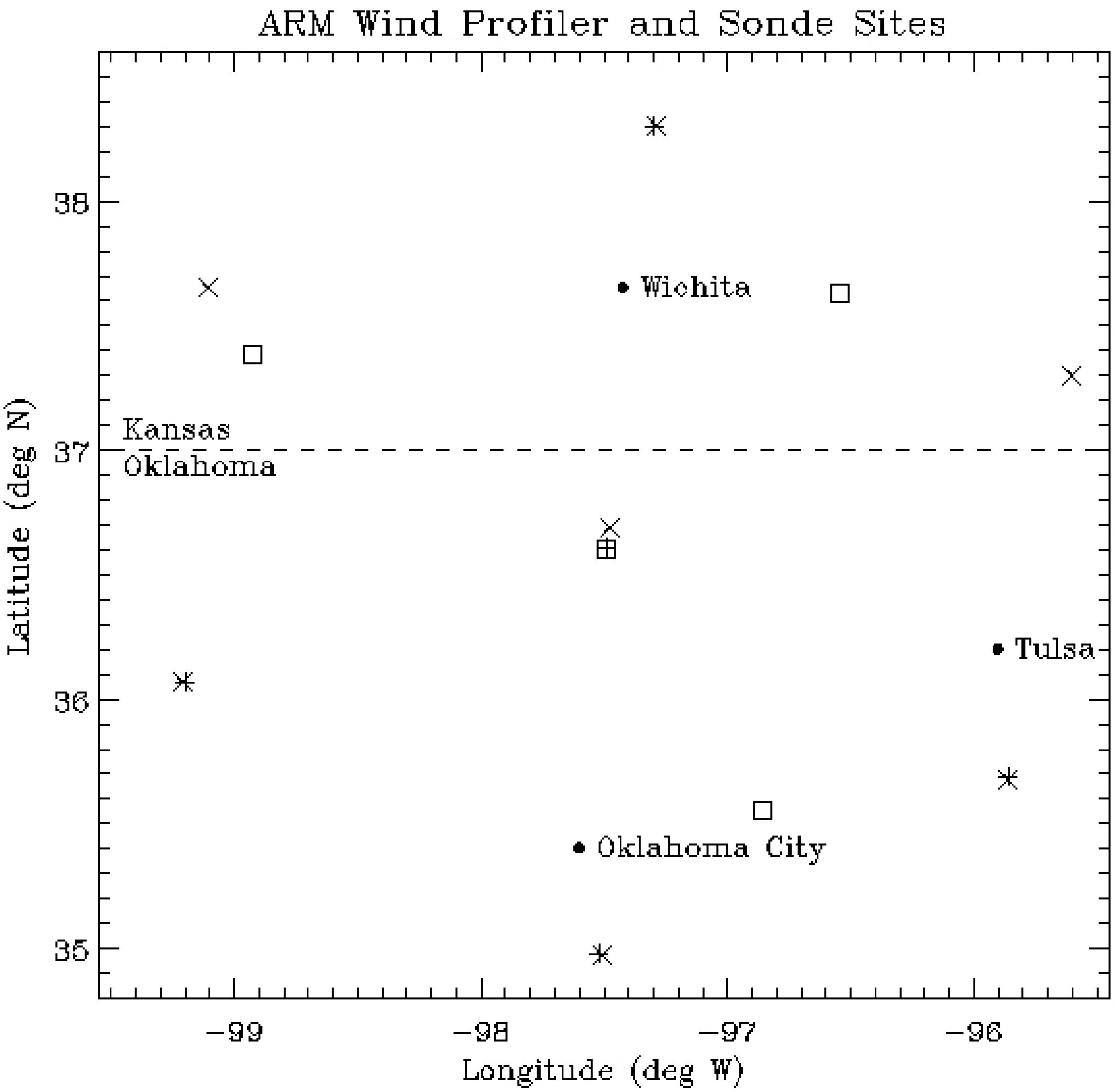


Figure 2. Location of ARM Upper Air Observations. + indicates sonde and AERI sites, × indicates NOAA Profiler sites, and □ 915 MHz RWP/ RASS sites. Note that some sites have multiple measurements, and the Central Facility has all three types.

sondes are launched every 3 hours at all 5 sites, the Central Facility and 4 boundary sites. In 2000 there were three IOP's that provided additional sonde data, March 1 to March 22, September 25 to October 8, and November 27 to December 22. The total number of sondes at each site is given in Table 5. The sonde netCDF files in the ARM archive provide latitude, longitude, altitude, pressure, temperature, and dew point temperature every two seconds during ascent and wind speed and direction every ten seconds. The ascent rate is typically about 5 m/ s, so the vertical resolution of the wind data is about 50 m. On November 24 a change in procedure started returning wind data every two seconds with the resolution changing to about 10 m.

Table 5. Number of Sondes at Each Site

Site	ID	Number
Central Facility	SDC1	1333
Hillsboro, KS	SDB1	439
Vici, OK	SDB4	443
Morris, OK	SDB5	458
Purcell, OK	SDB6	460

4.3.2 Radar Wind Profiler/Radio Acoustic Sounding System

The 915 MHz radar wind profiler (RWP)/ radio acoustic sounding system (RASS) operates by transmitting electromagnetic energy into the atmosphere and measuring the strength and frequency of back-scattered energy. It transmits in two different vertical planes and receives back-scattered energy from refractive index fluctuations that are moving with the mean wind. From the ARM netCDF files we extracted hourly vertical profiles of horizontal wind, and virtual temperature. There are two vertical resolutions in the data (dependent on power level); for lower heights the first level is typically 87 m above ground with a vertical spacing of about 60 m up to 2-2.5 km. For higher levels the lowest level is about 225 m with a spacing of 225 m up to 6 km.

4.3.3 NOAA Profiler Network

The NOAA Profiler Network (NPN) consists of 35 unmanned Doppler Radar sites located in 18 central states and Alaska; they provide hourly vertical wind profile data. Eleven of these sites also are equipped with RASS Systems that provide virtual temperature profiles. Seven of the NPN sites are located in the ARM SGP region, and six of these are equipped with RASS systems. Wind NPN profilers are designed to operate reliably and unattended in nearly all weather conditions. To reach the tropopause, they use a relatively long wavelength. The radars detect fluctuations in atmospheric density caused by turbulent mixing of volumes of air with slightly different temperature and moisture content. The resulting fluctuations of the index of refraction are used as a tracer of the mean wind in clear air. From the ARM data archive netCDF files we extracted vertical profiles of horizontal wind and virtual temperature for the seven sites. Because of the large wavelength used by the NPN radars, vertical resolution of these profiles is rather course; the lowest level is at 500 m with a spacing above that level of 250 m. Nevertheless, NPN data were consistently available and are a major component of the input data set used by ADAPT.

4.3.4 Atmospheric Emitted Radiance Interferometer

The atmospheric emitted radiance interferometer (AERI) measures the absolute infrared spectral radiance (watts per square meter per steradian per wavenumber) of the sky directly above the instrument. A calibrated sky radiance spectrum is produced every ten minutes. Among other things the AERI data can be used for calculating vertical atmospheric profiles of temperature and water vapor. In this study we used the vertical temperature profiles to calculate boundary layer heights. The AERI instruments are located at the same sites where sondes are launched, and these data were particularly useful because they provided high resolution temperature profiles when no sonde data were available.

5. METEOROLOGICAL DATA PROCESSING

5.1 Pasquill-Gifford (P-G) Stability Category

Both MACCS2 and RASCAL/ RATCHET require the Pasquill-Gifford (P-G) stability category in their input files, but the ARM data archive does not include this parameter. The ARM data archive does include the standard deviation of surface wind direction, σ_θ, for both the ARM and Oklahoma Mesonet surface sites. This parameter was converted into P-G stability category using the σ_θ method given in NRC's Regulatory Guide 1.23, "Onsite Meteorological Programs," and in chapter 6.4.4 of EPA (2000), available on the web at http:/ / www.webmet.com/ met_monitoring/ 644.html. Briefly, an initial P-G stability category is set based on σ_θ ($\sigma_\theta \geq 22.5$, A; $17.5 \leq \sigma_\theta < 22.5$, B; $12.5 \leq \sigma_\theta < 17.5$, C; $7.5 \leq \sigma_\theta < 12.5$, D; $3.8 \leq \sigma_\theta < 7.5$, E; $\sigma_\theta < 3.8$, F). This initial estimate is then modified based on wind speed (higher speeds giving P-G stability closer to neutral, category D) and daytime/ nighttime with the P-G category in the unstable to neutral range (A-D) during the day and the neutral to stable range (D-F) at night.

5.2 Mixing Height

Mixing height is another derived atmospheric parameter that is not directly archived in the ARM data set. MACCS2 selects its mixing height from an input list of eight mixing heights depending on season and time of day. The eight mixing heights are the average morning and afternoon mixing height for each season. In the current implementation, the larger of these two values (the afternoon height) is used by the code. RASCAL/ RATCHET calculates mixing height as a function of wind speed, stability, surface roughness, and latitude (Zilitinkevich 1972) for each meteorological station and for each hour. ADAPT requires mixing height for each hourly meteorological data set.

Della Monche (2002) examined several techniques for determining mixing height using available ARM data. The technique that performed best under the widest possible conditions was a technique by Heffter (1980) based on potential temperature profiles. The technique works in every stability regime, and in almost every case gave estimates of the mixing height that were at or above the mixing height as observed from an aircraft. Based on these results we adopted the Della Monche/ Heffter method to estimate mixing heights.

The Heffter method calculates potential temperature from the vertical profile of temperature and pressure available from the sonde and AERI data. Each profile is examined for the existence of a "critical inversion" which is assumed to mark the top of the mixed layer. A critical inversion is defined as the lowest inversion that meets the following two criteria:

$$\Delta\theta / \Delta z > 0.001 \text{ K/ m}$$

and

$$\theta_t - \theta_b > 2 \text{ K}$$

where $\Delta\theta / \Delta z$ is the potential temperature lapse rate and θ_t and θ_b are the potential temperature at the top and bottom of the critical inversion layer respectively; these criteria give the mixing height as that point in the inversion where the temperature is 2 K greater than the temperature at the inversion base. Lower and upper limits were placed on mixing height at 40 m and 3000 m respectively. In cases where the procedure failed to find a mixing height, the mixing height was set to the cloud base height if there was a cloud base, otherwise the mixing height was left undetermined and that site was not used. A single mixing height for each hour was computed as the average of the calculated valid individual mixing heights. These hourly average mixing heights were used in the ADAPT input files and were also seasonally averaged to provide daytime and nighttime seasonal mixing heights for MACCS2. The mixing height in ADAPT was assumed constant over the entire spatial domain. The cumulative number of hours with mixing heights less than a given height is shown in Figure 3.

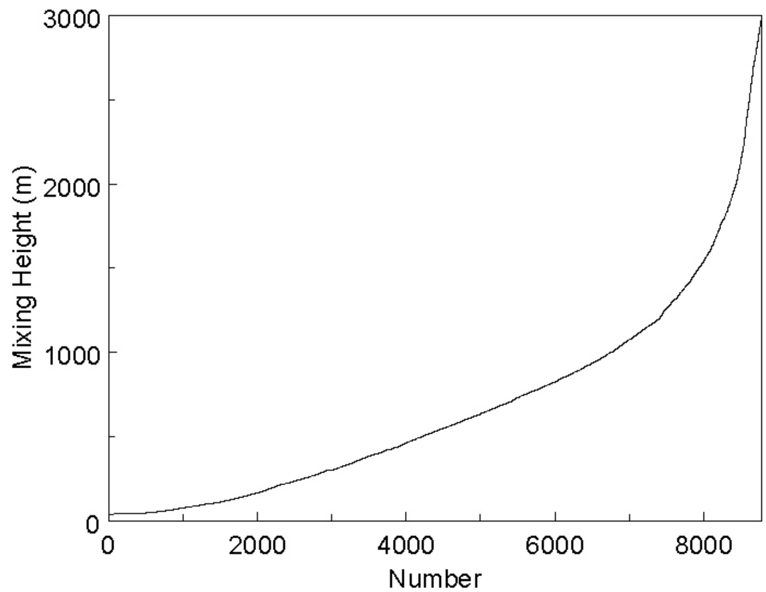


Figure 3. Cumulative Number of Hours with Mixing Heights less than a Given Height.

5.3 Low-Level Nocturnal Jet

The ARM SGP site lies almost in the center of the U. S. region with most frequent low-level nocturnal jets (Bonner 1968), and these could be an important transport mechanism for released material. Since only ADAPT/ LODI uses upper level wind data, these jets could lead to transport differences among the models. An example of a low level nocturnal jet is given in Figure 4 which is a plot of the lowest 1500 m of the RWP wind profile at the ARM Central Facility on the night of June 7, 2000. Note the increase

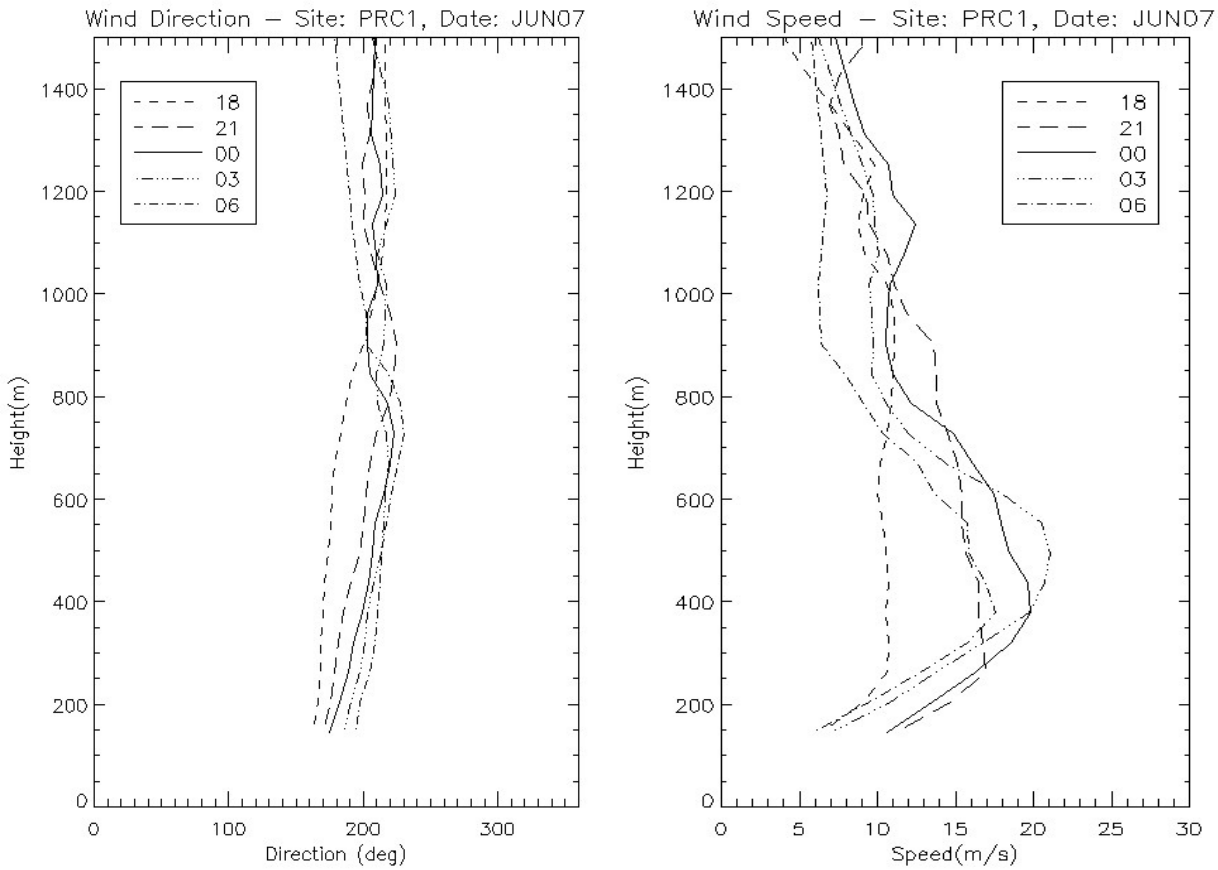


Figure 4. Example of a Nocturnal Jet. The left plot shows the vertical profile of wind direction and the right wind speed from the RWP at the ARM Central Facility on the night of June 7, 2000. Individual profiles at 1800, 2100, 0000, 0300, and 0600 local standard time show the increase in wind speed in the layer between 200 and 800 m.

in wind speed from a maximum of about 10 m/s at 1800 local standard time to over 20 m/s between midnight and 0300 in the layer from 200 to 800 m.

5.4 MACCS2 Input Meteorology File

The MACCS2 meteorology input file requires 8760 (365 days × 24 hours) hourly observations of wind speed and direction, stability category (A-F), and precipitation at the release site, plus eight (four seasons × day/night) mixing heights. The hourly observations were extracted from the ARM SMOS data at the Central Facility. Wind direction in degrees was converted to the sector the wind is blowing toward, and stability category was determined from the standard deviation of the horizontal wind direction as described above. The distribution of hours in each stability category is given in Table 6. When the Central Facility had missing data (67 of 13560 half hours), observations from the closest neighboring ARM SMOS station (E9 - Ashton, Kansas or E6 - Towanda, Kansas) were used. The eight mixing heights were determined as described above and are given in Table 7. Note, however, that MACCS2 rounds the data to the nearest 100 m.

Table 6. Number of Hours in Each Stability Category for MACCS2 Site

Category	Count
A	259
B	290
C	549
D	6122
E	1358
F	182

The ARM archive stores data using Coordinated Universal Time (UTC), what used to be referred to as Greenwich Meridian Time (GMT). Local Standard Time (LST) at the SGP site is UTC - 6 hours. So the first data in the ARM archive files for the year 2000 are for 1800 LST on December 31, 1999. However, since 2000 is a leap year, the last six hours of the 8760 come from December 31, 2000 data. The remaining 18 hours of December 31, 2000 data allow us to follow the transport and dispersion of releases that occur in the last few hours of the year in the ADAPT/ LODI calculation.

Table 7. Seasonal Average Mixing Heights (m)

Season \ Time	Morning	Afternoon
Winter	338.	788.
Spring	398.	1011.
Summer	276.	1311.
Autumn	366.	874.

5.5 RASCAL/RATCHET Input Meteorology Files

RASCAL/ RATCHET meteorology input uses observations from several surface stations in the vicinity of the release. In this study observations from the ARM SMOS sites at the Central Facility and the five other sites closest to the Central Facility (see Figure 1) were used. Hourly average wind speed, wind direction, temperature, and precipitation were extracted from the ARM data archive. Atmospheric stability was calculated from the standard deviation of the wind direction as described above. The distribution of stability categories for the six sites is given in Table 8, along with the total number of hours of meteorological data. The missing data periods are those times when neither of the two half hours that contribute to an hourly average was available. This data set also included data for the last 18 hours of December 31, 2000; data that was ignored for the MACCS2 data set.

Meteorological data for the Central Facility and the five other sites were combined into a single file for use by the RASCAL meteorological data processor. All available data for

Table 8. Number of Hours in Each Stability Category for RASCAL Sites

Station→ Stability↓	Central Facility	EF-7 Elk Falls	EF-9 Ashton	EF-11 Byron	EF-15 Ringwood	EF-20 Meeker
A	258	404	174	323	257	356
B	292	529	361	396	390	601
C	551	874	526	625	785	1023
D	6123	4145	5649	4855	5389	4399
E	1367	854	1365	1629	1060	1121
F	183	968	126	340	223	292
Total	8774	7774	8201	8168	8104	7792

each hour were used to generate the meteorological data fields used by RASCAL and RATCHET. No effort was made to replace missing values. If all values for a given parameter are missing, persistence is assumed, and the previous field is used.

5.6 ADAPT/LODI Input Files

ADAPT is designed to construct a three-dimensional wind field that agrees as closely as possible with all the available observations and is mass consistent. The choice of the ARM SGP site was driven primarily by our desire to have a meteorological data set that would define this wind field based completely on observations. ADAPT expects observations to be provided in two coordinated text files, an observ.met file that gives the height, wind speed, wind direction, temperature, dew point, and pressure observations for each station, and a stnloc.met file that gives the x, y, z_g, latitude and longitude of the station. The x and y position is given in the Universal Transverse Mercator (UTM) coordinates used by the meteorological grid, and z_g is the station altitude.

Table 9. Number of Hours vs Number of Valid Surface Observations.

Number of Observations	Number of Hours
89	3
90	0
91	0
92	1
93	2
94	12
95	27
96	217
97	552
98	1359
99	2659
100	3694
101	258

In this study the observ.met file included surface observations from the ARM SMOS and Oklahoma Mesonet sites and upper air observations from RWP and NPN profilers and sondes.

Since we have such a large set of meteorological observations, we put each hourly average set of observations in a separate input file. Most of the time nearly all the surface stations provide data; this is shown in Table 9. Note that there were 101 stations (15 ARM and 86 Oklahoma Mesonet) only through January 20 when one of the Oklahoma Mesonet stations was closed.

ADAPT requires at least one upper air sounding; it was the availability of a dense network of these profiles that led us to use the ARM SGP site for this study. Both the NPN and ARM 915 MHz RWP profiles are fairly reliable and provide valid data much of the time. The number of hours with valid profiles (out of 8784 hours) for each site is given in Table 10. The NPN profiles have fairly course vertical resolution, 250 m, and start well above the surface, 500 m. The RWP profiles have good vertical resolution and start near the surface, but they are prone to errors and many of them have limited vertical extent. The sonde profiles start near the ground and usually extend to great heights, but they are only available part of the time. Hourly ADAPT input meteorological data files include vertical profiles at each NPN and 915 MHz RWP site that had valid data and sonde data at each site where a sonde was launched within three hours of the ADAPT met time; i.e., the same sonde data could be included in up to six hourly ADAPT observ.met input files. The upper air part of these files could and occasionally did include profiles from all 16 sites (7 NPN, 4 RWP, and 5 sonde profiles); in the worst cases only two profiles were available. The number of hours (data sets) vs. the number of profiles is given in Table 11.

Table 10. Number of Hours vs. Number of Upper Air Profiles

Number of Profiles	Hours
2	7
3	23
4	25
5	4
6	0
7	19
8	217
9	670
10	1747
11	2529
12	2120
13	134
14	495
15	554
16	240

Table 11. Hours with Valid Data for Profiler and Sonde Sites

Site	ID	Hours with Valid Data
Hillsboro, KS	WX04	8274
Haviland, KS	WX06	8500
Neodoska, KS	WX07	6482
Lamont, OK	WX08	8264
Vici, OK	WX09	8266
Haskell, OK	WX10	8618
Purcell, OK	WX11	8156
Central Facility	PRC1	8434
Beaumont, KS	PRI1	8442
Medicine Lodge, KS	PRI2	8339
Meeker, OK	PRI3	6394
Central Facility, OK	SDC1	5847
Hillsboro, KS	SDB1	1387
Vici, OK	SDB4	1392
Morris, OK	SDB5	1435
Purcell, OK	SDB6	1437

6. DATA QUALITY ISSUES

Although the ARM SGP site has the largest amount and highest quality regional data available in the world, as we used the data we became aware of several data quality issues. These included ARM SMOS data archive files that were corrupted, NPN and RWP profiles that included very large wind speeds, and wind errors in sondes when the height levels were uneven.

6.1 SMOS Data

Each ARM SMOS netCDF file contains half-hour average data for one day at a particular site. The data for all variables for each half-hour are written sequentially. As we processed the data, occasionally we encountered a file that at some point in time contained incorrect values, almost as if a bit had been dropped or added. Rereading the file from the archive did not remedy the error. So, for the corrupt files, we extracted the good data and left the data for the rest of the day as missing. This problem occurred for about 75 of 5500 files. In some cases most of the data for a day was lost, in others only the last half hour. Even in the archive, not all files contain all 48 half-hours, and in some cases the data for a single day are split between two files. The processing algorithm was written to handle these anomalies.

6.2 NPN and 915 MHz RWP Data

The first time we ran the simulation, ADAPT gave frequent warning messages that observed wind speeds were greater than 150 m/ s, an unrealistically high value, especially since the greatest altitude included in the simulation is 6000 m. As we investigated theses winds, we discovered many additional instances of incorrect winds, with some of the bad values occurring near the surface. Since low levels winds are crucial for calculating the transport and dispersion of low altitude pollutant releases, we were compelled to scan the observed profiles for errors and attempt to correct them or remove the bad points.

The number of profiles in the data set is quite large, over 90,000. Since we are concerned mostly with wind, we wrote a code that displays wind speed and direction in adjacent panels and allows us to either accept the profile or make changes by specifying a new value for a layer, interpolating between layers, extrapolating from above or below, or interpolating between a specified lower and upper layer. We also had the option of completely deleting a profile, and we automatically deleted all profiles with fewer than four layers. The procedure used actually wrote a modification file for the observ.met file. Then, in another pass through the data, a new observ.met file with the modifications was produced for the simulation. It took about 10 weeks to look at all

90,000+ profiles and modify the incorrect ones. Samples of the more frequent errors and corresponding corrections are given in Figures 5-8.

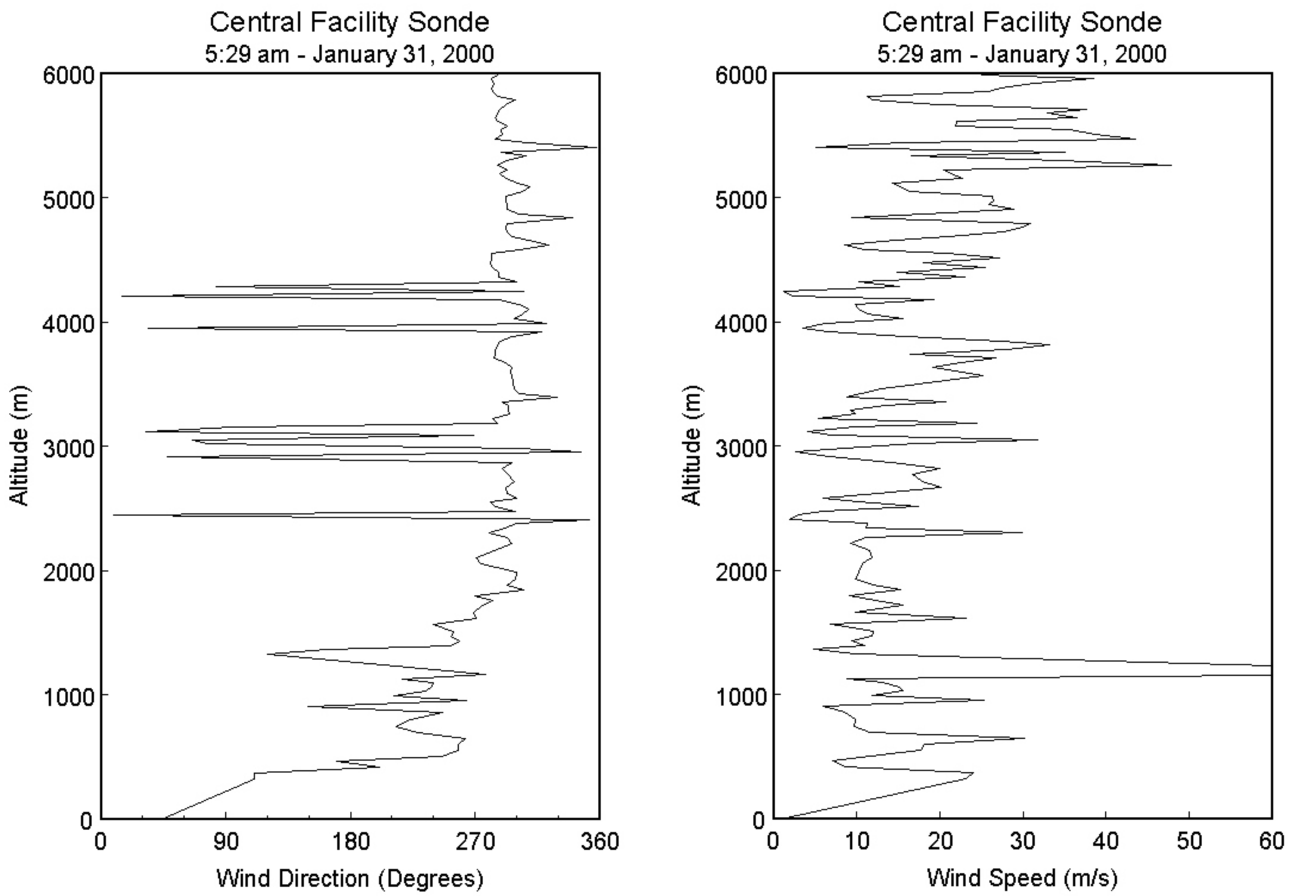
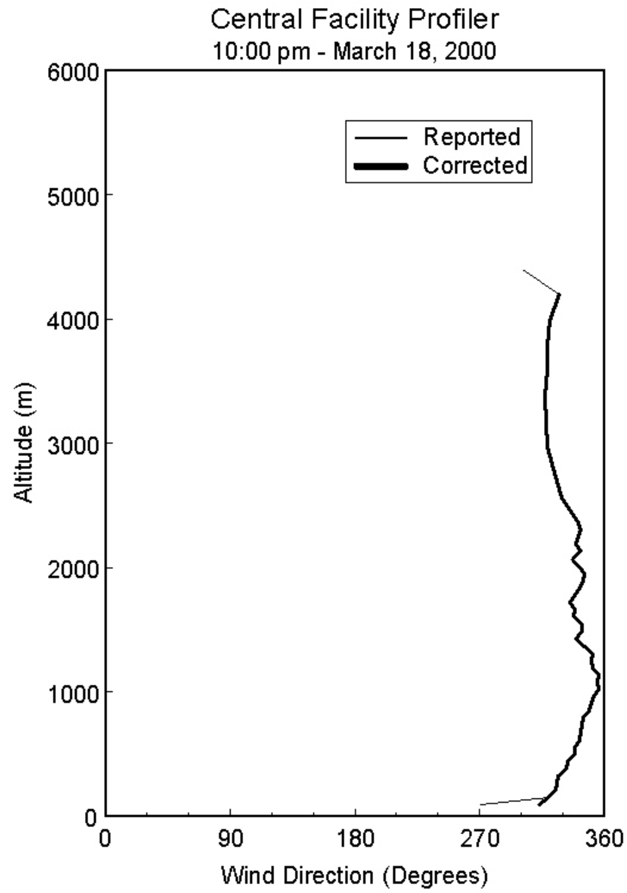


Figure 5. Central Facility Sonde Launched at 5:29 am CST on January 31, 2000. This is an example of a sonde that had to be deleted from the data set because it has so many errors.



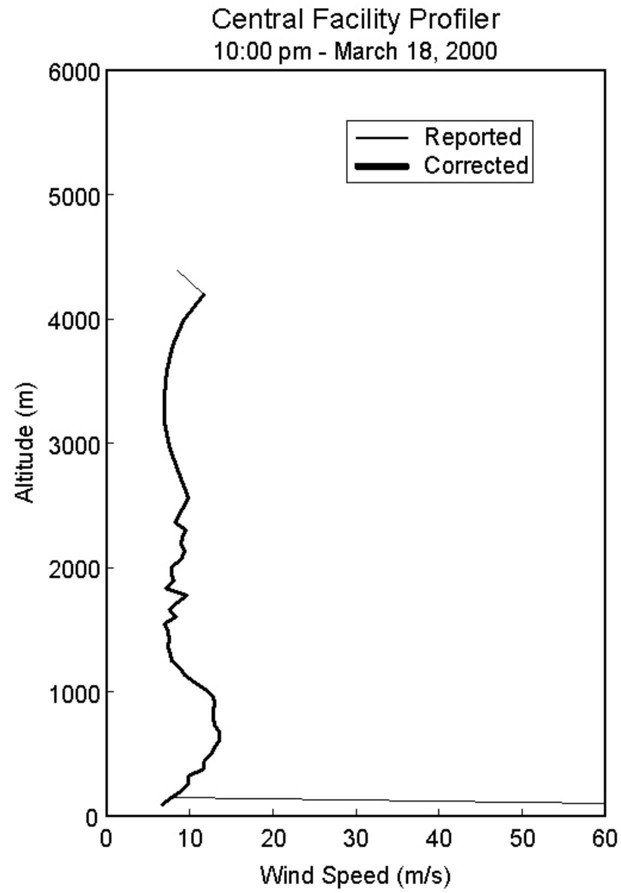


Figure 6. 915 MHz RWP Wind Profile for the Central Facility at 10:00 pm CST on March 18, 2000. This is an example case where the reported lowest level wind (77.5 m/ s) is wrong. The corrected profile is determined by extrapolating downward from the 2 levels above. Where the two profiles overlap only the heavy line shows.

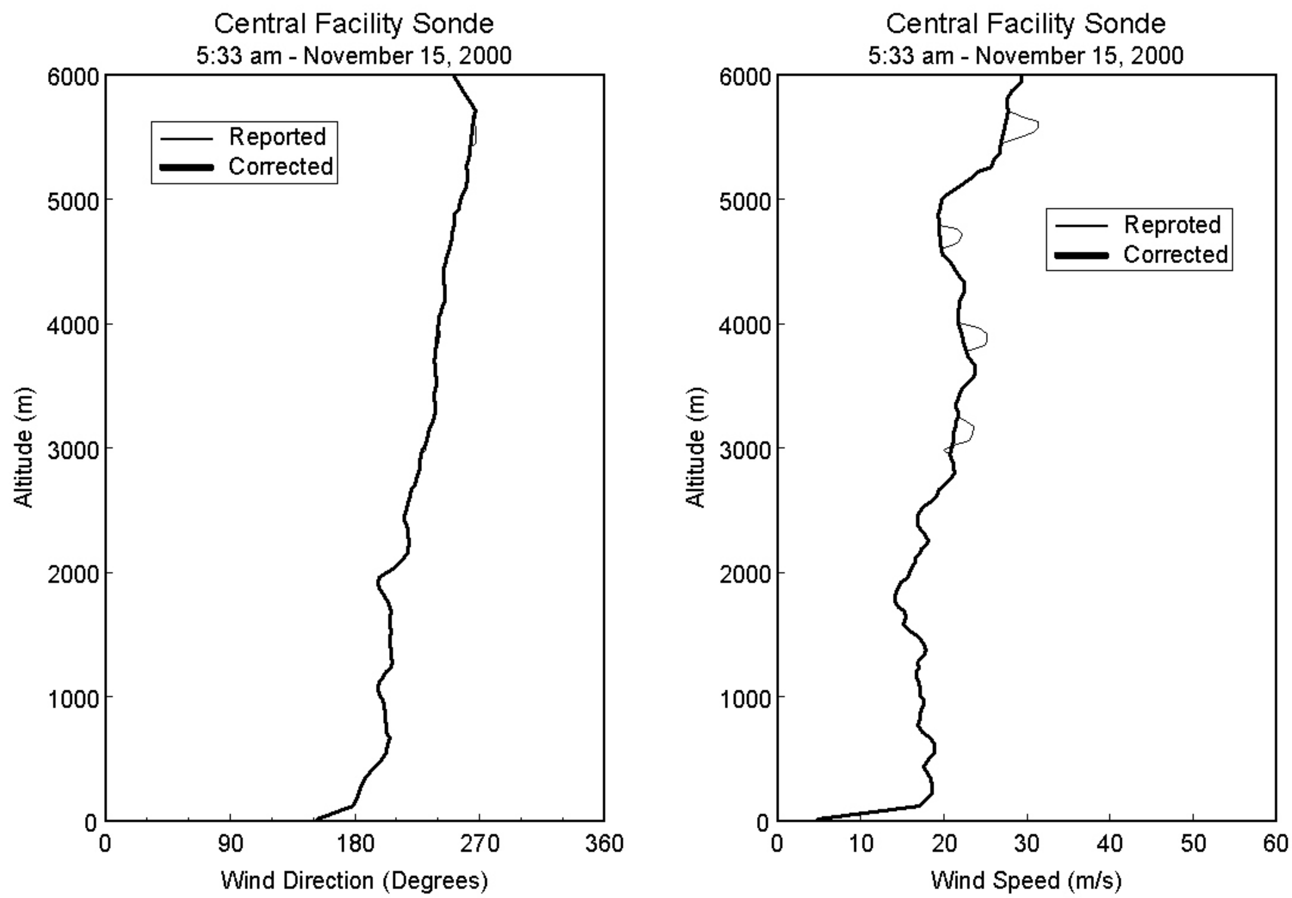


Figure 7. Central Facility Sonde Launched at 5:33 am CST on November 15, 2000. Quite a few of the sondes exhibited speed anomalies in an otherwise fairly smooth profile. They were often associated with a missing layer in the data. They were corrected by interpolating between the bottom and top of the anomaly. Note that direction was hardly affected.

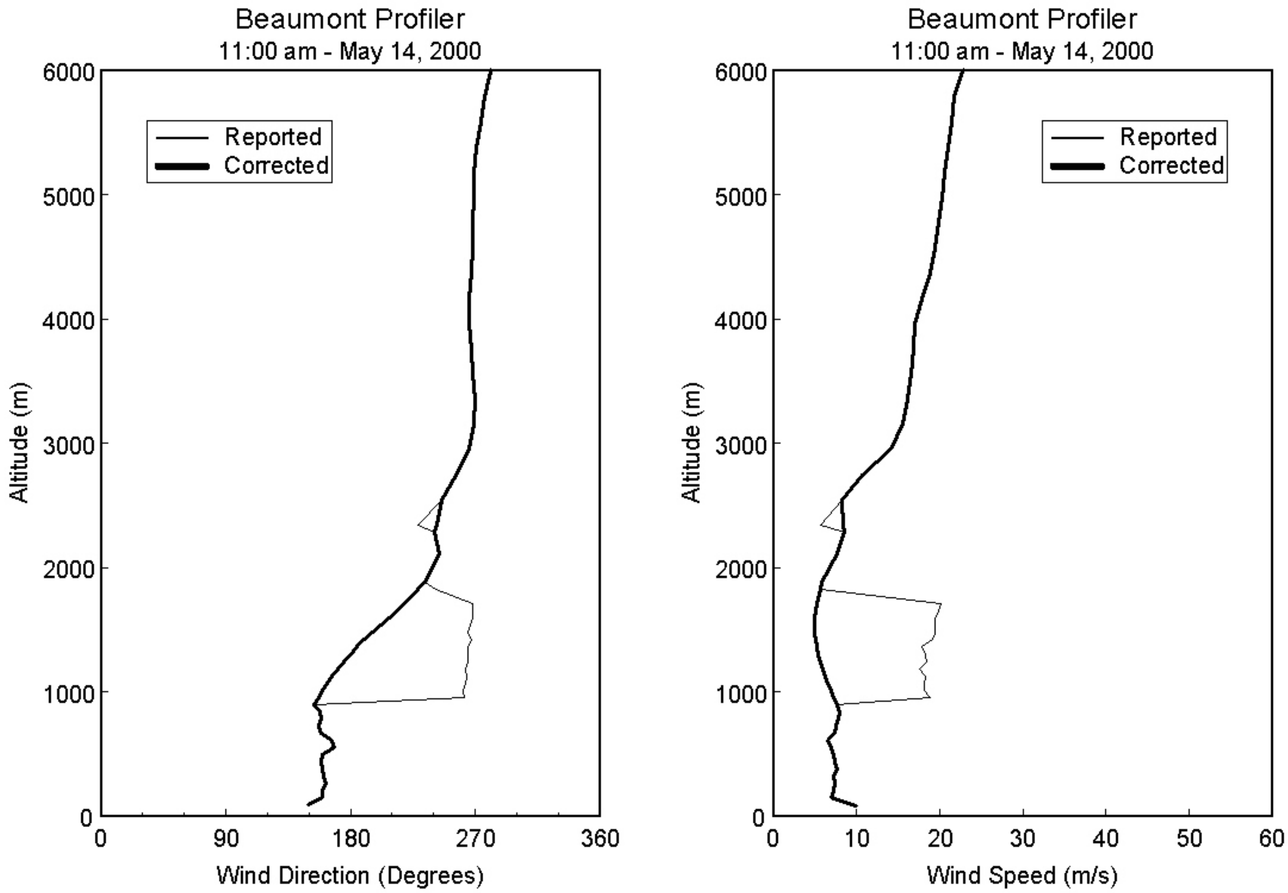


Figure 8. 915 MHz RWP Wind Profile for Beaumont at 11:00 am CST on May 14, 2000. This sounding exhibits an error seen occasionally with the 915 MHz RWP, having one or more layers where wind speed and direction are offset from the rest of the sounding. The correction resets values in the offset layer by interpolation. The second anomaly at 2400 m is seen frequently at this height where the high and low resolution radar modes merge.

7. SOURCE TERM

Each code requires that the user input a source term, that is, parameters giving the time and duration of the release, the height of the release, buoyancy of the released material, and release magnitudes of different radionuclides. This last input is described in all the codes as an inventory of each radionuclide at the start of the problem and a release fraction of several radionuclide chemical element groups. This formulation, which allows each code to account for radioactive decay of the various radionuclides from the start of the problem to the release of the material, is not needed for this study. Our source term was formulated to be as simple as possible while still allowing the ATD processes to be compared: we chose a single, long-lived radionuclide that does not deposit and a single, long-lived radionuclide that does deposit. Further, the inventory of each of these two radionuclides was arbitrarily chosen as 10^{16} Bq. This does not represent a realistic release from any NRC-licensed facility.

We chose only two radionuclides instead of tens of different radionuclides (as could be in a release from a severe accident at a nuclear power plant) because we wanted to avoid confounding the depositions and exposures with short-, medium-, and long-lived material, in case the comparison were to show unfavorable results. We believed that "trouble-shooting" the differences would be easier with only two radionuclides. As will be seen in the results section, this simplification was unnecessary.

The characteristics of the source term for this study are given in Table 12. The values of σ_y and σ_z, the initial size of the plume, are not usually considered part of the "source term," but since they influence the initial plume they are included here.

Table 12. Source Term Specification

Characteristic	Value
Location	ARM Central Facility
Time of release	0.0 s
Duration of release	1800 s, uniform
Amount of release, each nuclide	10^{16} Bq
Height of release	50 m
Buoyant energy	10^6 W

8. SIMULATION PROCEDURE

This study is aimed at evaluating the use of a simple atmospheric transport and dispersion model in predicting off-site consequences of large accidental releases from nuclear power plants and other NRC-licensed facilities. The primary metric chosen for comparison was the annual average integrated concentration in four arcs and sixteen compass directions around the assumed release point, the DOE ARM SGP Central Facility near Lamont, Oklahoma. The arcs were at distances of 14.5-16.1, 30.6-32.2, 78.8-80.5, and 159.3-160.9 km (9-10, 19-20, 49-50, and 99-100 miles); the compass directions were the sixteen 22.5 degree sectors from N clockwise around to NNW. Each model used a procedure to generate predicted annual average exposures (near surface air concentrations integrated during passage of the plume in Bq-s/ m^3) and depositions (total material deposited on the ground in Bq/ m^2) for these 64 areas using normal techniques.

8.1 MACCS2

MACCS2 was run in a single step that involved two of the three major modules in the code. The first module in the sequence is ATMOS, which calculates atmospheric transport and dispersion (ATD). ATMOS first bins all of the hours of the annual weather data into 36 bins, as discussed in section 3. It then selects weather trials randomly from these bins. In this case the number of weather trials was limited to 610 to keep the CPU requirements for ADAPT/ LODI from being excessive. However, 610 weather trials are more than enough to attain valid statistics, especially for the mean values that are presented in this study. After selecting the weather trials, ATMOS calculates the atmospheric transport and dispersion for each trial in the set. The EARLY module, which calculates emergency response and acute health effects, would not have been needed except that it also contains the logic to perform wind rotations and the output capability that was required for comparison with the other codes.

8.2 RASCAL/RATCHET

Meteorological data processing involved three steps. In the first step the full year of meteorological data for the six sites was combined into a single file with data in the format required by the RASCAL meteorological data processor; in the second step the meteorological data file was divided into twelve monthly files. Each monthly file contained data for the month plus data for the first two days of the following month. These two steps required only a few seconds of computer time. The third step was running the RASCAL meteorological processor. The processor created sets of meteorological data fields for three model domains – 32.2 km (20 miles) on a side, 80.5 km (50 miles) on a side, 160.9 km (100 miles) on a side – for each month.

8.3 ADAPT/LODI

The ADAPT/ LODI model system is designed to produce rapid and accurate estimates of downwind concentrations from accidental releases of hazardous and toxic pollutants. The general approach used in this study was to treat each postulated release as a separate event, and, after running all cases, calculate the average exposure and deposition from the individual cases weighted by their individual frequencies. The individual cases were 610 releases at times and with weights (frequencies) identified by MACCS2 as representative of the entire year's meteorology. Since the procedure was highly repetitive, the computer processing was accomplished using a series of scripts.

8.3.1 Grids

Both ADAPT and LODI perform their calculations using grids that define a frame of reference in the vicinity of the release site. Two grids were used in this study, a three-dimensional meteorology grid and a two-dimensional concentration (exposure and deposition) grid.

Table 13. Meteorology Grid Vertical Levels and Corresponding Central Facility Altitudes (MSL).

Layer	Sigma	Altitude (m)
1	0.	312
2	0.003730	332
3	0.007927	355
4	0.012651	380
5	0.017967	409
6	0.023950	442
7	0.030683	479
8	0.038261	520
9	0.046789	566
10	0.056387	619
11	0.067189	678
12	0.079345	744
13	0.093026	818
14	0.108423	902
15	0.125751	997
16	0.145252	1103
17	0.167199	1222
18	0.191898	1357
19	0.219696	1508
20	0.250979	1679
21	0.286187	1871
22	0.325810	2087
23	0.370402	2329
24	0.420587	2603
25	0.477067	2911
26	0.540629	3257
27	0.612165	3647
28	0.692672	4085
29	0.783276	4579
30	0.885244	5134
31	1.000000	5760

The meteorology grid specifies the locations where gridded meteorology is defined by ADAPT and provides a frame of reference for transport and dispersion of LODI parcels. It has a uniform 4 km spacing in the horizontal covering a square area 400 km on a side centered at the ARM SGP Central Facility. In the vertical it uses a non-uniform terrain- following sigma coordinate (A sigma coordinate gives height as a fractional distance between the surface and the top of the domain, 5760 m in this case.) with greater resolution near the ground, and courser resolution aloft. The bottom of the grid follows the topography while the top is at a constant elevation of 5760 m above mean sea level (MSL). The list of sigma levels is

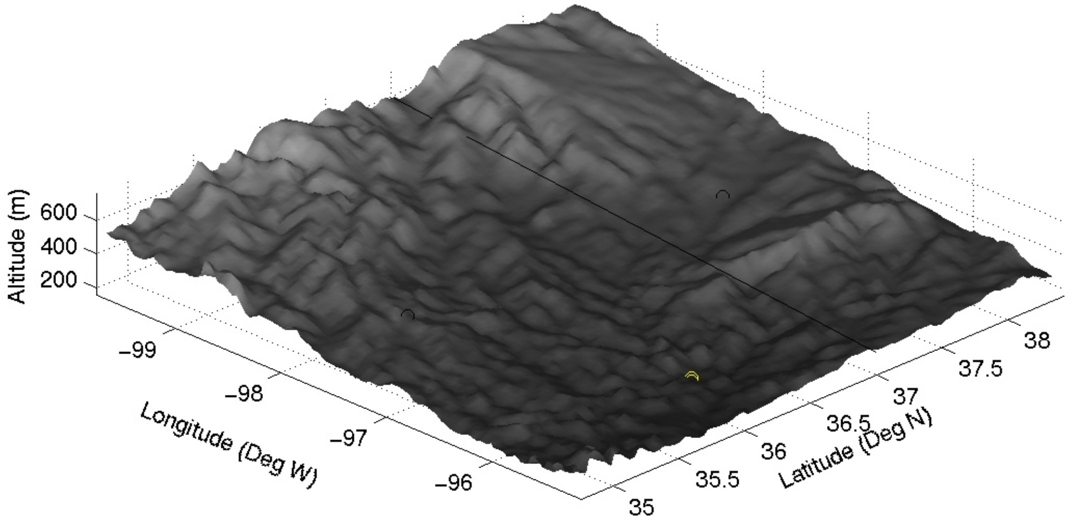


Figure 9. Topography of the ARM SGP Site. The view is from the southeast looking northwest. The black line at 37° N indicates the Oklahoma/ Kansas border. Black half circles indicate the locations of Oklahoma City and Wichita, and a light one Tulsa. The range of elevations is from 153 to 760 m above sea level.

given in Table 13, and the topography of the region is illustrated in Figure 9. Because of the vertical stretching in the plot, the topography appears more rugged that it is; the total change in elevation across the domain is about 600 m over a distance of 400 km, for a mean slope 1.5 m/ km. The general slope is from the northwest to the southeast, but there are several river valleys and other irregularities in the terrain.

A concentration grid is used by LODI to calculate and accumulate the exposure and deposition during a run. For this study it has a uniform spacing of one km and covers a square region 350 km on a side centered on the ARM SGP Central Facility. The final result of a LODI simulation is the exposure and deposition of emitted materials at the 350 by 350 points of the concentration grid.

8.3.2 Solution Steps

The script that runs the cases allows one to process all 610 cases in sequence or start with any given case and run a specified number. It also assumes that the ADAPT meteorology input files based on the ARM SGP data are already prepared. The steps are the following:

1. Read the case start times (Julian day and hour) from the weather data file provided by MACCS2. The case number is used as an index for saved results.

2. Loop over the requested cases (Steps 3-6).

3. Set the current month and day. ADAPT and LODI use dates/ times in the format yyyyMMMdd_hhmmss where yyyy is the year, MMM is the three-character month, dd is the day, hh is the hour and the minutes and seconds (mm and ss) are both 00 for this problem because we use only hourly meteorological data and hourly release times.

4. Delete ADAPT output/ LODI input meteorology files from hours prior to this release. These three-dimensional data files are quite large (23 Mb each), and since we process dates sequentially, those files for times prior to the release time are no longer needed. We keep those files that were created for the previous run and are still needed for this run. Of course, the first case has no unneeded files to delete.

5. Create ADAPT output/ LODI input meteorology files for the next 48 hours. To be sure we have accurate concentrations, all the LODI parcels need to exit the 400-km square domain by the end of the run. In some cases 24 hours was too short, so we used 48 hours. Since LODI's runtime depends directly on the number of remaining parcels, there is no time penalty for running too long. This step runs ADAPT repeatedly. The meteorology files are pre-prepared, and the ADAPT namelist file is created by the script. The key mixing height parameter is read from the hourly mixing height file prepared while processing the ARM meteorology data by the procedure described in section 5.2.

6. Run LODI to calculate the exposures and deposition for this case. The LODI wind and turbulence data come from the files just produced by the previous ADAPT runs and the namelist files are created in the script. The scavenging rate is read from a file that translated hourly precipitation rates for the ARM Central Facility into the appropriate scavenging rates as given in section 3.3.2.2. In these simulations 25,000 LODI parcels were tracked for each species; this is at the lower range of the typical number of parcels experience has shown gives correct concentrations. The main outputs from LODI for each case are two files giving exposures for the depositing and non-depositing species and one file of deposition for the depositing species.

7. The exposures and depositions calculated by LODI are processed by a smoothing function. Concentrations in LODI are derived by periodically sampling the position and properties of parcels. With a limited number of parcels, concentrations can be uneven, particularly at great distances from the source, and plots based on these concentrations are often ragged. Using a 1-2-1 smoothing function produces the smoother plots we expect without changing the accuracy of the solution.

8. Reduce the 350 by 350 one-kilometer resolution exposures and depositions to the arc/ sector values. This was done by simply constructing a list of points in the concentration grid that were within each arc/ sector and finding the average exposure or deposition for these points. For individual arc/ sectors at 16.1, 32.2, 80.5, and 160.9 km (10, 20, 50, and 100 miles), the number of points was between 9 and 12, between 19 and 21, between 40 and 52, and between 101 and 106, respectively.

9. Calculate the annual average exposures and deposition as the weighted average of the 610 individual cases.

We also evaluated performing the last two steps in reverse order, calculating the weighted average annual exposure on the 350 by 350 grid, and then determining the arc/ sector values. Both methods give the same result.

8.4 Computer Time Requirements

8.4.1 MACCS2

Performing all 610 weather trials with the MACCS2 code required less than 1 minute of CPU time. For this problem, only the ATMOS and EARLY modules were used; long term consequences calculated in CHRONC were not needed and so were not performed. Otherwise, MACCS2 was run in the standard way, which involves weather binning and wind rotation. Weather binning is described in section 3. Wind rotation involves accounting for the possibility that the wind might have been blowing in a different direction than the one corresponding to the beginning of the weather trial. In the wind rotation mode, MACCS2 performs a calculation for each of the 16 compass directions for each weather trial. Each of these calculations is weighted by the probability that the wind might have been blowing in that direction, as determined by performing statistics on the weather file. (Wind rotation is described further in section 4.) Thus, the 610 weather trials performed by MACCS2 accounted for 8760 possibilities.

8.4.2 RASCAL/RATCHET

Processing the meteorological data to create the input files for RASCAL required about 16 min of computer time and resulted in 36 files with an average size of about 12.5 Mb. RASCAL and RATCHET were run in batch mode on a networked 3 GHz PC with 1 Gb RAM. Each case was run three times, once for each model domain. The total time required to run RASCAL for all 610 releases for the three model domains was about 46 min (~1.5 s per release). About 65 min were required for the RATCHET runs (~2.2 s per release).

8.4.3 ADAPT/LODI

ADAPT and LODI were run on a DEC computer with 1 GHz alpha processors. ADAPT runs that produced one hourly meteorology data set took an average of 40 s with a range of 37-52 s. Each LODI run that produced exposures and depositions for one of the 610 cases used an average of 138 s with a range of 51 to 360 s. The entire simulation, made up of 8778 ADAPT runs and 610 LODI runs, took 435300 s (121 hours) of CPU time.

9. WIND CHARACTERISTICS OF THE ARM SGP SITE

The wind and its variability is the most important parameter in this study, and one of the best ways to summarize winds at a location is with a wind rose that shows the relative frequency of winds with particular directions and speeds at a given site. The wind rose for the surface data (10 m measurement height) at the ARM SGP Central Facility near Lamont, OK for the year 2000 is shown in Figure 10. This is the only wind data used by MACCS2 to calculate exposure and deposition. It is also important to point out, especially to those familiar with MACCS2, that the wind roses plotted here are in the standard format where the arms point in the direction the wind is coming from rather than using MACCS2's convention showing the direction the wind is blowing towards. Figure 10 shows a very large predominance of southerly and south-southeasterly winds; nearly half the time the wind is from the southeast through south-southwest. When the wind is not from the south it is most often from the north. Winds predominately from the east (12.0%) and west (6.7%) occur relatively infrequently.

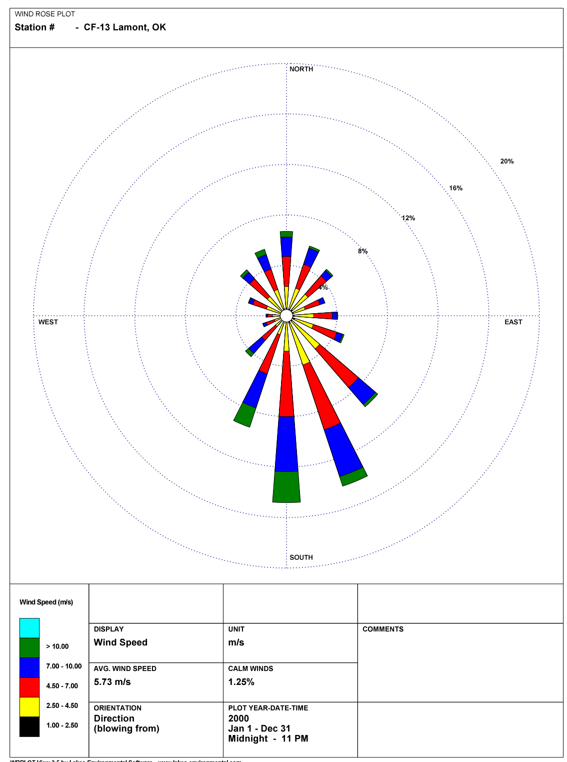


Figure 10. Wind Rose for the ARM Central Facility at Lamont, OK. The speed ranges in m/ s are 1-2.5, 2.5-4.5, 4.5-7, 7-10, >10. Wind speed is less than 1 m/ s 1.25% of the time. Wind direction is the direction the wind is blowing from. The circles are at 4, 8, 12, 16, and 20%. There are 8774 valid hourly surface (10 m) wind observations at this site. The average wind speed is 5.73 m/ s.

The seasonal variability of the winds at the Central Facility is shown by the surface wind rose plots for each season in Figures 11-14. In the summer the wind blows with a southerly component (direction from southwest through southeast) over 70% of the time, while in winter the frequency of winds with a northerly component (36%) is nearly equal to the frequency of winds with a southerly component (39%).

While MACCS2 does not take the spatial variability of wind into account, RASCAL/ RATCHET and ADAPT/ LODI do. RASCAL/ RATCHET uses the five additional ARM surface sites closest to

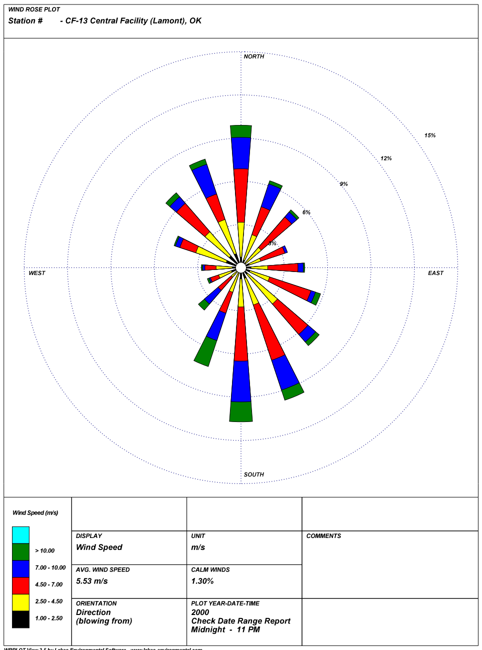


Figure 11. Surface Wind Rose for the ARM Central Facility for Winter, 2000.

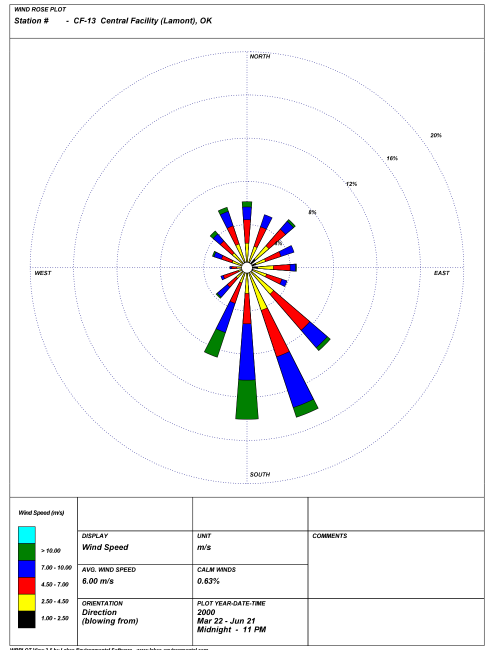


Figure 12. Surface Wind Rose for the ARM Central Facility for Spring, 2000.

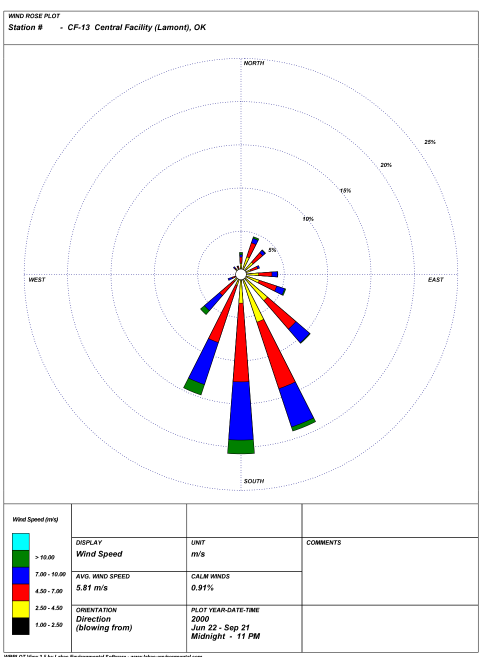


Figure 13. Surface Wind Rose for the ARM Central Facility for Summer, 2000.

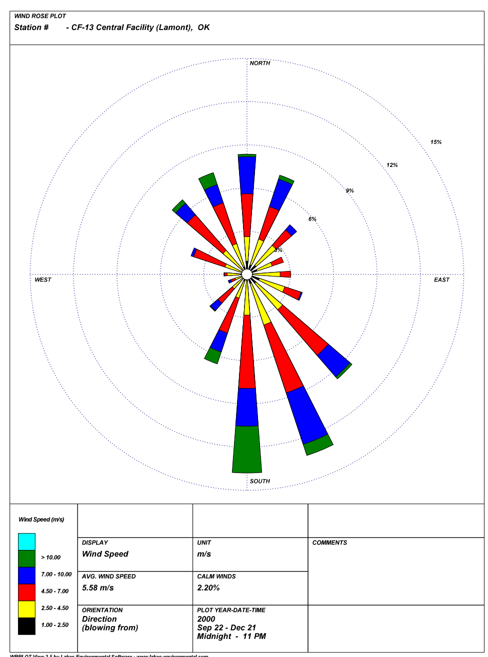


Figure 14. Surface Wind Rose for the ARM Central Facility for Autumn, 2000.

the Central Facility. The wind roses for these sites for the year 2000 are shown in Figures 15-19. While all these sites have wind roses similar to each other and to the Central Facility, there are differences that are probably due to natural variability and perhaps local effects such as surface conditions and terrain. All the sites have a strong

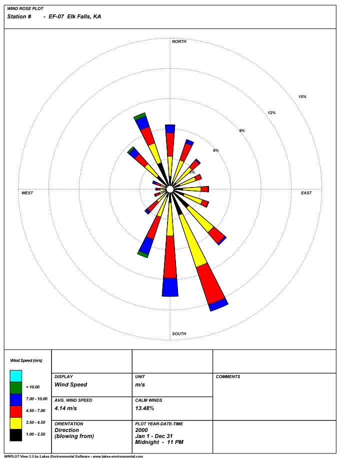


Figure 15. Surface Wind Rose for the Elk Falls, KA Site.

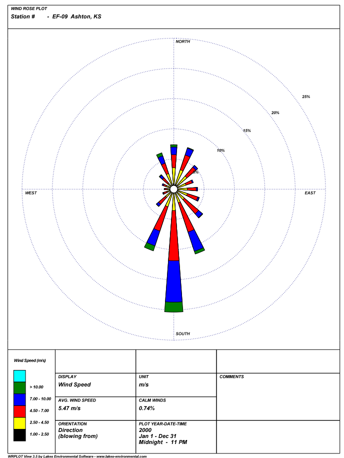


Figure 16. Surface Wind Rose for the Ashton, KA Site.

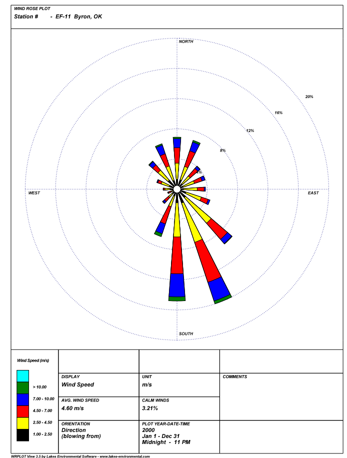


Figure 17. Surface Wind Rose for the Byron, OK Site.

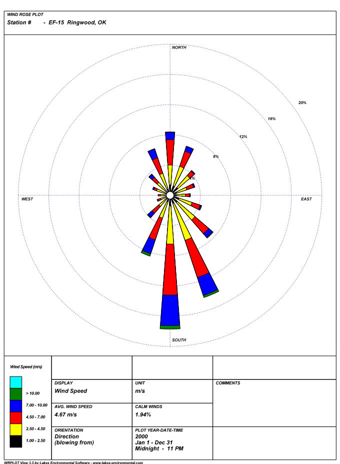


Figure 18. Surface Wind Rose for the Ringwood, OK Site.

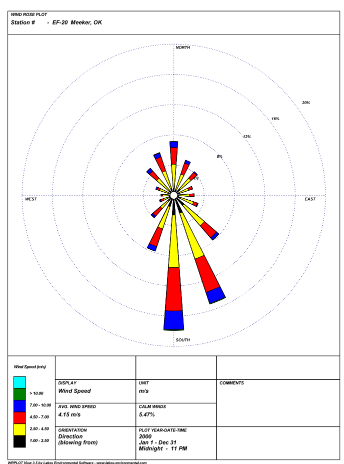


Figure 19. Surface Wind Rose for the Meeker, OK Site.

The speed ranges are 1-2.5, 2.5-4.5, 4.5-7, 7-10, and >10 m/ s. Wind speeds less than 1 m/ s occur 13.5% (Elk Falls), 0.7% (Ashton), 3.2% (Byron), 1.9% (Ringwood) and 5.5% (Meeker) of the time. Wind direction is the direction the wind is blowing from. The circles are at multiples of 3% (Elk Falls), 5% (Ashton), and 4% (Byron, Ringwood, and Meeker). There are 7774 (Elk Falls), 8201 (Ashton), 8166 (Byron), 8104 (Ringwood), and 7792 (Meeker) valid hourly surface (10 m) wind observations. The average wind speeds are 4.14 m/ s (Elk Falls), 5.47 (Ashton), 4.60 (Byron), 4.67 (Ringwood), and 4.15 (Meeker).

peak in wind frequency associated with southerly flow. At all the additional sites wind speeds are lower than at the Central Facility.

In addition to many more surface sites, ADAPT/ LODI uses upper air wind data from profilers and sondes. Wind roses from the 915 MHz profiler at its lowest height of 87 m are shown in Figures 20-23. Valid data from the Central Facility profiler at the lowest

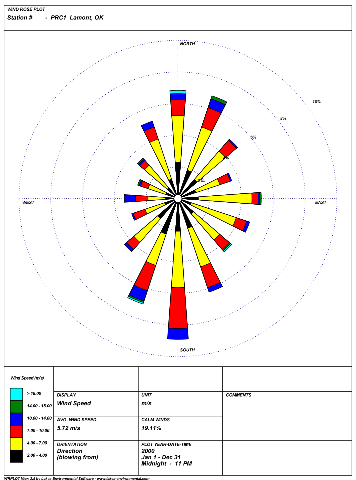


Figure 20. Wind Rose from 915 MHz Profiler at 87 m Height at Lamont, OK

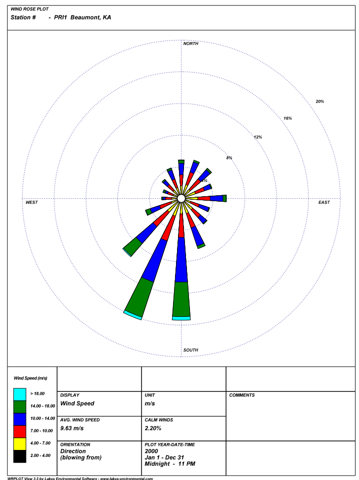


Figure 21. Wind Rose from 915 MHz Profiler at 87 m Height at Beaumont, KA.

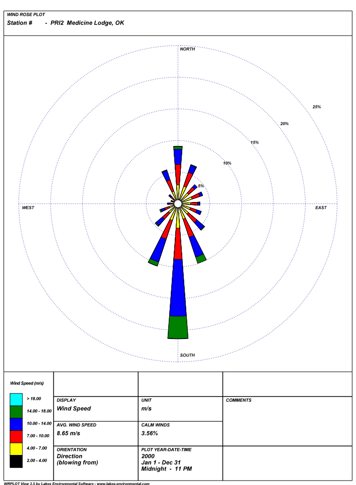


Figure 22. Wind Rose from 915 MHz Profiler at 87 m Height at Medicine Lodge, KA.

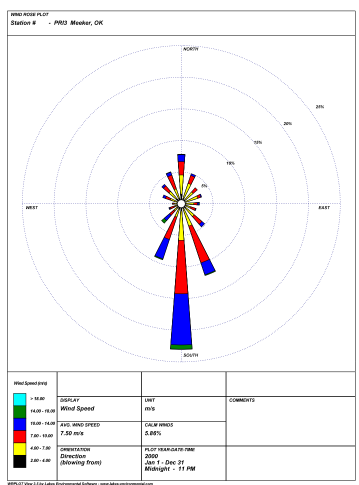


Figure 23. Wind Rose from 915 MHz Profiler at 87 m Height at Meeker, OK.

The speed ranges are 2-4, 4-7, 7,10, 10-14, 14-18, and >18 m/ s. Wind speeds less than 2 m/ s occur 19.1% (Lamont), 2.2% (Beaumont), 3.6% (Medicine Lodge), and 5.9% (Meeker) of the time. Wind direction is the direction the wind is blowing from. The circles are at multiples of 2% (Lamont), 4% (Beaumont), and 5% (Medicine Lodge and Meeker). There are 1010 (Lamont), 4633 (Beaumont), 7701 (Medicine Lodge), and 1979 (Meeker) valid hourly wind observations at 87 m. The average wind speeds are 5.72 m/ s (Lamont), 9.63 (Beaumont), 8.65 (Medicine Lodge), and 7.50 (Meeker). The Central Facility, with a rather small number of observations, does not seem to represent the year very well.

height are often missing (valid wind data are available for only 1010 out of 8778 hours), and the data do not seem to represent the entire year very well. Fortunately, sondes are frequently available at this site to make up for the lack of profiler data. The other profilers provide 87 m wind data most of the time and the winds are representative. Southerly winds dominate, and wind speeds are higher than at the surface. A final set of wind roses, for a height of 500 m at the Central Facility, is shown in Figure 24, which provides the observations from the 915 MHz profiler, and Figure 25, which provides the data from the NOAA wind profiler network. These are measurements of the same quantity by two different instruments. The plots are quite similar, but they also exhibit differences reflecting the variation in the winds and the inaccuracy of wind profiling

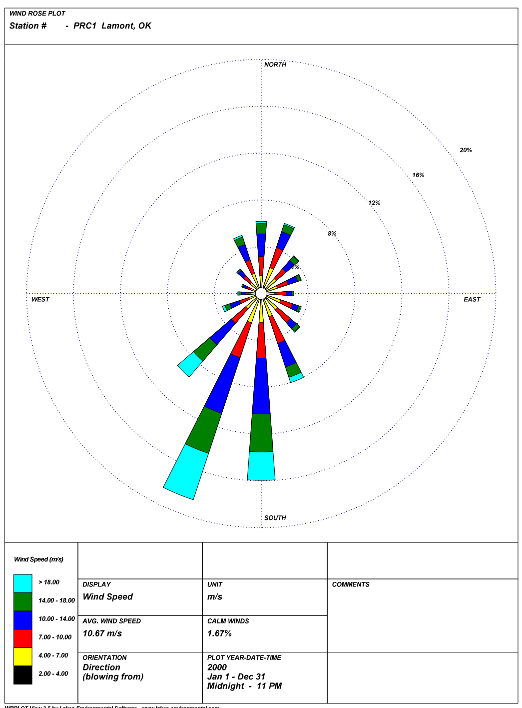


Figure 24. Wind Rose from 915 MHz Remote Wind Profiler (RWP) at 495 m height at Lamont, OK (Central Facility).

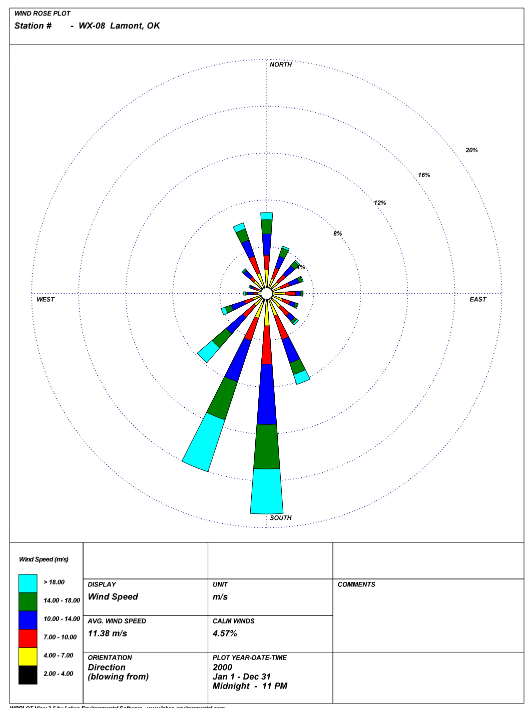


Figure 25. Wind Rose from NOAA Wind Profiler (NWP) at 500 m Height at Lamont, OK (Central Facility).

The speed ranges in these figures are 2-4, 4-7, 7,10, 10-14, 14-18, and >18 m/ s. Wind speeds less than 2 m/ s occur 1.7% (RWP) and 4.6% (NWP) of the time. Wind direction is the direction the wind is blowing from. The circles are at 4, 8, 12, 16, and 20%. There are 7490 (RWP) and 8102 (NWP) valid hourly wind observations at 500 m.

instruments. At this mid-level of the atmosphere the winds are stronger than at the surface and on average have veered (rotated clockwise) from the predominant surface direction a bit east of south to a direction a bit west of south. If wind speed and direction are important parameters in controlling the arc and arc/ sector annual average exposure and deposition, this change in wind direction could be important because some of the released material may be transported at heights several hundred meters above the surface.

10. RESULTS

Our primary goal is to provide an evaluation of the atmospheric transport and dispersion (ATD) modules in MACCS2, averaged over a representative meteorological data set, and to enable a discussion about their continued use for NRC purposes. The evaluation is done by comparing results from MACCS2 to those from ADAPT/ LODI, a complex state-of-the-art ATD code. In addition results from RASCAL and RATCHET were included in the study. The primary metrics of comparison are the arc and arc-sector annual average exposure and deposition derived from a set of 610 representative releases during the year 2000 at the DOE ARM SGP site.

To add validity to the study the results were obtained using the models in their normal modes. Each model was run by personnel who normally utilize these models, and all simulations were done independently and without adjustment. In order to make the best possible comparison of the ATD components, we chose a dry deposition velocity and specified washout coefficients, based on normal properties of the models, that gave the same or very similar removal rates, and these choices were made before the model runs started. The same set of 610 release times, derived from MACCS2's normal selection criteria, was used by all models. Each code used hourly meteorological data and ran each case until all the released material exited the 160.9-km (100-mile) radius domain, 80.5-km (50-mile) radius for RASCAL/ RATCHET. The characteristics of the release – location, start time, duration, amount of depositing and non-depositing species, height, and heat energy of release – were identical for all models.

10.1 Arc Averages

The annual average exposures for the depositing and non-depositing species and the annual average deposition for arcs at distances of 14.5-16.1, 30.6-32.2, 78.8-80.5, and 159.3-160.9 km (9-10, 19-20, 49-50, and 99-100 miles) from the source are given in Tables 14-16. In all cases the arc average exposures and depositions for MACCS2, RASCAL, and RATCHET differ from LODI by less than a factor of two (ratio between 0.5 and

Table 14. Non-Depositing Species Arc Average Exposure (Bq-s/ m^3) and Ratio to LODI

Model	16.1 km (10 mi)	32.2 km (20 mi)	80.5 km (50 mi)	161 km (100 mi)
MACCS2	8.02e7 (1.58)	2.39e7 (1.01)	4.77e6 (0.64)	1.80e6 (0.65)
RASCAL	7.32e7 (1.45)	3.09e7 (1.30)	8.41e6 (1.12)	
RATCHET	3.24e7 (0.64)	1.33e7 (0.56)	3.59e6 (0.48)	
LODI	5.06e7 (1.00)	2.36e7 (1.00)	7.49e6 (1.00)	2.75e6 (1.00)

Table 15. Depositing Species Arc Average Exposure (Bq-s/ m^3) and Ratio to LODI

Model	16.1 km (10 mi)	32.2 km (20 mi)	80.5 km (50 mi)	161 km (100 mi)
MACCS2	5.18e7 (1.41)	1.40e7 (1.05)	2.49e6 (0.81)	7.86e5 (0.89)
RASCAL	5.91e7 (1.61)	2.01e7 (1.50)	3.94e6 (1.28)	
RATCHET	2.89e7 (0.79)	1.09e7 (0.81)	2.69e6 (0.88)	
LODI	3.68e7 (1.00)	1.34e7 (1.00)	3.07e6 (1.00)	8.86e5 (1.00)

Table 16. Arc Average Deposition (Bq/ m^2) and Ratio to LODI

Model	16.1 km (10 mi)	32.2 km (20 mi)	80.5 km (50 mi)	161 km (100 mi)
MACCS2	5.57e5 (1.21)	1.53e5 (0.96)	2.87e4 (0.78)	8.96e3 (0.83)
RASCAL	7.20e5 (1.56)	2.34e5 (1.46)	4.71e4 (1.29)	
RATCHET	3.10e5 (0.67)	1.06e5 (0.66)	2.63e4 (0.71)	
LODI	4.62e5 (1.00)	1.60e5 (1.00)	3.67e4 (1.00)	1.08e4 (1.00)

2.00), except RATCHET at 80.5 km (50 miles) for the non-depositing species. MACCS2's exposure and deposition values have a tendency to be higher close to the source and lower at distances of 80.5 and 160.9 km (50 and 100 miles). RASCAL and RATCHET have the same tendency, but with smaller magnitude. RASCAL consistently has higher and RATCHET lower exposures and depositions than LODI. Ratios of RASCAL to RATCHET exposures and depositions are often larger than two; this is attributed to faster vertical dispersion in RATCHET's new and more complex dispersion model.

The agreement among these models is gratifying. The explanation seems to be related to the fact that arc averaging minimizes the importance of transport since released material must move away from the source and after some transit time cross the arcs at 16.1, 32.2., 80.5, 160.9 km (10, 20, 50, and 100 miles). Dispersion and deposition are both related to travel time. The non-depositing species is subject only to vertical and horizontal dispersion and transport, and, after an initial period, is well mixed throughout the boundary layer. Large differences in exposure would require large differences in mixing heights among the models, but MACCS2 used the seasonal average mixing heights derived from the hourly mixing heights used by LODI so the differences are not large. In addition the dry and wet deposition rates were chosen to be similar; therefore, as long as the transit times are similar, there should not be large differences in depositing species exposures either. The fact that the largest differences are between RASCAL and RATCHET which have the same plume trajectory and differ only in the dispersion parameterization tends to support this argument.

10.2 Arc-Sector Averages

The second metric chosen for comparison is the annual average arc-sector exposure and deposition. The same 1.6 km (one mile) wide arcs at 16.1, 32.2, 80.5, and 160.9 km (10, 20, 50, and 100 miles) and the sixteen 22½ degree directional sectors from north clockwise through north-northwest provide 64 values for MACCS2 and ADAPT/ LODI (48 for RASCAL/ RATCHET) of exposure for the non-depositing material and 64 (48) values of exposure and deposition for the depositing material. Exposure for the non-depositing species is plotted and compared with the bar graphs in Figures 26-29. Similar plots of exposure for the depositing material are shown in Figures 30-33 and of deposition in Figures 34-37. In all these plots the sector to the north is repeated on both sides of the plot denoted N and N2. These plots show the angular distributions of the released material in addition to the decrease of exposure and deposition with distance. All models produce similar angular distributions that reflect the mean annual wind cycle. The largest concentrations are to the north, with a secondary maximum to the south; a relatively small amount of material goes west and especially east.

The arc-sector exposures and depositions for MACCS2 are generally within a factor of two of the corresponding values for the state-of-the-art model, LODI. Of the 192 exposures and depositions (4 arcs, 16 sectors, 2 exposures and 1 deposition), only nine are more than twice as large – all in the 16.1-km (10-mile) arc – and 12 are less than half as large, – four in the 80.5-km (50-mile) and eight in the 160.9-km (100-mile arc) – and these are usually in sectors where the exposure or deposition is smaller. The higher values close in and lower values at greater distances for MACCS2 correspond to the same trend noted for the arc average exposure and deposition. Differences greater than a factor of three are seen only twice, both for the non-depositing material; these are in the WSW sector of the 80.5-km (50-mile) arc (ratio = 0.31) and in the NNE sector of the 160.9-km (100-mile) arc (ratio = 0.33).

RASCAL and RATCHET arc-sector exposures and depositions have many more values differing by more than a factor of two from LODI, but this is partly related to the fact that RASCAL tends to consistently produce higher and RATCHET lower values than LODI. RASCAL has 33 of 144 exposures and depositions (3 arcs, 16 sectors, 2 exposures and 1 deposition) more than twice as large as LODI, and none less than half as large. Ten of these are more than three times as large as LODI. RATCHET has three of 144 exposures and depositions more than twice as large as LODI and 33 less than half as large. Of these 33, ten are less than one-third as large as LODI.

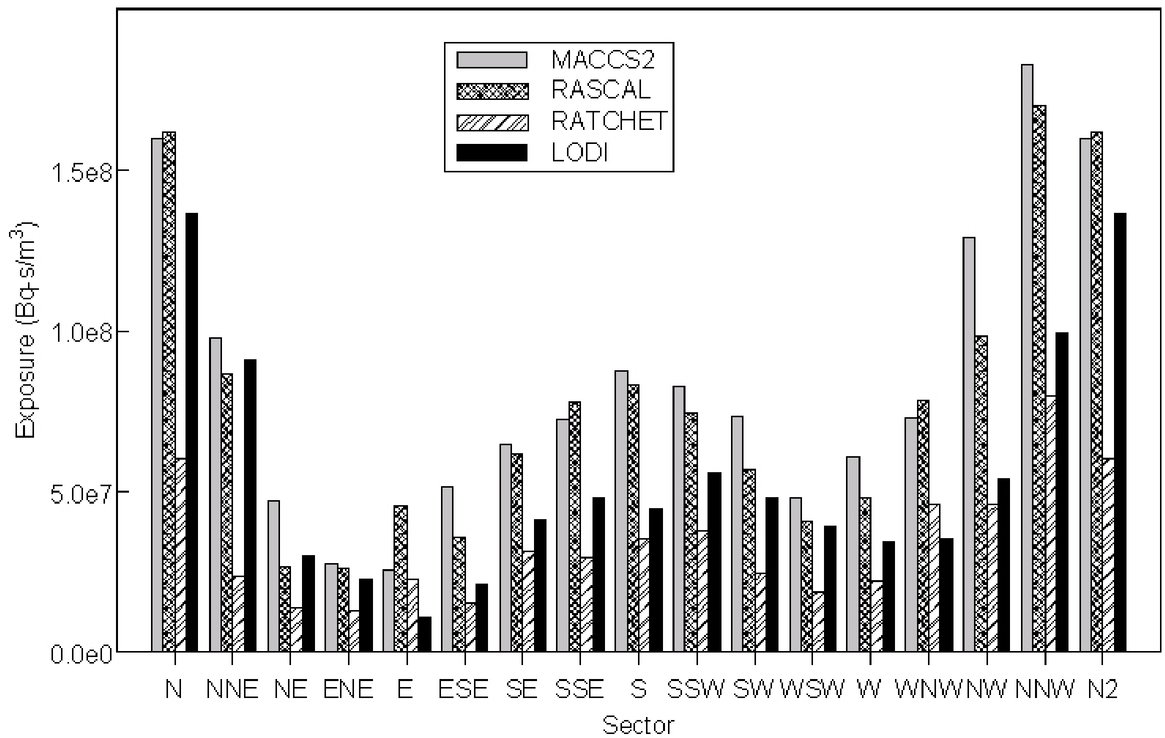


Figure 26. Arc-Sector Exposure for Non-Depositing Species on 16.9-km (10-mile) Arc.

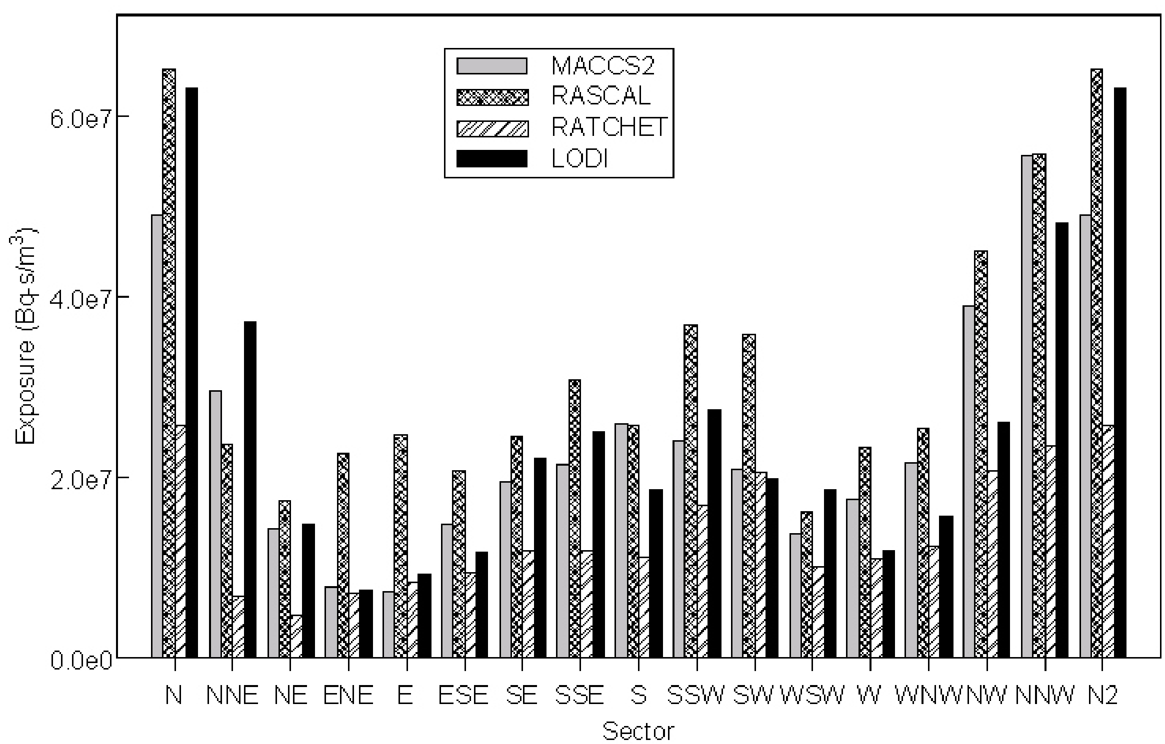


Figure 27. Arc-Sector Exposure for Non-Depositing Species on 32.2-km (20-mile) Arc.

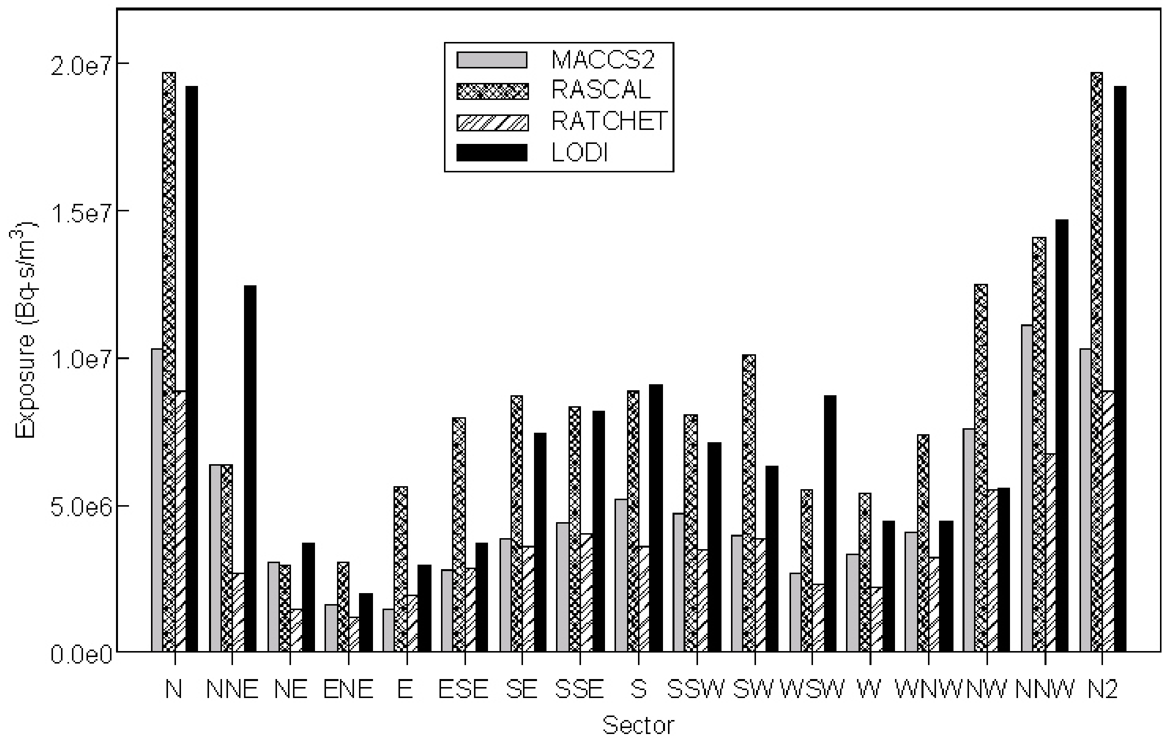


Figure 28. Arc-Sector Exposure for Non-Depositing Species on 80.5-km (50-mile) Arc.

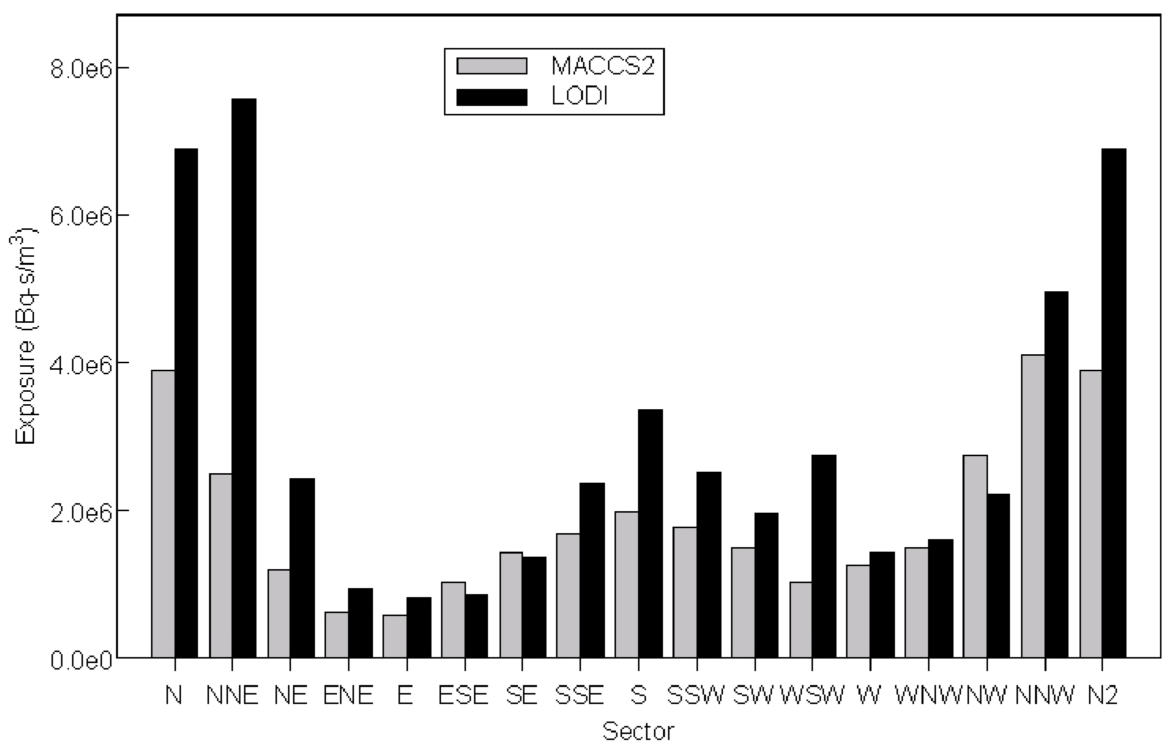


Figure 29. Arc-Sector Exposure for Non-Depositing Species on 160.9-km (100-mile) Arc.

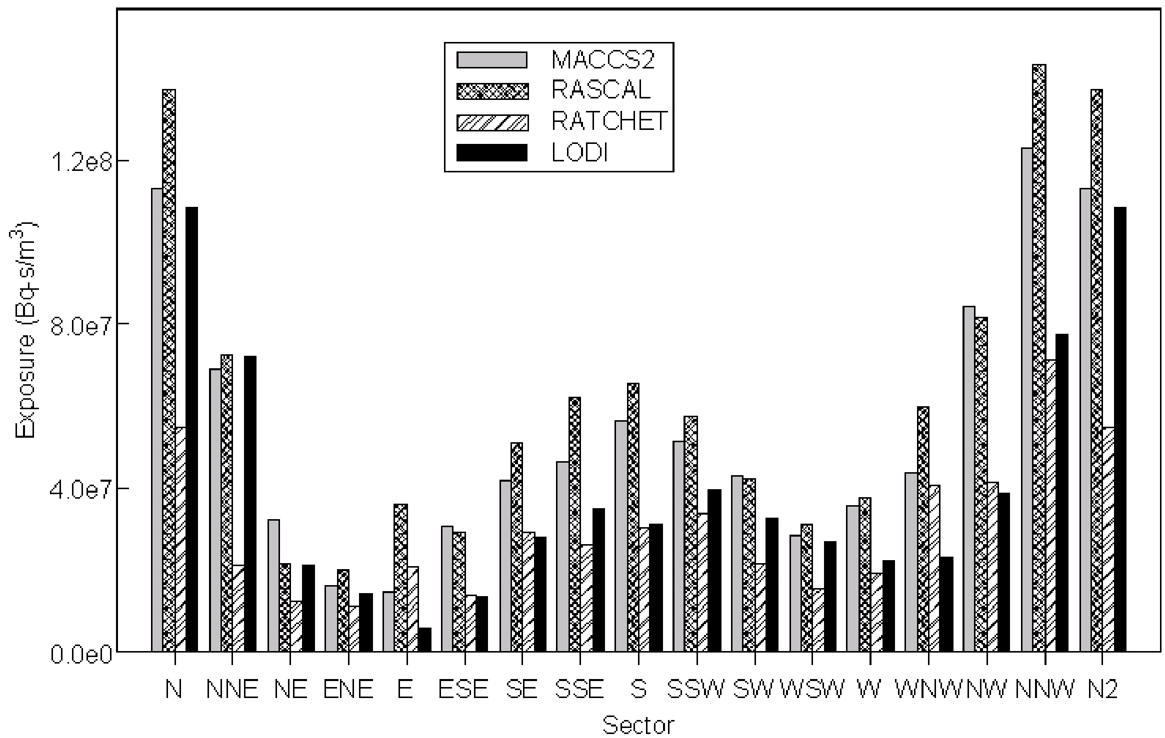


Figure 30. Arc-Sector Exposure for Depositing Species on 16.1-km (10-mile) Arc.

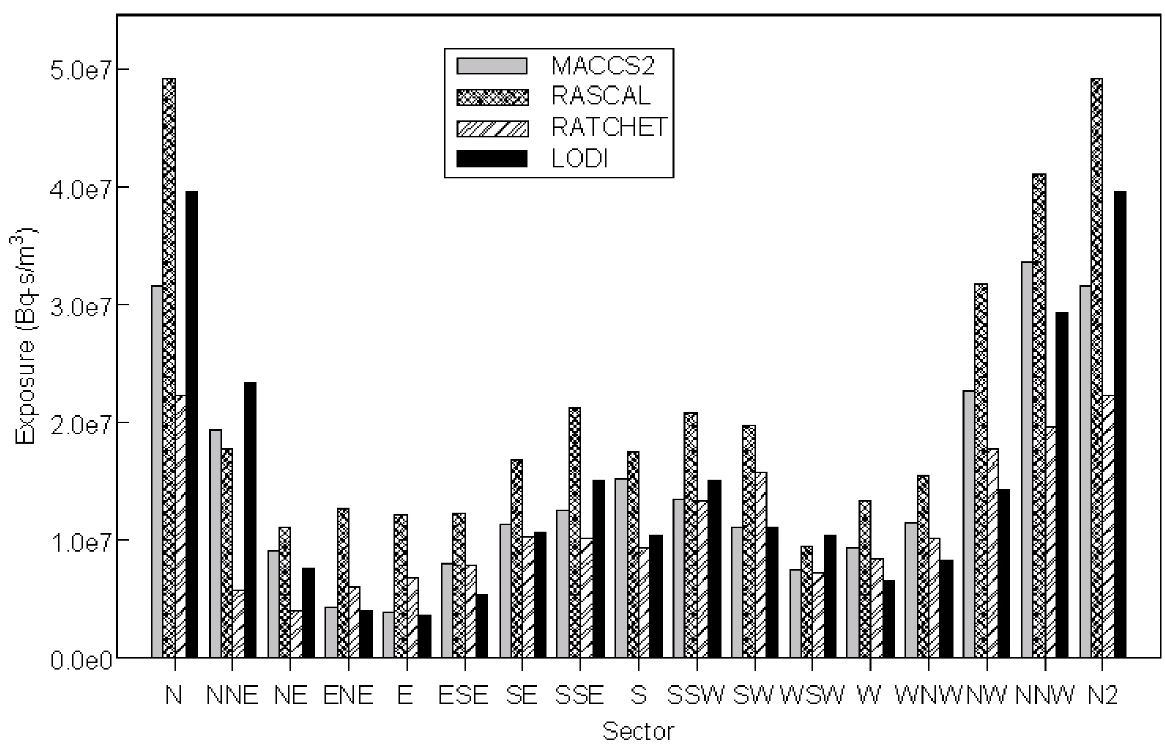


Figure 31. Arc-Sector Exposure for Depositing Species on 32.2-km (20-mile) Arc.

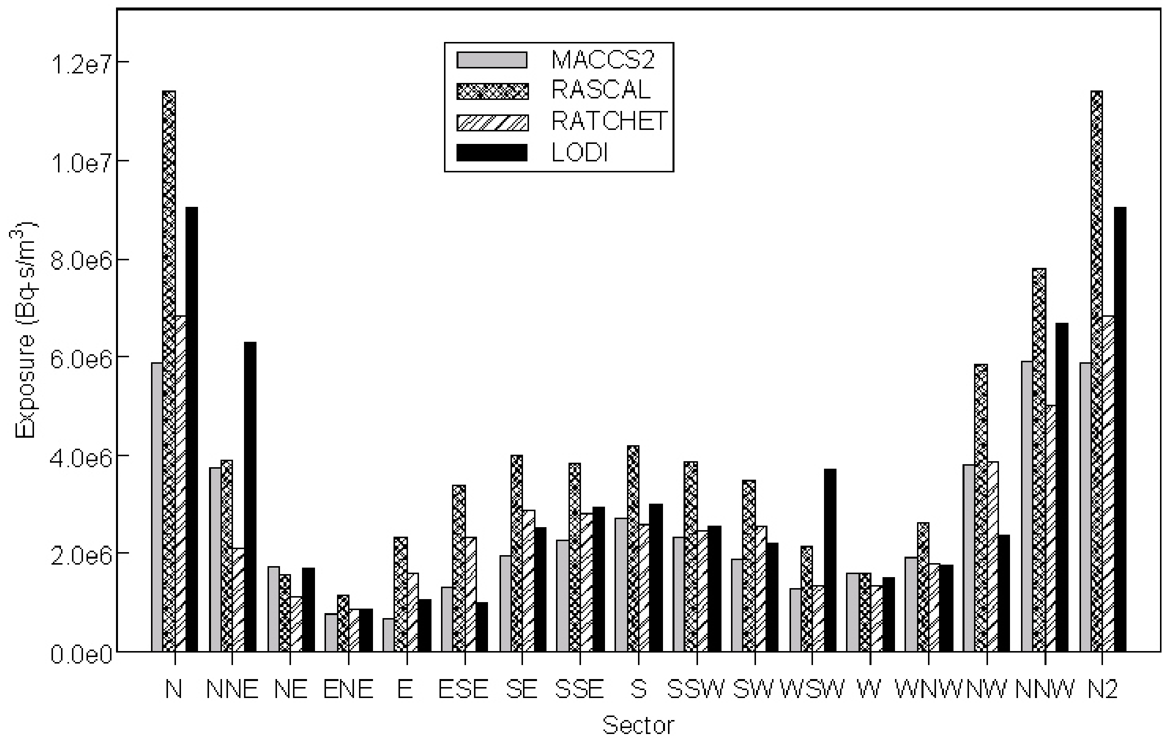


Figure 32. Arc-Sector Exposure for Depositing Species on 80.5-km (50-mile) Arc.

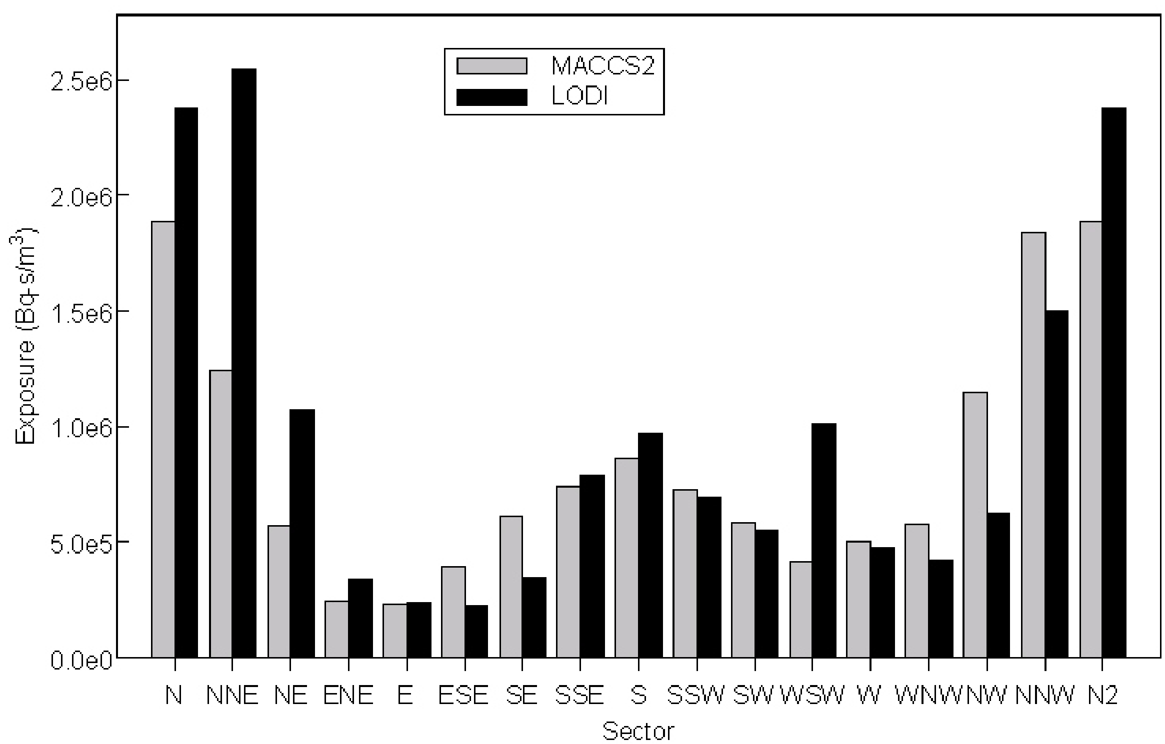


Figure 33. Arc-Sector Exposure for Depositing Species on 160.9-km (100-mile) Arc.

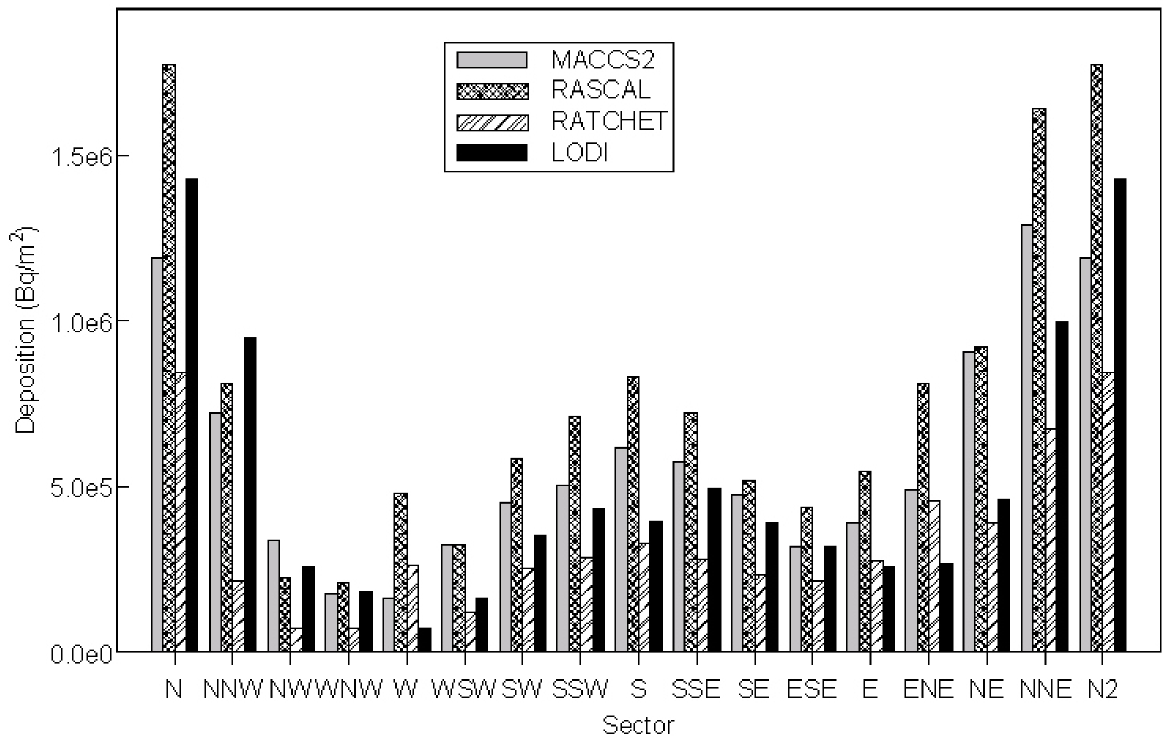


Figure 34. Arc-Sector Deposition on 16.1-km (10-mile) Arc.

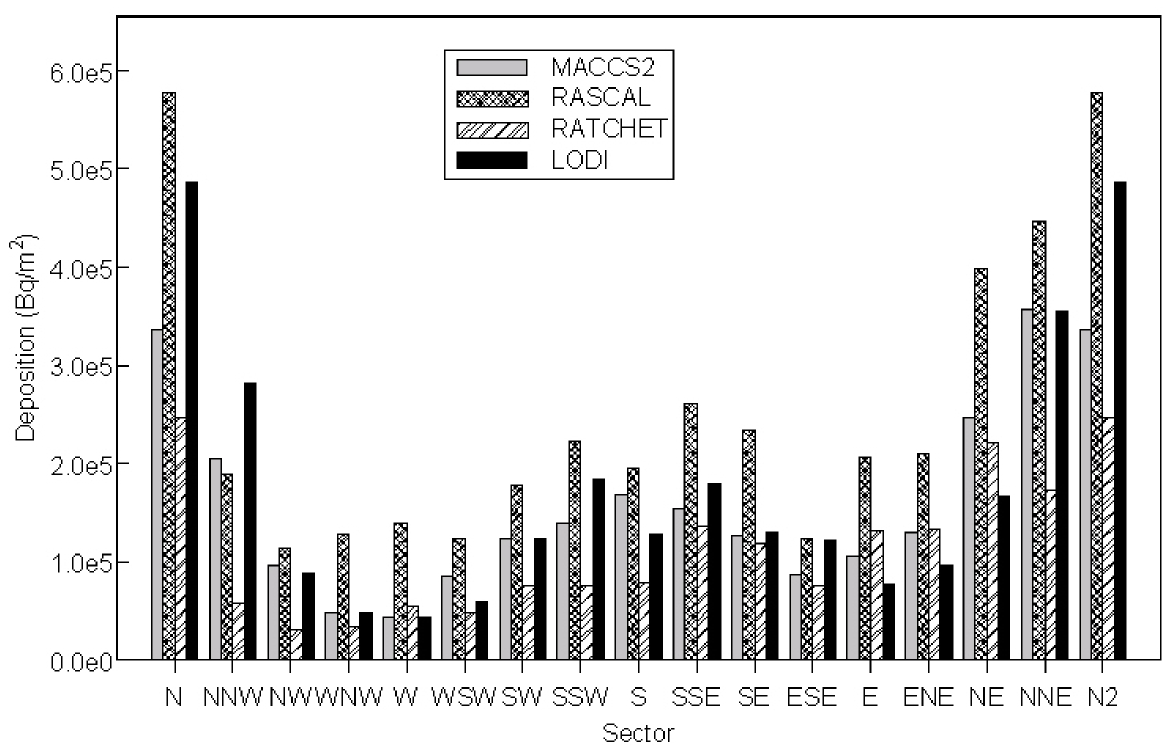


Figure 35. Arc-Sector Deposition on 32.2-km (20-mile) Arc.

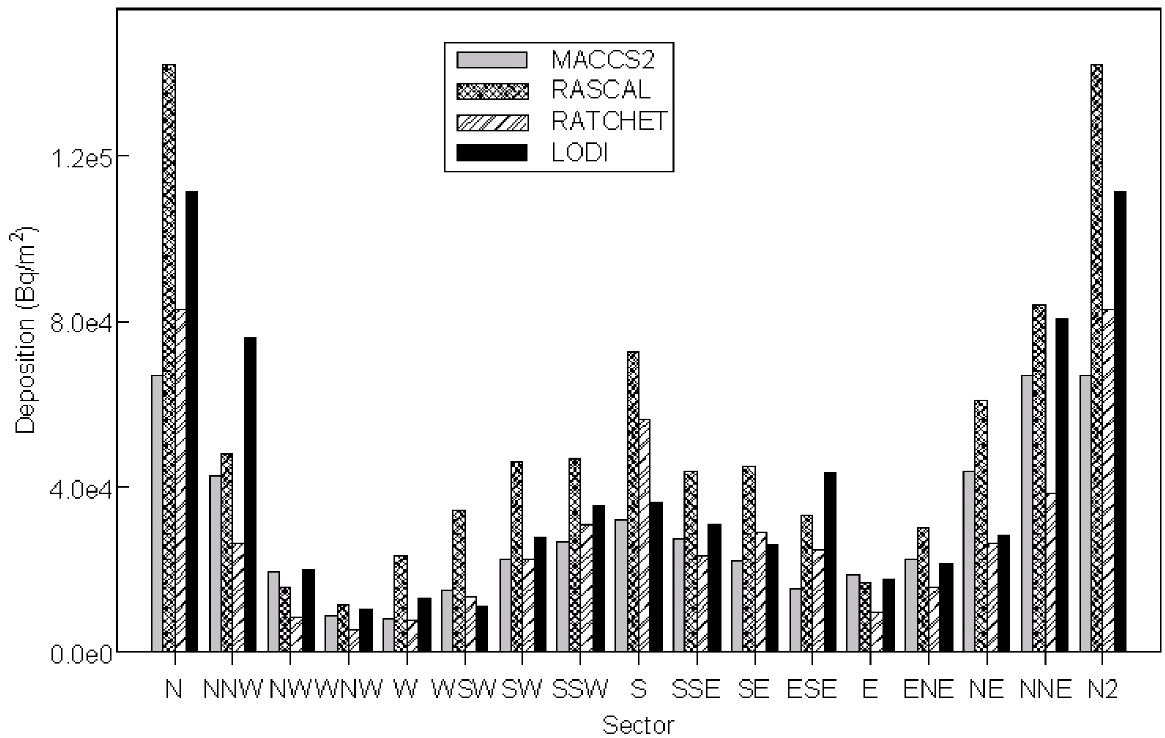


Figure 36. Arc-Sector Deposition on 80.5-km (50-mile) Arc.

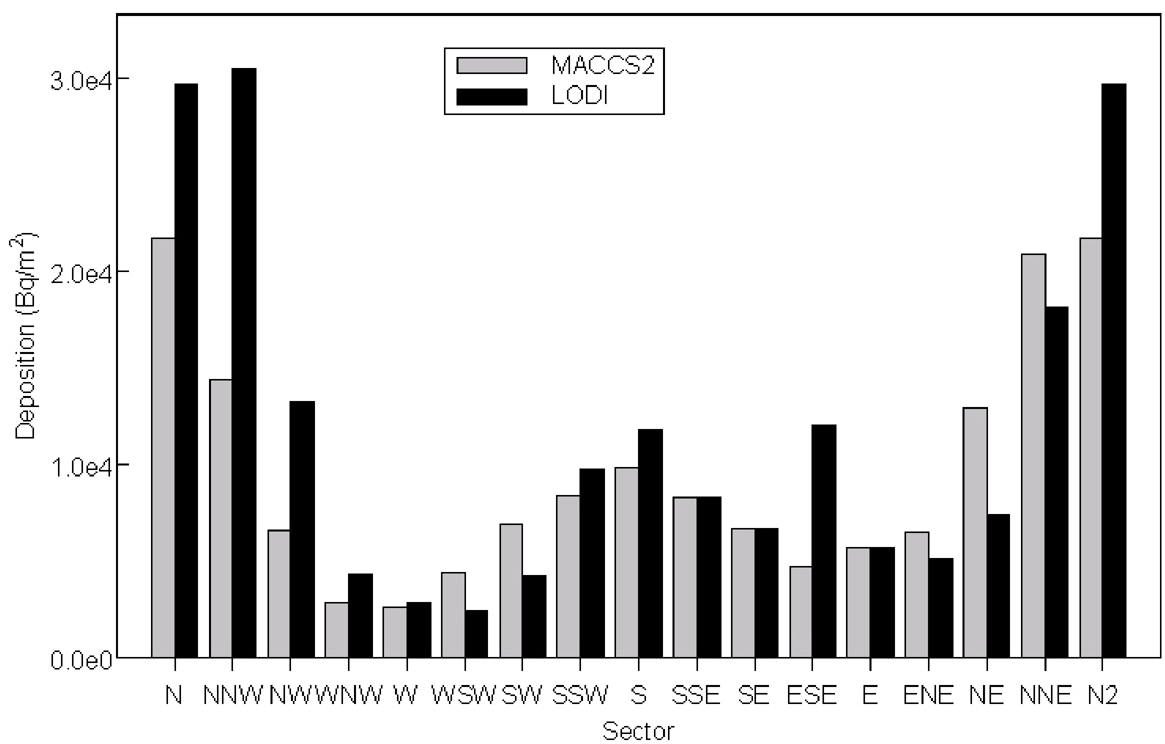


Figure 37. Arc-Sector Deposition on 160.9-km (100-mile) Arc.

Because each model has a different arc average exposure and deposition, it is difficult to portray how closely the angular distributions actually agree. Figures 38-49 show the angular distributions normalized by each model's arc average concentration. The ordinate in these plots is logarithmic so that multiplicative changes are proportional to distance, *i.e.,* a value twice the average is just as far above the average line as a value half the average is below, and a value four times the average is twice as far above the average line as a value twice the average. These figures also include the north sector on both sides.

The angular distributions of exposure and deposition are quite similar for all models and again reflect the distribution of the wind. The highest values are to the north where the exposure or deposition is 2-3 times the average; intermediate values, near the average, occur in southerly directions; lower values, from one-half to three-quarters of the average, occur to the west of the source; and the lowest values, often less the one-half the average, occur to the east, corresponding to infrequent westerly winds. The largest differences in normalized exposure and deposition occur in sectors to the east and west where the values of exposure and deposition are smaller.

In general, the angular distribution from MACCS2 seems to correspond more closely with LODI than RASCAL or RATCHET. This is a bit surprising since RASCAL and RATCHET follow individual plumes more closely than MACCS2, and the annual distributions are averages of individual plumes from the 610 releases just like LODI. Where local maxima (minima) of the curves are displaced, it is often by only one sector; that could be a result of individual plumes taking slightly different tracks and showing up in neighboring sectors. LODI also makes use of upper-level wind data; therefore, wind direction shear with height would be represented in LODI but not in the other models. For most plumes from individual releases, exposure and deposition are confined to two or three sectors. The differences in normalized distributions do not increase with distance, in fact they may even decrease. Larger differences in deposition are probably due to relatively infrequent large rain events occurring at different locations. Heavy rain over a period of an hour can deposit most of the depositing material in a local area and largely deplete the plume.

10.3 Two-Dimensional Exposure and Deposition

While not a primary metric of comparison, it is interesting to examine the two-dimensional exposure and deposition plots from each model; these are shown in Figures 50-52. The differences in these plots are only partly due to differences in results; they also depend on the location and spacing of the data used to construct them and to particular features of the models. The MACCS2 plots are based on radial/ sector exposure (deposition) data, specifically, 29 not very evenly spaced radii from 0.16 to 320.8 km (0.1 to 200 miles) and 16 sectors. In these figures the data are plotted for radii

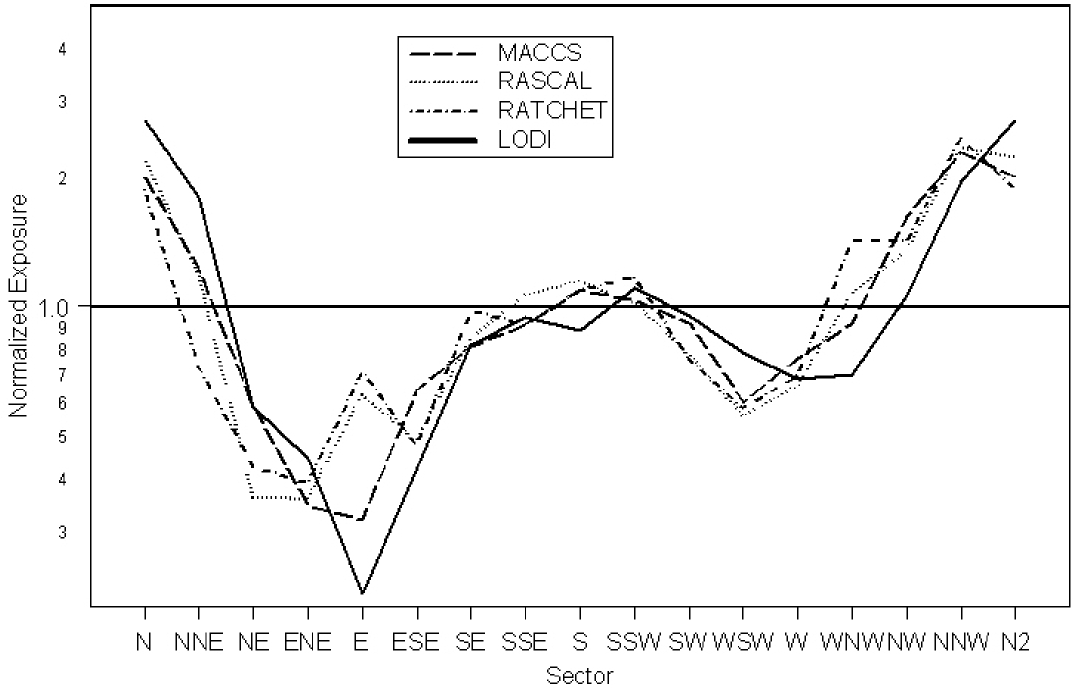


Figure 38. Normalized Exposure for Non-Depositing Material on the 16.1-km (10-mile) Arc.

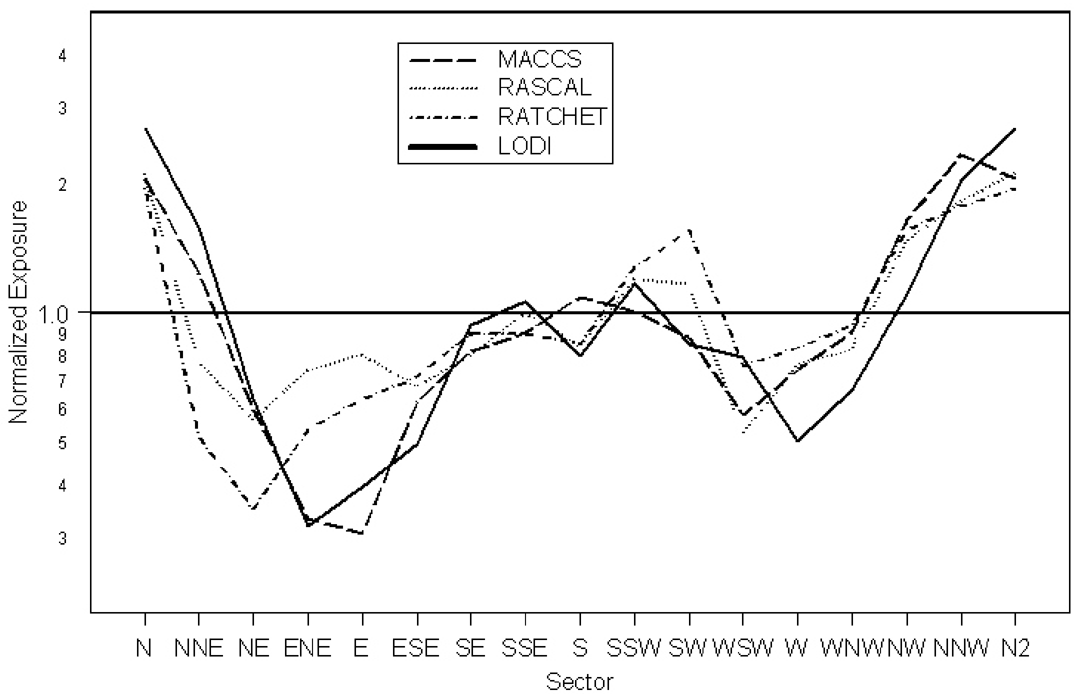


Figure 39. Normalized Exposure for Non-Depositing Material on the 32.2-km (20-mile) Arc.

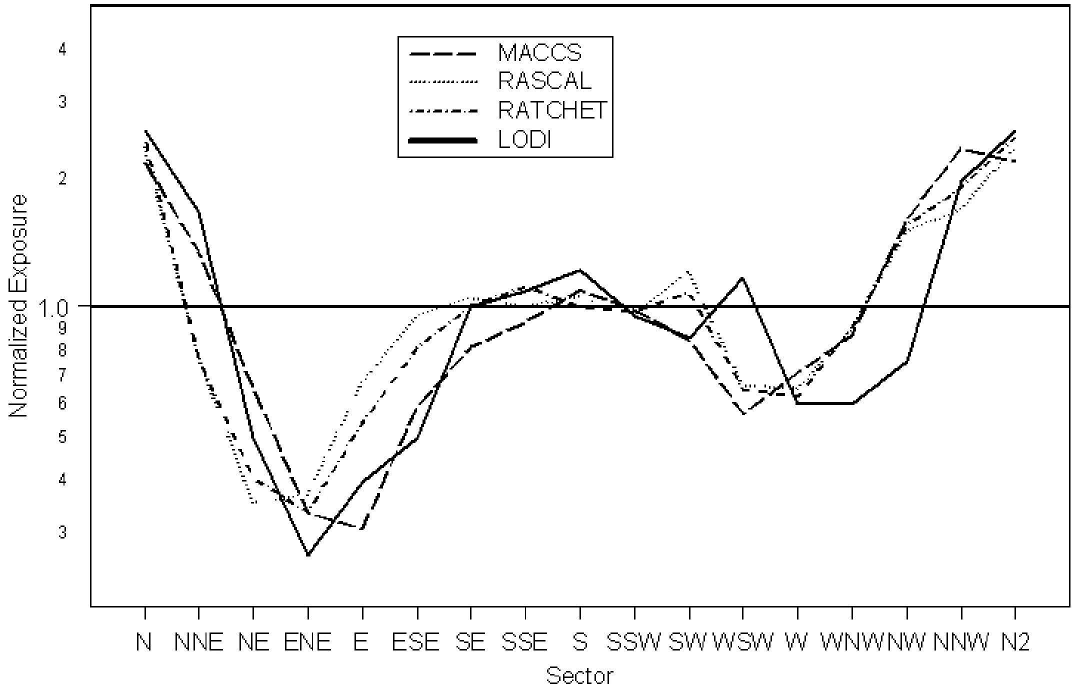


Figure 40. Normalized Exposure for Non-Depositing Material on the 80.5-km (50-mile) Arc.

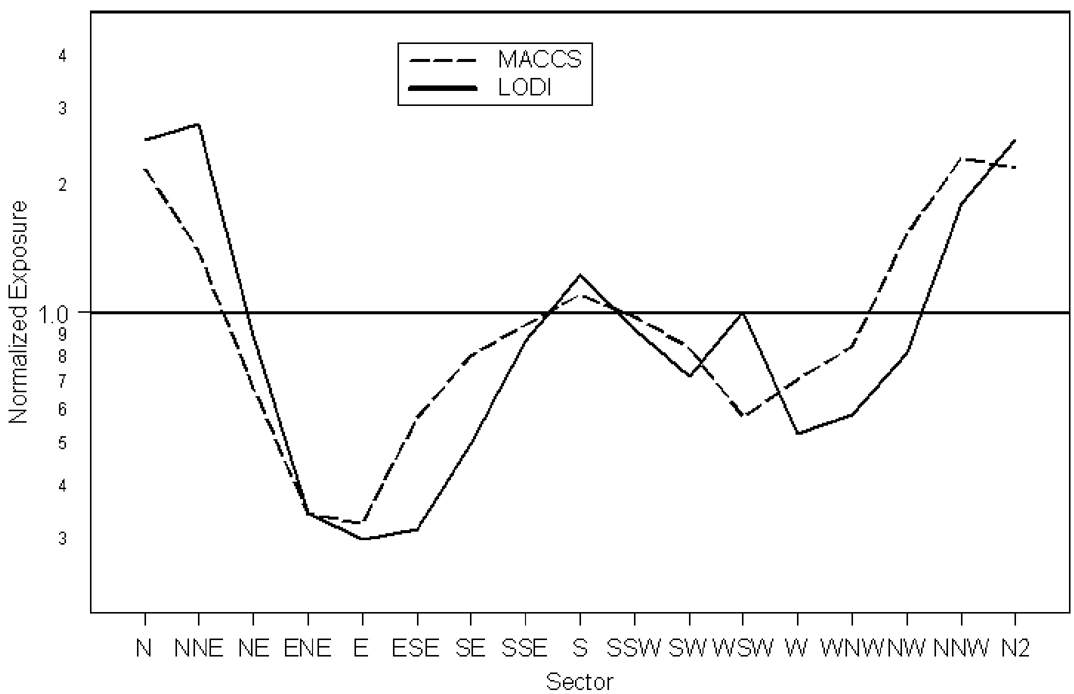


Figure 41. Normalized Exposure for Non-Depositing Material on the 160.9-km (100-mile) Arc.

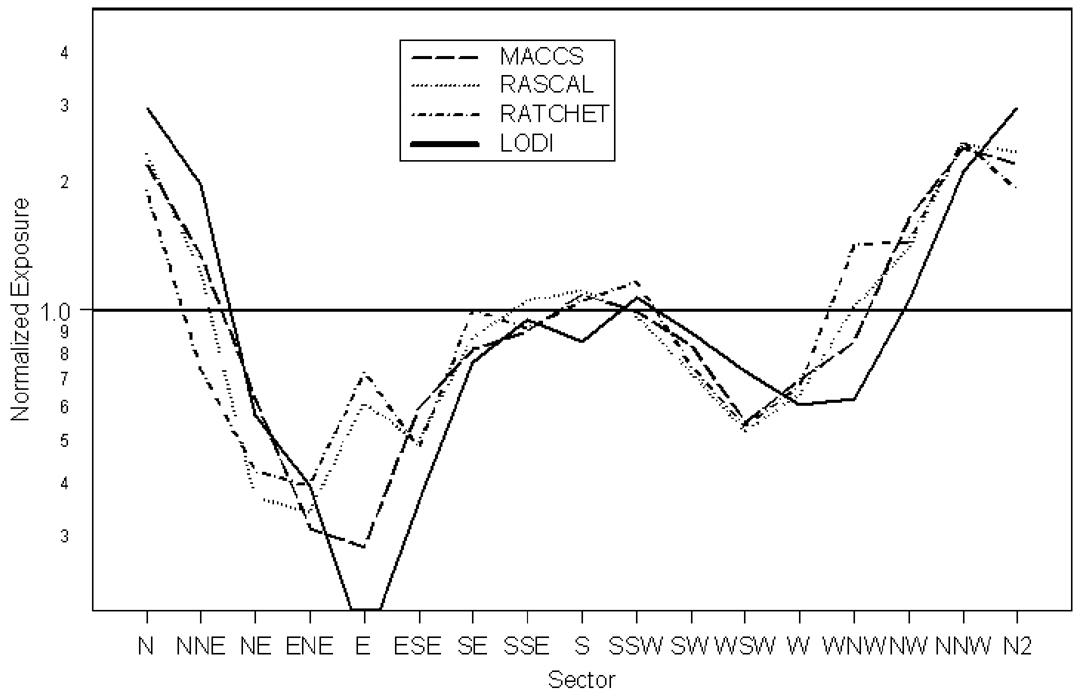


Figure 42. Normalized Exposure for Depositing Material on the 16.1-km (10-mile) Arc.

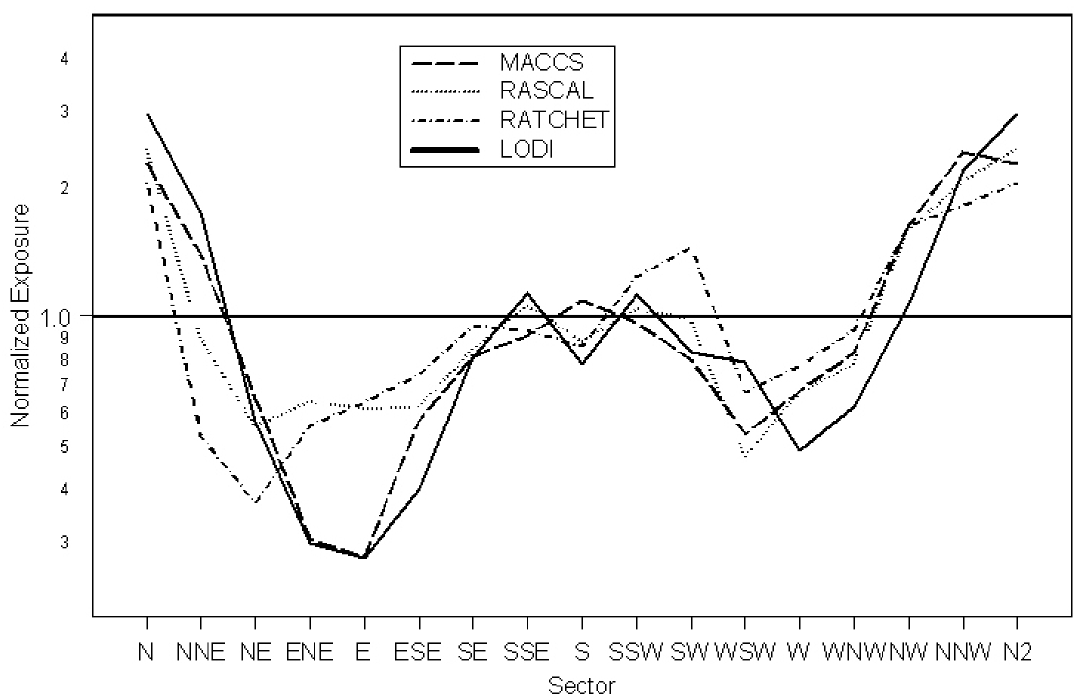


Figure 43. Normalized Exposure for Depositing Material on the 32.2-km (20-mile) Arc.

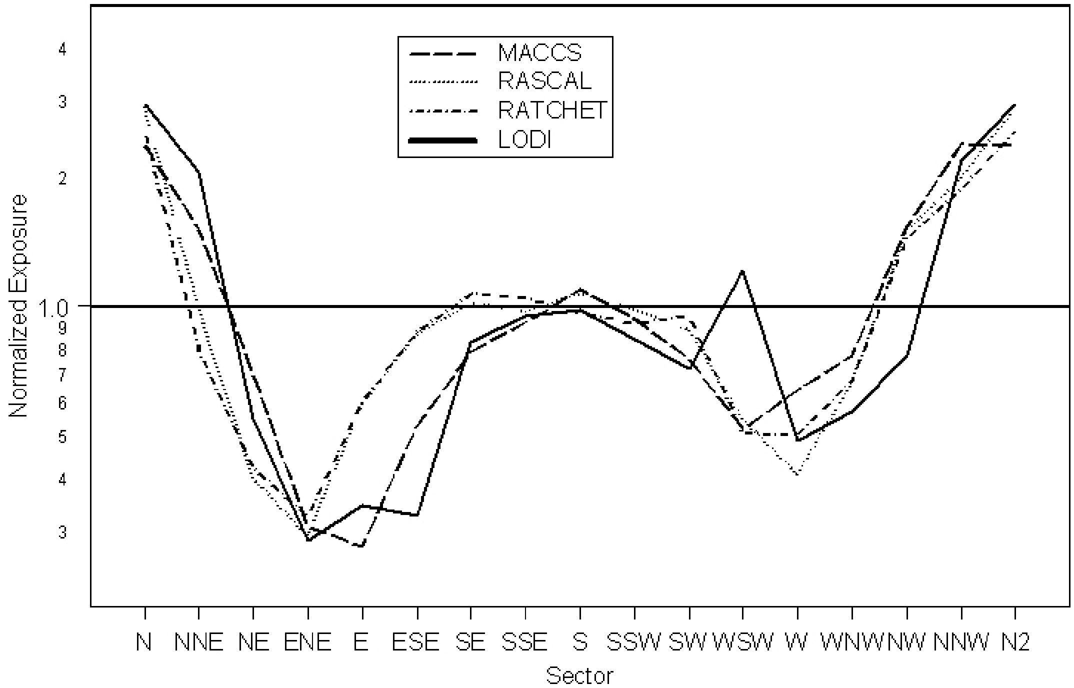


Figure 44. Normalized Exposure for Depositing Material on the 80.5-km (50-mile) Arc.

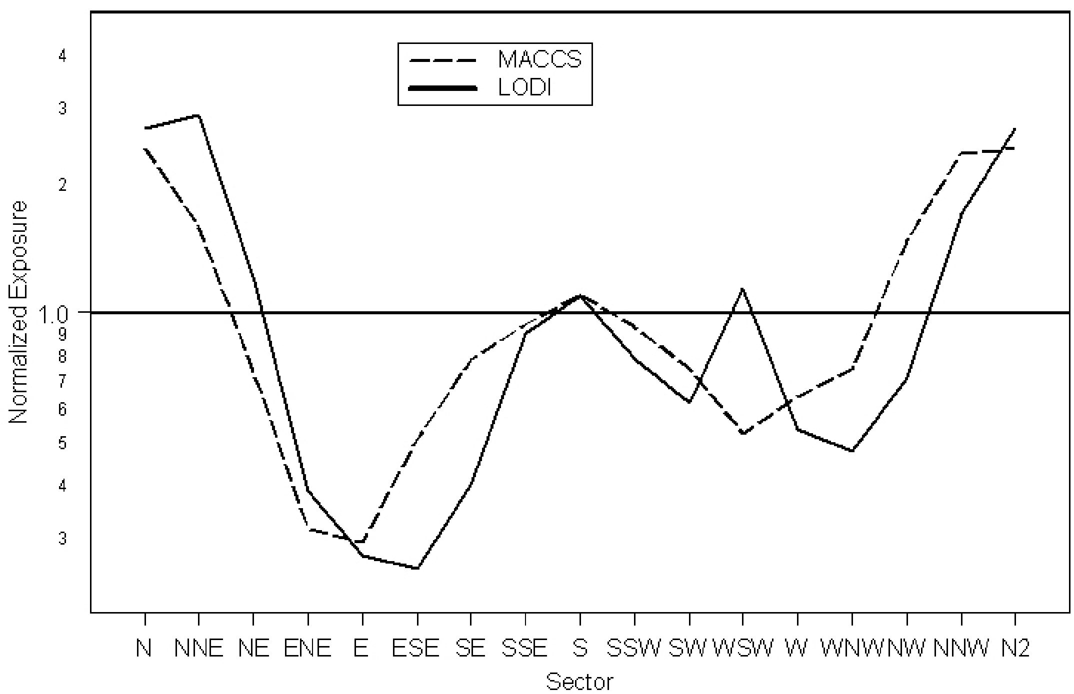


Figure 45. Normalized Exposure for Depositing Material on the 160.9-km (100-mile) Arc.

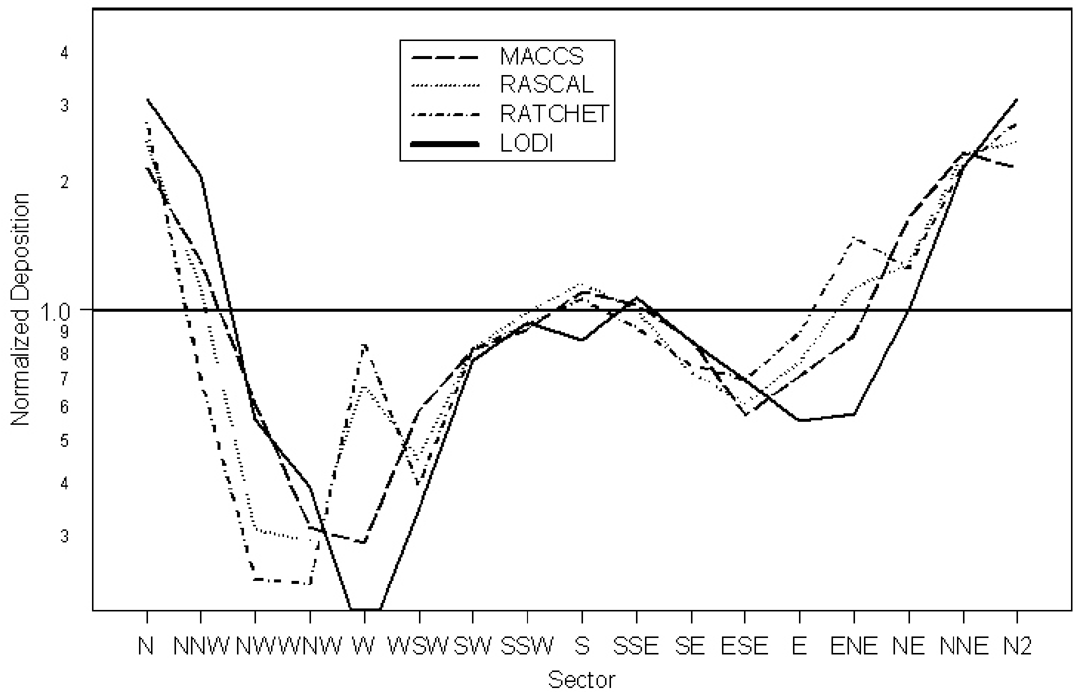


Figure 46. Normalized Deposition on the 16.9-km (10-mile) Arc.

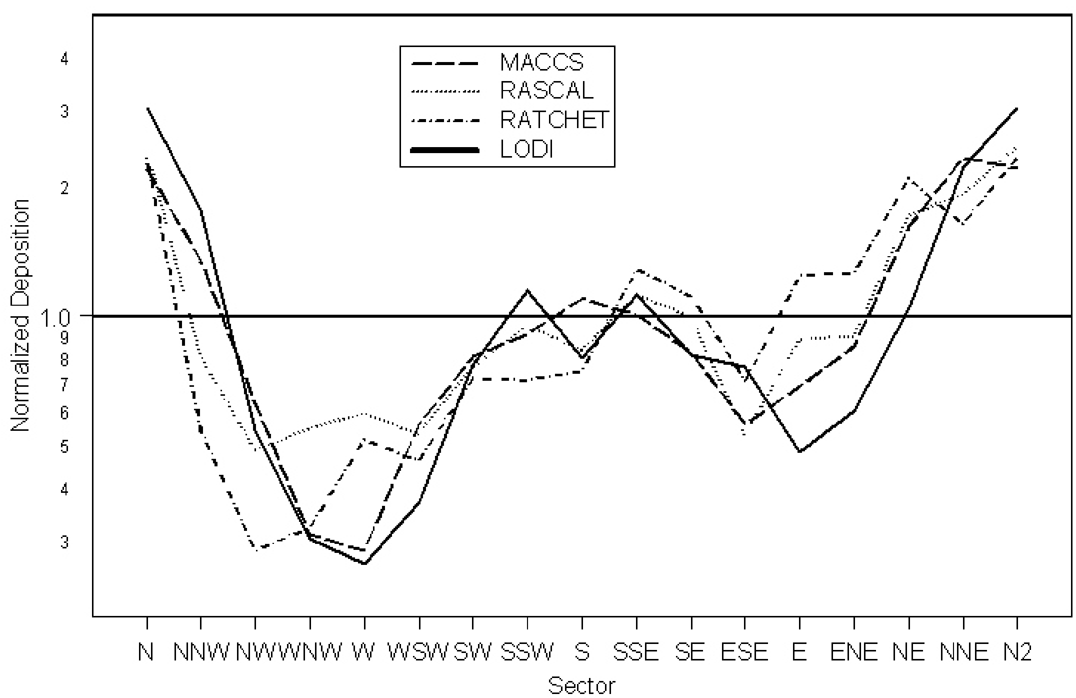


Figure 47. Normalized Deposition on the 32.2-km (20-mile) Arc.

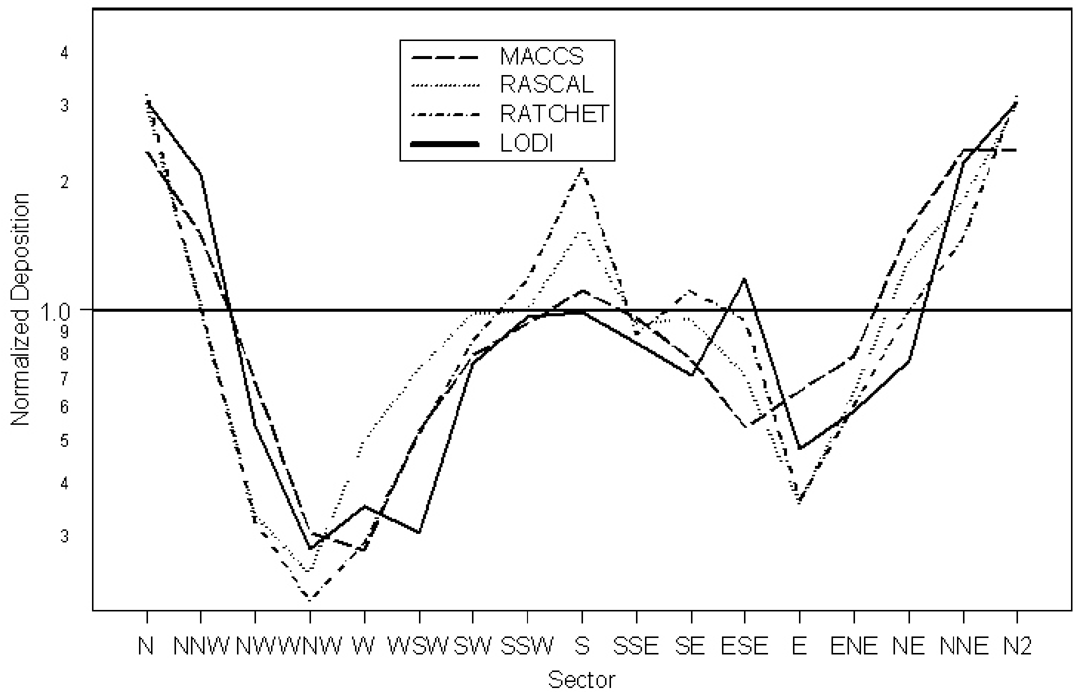


Figure 48. Normalized Deposition on the 80.5-km (50-mile) Arc.

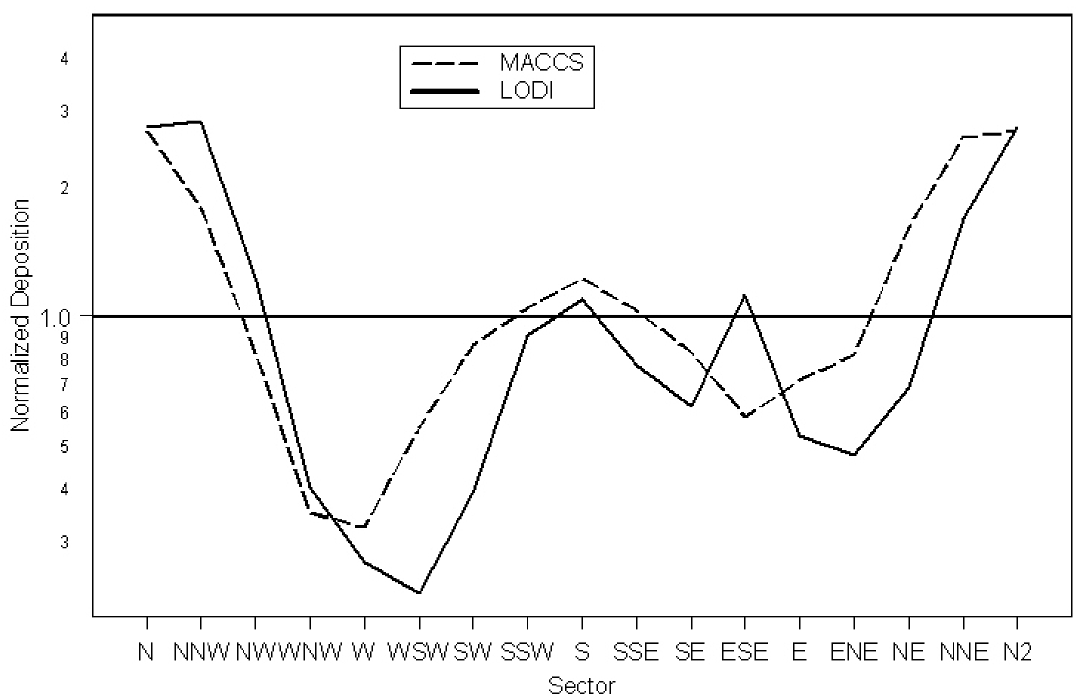


Figure 49. Normalized Deposition on the 160.9-km (100-mile) Arc.

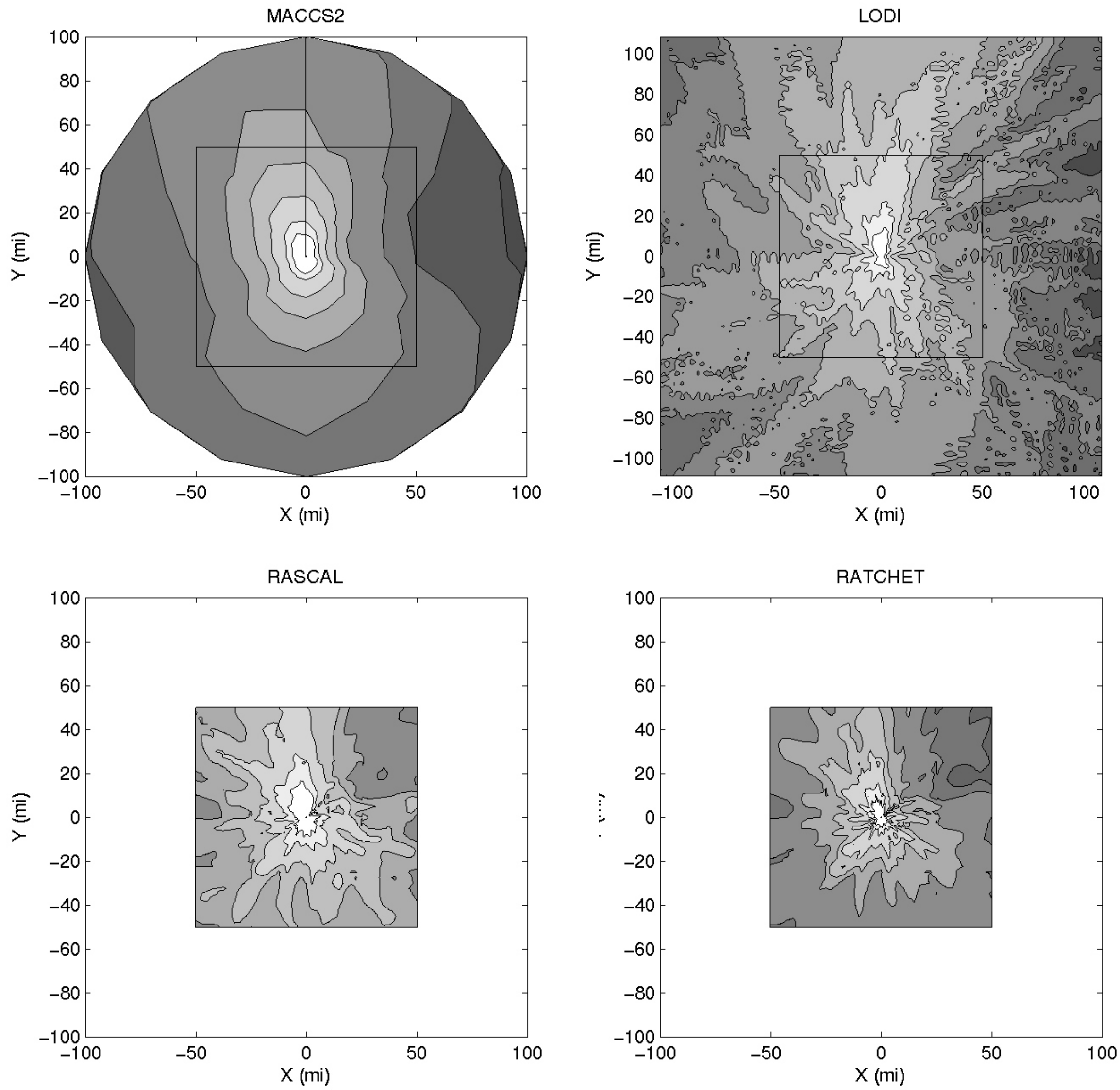


Figure 50. Annual Average Exposure for Non-Depositing Species. Contour levels are 10^8, 5×10^7, 2×10^7, 10^7, 5×10^6, 2×10^6, 10^6, 5×10^5, 2×10^5, 10^5, and 5×10^4 Bq-s/ m^3. Results for each model are as indicated. Note that RASCAL and RATCHET only provide data within 80.5 km (50 miles) of the source.

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from 0 to 160.9 km (100 miles), 25 radii. RASCAL and RATCHET data are in three grids: an inner grid with a spacing of 0.8 km (0.5 miles) over a range from -16.1 to +16.1 km (-10 to +10 miles), an intermediate grid with a spacing of 2 km (1.25 miles) over a range from -40.2 to +40.2 km (-25 to +25 miles), and an outer grid with a spacing of 4 km

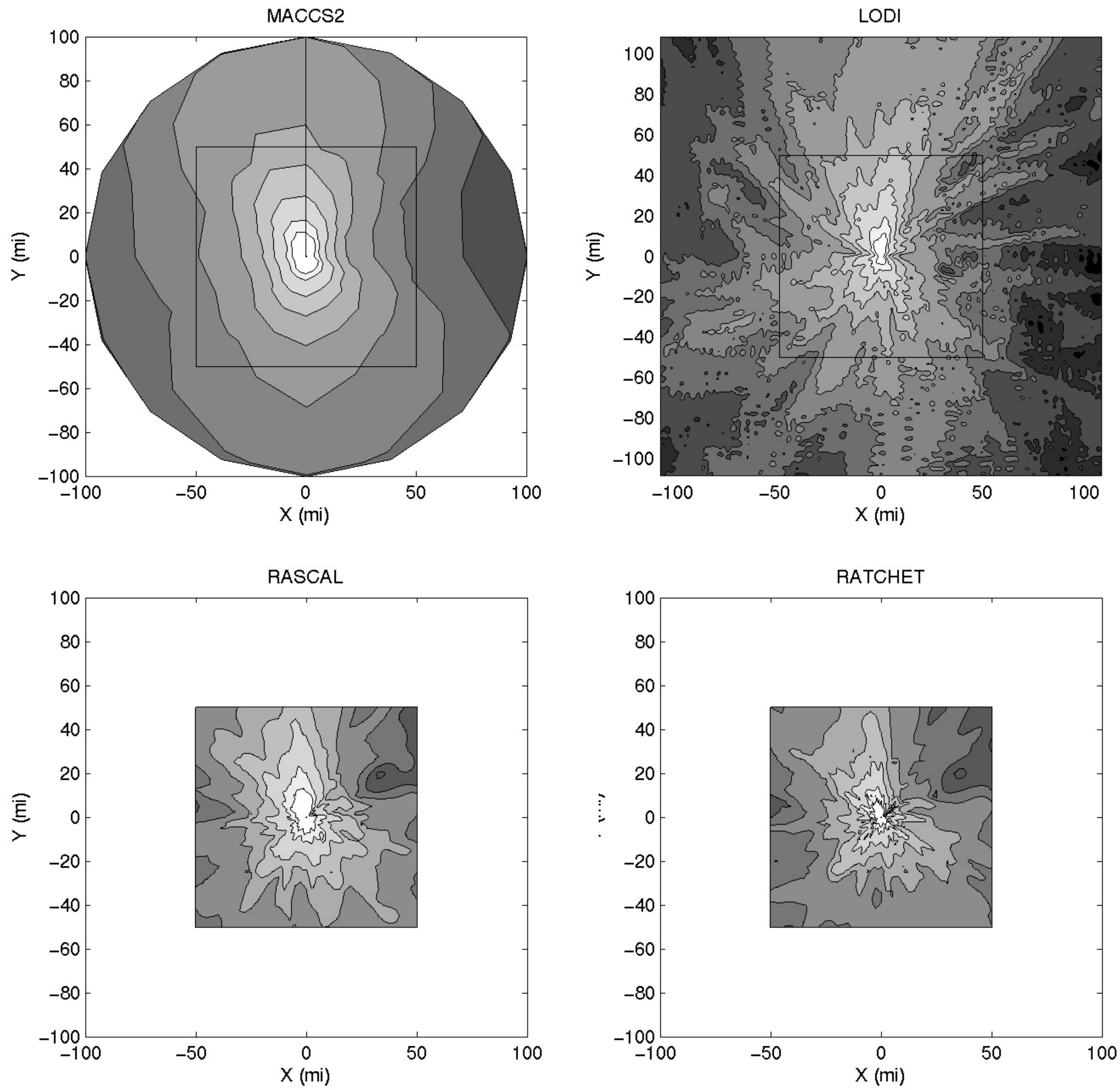

Figure 51. Annual Average Exposure for Depositing Species. Contour levels are 10^8, 5×10^7, 2×10^7, 10^7, 5×10^6, 2×10^6, 10^6, 5×10^5, 2×10^5, 10^5, and 5×10^4 Bq-s/ m^3. Results for each model are as indicated. Note that RASCAL and RATCHET only provide data within 80.5 km (50 miles) of the source.

(2.5 miles) over a range from -80.5 to +80.5 km (-50 to +50 miles). The data for LODI are from the concentration grid with a spacing of 1 km over a range from -175 to +175 km (-109 to +109 miles) from the source. Since we are primarily interested in the

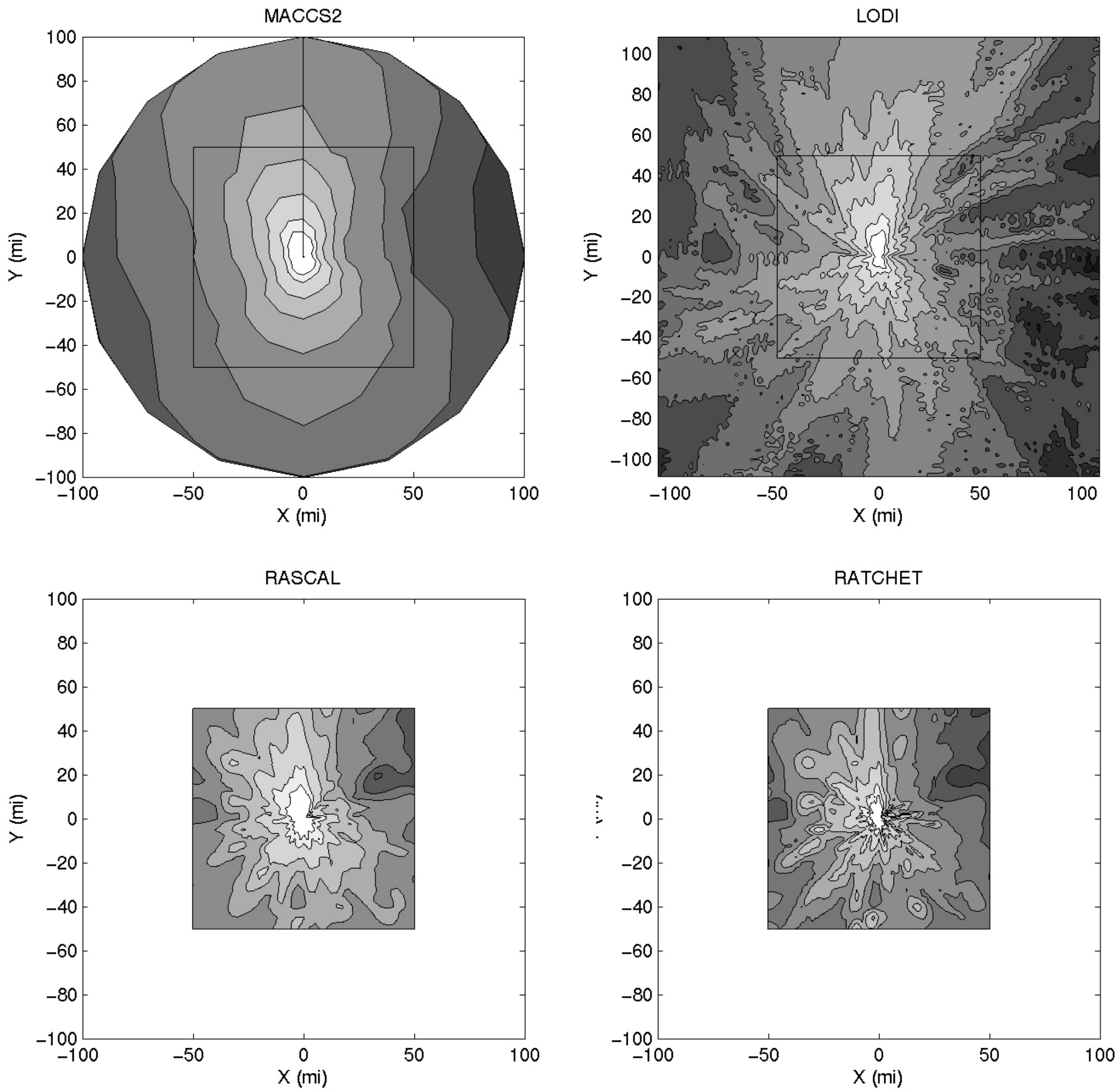

Figure 52. Annual Deposition. Contour levels are 10^6, 5×10^5, 2×10^5, 10^5, 5×10^4, 2×10^4, 10^4, 5×10^3, 2×10^3, 10^3, and 5×10^2 Bq-s/ m^3. Results for each model are as indicated. Note that RASCAL and RATCHET only provide data within 80.5 km (50 miles) of the source.

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distribution over the 8-160.9 km (5-100 mile) range, the highest values close to the source are not contoured. Also note that RASCAL and RATCHET plots cover only a 80.5-km (50-mile) square about the source while LODI and MACCS2 go out 160.9 km

(100 miles). The smooth contours in the plots for MACCS2 are a result of the solution technique, the assumed straight line transport, and the wide spacing of the data points (400 points). The LODI figures include some high frequency noise that is a feature of mapping parcels to a grid, especially a high-density (closely-spaced) concentration grid (122,500 individual exposures or depositions are used in constructing the contour plots). RASCAL, RATCHET, and LODI all show features in these annual averages that appear to preserve individual plumes, and there seems to be general agreement about the direction of these plumes. The RASCAL and RATCHET data are in quite close agreement except for the magnitude of the exposure or deposition. This is expected since these models are very closely related and the main difference is the turbulent diffusion formulation. RASCAL and RATCHET also have isolated downwind high deposition contours that are not present in MACCS2 or LODI plots. These are presumably due to rapid wet deposition when rain occurs several hours after the release. The closer spacing of the contours for MACCS2 compared with LODI, as one moves away from the release location, is evidence of the more rapid decrease of exposure and deposition with distance for MACCS2. In general, the similarities in the distributions of exposure and deposition shown by these plots are greater than the differences, particularly when consideration is given to the different density (closeness of spacing) of the underlying data. The more complex models certainly show more detail in structure; however, the smoothed distribution still show the common features that we noted in the previous sections on arc and arc-sector averages.

10.4 Summary of Results

All of the arc average and the great majority of the arc-sector average exposures and depositions are within a factor of two when comparing MACCS2 to the state-of-the-art model, LODI. Similar comparisons of RASCAL and RATCHET to LODI also have most exposures and depositions within a factor of two of LODI. In fact the largest differences in results are between the closely related RASCAL and RATCHET models.

We can identify at least two caveats to the discussion of model differences. First, this study was performed in an area with smooth or favorable terrain and persistent winds although with structure in the form of low-level nocturnal jets and severe storms. In regions with complex terrain, particularly if the surface wind direction changes with height, caution should be used. Second, MACCS2 predicts a too rapid decrease of exposure with distance; this should be considered when MACCS2 is used to estimate consequences at distances greater than 321.8 km (200 miles). However, this second caveat is tempered by the fact that the majority of the deposition (and exposure to depositing material) is within this 321.8-km (200-mile) distance.

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APPENDIX A - CONTENTS OF DATA CD

The CD included with this report includes the following:

1) FORTRAN source codes used to read ARM data from the netCDF files and provide input files of meteorological observations for use by MACCS2, RASCAL/ RATCHET, and ADAPT/ LODI,
2) FORTRAN source codes used to convert LODI gridded data to arc-sector exposure and deposition and to calculate the annual weighted average,
3) C shell scripts that cycled through the 610 cases, running ADAPT to provide the wind fields and LODI to produce the integrated exposure and deposition,
4) IDL procedures used for quality control analysis and modification of ADAPT input meteorological observation files,
5) some sample ADAPT and LODI input and output files,
6) some sample individual case and annual average arc-sector concentration files,
7) meteorological data files provided to MACCS2 and RASCAL/ RATCHET,
8) hourly mixing heights and scavenging rates used by ADAPT/ LODI,
9) the list of 610 weather trials and their associated weights,
10) MATLAB m-files used for 2D exposure and deposition plots,
11) C shell script used to cycle through the smoothing of LODI exposures and depositions and a sample input file,
12) sample smoothed exposure and deposition data,
13) file lists for each type of arm data.

Many of the source codes and scripts locate files within the specific directory structure that was used at LLNL for this project. The CD uses this same directory structure to organize the files. On the computer used for this project the directory structure given below is a subdirectory in my home directory, / u/ cmole/ nrc. The files were transferred directly from a UNIX system so the files may not be completely compatible with a Windows PC. The subdirectory structure is as follows:

adaptdata	- observed meteorology ASCII input files for ADAPT
adaptrun	- ADAPT run directory (adapt_run.scr, input namelist file, ADAPT output log file
armdata	- ARM data directory (no files)
60wpdn	- NOAA weather profile netCDF data files
915rwp	- 915 MHz ARM profiler netCDF data files
aeri	- AERI data directory (no files)
B1	- AERI netCDF data files for Hillsboro, KA
B4	- AERI netCDF data files for Vici, OK
B5	- AERI netCDF data files for Morris, OK

B6	- AERI netCDF data files for Purcell, OK
C1	- AERI netCDF data files for Central Facility
okm	- Oklahoma Mesonet netCDF data files
smos01	- SMOS netCDF data files for Larned, KA
smos03	- SMOS netCDF data files for Le Roy, KA
smos04	- SMOS netCDF data files for Plevna, KA
smos05	- SMOS netCDF data files for Halsted, KA
smos06	- SMOS netCDF data files for Towanda, KA
smos07	- SMOS netCDF data files for Elk Falls, KA
smos08	- SMOS netCDF data files for Coldwater, KA
smos09	- SMOS netCDF data files for Ashton, KA
smos11	- SMOS netCDF data files for Byron, OK
smos13	- SMOS netCDF data files for Central Facility (Lamont, OK)
smos15	- SMOS netCDF data files for Ringwood, OK
smos20	- SMOS netCDF data files for Meeker, OK
smos21	- SMOS netCDF data files for Okmulgee, OK
smos24	- SMOS netCDF data files for Cyril, OK
smos25	- SMOS netCDF data files for Seminole, OK
sonde	- Sonde netCDF data files
ascondata	- Arc-sector concentration data for each of 610 cases
codes	- Directory for most of the codes (no files)
arac2maccs	- Fortran source codes for converting results from rectangular grid to arc-sectors and averaging results over 610 cases
arm2arac	- Fortran source codes for reading ARM data and preparing ADAPT observed meteorology data files
qc	- IDL source codes for displaying and correcting observed meteorology data files
gridgen	- ADAPT/ LODI grid netCDF files
lodiout	- LODI input namelist files and output files (run log, particle position, exposure, deposition for each case)
lodirun	- LODI run directory (run_cases.scr, lodi_run.scr, incrdat8, jd2md, WeatherTrials.txt, scav_rate.txt)
results	- MATLAB source codes for 2D concentration plots
smoothdata	- Slightly smoothed gridded exposure and deposition netCDF files
smoothing	- Smoothing run directory (smooth_cases.scr, input file)
surfacedata	- Surface data files sent to PNL for RASCAL/ RATCHET and Sandia for MACCS2