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SIMULATION OF OZONE FORMATION IN THE MIDDLE TENNESSEE AREA

A Thesis

Presented for the

Master of Science

Degree

The University of Tennessee, Knoxville

Nianjun Zhou

May 1992

ACKNOWLEDGEMENTS

I would like to express my sincere gratitude to Dr. Wayne Davis and Dr. Terry Miller for their generous guidance and kind help in preparing this thesis. Finally, I would like to thank all my friends for helping me finish the job.

ABSTRACT

This thesis discusses the methods for simulation of ozone formation in the middle Tennessee area for the summer time of the base year of 1988. Two photochemical models developed by Systems Applications Incorporated were used for the modeling purposes. They were the OZIPM-4 model and the Urban AIRSHED model.

As a photochemical trajectory model, the OZIPM-4 model was used first to find the ozone profiles at Hendersonville, TN where a monitoring station is located. The inputs of the model included the hourly emissions (kg/sq-km) of volatile organic compounds and nitrogen oxides by chemical species, the meteorological conditions, the aloft ozone concentration and initial air quality conditions.

The meteorological conditions used in the simulations (wind velocity, temperature and relative humidity) were determined by analyzing the ten highest days of ozone concentrations in the middle Tennessee area for 1986, 1987, and 1988. The trajectories of air parcels passing over the Hendersonville air monitoring site were determined based on the chosen wind field for the ozone formation.

Obviously, different air parcels arrived at Hendersonville at different times. The simulations of ozone formation of those air parcels allowed the development of the ozone concentration profile verse time for the Hendersonville site. The air parcel was initiated at 6:00 AM with the chosen initial

conditions and picked up the hourly emissions of pollutants as it moved toward the Hendersonville site. The approach was basically one of finding a solution in an Eulerian Coordinate System by solving it in a Lagrangian Coordinate System. The research indicated that ozone formation was sensitive to wind field, mixing height, initial conditions, anthropogenic emissions, biogenic emissions and aloft ozone concentration. The results showed that the largest single contribution to ozone formation was from mobile sources.

Finally the Urban AIRSHED model, a numerical grid model, was used to simulate the physical and chemical processes of ozone formation using a 20 x 20 x 3 grid system with 5 km x 5 km horizontal resolution. Vertically, the region was divided into three layers, two layers below the mixing height and one layer above it. The model showed that the ozone peak formed in the later afternoon near Hendersonville if wind direction was from southwest to northeast. It was interesting that an ozone hole was found from the output results, which was located at a large nitrogen oxides source. The discovered ozone hole illustrated the scavenging effects of nitrogen oxides.

The results obtained from the two models were compared. A discussion of the advantages and disadvantages of the two models was included after detailed analyses of the simulation processes and the outputs of the two models.

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ACRONYMS

AIRSHED	A Photochemical Model Developed by SAI
CBD	Center of Business District
CBM-IV	Carbon Bond IV Mechanism
CO	Carbon Monoxide
EPA	Environmental Protection Agency
EKMA	Empirical Kinetics Modeling Approach
LDT	Local Daylight Saving Time
NAAQS	National Ambient Air Quality Standard
NMOC	Nonmethane Organic Compound
NOx	Nitrogen Oxides
NWS	National Weather Service
OZIPM-4	A Photochemical Model Developed by SAI
SAMS	SIP Air Pollution Management System
SCC	Standard Classification Codes
SAI	Systems Applications Incorporated
SIP	State Implementation Plan
UTM	Universal Trans-Mercator
UTK	University of Tennessee at Knoxville

ACRONYMS (CONTINUED)

VOC	Volatile Organic Compound

1.0 INTRODUCTION

As a result of violation of the National Ambient Air Quality Standard (NAAQS) for ozone from 1986 to 1988 in the Nashville, TN metropolitan area, EPA has required the state of Tennessee to revise its State Implementation Plan (SIP) to include a program for meeting the standard by 1996. In order to aid in understanding ozone formation and to help determine ozone control strategies, a research program was carried out to perform comprehensive emission inventories and modeling studies of the area. The program, funded by the Tennessee Department of Health and Environment, was conducted by the Department of Civil Engineering, UTK under the direction of Dr. Wayne T. Davis.

Because of relatively high levels of emissions from point, area, mobile and biogenic sources of VOCs and NOx, unacceptable ozone levels had been formed under certain meteorological conditions in the middle Tennessee area from the 1986 to 1988 period. In order to assess whether the region would be in compliance with the ozone air quality standard in the future, it was necessary to be able to predict the changes of peak ozone concentration in response to proposed changes in source emissions. This requires the simulation of ozone formation by air quality models.

The emission inventories developed by UTK and Davidson County [1,2] were used as the basis for the the computer simulation discussed in this thesis. It was necessary to spatially allocate the emissions of VOC and NOx from emission sources, to speciate the emissions by chemical species, and to distribute the speciated emissions on a hourly basis, after

which modeling was conducted using the OZIPM-4 and the Urban AIRSHED models in the middle Tennessee area. The purpose of the modeling was to verify that a sufficient inventory had been completed and that meteorological conditions were sufficiently understood to allow the prediction of the observed ozone exceedances which occurred in the 1986 - 1988 period. By demonstrating this ability, one can then use the models with future projected inventories to predict future violations of the ozone standard and to test potential control strategies which might be required to meet the standard.

1.1 Literature Review

Theoretically, an air quality model is a mathematical description and simulation of atmospheric transport, diffusion and chemical reactions of pollutants [3]. It operates on a set of inputs which include emissions, topography, and meteorology of an area and produces outputs which describe the air quality of the study area. An air quality model can be classified as a box model, trajectory model, or grid model. The box model is the simplest of the mathematical models. The concept of a box model is that pollutant concentrations in a box are assumed spatially homogeneous and instantaneously mixed, thus only chemical reactions are considered. The trajectory model is based on the atmospheric chemical reaction equations, but unlike the box model which uses a fixed box, it uses a moving box along with a moving coordinate system called the Lagrangian Coordinate System to describe the transport of pollutants. The grid model employs a fixed Cartesian reference system called the Eulerian Coordinate

System for describing atmospheric chemical reactions and atmospheric dynamics including transport and diffusion of pollutants. The simulated region is bounded on the bottom by the ground, on the top by the mixing height, and on the sides by the east-west and north-south boundaries. The basis for the grid model is the equations including atmospheric transport, diffusion and chemical reactions, which express the conservation of mass of each pollutant in a turbulent fluid in which chemical reactions occur [3].

In spite of impressive improvements in air quality in the United States since 1970, the reduction of urban ozone level has proven particularly intractable [4,5], thus further efforts are required to reduce unacceptable ozone levels. The development of photochemical air quality models for ozone formation can be traced back to 1969. EPA recommends two possible modeling approaches which can be used as tools to assist with a better understanding of the relationship between emissions and formation of ozone. The results of the simulation can be used to formulate the SIP to achieve the NAAQS for ozone. The first model is called the Empirical Kinetic Modeling Approach (EKMA) proposed by EPA in the middle 1970s and this approach utilizes a trajectory model. The other modeling approach is based on a grid-based photochemical air quality model, the Urban AIRSHED model.

The EKMA Method

The EKMA method (i.e. the OZIPM-4 Model) was developed by Systems Application Incorporated (SAI) as a procedure to relate levels of peak ozone to levels of VOC and NOx emissions. In March of 1981, EPA issued guidelines for applying the EKMA

method. It utilizes a set of isopleths that depict peak ozone concentrations as a function of the following parameters: morning concentrations of VOCs and NOx, emissions of VOCs and NOx during the day, meteorological conditions, and reactivity of different VOCs mixtures. Since 1984, a newer chemical mechanism, Carbon Bond IV Mechanism (CBM-IV), has been developed and is being utilized by EKMA [6]; 82 chemical equations are used by the method.

In the OZIPM-4 model, an air box containing ozone and its precursors is transported along a chosen trajectory. Supposedly, the horizontal dimensions of the box are such that the concentration gradients are small enough to make the horizontal exchange of air between the box and its surroundings insignificant. This means that the effect of diffusion is ignored by the model. The air within the parcel is assumed to be uniformly mixed at all times. The height is defined from the ground to the mixing height. Generally, the trajectory is defined so that the simulated box of air arrives at the site observing the daily maximum ozone concentration at the time of the observed maximum. As the box moves, it absorbs emissions of ozone precursors. The emissions are assumed to be mixed uniformly within the box.

At the beginning of a simulation, the box is assumed to contain initial concentrations of NMOC, NO, NO_2 and ozone. As time progresses, the height of the box can change because of variations in mixing height. This height is assumed to change with time during a period and to be constant before and after the period, which is decided by the inputs of the model. As the mixing height increases, air as well as ozone and ozone precursors located above the previous mixing height are mixed in, at the same time the volume of the box increases. Air

above from the mixed layer is mixed in. Ozone and its precursors mixed in are assumed to be instantaneously mixed throughout the box.

Concentrations of NMOC species, NO, NO_2 and ozone, within the box are physically decreased by dilution due to the rise in the mixing height, and physically increased both by entrainment of pollutants transported from aloft and by new emissions from ground-level and elevated sources. All species are allowed to react chemically according to the CBM-IV kinetic mechanism. Photolysis rates are functions of the intensity and spectral distribution of sunlight, and vary diurnally according to the time of year and the location.

The Urban AIRSHED Model

The Urban AIRSHED model was developed by SAI, and is used to simulate the numerous physical and chemical processes of ozone and its precursors and yield the concentrations of ozone and other reactive or inert air pollutants. The physical and chemical processes which take place in the atmosphere are treated grid by grid. The physical dynamic processes include the transport and diffusion of the pollutants. The model uses recognized turbulent diffusion theory. The photochemical mechanism is the same mechanism used by the OZIPM-4 model [3,4].

As a complex, gradient transport type model, it employs photochemical reaction equations, an hourly varying wind field, emission rates, and meteorological conditions to calculate three dimensional ozone concentrations. Based on similarity theory, turbulence diffusion coefficients were

calculated as a function of atmospheric stability, and the Urban AIRSHED model incorporates formulations for the coefficients.

The Urban AIRSHED model requires 13 input files. With the exception of certain physical or chemical parameters, the inputs are hourly grid based physical, chemical or emissions related variables. According to the characteristics of contents of these files, they can be categorized as to whether they relate to air quality, meteorology, emissions, chemical reaction parameters or simulation control.

The files related to air quality supply the background information on the air quality of the simulated region for the surrounding and top boundary. The meteorology files specify the hourly temperature of each grid of the surface layer, the hourly mixing height, three dimensional wind field and other required miscellaneous physical parameters. There are two emissions related files: ground level sources and point sources. The file for ground level sources gives the information of hourly grid based speciated emissions of VOCs, NOx and CO from area, mobile and biogenic sources since these are assumed to be ground level sources. The file related to emissions from point sources contains the information on location, stack height, and hourly speciated emissions from these sources.

At the beginning of a simulation, the initial concentrations of ozone and other chemicals of each grid begin to change due to chemical reactions, transport and diffusion. The entire time period of interest is sliced into very tiny time increments. The changes in concentrations are calculated grid by grid and increment by increment. The concentrations at the

end of an increment are calculated to be the concentrations at the beginning of the increment less the changes in the concentrations which occurred during the increment. The changes are caused by these things: chemical reactions, transport, diffusion and emissions. The changes due to the chemical reactions are determined by the concentrations of the pollutants at the beginning of the increment and the chemical reaction rates. The changes because of the transport are calculated according to the pollutants moved in and out by the wind. The changes depend on the concentrations of the pollutants in the grid and its neighbor grids and also the wind direction and speed. The changes resulting from the diffusion are dependent on the differences of the concentration of the grid with the neighbor grid and the characteristics of turbulence, since the diffusion coefficients are determined by the characteristics of turbulence. The emissions of precursors also change the concentrations inside the grid. It is assumed that the emitted precursors are rapidly mixed throughout the grid cell. Vertically, the study region can be separated into layers above and below the mixing height.

The Urban AIRSHED model provides three output files. One of the them is related to the internal calculation process and how the computer simulates the physical and chemical processes of ozone formation. The others give the results of the simulation, namely, the concentrations of ozone and other pollutants. These concentrations are given as hourly average concentrations and instantaneous concentrations of ozone and other pollutants at the beginning of each hour.

The Urban AIRSHED model has been labeled as EPA preferred and as a result the Urban AIRSHED model has been applied to various urban areas including Los Angeles and 15

other cities in the U.S. and abroad. Much of the current interest in the model arises from the need to calculate ozone concentrations as a part of various environmental assessment studies, such as federally required SIP and New Source Reviews. The results of recent application studies indicate that the Urban AIRSHED model provides a sound, practical, and effective means for analyzing a variety of regional air quality problems [4].

1.2 The Principle of Ozone Formation

Ozone is an unstable and reactive chemical, and it is very destructive to the environment, especially to plants and humans. In the troposphere part of the atmosphere, ozone is formed from reactive precursors such as VOCs and NOx with sunlight. When NO_2 is initially present, NO and free oxygen radicals O are formed by NO and oxygen reacting with sunlight (ultraviolet radiation with a wavelength of 430 $x10^{-9}$ meters) as given in equation (2) [7]. Ozone is formed by the reaction of free oxygen radicals and oxygen as shown in equation (3). As a reactive species, ozone continues reacting with NO and thus, NO performs as a scavenger of ozone. If there are no other pollutants available, only a small ozone concentration can be formed.

$$2\,NO + O_2 \longrightarrow 2\,NO_2 \qquad (1)$$

$$NO_2 + \text{sunlight} \longrightarrow NO + O \qquad (2)$$

$$O + O_2 \longrightarrow O_3 \qquad (3)$$

$$O_3 + NO \longrightarrow NO_2 + O_2 \qquad (4)$$

When VOCs and CO are introduced. The reactions are different.

$$R + O_2 \longrightarrow R\text{-}O_2 \quad (5)$$

$$R\text{-}O_2 + NO \longrightarrow RO + NO_2 \quad (6)$$

$$RO + NO_2 \longrightarrow R\text{-}NO_2 + O \quad (7)$$

$$O + O_2 \longrightarrow O_3 \quad (8)$$

R, R-O, $R\text{-}O_2$, and O are free radicals. Reaction (6) removes NO from the reaction sequence. The NO concentration decreases allowing the ozone concentration to increase. Smaller concentrations of VOCs and NOx mean less ozone formation and lower ozone concentrations [7]. It should be noted that reactions represented by equations (1) - (8) are temperature-dependent and some of them are solar radiation-dependent. Hence, higher temperatures and an increase in the intensity of the solar radiation will cause faster reaction rates.

1.3 Objectives of the Thesis

The research was separated into six parts which are listed as follows:

a. to design a grid coordinate system for the study area;

b. to allocate sources for each grid and to speciate the sources of VOCs and NOx;

c. to analyze ozone violations occurring on the ten highest ozone days from 1986 to 1988 and the corresponding meteorological data;

d. to simulate ozone formation by using the OZIPM-4 model;

e. to find the reasons resulting in unacceptable ozone level formation; and

f. to simulate ozone formation by using the Urban AIRSHED model.

The study area was determined to include (1) Davidson County; (2) the seven surrounding counties: Cheatham, Dickson, Robertson, Rutherford, Sumner, Williamson and Wilson; and (3) a 25 mile extension area beyond the boundary of the seven counties. A detailed description of the area can be found in Section 2.

In order to simulate ozone formation, it was necessary to allocate and speciate the VOC and NOx sources. Allocation of sources is defined as spatially and temporally assigning the emissions from pollutant sources to each grid. Speciation is defined as speciating the emissions from pollutant sources by chemical species.

For a better understanding of the problem, the historical data of ozone pollution from 1986 to 1988 were analyzed, especially the ten days of highest ozone concentrations during the period and the correspondent meteorological data. This defined a set of meteorological conditions which were used as the inputs to the OZIPM-4 model and the Urban AIRSHED model.

Once air quality and meteorological data were collected and analyzed, the OZIPM-4 model was used to simulate the ozone formation. Different scenarios were used to represent different simulation conditions, such as different wind fields, temperature profiles, or aloft ozone concentrations. Each scenario provided an ozone profile at the Hendersonville site where the majority of the ozone violation were observed. There were four categories of emission sources: point, area, mobile and biogenics. The contribution of each category was analyzed for downtown Nashville.

In order to estimate the influences of different factors on ozone formation, sensitivity analyses were performed on meteorology and boundary conditions. Factors of temperature, mixing height, wind field and aloft ozone concentration were analyzed to better understand the reasons for the ozone violations. The meteorological inputs and aloft ozone concentrations were revised in an attempt to improve model performance. Finally, the model-predicted ozone concentrations were compared with observed concentrations measured at the monitoring stations in an effort to determine if the OZIPM-4 model could be used to simulate the air quality at the Hendersonville site.

A three dimensional region with a 20 x 20 x 3 grid system was chosen for the simulation of ozone formation by using the Urban AIRSHED model. It covered the Nashville metropolitan area and extended into neighboring counties. The 20 x 20 grid area was smaller than the study area mentioned above in order to reduce the CPU time needed for the simulation. The same meteorological data used by the OZIPM-4 model were used by the Urban AIRSHED model. Unlike the OZIPM-4 model, the Urban AIRSHED model required hourly

speciated emissions for each grid. The simulation of ozone formation provided the detailed patterns of how the ozone was formed and transported. Compared with the OZIPM-4 model, the need for detailed data on the hourly rates and composition of emissions from each grid was one of the most time consuming and expensive requirements of using the Urban AIRSHED model.

2.0 THE DESIGN OF COORDINATE SYSTEMS FOR THE MIDDLE TENNESSEE AREA

The first requirement of the research was to define the study area, because the emission inventories and the simulation of ozone formation had to focus on a chosen area. The extent of the study would only include all areas contributing to the ozone violations of the Nashville Metropolitan area.

The purpose of the overall research program was to find the reasons for formation of unacceptable ozone levels and predict the changes of the peak ozone concentrations in response to the proposed control strategies. Because of the movement of atmospheric pollutants and the nature of photochemical reactions, the highest ozone concentrations were usually observed downwind from the Nashville Metropolitan area. Thus the study area can not be limited only to the metropolitan area; some surrounding areas had to be included in order to consider the influences resulting from the movement of pollutants.

2.1 Description of the Middle Tennessee Area

The study area was separated into three sub-areas according to the geographic locations and influences on the ozone formation of the middle Tennessee area as shown in Figure 2-1:

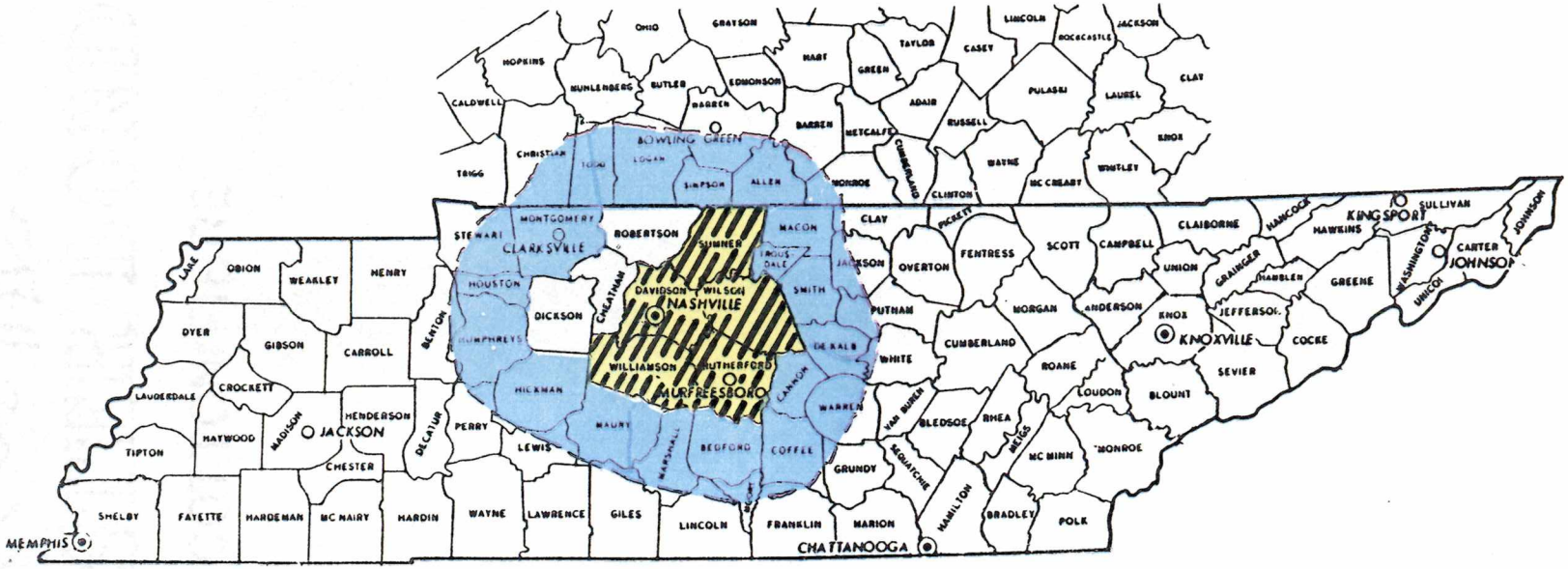


Figure 2-1. The Map of the Middle Tennessee Area

1. Davidson County, where the Nashville metropolitan area is located and listed as a non-attainment county, was the core of the study area.

2. In 1988, the seven counties which encompass Davidson County were called surrounding area (Figure 2-1). These counties were initially designated as non-attainment or proposed non-attainment counties. Since the initiation of the study, five counties of the middle Tennessee area have been officially designated as part of the non-attainment area by EPA. They are Davidson, Wilson, Rutherford, Williamson, and Sumner[1].

3. The 25 mile extension area of the surrounding area was called the affected area. Sources of VOCs, NOx, and CO with emitting greater than or equal to 100 tons/year were included as part of the inventory.

2.2 The Description of Coordinate Systems

The next step was to build a grid system for the study area. The inventories and modeling required a Cartesian coordinate system, which could be used to develop the grid system. The Cartesian Coordinate System selected for use was the Universal Trans-Mercator (UTM) system. Based on the UTM system, a grid system consisted of 5 km x 5 km squares. The grid system was crucial because the inventories of mobile sources, the speciation and allocation of point, area, and mobile sources, and the modeling ozone formations were based on the grid system.

In the UTM system, any point on the earth is defined by three numbers (northing, easting, zone). In particular, the middle Tennessee area is located in zone 16 of the UTM system [8]. The origin of the grid coordinate system for this study was located at (northing 3900, easting 432, zone 16) of the UTM system. The entire study area was divided into small squares with the area of 5 x 5 sq-km to create a grid system, thus a grid was used to define a 5 x 5 sq-km area rather than to define a point. Each grid was assigned a pair of grid numbers called x-east number and y-north number according to the following principles:

1. Grid (1,1) referred to the grid on the upper right of the origin of the grid system, such that the origin was located in the lower left corner of grid (1,1) [9].

2. If a grid number was (i,j), then (i+1, j) was the neighbor grid to the east.

3. If a grid number was (i,j), then (i, j+1) was the neighbor grid to the north.

Based on the principles just mentioned above, the grid system was built for the study area defined in Section 2.1. The range of grid coordinates for the middle Tennessee area was, x-east direction, from -5 to 41; y-north direction, from 0 to 41. Thus the study area was covered by the rectangular area with grid numbers x-east direction from -5 to 41 and y-north direction from 0 to 41. Because some of the grids of the rectangular area did not lie within the study area, a variable called 'type' was introduced. Type 1 referred to the grids in Davidson County and the seven surrounding counties, type 2 referred to the grids in the affected area (25 mile extension),

and type 3 referred to the grids beyond the study area (Table B-1).

Example maps which show the grid system of the middle Tennessee area can be found in Section 7.1.

2.3 The Usage of these Coordinate Systems

Grid based and speciated emissions of ozone precursors were required by ozone simulations, thus all point, area and mobile sources were separated and allocated on a grid basis for modeling purposes.

For a point source, its location was defined by its longitude and latitude. The earth is basically an ellipse. A pair of longitudinal and latitudinal degrees (geodetic coordinates) can define any point on the earth. Because the location of point sources were given by the geodetic system, and the UTM system was used to design the grid system, a transformation between these systems was required. A coordinate transformation was needed for each source. A FORTRAN program titled 'Universal Transverse Mercator Conversion' was used to convert geodetic coordinates to UTM coordinates or vice-versa [8]. For each point source, the execution of the program provided the relevant UTM coordinates, which were used to decide which grid the point source was located in.

Area sources were investigated on a county-wide basis [1,2]. The allocation of these emissions to each grid was needed. A map of the middle Tennessee was used to help allocate the emissions. As pointed out above, either grid numbers or the coordinates of the lower left corner of the grid

can be used to identify the grid. The emissions from area sources were allocated to each grid according to land use. The area sources were grouped as population-based, rural-based, aircraft-based, or railroad-based sources and allocated on this basis to each grid. From the grid based map, the locations of railroad, airports, and rural areas were easily identified. The population of each grid for 1988 was determined based on the method discussed in Appendix A.

The emission inventory for mobile sources was compiled using the grid system. For each grid, the total mileage of roadways and the average daily traffic for each road were used to calculate total vehicle-miles of travel for each of five functional categories of roadways: interstates, U.S. routes (major arterials), state primary highways (minor arterials), state secondary highways (collectors) and local roads.

The maps related to the traffic information were provided on the county basis, and were scaled by the geodetic system only. The UTM coordinates of the left corner of each grid were transformed to the geodetic system. Therefore, the relevant longitudinal and latitudinal degrees were found, which were used to scale the map of each county and to give the map of each grid.

In total, three coordinate systems were used for the research. The three pairs of the coordinates were the grid numbers, the UTM coordinates and the geodetic coordinates of the left lower corner of the grid. With the application of the mentioned FORTRAN program, a dBASE III PLUS file was developed to provide the transformations of all three pairs of coordinates for each grid. Table B-1 of Appendix B provides an

example of the transformations which were extracted from the dBASE III PLUS file.

3.0 ALLOCATION AND SPECIATION OF POLLUTANT EMISSIONS FOR THE MIDDLE TENNESSEE AREA

Both the OZIPM-4 model [6] and the Urban AIRSHED model [10] require the information on the spatial and temporal emissions by chemical species as inputs. This section will use the OZIPM-4 model as an example to show how to speciate and allocate the emission sources. For the OZIPM-4 model, the required inputs are the hourly emissions (by mole) of eight chemical species of VOCs and two species of NOx for each grid.

The necessary data for speciation were supplied by UTK [1] and Davidson County [2]. The university provided the comprehensive inventories of point, area, and mobile sources of the seven surrounding counties, and point sources emitting larger than 100 (ton/yr) in the 25 mile extension area. The detailed definition of the research area was provided in Section 2.1. Davidson County Department of Air Pollution Control supplied the inventory for Davidson County [2].

There are eight chemical species of VOCs and two of NOx used by the OZIPM-4 model as its inputs. The names and molecular weights of these chemical species are listed in Table 3-1.

Regardless of whether it was a point, area, or mobile source, the speciation process for the emissions of the source was accomplished by three steps. The steps were: 1) to determine the grid in which the source was located, 2) to calculate the daily emissions (by mole) of each chemical species of VOCs or NOx for the source in the summer season,

Table 3-1. The Molecular Weights of VOCs and NOx

Class	Species	Molecular Weights
VOC	OLE	26
	PAR	14
	TOL	92
	XYL	106
	FORM	30
	ALD2	29
	ETH	28
	ISOP	68
NOx	NO	30
	NO2	46

and 3) to allocate the daily emission of each species to hourly emissions.

The Urban AIRSHED model contained several data files designed for preparing emission related files for the model [11]. Two of these files were NSC.EPA and SPECIT.EPA. These two files were used to find the VOC and NOx speciation coefficients. From the NSC.EPA file, each SCC code was assigned a hydrocarbon speciation profile code. Furthermore, a set of speciation coefficients related to each hydrocarbon profile code was provided by the SPELIC.EPA file. The coefficients were the speciation coefficients for VOC and NOx.

Originally as two main frame files, these were transferred from the UTK VAX/VMS system to an IBM-PC computer. Several dBASE III PLUS programs were developed to create a file named VOCSPEC.DBF. For a given SCC code, the file could provide the corresponding speciation coefficients of the eight species of VOCs [11].

There were only two speciation coefficients required for speciation for a NOx source with a given SCC code. The speciation coefficients provided by the SPECIT.EPA for all SCC code were the same. Table 3-2 lists the speciation coefficients used for NOx sources.

3.1 Speciation of Point Sources

The information on point sources was stored in a dBASE III PLUS file called NASHTOT.DBF, which was developed by combining the inventory results provided by UTK and Davidson County.

Table 3-2. The Speciation Coefficients for NOx Sources

Species	Coefficients (mole/gram)
NO	0.196667
NO2	0.002174

VOC Speciation

For a VOC point source, the speciation of its emissions required both the information for the source and the speciation coefficients related to the source. NASHVOC.DBF, as a dBASE III PLUS file extracted from NASHTOT.DBF, contained information on all VOC point sources for the study area. The daily emissions by mass of each point source and its location (latitude and longitude) were given in the file. Each point source had a unique SCC code [11] provided by NASHVOC.DBF. This code was used to determine the needed speciation coefficients. Thus the daily emissions of each species were found by multiplying the daily emissions by the relevant coefficient.

Finally, the daily emissions of each chemical were allocated to hourly emissions. It was assumed that the emissions of a point source were distributed evenly throughout the operating time. As pointed out above, the information for each point source was provided by the dBASE III PLUS file, NASHVOC.DBF. This file provided the number of operating hours of each day. For a given value of operating hours, the operating time would be specified using a table in the appendix of [11]. For example, a value of eight operating hours meant an operating time spanning from 8:00 A.M. to 4:00 P.M.

For each operating hour, the temporal distribution coefficient of each hour was calculated and stored in a dBASE III PLUS program called TIMEDIS.PRG. Thus the hourly emissions of a chemical species for a point source were found by multiplying the daily emission by the relevant distribution coefficient provided by TIMEDIS.PRG.

A flow chart of the speciation and the allocation is given in Figure 3-1.

NOx Speciation

Basically, the procedure of speciation of NOx was the same as VOC's. An exception was that there were eight categories of VOCs needed to be speciated, whereas NOx was speciated to only two: NO and NO_2. NASHNOX.DBF, like NASHVOC.DBF, was a file extracted from NASHTOT.DBF. The file had the inventory information of all NOx point sources. Similarly, the assignment of each point source to the relevant grid was accomplished by calculating the grid numbers using the corresponding latitude and longitude. After speciation of the daily emissions of NOx based on the coefficients listed in Table 3-2, the hourly emissions of NO or NO_2 were found by multiplying the daily emissions of NO or NO_2 by the temporal distribution coefficient for the hour.

3.2 Area Sources

The inventories related to the area sources were investigated and were initially prepared on a county-wide basis. The inventories of the seven surrounding counties were provided by UTK, whereas the inventory of the Davidson County area was prepared by Davidson County Department of Air Pollution Control.

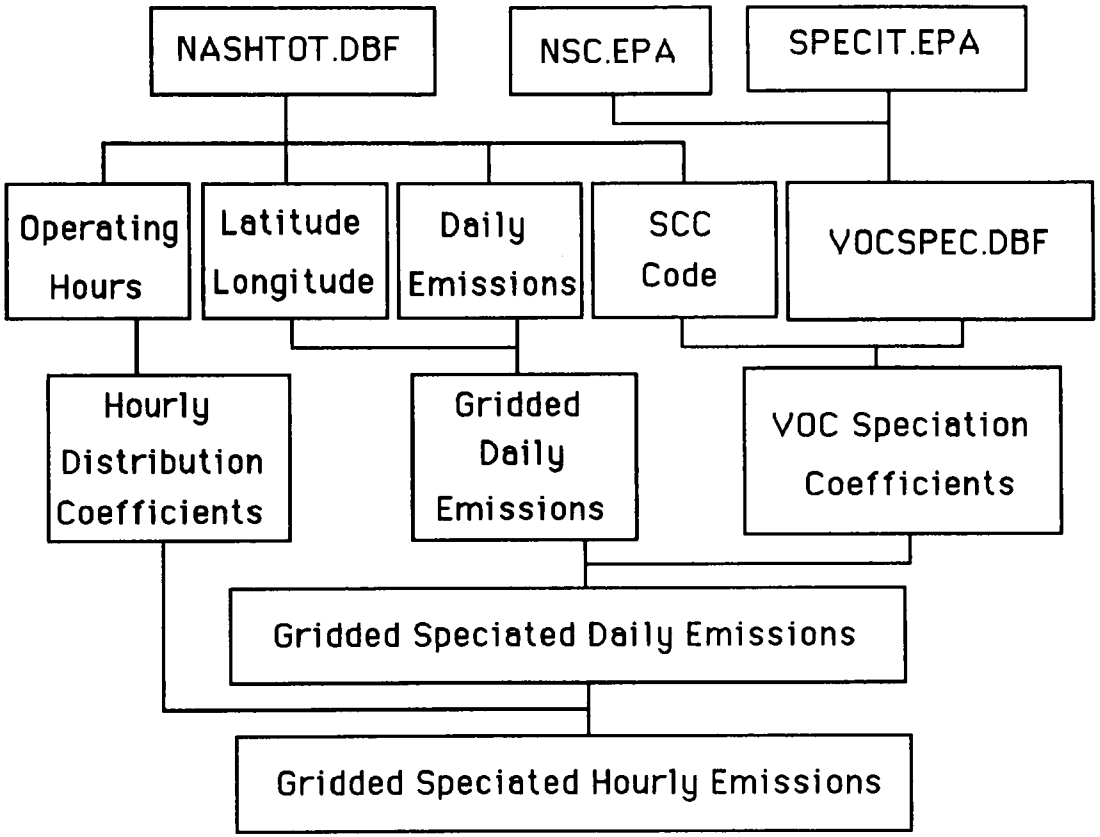


Figure 3-1. The Speciation and Allocation of the VOC Point Sources

1) The Seven Surrounding Counties

Table 3-3 provides a list of 44 source categories related to the pollutant emissions from area sources of the surrounding area. Based on the information previously provided [12], these categories had been divided into five groups. They were: population-based, rural-based, aircraft-based, railroad-based, and recreational boat-based emissions. The results of the inventories supplied by UTK provided all VOC and NOx emissions of all these categories for each of the seven counties [1]. Population-based and recreational boat-based sources were assumed to be emitted evenly over an eight-hour period (8:00 A.M.-4:00 P.M.). Aircraft-based and railroad based sources were assumed to be distribute evenly over twenty-four hours [12]. The rural-based emissions group included five categories: motorcycles, pesticide application, farm equipment, forest fires and non-forest fires. All the categories except forest fires and non-forest fires were assumed to be emitted over eight hours evenly; forest and non-forest fires were assumed to be emitted evenly for twenty-four hours [12].

VOCs Speciation Coefficients for the Surrounding Counties

The daily emissions of each VOC category for each county are listed in Table 3-4. As in the case of emissions from point sources, the emissions of area sources had to be speciated and allocated. From Appendix A1 of [12], for each grid, the daily emissions of VOCs of each group mentioned were provided.

Table 3-3. The Categories of Area Sources of the Seven Surrounding Counties

NO.	PROFILE NO.	CATEGORY CONTENT	GROUP
1	1190	TANK TRUCK UNLOADING	POPULATION BASED
2	1190	UNDERGROUND TANK BREATHING	POPULATION BASED
3	1190	GAS TRUCKS IN TRANSIT	POPULATION BASED
4	1196	COMMERCIAL DRY CLEANING	POPULATION BASED
5	1196	COIN OP DRY CLEANING	POPULATION BASED
6	1195	DECREASING COLD CLEANING	POPULATION BASED
7	1016	ARCHITECTURAL SURFACE COATING	POPULATION BASED
8	1194	AUTO REFINISHING	POPULATION BASED
9	1191	GRAPHIC APPLICATION	POPULATION BASED
10	76	PESTICIDE APPLICATION	RURAL BASED
11	197	COMMERCIAL/CONSUMER SOLVENT USE	POPULATION BASED
12	202	MUNICIPAL SOLID WASTE LANDFILL	POPULATION BASED
13	9022	PUBLIC WATER TREATMENT	POPULATION BASED
14	195	NATURAL GAS-RESIDENTIAL	POPULATION BASED
15	1185	COAL-RESIDENTIAL	POPULATION BASED
16	2	DISTILLATE OIL AND KEROSENE-RES	POPULATION BASED
17	1	RESIDUAL OIL-RESIDENTIAL	POPULATION BASED
18	195	LPG-RESIDENTIAL	POPULATION BASED
19	3	NATURAL GAS-COMMERCIAL	POPULATION BASED
20	1178	COAL-COMMERCIAL	POPULATION BASED
21	2	DISTILLATE OIL AND KEROSENE-COMM	POPULATION BASED
22	1	RESIDUAL OIL-COMMERCIAL	POPULATION BASED

Table 3-3. (Continued)

NO.	PROFILE NO.	CATEGORY CONTENT	GROUP
23	3	LPG-COMMERCIAL	POPULATION BASED
24	3	NATURAL GAS-INDUSTRIAL	POPULATION BASED
25	1185	LPG-INDUSTRIAL	POPULATION BASED
26	2	DISTILLATE OIL AND KEROSENE-IND	POPULATION BASED
27	1	RESIDUAL OIL-INDUSTRIAL	POPULATION BASED
28	3	LPG-INDUSTRIAL	POPULATION BASED
29	1201	RAILROAD	RAILROAD BASED
30	1186	RECREATIONAL BOATS	RECREATIONAL BOATS
31	1186	MOTORCYCLES	POPULATION BASED
32	1201	FARM EQUIPMENT	RURAL BASED
33	1186	CONSTRUCTION EQUIPMENT	POPULATION BASED
34	1186	INDUSTRIAL EQUIPMENT	POPULATION BASED
35	1186	LAWN AND GARDEN EQUIPMENT	POPULATION BASED
36	1099	AIRCRAFT	AIRCRAFT BASED
37	122	ON-SITE INCINERATION-RESIDENTIAL	POPULATION BASED
38	122	ON-SITE INCINERATION-COMMERCIAL	POPULATION BASED
39	122	ON-SITE INCINERATION-INDUSTRIAL	POPULATION BASED
40	307	FOREST FIRES	RURAL BASED
41	307	NON-FOREST FIRES	RURAL BASED
42	121	OPEN BURNING-RESIDENTIAL	POPULATION BASED
43	121	OPEN BURNING-COMMERCIAL	POPULATION BASED
44	121	OPEN BURNING-INDUSTRIAL	POPULATION BASED

Table 3-4. The VOC Emissions of the Seven Surrounding Counties (ton/day)

No.	Cheatham	Dickson	Robertson	Rutherford	Sumner	Williamson	Wilson	Total	Profile
1	0.3188	0.4179	0.5181	1.3269	1.2308	0.9366	0.8225	5.5716	1190
2	0.0277	0.0363	0.0451	0.1154	0.1070	0.0814	0.0715	0.4844	1190
3	0.0078	0.0102	0.0126	0.0323	0.0300	0.0228	0.0200	0.1357	1190
4	0.0670	0.0868	0.1083	0.2803	0.2563	0.1975	0.1725	1.1687	1196
5	0.0206	0.0267	0.0333	0.0862	0.0788	0.0608	0.0531	0.3595	1196
6	0.1288	0.1668	0.2083	0.5389	0.4928	0.3798	0.3317	2.2471	1195
7	0.2201	0.2850	0.3557	0.9208	0.8420	0.6489	0.5668	3.8393	1016
8	0.0978	0.1268	0.1582	0.4096	0.3745	0.2887	0.2521	1.7077	1194
9	0.0412	0.0534	0.0666	0.1725	0.1577	0.1215	0.1062	0.7191	1191
10	0.0581	0.1075	0.4921	0.2523	0.2735	0.2735	0.1665	1.6235	76
11	0.2319	0.3003	0.3747	0.9701	0.8870	0.6837	0.5971	4.0448	197
12	0.0012	0.0035	0.0008	0.0107	0.0003	0.0012	0.0025	0.0202	202
13	0.0078	0.0226	0.0497	0.1231	0.0573	0.0309	0.0608	0.3522	9022
14	0.0005	0.0007	0.0008	0.0022	0.0020	0.0015	0.0014	0.0091	195
15	0.0005	0.0007	0.0008	0.0021	0.0019	0.0015	0.0013	0.0088	1185
16	0.0000	0.0001	0.0001	0.0002	0.0002	0.0001	0.0001	0.0008	2
17	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1
18	0.0001	0.0001	0.0001	0.0003	0.0003	0.0002	0.0002	0.0013	195
19	0.0002	0.0007	0.0006	0.0037	0.0022	0.0031	0.0015	0.0120	3
20	0.0000	0.0001	0.0001	0.0004	0.0002	0.0003	0.0002	0.0013	1178
21	0.0000	0.0001	0.0001	0.0004	0.0002	0.0003	0.0002	0.0013	2
22	0.0000	0.0000	0.0000	0.0001	0.0001	0.0001	0.0000	0.0003	1

Table 3-4. (Continued)

No.	Cheatham	Dickson	Robertson	Rutherford	Sumner	Williamson	Wilson	Total	Profile
23	0.0000	0.0000	0.0000	0.0001	0.0001	0.0001	0.0000	0.0003	3
24	0.0014	0.0015	0.0027	0.0117	0.0064	0.0042	0.0045	0.0324	3
25	0.0104	0.0116	0.0201	0.0879	0.0481	0.0315	0.0335	0.2431	1185
26	0.0001	0.0001	0.0001	0.0005	0.0003	0.0002	0.0002	0.0015	2
27	0.0000	0.0000	0.0001	0.0002	0.0001	0.0001	0.0001	0.0006	1
28	0.0000	0.0000	0.0001	0.0004	0.0002	0.0001	0.0001	0.0009	3
29	0.1272	0.1422	0.1173	0.1551	0.2264	0.2055	0.1653	1.1390	1201
30	0.4595	0.4847	0.4375	1.2740	1.6837	0.8529	1.2448	6.4371	1186
31	0.0083	0.0102	0.0103	0.0573	0.0329	0.0237	0.0212	0.1639	1186
32	0.0881	0.1629	0.7459	0.3820	0.4145	0.3599	0.2524	2.4057	1201
33	0.0000	0.0000	0.0000	0.1881	0.0583	0.3417	0.1118	0.6999	1186
34	0.0203	0.0239	0.0433	0.1811	0.0986	0.0725	0.0686	0.5083	1186
35	0.2197	0.2844	0.3549	0.9189	0.8402	0.0475	0.5656	3.2312	1186
36	0.0000	0.0080	0.0080	0.4840	0.0160	0.0080	0.0000	0.5240	1099
37	0.0147	0.0191	0.0238	0.0616	0.0563	0.0434	0.0379	0.2568	122
38	0.0025	0.0033	0.0041	0.0106	0.0097	0.0075	0.0065	0.0442	122
39	0.0031	0.0034	0.0060	0.0259	0.0142	0.0093	0.0099	0.0718	122
40	0.0775	0.0963	0.1726	0.3297	0.4226	0.0070	0.2618	1.3675	307
41	0.0121	0.0189	0.0584	0.0222	0.0288	0.0034	0.0471	0.1909	307
42	0.0994	0.1287	0.1606	0.4158	0.3802	0.2930	0.2559	1.7336	121
43	0.0023	0.0030	0.0037	0.0096	0.0088	0.0068	0.0059	0.0401	121
44	0.0011	0.0012	0.0021	0.0091	0.0051	0.0033	0.0035	0.0254	121

For each group, a set of speciation coefficients had to be found in order to give the speciated emissions of VOCs for each grid. Each category was given a profile code (Table 3-3), the corresponding speciation coefficients for the code were provided by the dBASE III PLUS file VOCSPEC.DBF (Table B-2, Appendix B). The daily emissions for each group consisted of the emissions from those categories belonging to the group. The method of weighted average was used to find the speciation coefficients for the group by using the relevant coefficients of the categories.

The population-based daily emissions were the sum of the emissions from 36 categories of VOCs (Table 3-3). For a given county, if E_i (i=1 to 36) was the emitted VOCs by mass of the i-th population-based category in Table 3-4, and a_{ij} was the speciation coefficient of the j-th (j=1 to 8, Table 3-1) chemical species for i-th VOCs pollutant given in Table B-2, then

$$a_j = \frac{\Sigma E_i a_{ij}}{\Sigma E_i} \qquad (9)$$

The values of a_j (j=1 to 8) were the weighted average speciation coefficients for population-based emissions. Table 3-5 provided the weighted average speciation coefficients for the seven counties.

Because it was not possible to simply assume that the rural-based emissions for each grid were emitted over 24 hours evenly, two sets of speciation coefficients for rural-based emissions were determined for each county. One was for

Table 3-5. The Speciation Coefficients for Population-Based Emissions (The Seven Surrounding Counties)

County	Cheatham	Dickson	Robertson	Rutherford	Sumner	Willamson	Wilson
OLEMOLE	0.00269173	0.00268528	0.00264843	0.00254417	0.00265261	0.00251265	0.00259878
PARMOLE	0.10425725	0.10381206	0.10235205	0.09882645	0.10274800	0.09022843	0.10086707
TOLMOLE	0.00456677	0.00456708	0.00448566	0.00427299	0.00450002	0.00462475	0.00438317
XYLMOLE	0.00431710	0.00432680	0.00424490	0.00403955	0.00426224	0.00430958	0.00414803
FORMMOLE	0.00019302	0.00019139	0.00018911	0.00018467	0.00019016	0.00014327	0.00018778
ALD2MOLE	0.00123756	0.00123016	0.00121528	0.00119787	0.00122679	0.00068227	0.00121689
ETHMOLE	0.00089180	0.00090170	0.00092891	0.00095165	0.00090989	0.00085881	0.00093520
ISOPMOLE	0.00000683	0.00000677	0.00000671	0.00000671	0.00000681	0.00000146	0.00000684

the emissions from 8:00 A.M. to 4:00 P.M., the other was the emissions from 4:00 P.M. to 8:00 A.M.

Similarly, Equation (9) was used to determine the speciation coefficients of the rural-based emissions from 8:00 A.M. to 4:00 P.M. for each county. Because the rural-based group only contained five categories, the range of i was from 1 to 5 in Equation (9) instead of from 1 to 36. The speciation coefficients are listed in Table B-3 (Appendix B) for all the seven counties. It should be noted that the emitted VOC values (Ei) used for forest and non-forest fires were one-third of the values provided in Table 3-4, because forest and non-forest fires were logically assumed to occur evenly over twenty-four hours, rather than evenly over eight hours. The speciation coefficients for rural-based emissions from 8:00 A.M. to 4:00 P.M. are shown in Table B-3.

From 4:00 P.M. to 8:00 A.M., only forest and non-forest fires categories contributed to rural-based emissions. Because the emissions of forest and non-forest fires had the same profile code, i.e. code 307 (Table 3-3), the speciation coefficients referred to code 307 in Table B-2 were the speciation coefficients for rural-based emissions from 4:00 P.M. to 8:00 A.M.

The profile codes for aircraft-based, railroad-based, and recreational boat-based were 1099, 1201, and 1186. Each of the three groups consisted of only one category (Table 3-3). The speciation coefficients for these groups are given in Table B-2 by relating the corresponding profile codes to the coefficients given in Table 3-3. These coefficients are listed in Table B-4.

VOC Speciation and Allocation for the Seven Surrounding Counties

The speciation coefficients for each grid were used to speciate the daily emissions of VOCs of the group for each grid. Furthermore, the speciated emissions of each group were temporally allocated to give the hourly emissions.

For the population-based group, the daily emissions of a VOC species for a given grid were found by multiplying the daily emissions by the relevant speciation coefficients of the county where the grid was located. The pollutants from sources of population-based group were assumed to be emitted evenly over eight hours from 8:00 A.M. to 4:00 P.M. The hourly emissions for each VOC species from 8:00 A.M. to 4:00 P.M. were the daily emissions divided by eight, and the hourly emissions from 4:00 P.M. to 8:00 A.M. were assumed to be zero.

For the rural-based group, the pollutants could be assumed to be emitted evenly from 8:00 A.M. to 4:00 P.M. and from 4:00 P.M. to 8:00 A.M.. Therefore, the emissions of the two periods needed to be calculated first from the daily VOC emissions. Two coefficients RU1 and RU2 were introduced, these were the mass ratios of the emissions from 8:00 A.M. to 4:00 P.M. and 4:00 P.M. to 8:00 A.M. over the overall daily rural emissions, respectively. The coefficients were county-based variables. The following was the formula used to calculate RU1 and RU2 coefficients. Naturally, the sum of RU1 and RU2 was equal to 1. In fact, among all categories of the rural-based group, only forest and non-forest fires were assumed to emit evenly over 24 hours. For the categories of forest and non-forest fires, the emissions from 4:00 P.M. to 8:00 A.M.

were two thirds of the overall daily emissions from forest and non-forest fires. The results are listed in Table B-5 (Appendix B).

$$RU2 = \frac{2*(\text{sum of emissions of forest and non-forest fires})/3}{(\text{sum of emissions of the rural-based group})} \quad (10)$$

$$RU1 = 1 - RU2 \quad (11)$$

By using RU1 and RU2, the emissions from 8:00 A.M. to 4:00 P.M. and from 4:00 P.M. to 8:00 A.M. for a grid could be found. Thus the hourly speciated emissions of each VOCs species were found by speciating the rural-based emissions from 8:00 A.M. to 4:00 P.M. or from 4:00 P.M. to 8:00 P.M. distributing the speciated emissions evenly over eight hours or over sixteen hours, respectively.

The hourly speciated results for aircraft-based, railroad-based, and recreational boat-based groups were calculated using the same method. The only difference was that the emissions from aircraft-based group and railroad-based VOCs were assumed to be emitted over 24 hours evenly and the emissions from recreational boat-based group were only emitted over eight hours evenly.

Finally, the hourly emissions of each species for each hour were the sum of all the corresponding hourly speciated emissions of all five groups.

A flow chart of the speciation and the allocation is given in Figure 3-2.

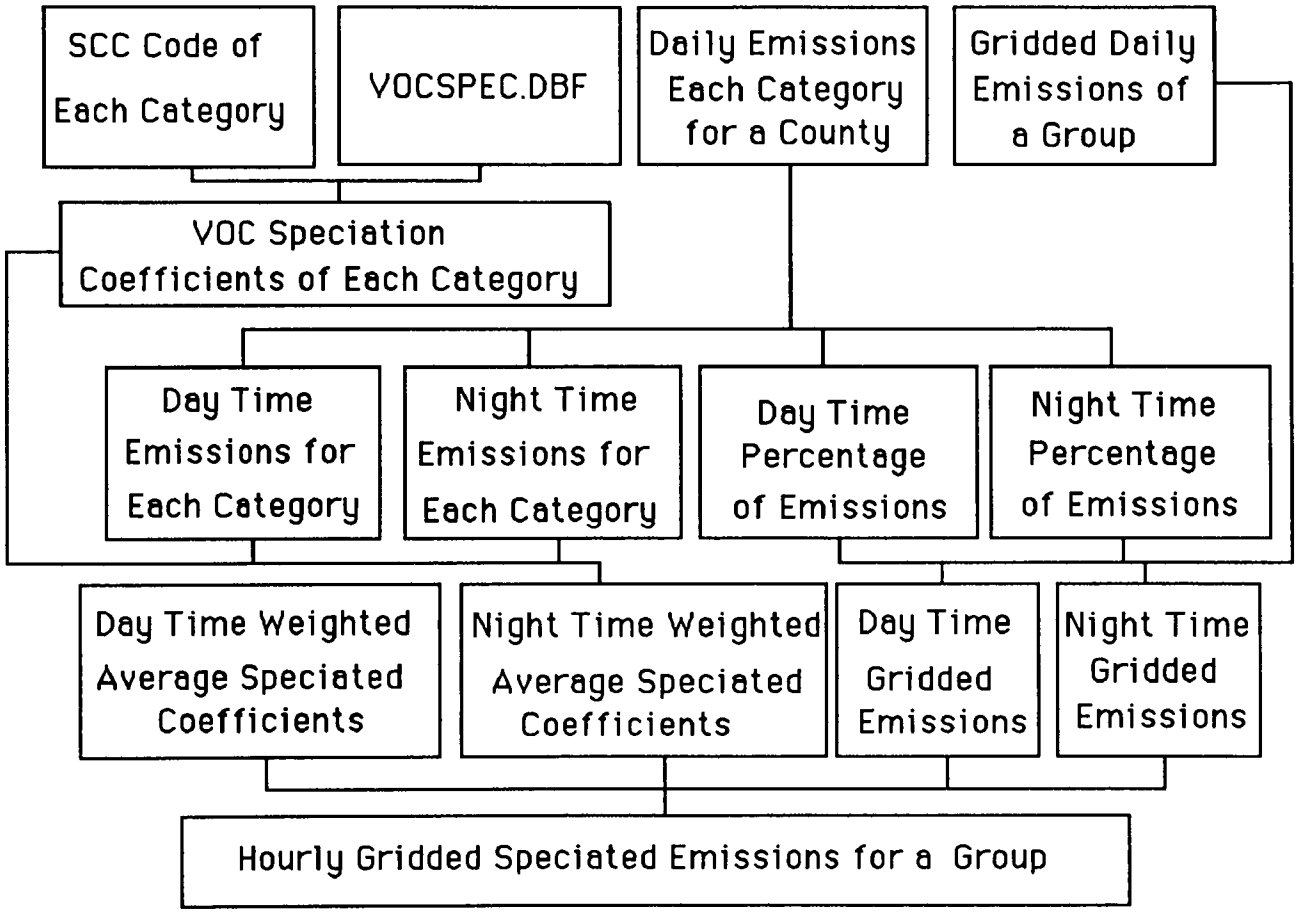


Figure 3-2. The Speciation and Allocation of the VOC Area Sources (the Seven Surrounding Counties)

NOx Speciation and Allocation for the Seven Surrounding Counties

The NOx sources, like VOCs sources, were investigated according to the categories listed in Table 3-3. These categories were separated into five groups [12]: population-based, rural based, aircraft-based, railroad-based and recreational boat-based sources. The daily emissions of each grid for the group were given by [12]. The emissions from population-based, aircraft-based, railroad-based and recreational boat-based sources were assumed to be emitted evenly over 8 hours, 24 hours, 24 hours, and 8 hours, respectively. The allocation for NOx sources was finished the same as the allocation for VOC sources. Table B-5 gives the temporal distribution coefficients of the emissions of the rural-based group from 8:00 A.M. to 4:00 P.M. and from 4:00 P.M. to 8:00 A.M.. Thus the hourly emissions of each group for each grid were found. With the application of the same procedure of speciating VOCs, the hourly emissions of NO and NO_2 were found for each group. By summing the hourly emissions of NO and NO_2 for all the groups, the hourly emissions by mole of NO and NO_2 for each grid were determined.

2) Davidson County

Davidson County [2] provided the inventories for VOC and NOx sources. From the information provided by [12], the daily emissions of VOCs and NOx for each grid of the county were given. The temporal allocation and the speciation coefficients

for VOCs and NOx were needed in order to allocate and speciate the emissions.

Speciation and Allocation of VOC Sources

The weighted average method was used again to find the speciation coefficients needed for speciation. There were a total of 44 categories of emission sources (Table 3-6). They were separated into two groups. One group dealt with sources emitted evenly over eight hours while the other group dealt with those emitted over 24 hours. Two sets of temporal allocation and speciation coefficients were found for the time periods from 8:00 A.M. to 4:00 P.M. and from 4:00 P.M. to 8:00 A.M.. From Table 3-6, the emissions from the group emitted over 8 hours and 24 hours were 15207.550 ton/yr and 1091.136 ton/yr, respectively. Thus, the fraction of emissions from 8:00 A.M. to 4:00 P.M. over the total daily emissions was:

$$\frac{15207.550+1091.136/3}{15207+1091.136} = 0.955$$

The fraction of emissions from 4:00 P.M. to 8:00 A.M. was:

$$1- 0.955 = 0.045$$

Table B-6 (Appendix B) lists the speciation coefficients of each category and its emissions over the daytime (From 8:00 A.M. to 4:00 P.M.). The weighted average speciation coefficients for the day time and night time are listed in Table B-7 (Appendix B).

Table 3-6. The VOC Emissions of Davidson County (ton/yr)

CATEGORY	EMISSIONS	PROFILE CODE	OPERATING HOURS
GASOLINE AND CRUDE OIL STORAGE (FIXED ROOF)	0.904	297	8
VOL STROAGE	3.730	9024	8
VOL TRANSFER (OTHER)	9.950	9024	8
GASOLINE BULK PLANTS	4.116	9024	8
SERVICE STATIONS (TANK TRUCK UNLOADING)	389.667	1190	8
SERVICE STATIONS (VEHICLE REFUELING)	2656.730	1100	8
SERVICE STATIONS (TANK BREATHING LOSSES)	266.745	1190	8
SERVICE STATIONS (TANK TRUCKS IN TRANSIT)	94.566	1190	8
INORGANIC CHEMICAL MANUFACTURE	0.301	0	8
PLASTIC PRODUCTS MANUFACTURER	9.500	9005	8
OTHERS	35.741	0	8
PAPER PRODUCTS	9.739	1189	8
MISCELLANEOUS METAL PRODUCTS	18.273	9009	8
PLASTIC PRODUCTS	6.024	9014	8
OTHERS	18.642	0	8
ARCHITECTURAL COATINGS	1291.163	1016	8
AUTO REFINISHING	584.600	1194	8
OTHERS	3.414	0	8
SOLVENT METAL CLEANING (COLD CLEANERS)	682.876	1081	8
DRY CLEANING (PERCHLOROETHYLENE)	409.270	1196	8
ADHESIVES	16.566	1088	8
CONSUMER/COMMERCIAL SOLVENT USE	1815.795	197	8

Table 3-6. (Continued)

CATEGORY	EMISSIONS	PROFILE CODE	OPERATING HOURS
MUNICIPAL WASTE LAND FILLS	8.720	202	8
OPEN BURNING (ON-SITE INCINERATION)	2.106	122	8
OPEN BURNING (RESIDENTIAL)	25.871	121	8
COMMERCIAL/INSTITIONAL	0.613	1085	8
COMMERCIAL BAKERIES	158.434	1085	8
PESTICIDE APPLICATION	5.930	76	8
STA. EXTERNAL COMBUSTION (COAL)	18.832	1185	8
STA. EXTERNAL COMBUSTION (FUEL OIL)	3.207	2	8
STA. EXTERNAL COMBUSTION (NATURAL GAS)	43.574	3	8
STA. EXTERNAL COMBUSTION (LP GAS)	2.906	4	8
STA. EXTERNAL COMBUSTION (FOREST FIRES)	39.909	307	24
STA. EXTERNAL COMBUSTION (STRUCTURE FIRES)	74.000	307	24
WASTE DISPOSAL COMBUSTION	0.003	307	8
OTHER VOCs SOURCES	3959.870	0	8
NON-HIGHWAY VEHICLES (RAIL)	694.001	1201	24
NON-HIGHWAY VEHICLES (AIRCRAFT)	283.226	109	24
NON-HIGHWAY VEHICLES (VESSELS)	987.774	1186	8
NON-HIGHWAY VEHICLES(OFF-HIGHWAY MOTORCYCLES)	51.378	1189	8
NON-HIGHWAY VEHICLES(FARM EQUIPMENT)	4.423	1201	8
NON-HIGHWAY VEHICLES(CONSTRUCTION EQUIPMENT)	773.571	1186	8
NON-HIGHWAY VEHICLES(INDUSTRIAL EQUIPMENT	289.425	1186	8
NON-HIGHWAY VEHICLES(LAWN AND GARDEN EQUIPMENT	542.601	1201	8

With the two sets of speciation coefficients, the emissions of each species for a chosen grid were calculated. By distributing the results evenly over eight or sixteen hours, the hourly emissions of the species for each grid were determined.

A flow chart of the speciation and the allocation is given in Figure 3-3.

NOx Speciation and Allocation for Davidson County

NOx emissions of Davidson County are listed in Table 3-7. The emissions from the sources emitted over eight hours evenly were 5574.604 tons/yr, and from the sources emitted over twenty-four hours 3430.819 tons/yr. Then, the fraction of emissions from 8:00 A.M. to 4:00 P.M. over the total emissions was:

$$\frac{5574.604 + 3430.819/3}{5574.604 + 3430.819} = 0.746$$

The fraction of emissions from 4:00 P.M. to 8:00 A.M. was,

$$1 - 0.746 = 0.254$$

Similarly, the hourly emissions of NO and NO_2 for each grid were calculated using the same method for VOC sources.

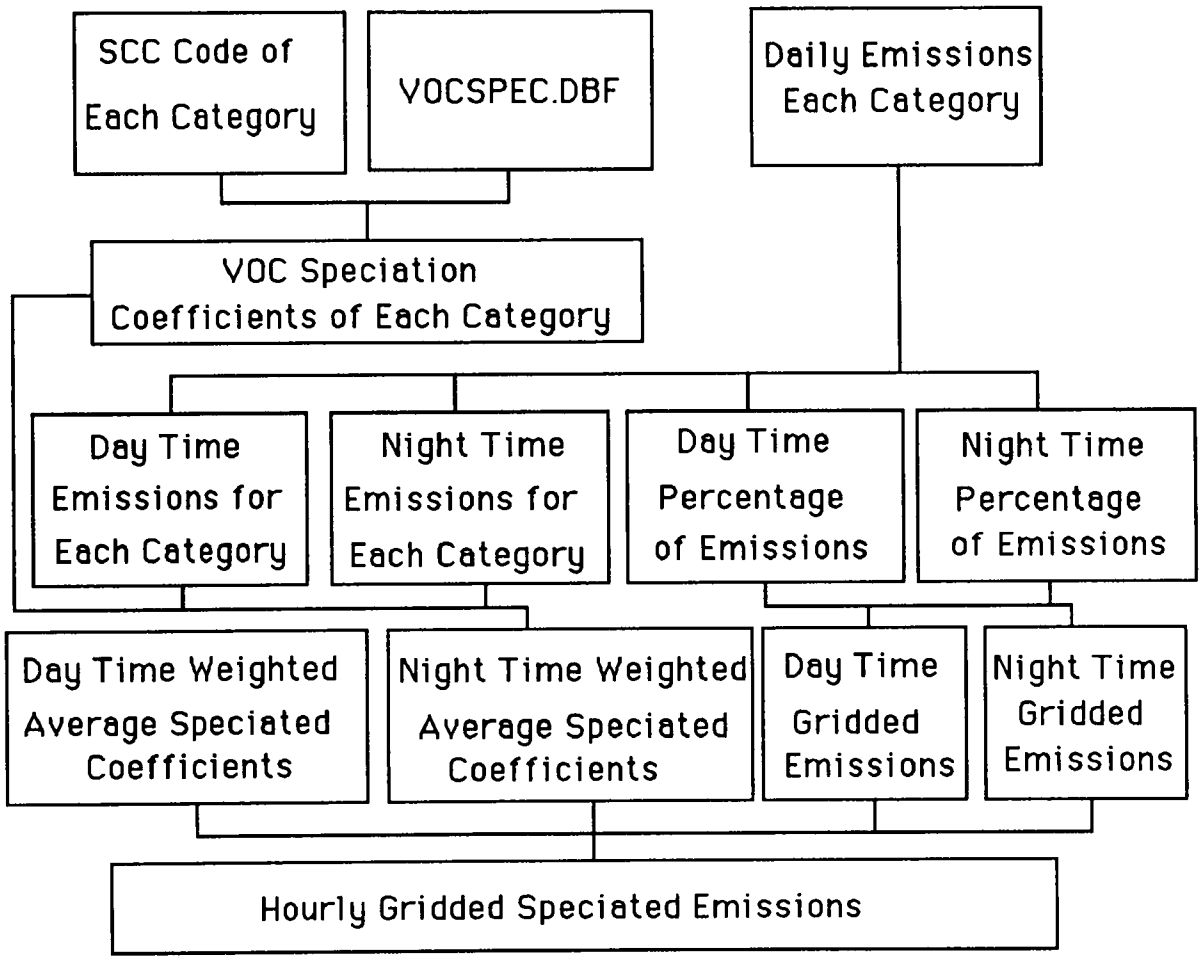


Figure 3-3. The Speciation and Allocation of the VOC Area Sources (Davidson County)

Table 3-7. The NOx Emissions of Davidson County (ton/yr)

CATEGORY	EMISSIONS	PROFILE CODE	OPERATING HOURS
INDUSTRIAL BOILERS	542.031	297	8
COMMERCIAL/INSTIT./RESIDENTIAL	1127.089	9024	8
WASTE DISPOSAL	72.703	9024	8
OPEN BURNING	8.707	9024	8
MINERAL PRODUCTS (CEMENT)	0.002	1190	8
MINERAL PRODUCTS (GLASS)	14.056	1100	8
MINERAL PRODUCTS (OTHERS)	34.773	1190	8
NON-HIGHWAY VEHICLES (RAIL)	2731.784	1190	24
NON-HIGHWAY VEHICLES (AIRCRAFT)	699.035	0	24
NON-HIGHWAY VEHICLES (VESSELS)	485.745	9005	8
NON-HIGHWAY VEHICLES (OTHERS)	3289.498	0	8

Section 3.3 Speciation and Allocation of Mobile Sources

The daily emissions of VOCs and NOx for each grid of Davidson County can be found in Appendix A-4 of [2], and the hourly emissions of VOCs and NOx for the seven surrounding counties were provided by UTK.

VOC Speciation of Mobile Sources for the Seven Surrounding Counties

For mobile sources, there were three categories of emissions: gasoline exhaust, gasoline evaporation and refueling, and diesel vehicles. The VOCs speciation coefficients for these categories were different. The hourly emissions of each category for a grid were found first by separating the hourly emissions given by UTK. Then the hourly emissions of each category were speciated and summed up to get the hourly speciated emissions for each species.

The inventories only provided the hourly emissions of VOCs and NOx for each grid. The mass distribution ratios for the three categories were needed in order to find the hourly emissions of each category. By running the MOBILE-4 [13] model under the speed of 19.6 miles/hr (Average Speed of Federal Test Procedure), these ratios was calculated with some simple mathematical calculations (Table 3-8). Thus the hourly emissions of each category for each grid were the hourly emissions of the grid multiplied by the relevant ratio.

Three sets of speciation coefficients, provided by VOCSPEC.DBF, were used (Table B-8, Appendix B). They were,

Table 3-8. The Hourly Mass Distribution Ratios

Time (hour)	Gasoline Exhasut	Gasoline Evaportion	Diesel Exhaust
00:00-01:00	0.459913	0.517442	0.022234
01:00-02:00	0.481000	0.497024	0.022457
02:00-03:00	0.489617	0.486893	0.022593
03:00-04:00	0.494951	0.481968	0.022730
04:00-05:00	0.498348	0.478551	0.022776
05:00-06:00	0.501758	0.475847	0.022823
06:00-07:00	0.492322	0.483909	0.022684
07:00-08:00	0.459032	0.517840	0.022190
08:00-09:00	0.455234	0.523151	0.021104
09:00-10:00	0.430902	0.548646	0.019188
10:00-11:00	0.405527	0.576977	0.017374
11:00-12:00	0.387798	0.595705	0.016194
12:00-13:00	0.377947	0.606705	0.015499
13:00-14:00	0.374659	0.609915	0.015205
14:00-15:00	0.375289	0.608249	0.015330
15:00-16:00	0.373334	0.610978	0.015143
16:00-17:00	0.377947	0.606705	0.015499
17:00-18:00	0.387260	0.596110	0.016170
18:00-19:00	0.403097	0.579246	0.017214
19:00-20:00	0.425121	0.554802	0.018771
20:00-21:00	0.436454	0.541918	0.019660
21:00-22:00	0.449636	0.530132	0.020599
22:00-23:00	0.456275	0.521371	0.021426
23:00-24:00	0.458397	0.520469	0.021802

the coefficients for (1) the emissions from the exhaust of light duty gasoline vehicles (LDGV), (2) the emissions from evaporation and refuel of light duty gasoline vehicles (LDGV), and (3) the emissions from heavy duty diesel vehicles [11].

For each grid, the hourly emissions of a category for a VOC species were the hourly emissions of VOCs of the grid multiplied by the corresponding mass distribution ratio in Table 3-8 and the speciation factor in Table B-8. The sum of all three categories provided the hourly emissions of the species. A flow chart of the speciation and the allocation is given in Figure 3-4.

NOx speciations were accomplished in the same manner.

Speciation of Mobile Sources of Davidson County

For each grid, the daily emissions of VOCs and NOx for mobile sources were provided [2]. Compared with the speciation for the surrounding area, an extra step of temporal allocation was needed. A flow chart of the speciation and the allocation is given in Figure 3-5. Because of the lack of temporal distribution coefficients for Davidson County, the coefficients developed for Rutherford County were used. By using the hourly emissions information of VOCs and NOx of Rutherford County, the temporal distribution factors for VOCs and NOx were found and given in Table 3-9 and Figures 3-6 and 3-7. The reason for choosing Rutherford County was that it was the second most industrialized county in the middle Tennessee area. The coefficients for Rutherford County were the best coefficients available. After allocating the daily

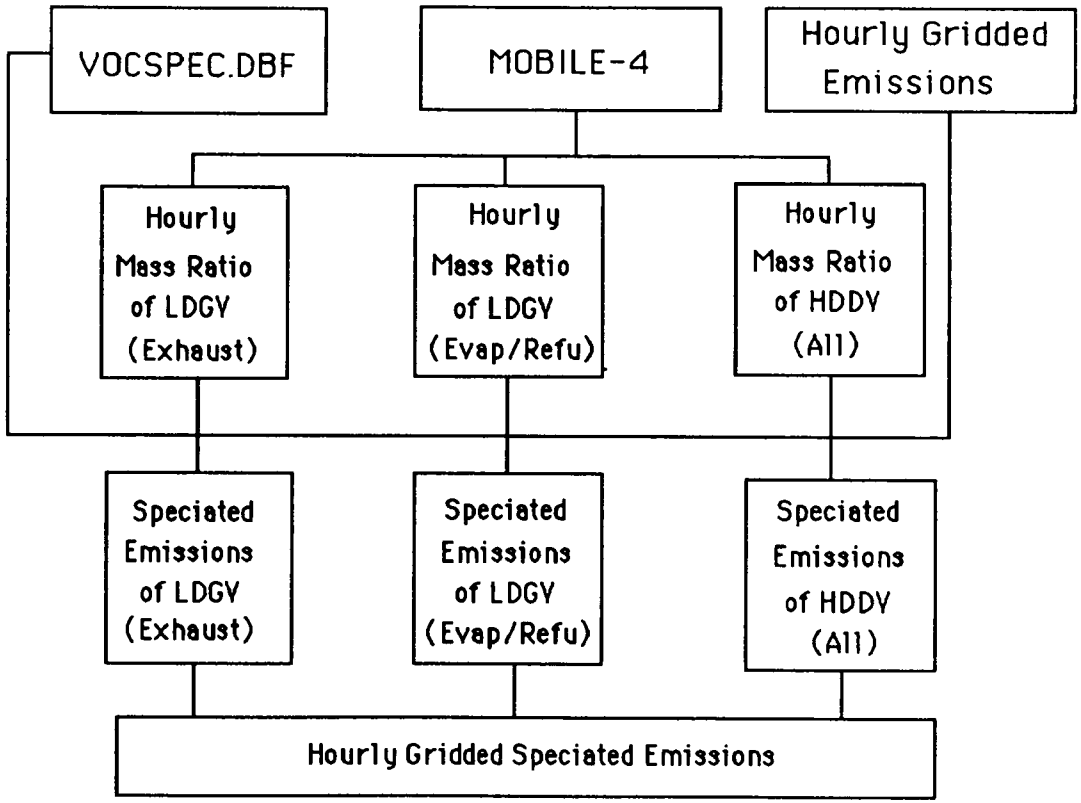


Figure 3-4. The Speciation of the VOC Mobile Sources (the Seven Surrounding Counties)

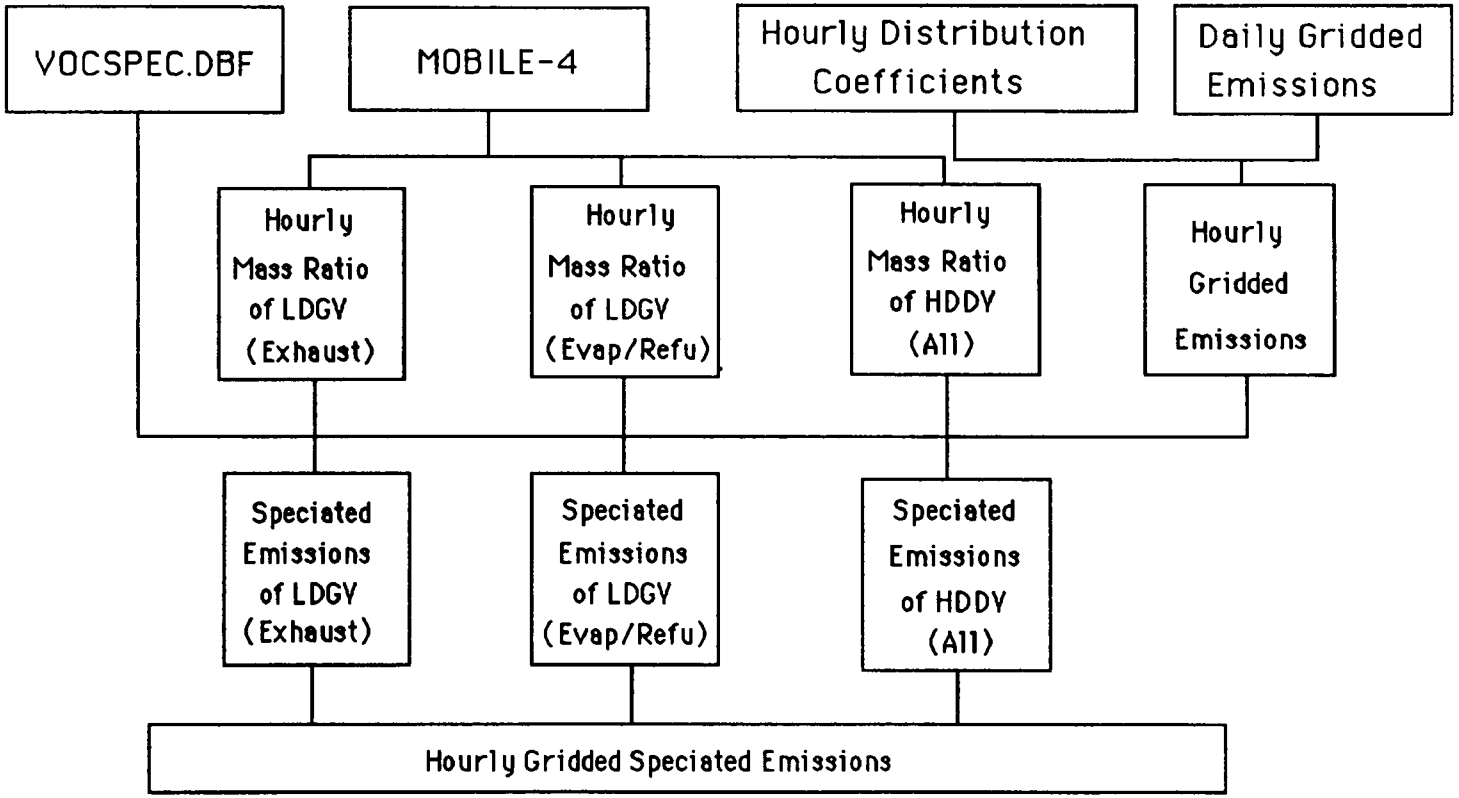


Figure 3-5. The Speciation of the VOC Mobile Sources (Davidson County)

Table 3-9. The Temporal Allocation Coefficients

(Rutherford County)

Time	VOC	NOx
00:00-01:00	0.01953	0.02568
01:00-02:00	0.01295	0.02107
02:00-03:00	0.00669	0.01546
03:00-04:00	0.00564	0.01374
04:00-05:00	0.00549	0.01364
05:00-06:00	0.00734	0.01494
06:00-07:00	0.01728	0.02624
07:00-08:00	0.04638	0.04992
08:00-09:00	0.05287	0.05985
09:00-10:00	0.04359	0.05398
10:00-11:00	0.04520	0.05241
11:00-12:00	0.05240	0.05447
12:00-13:00	0.06182	0.05202
13:00-14:00	0.06752	0.05514
14:00-15:00	0.06733	0.05385
15:00-16:00	0.07101	0.05724
16:00-17:00	0.06633	0.05916
17:00-18:00	0.07327	0.05826
18:00-19:00	0.06122	0.05826
19:00-20:00	0.06365	0.05002
20:00-21:00	0.04946	0.04608
21:00-22:00	0.04296	0.04013
22:00-23:00	0.03451	0.03621
23:00-24:00	0.02556	0.03218

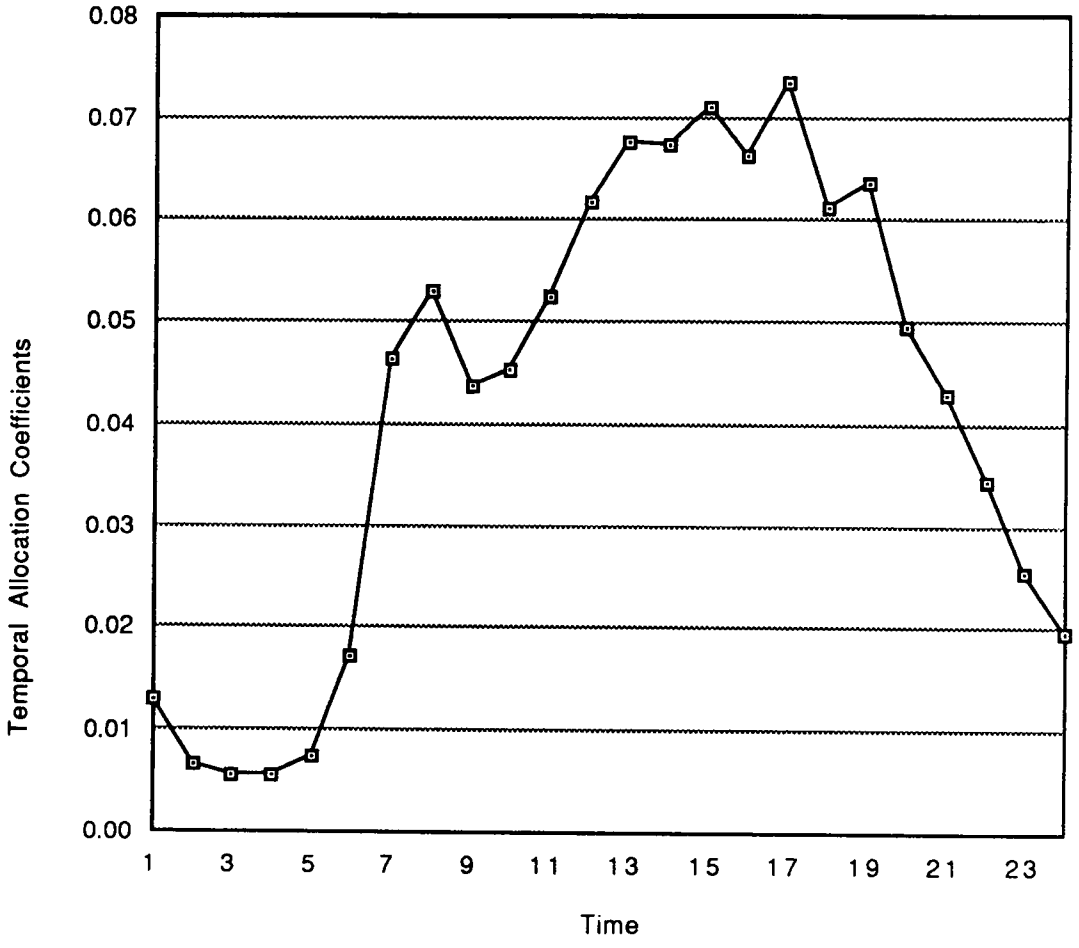


Figure 3-6. The Temporal Allocation Coefficients for Mobile Sources (VOC) (Rutherford County)

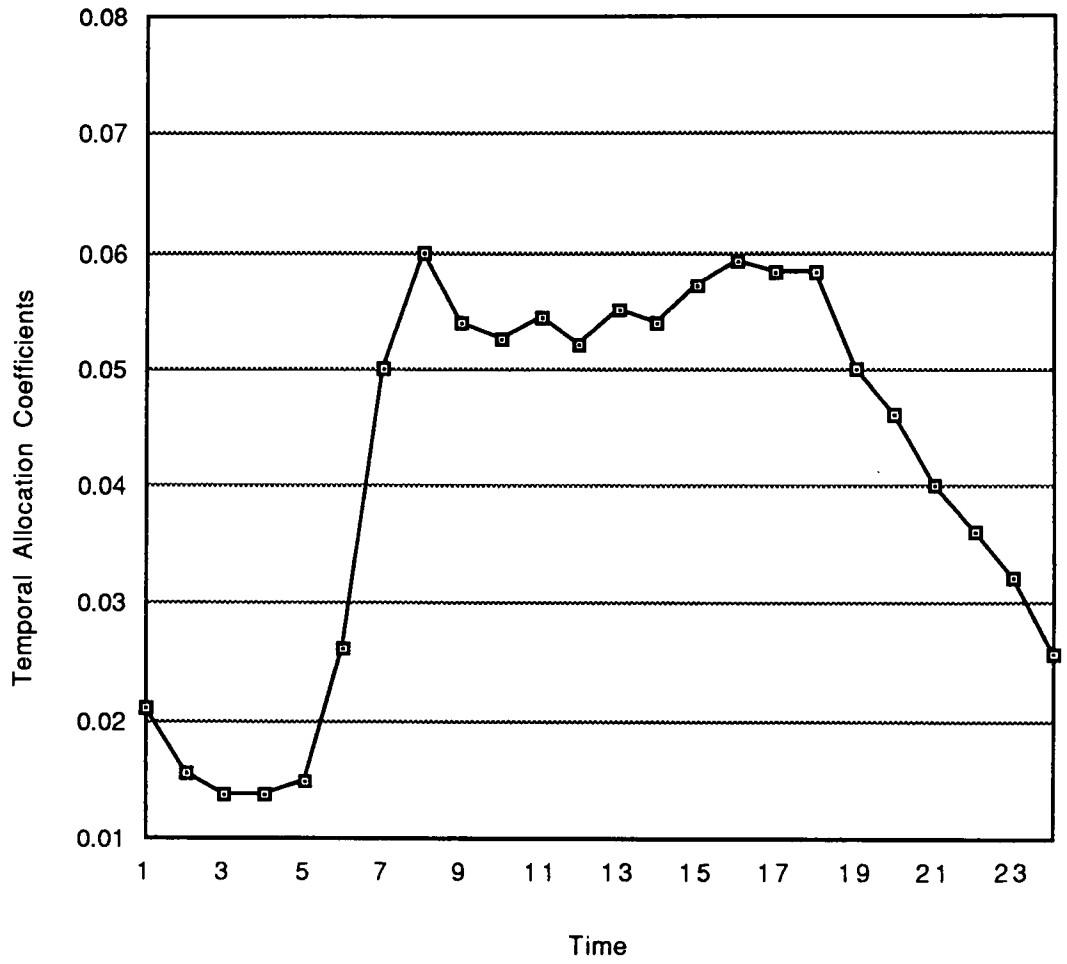


Figure 3-7. The Temporal Allocation Coefficients for Mobile Sources (NOx) (Rutherford County)

emissions of VOCs and NOx to hourly emissions, the speciation of VOCs and NOx for Davidson County was done using the same procedure as the speciation for the seven surrounding counties.

4.0 OZONE VIOLATIONS IN THE MIDDLE TENNESSEE AREA

The formation of ozone is a large concern in the Nashville metropolitan area and the seven surrounding counties. There are seven monitoring stations located in the study area. An exceedance is defined as a one-hour average of ozone concentration which is higher than the current 0.12 ppm NAAQS for ozone [7,10]. An area is considered in violation of the ozone standard if there is more than one exceedance per year. In general, this is reviewed on a rolling three year basis such that an area is classified non-attainment area if there are more than three exceedances in any three year period.

Table 4-1 lists the ten highest ozone violations from 1986 to 1988 [7]. Table B-9 (Appendix B) gives the detailed ozone monitoring data for these days. The contours of the maximum and minimum ozone concentrations observed at each hour for the ten highest days is shown in Figure 4-1. Although the peaks of ozone concentrations occurred as early as at 11:00 AM, or as late as at 6:00 PM, the peaks were generally observed in the late afternoon (Tables 4-1 and B-9). During the evening hours the ozone concentration declined back to a low level (Table B-9) due to scavenging by other pollutants and the lack of sunlight.

4.1 Precursor Emissions and Meteorological Conditions

A logical question is why there were ozone exceedances in the middle Tennessee area. An ozone exceedance occurs because of relative high emissions of ozone precursors

Table 4-1. The Ten Highest Ozone Violations

Date	Max Ozone Conc. (ppm)	Time	Max Temperature (F)	Wind Speed (m/sec)	Wind Direction	Location
87-08-03	0.150	12:00	99	9.8	SW	Hendersonville
88-06-20	0.145	11:00	98	9.3	NW	East Health
87-08-25	0.143	14:00	96	9.3	SW	Hendersonville
86-08-25	0.142	17:00	91	8.2	S	Hendersonville
86-06-22	0.139	11:00	96	10.5	SW	Hendersonville
86-07-24	0.138	13:00	99	6.9	W	Hendersonville
88-06-14	0.138	16:00	95	7.1	NW	Hendersonville
88-07-09	0.138	11:00	103	13.0	ESE	Hendersonville
88-08-01	0.138	11:00	98	6.6	S	Hendersonville
88-05-27	0.137	17:00	83	7.4	SW	Hendersonville

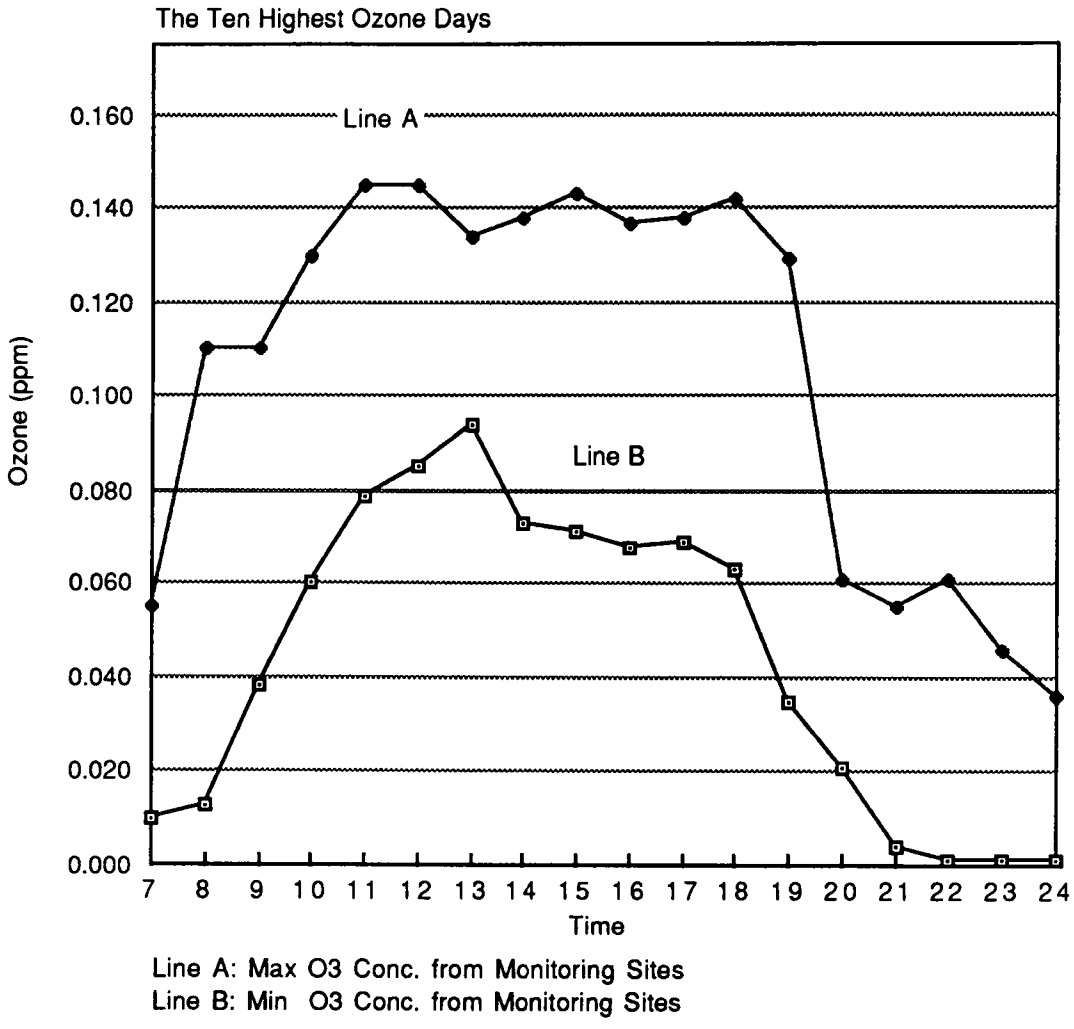


Figure 4-1. The Ozone Concentration Contours

combined with the various meteorological conditions such as wind speed, wind direction, temperature, and mixing height.

VOC and NOx Emissions

In the Nashville metropolitan area, the morning rush hour starts around 6:30 AM. The concentration of NO begins to increase rapidly because motor vehicle emissions increase. The rapid oxidation of NO to NO_2 causes the NO concentration to decrease. When the sun rises, the solar intensity increases. The oxidation of NO and the increasing solar intensity initiates ozone formation. The evening rush hour did not produce high ozone concentrations because of the lack of solar intensity. The percentages of emissions from point, area, and mobile sources in the middle Tennessee area were 17.7%, 27.8% and 54.5% for anthropogenic emissions of VOCs; and 29.4%, 20.2% and 50.4% for NOx [1]. Obviously, the major emissions of VOCs and NOx were from mobile sources, therefore ozone formation depends heavily on the amount of vehicular traffic.

Wind Speed and Wind Direction

Nine of the ten exceedances in the middle Tennessee area occurred at Hendersonville (Table 4-1), which was located northeast of downtown Nashville about 24 km from the Center of Business District (CBD). The prevailing wind directions in the summer were primarily from southwest to northeast thus moving pollutants downwind away from the urban area and into the surrounding area. Therefore, the highest ozone concentrations were observed at Hendersonville rather than at downtown Nashville.

Table 4-1 provides the average wind direction and wind speed from 6:00 AM to the time of day that the ozone concentration peaked for each of the ten highest ozone days. Table B-10 (Appendix B) shows the hourly wind speeds and directions on the ten highest ozone days. Figure 4-2 shows the profile of the hourly average wind speeds of the ten days.

Temperature

Temperature was one of the most significant meteorological factors in ozone formation [7] because all the exceedances were observed in summer seasons. The average of the maximum temperatures of these days was 96 °F. Table 4-1 lists the highest temperatures of these days of highest ozone while Table B-11 (Appendix B) provides the hourly temperatures of these days. Figure 4-3 gives a profile of the hourly average temperatures based on the information of Table B-11.

Table B-12 (Appendix B) provides the hourly relative humidities and water concentrations of these days, and Figure 4-4 gives the profile of the hourly average humidity of the ten days.

Mixing Height

The mixing height is defined as the top of surface-based layer of air which is well-mixed due to mechanical and thermal turbulence. The rate of dilution of atmospheric pollutants was governed by the diurnal change of mixing height. Therefore, the mixing height was also a very important

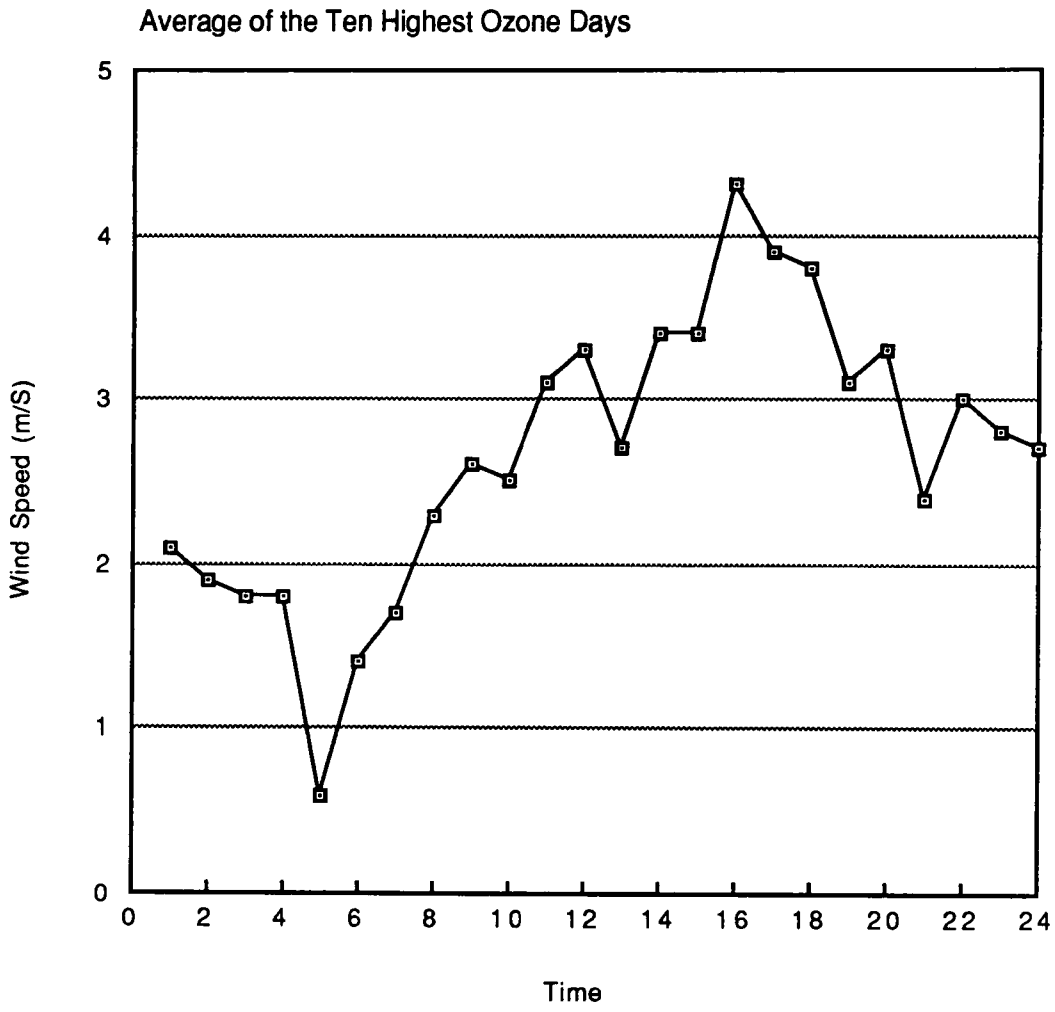


Figure 4-2. The Wind Speed Profile

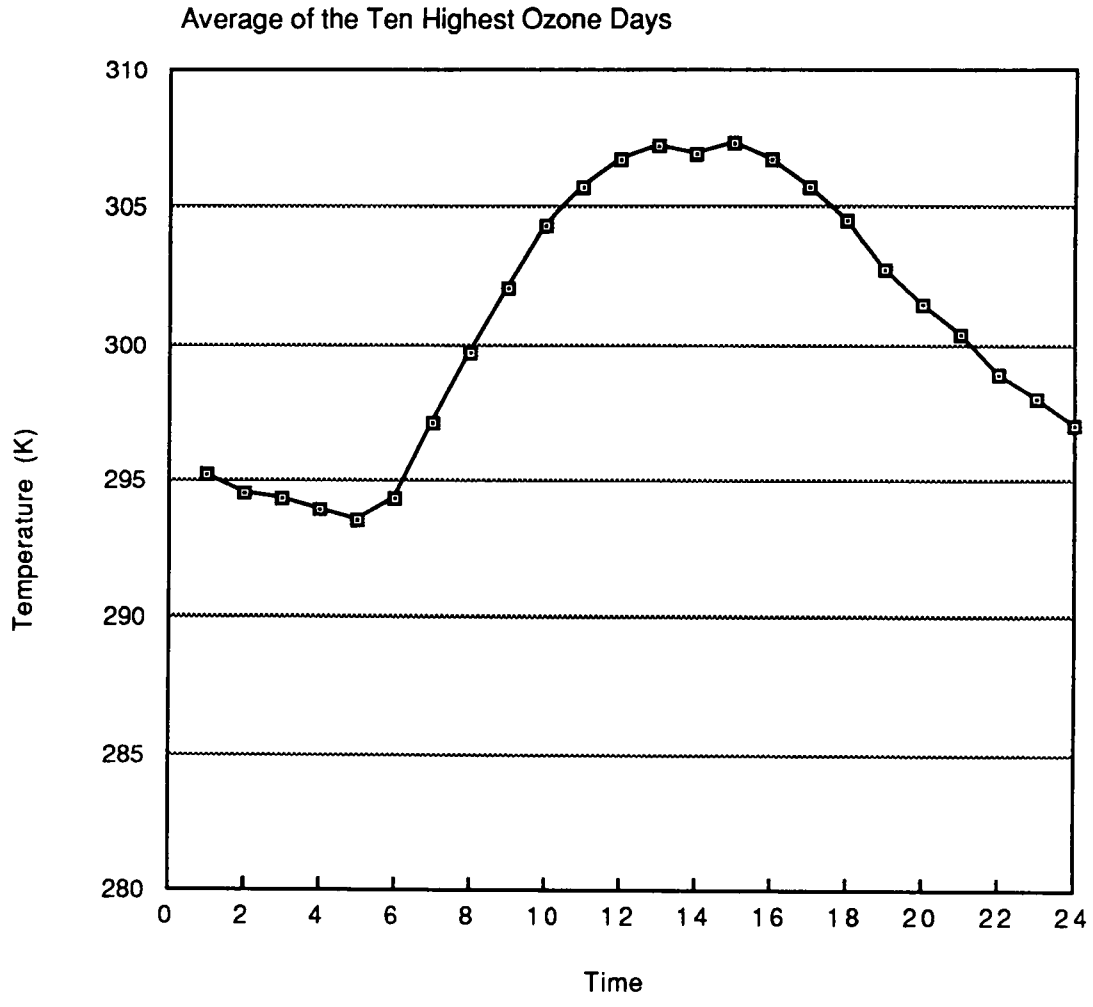


Figure 4-3. The Temperature Profile

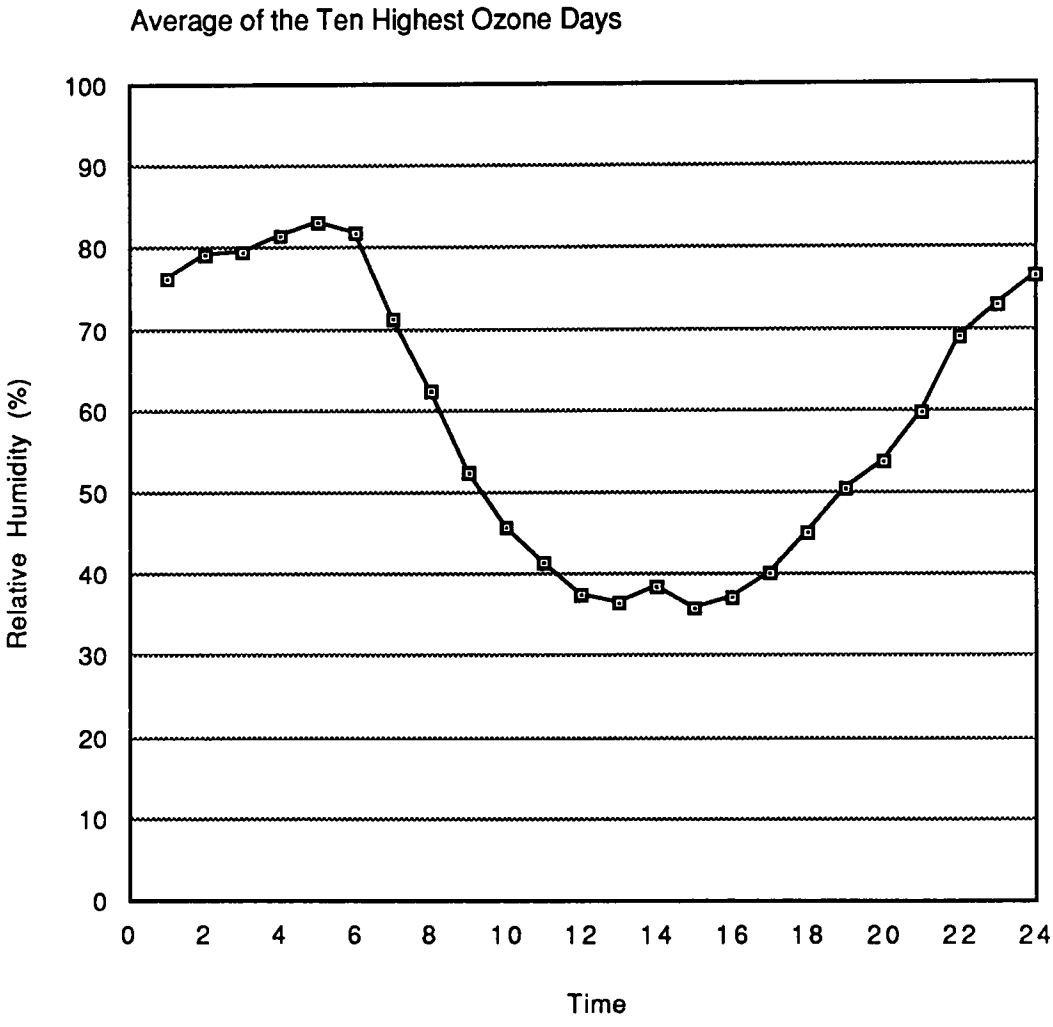


Figure 4-4. The Relative Humidity Profile

meteorological factor in ozone formation. The National Weather Service (NWS) provided the mixing heights of mornings and afternoons of the highest ozone days. The information related to mixing height is listed in Table 4-2.

Table 4-2. The Mixing Heights of the Ten Highest Ozone Days
(meter)

Date	Morning	Afternoon
87-08-03	281	2359
88-06-20	267	2881
87-08-25	158	2273
86-08-25	166	1968
86-06-22	155	2431
86-07-24	268	2272
88-06-14	135	2668
88-07-09	232	3773
88-08-01	311	2141
88-05-27	63	1925
Average	204	2407

5.0 SIMULATIONS OF OZONE FORMATION USING THE OZIPM-4 MODEL

The highlights of the study were the simulations of ozone formation. The purposes of these were threefold: (1) to simulate ozone formation for the middle Tennessee area using meteorological and emissions data, (2) to validate the OZIPM-4 model by comparing the results from simulations with the results from monitoring stations, and (3) to discuss ozone formation by sensitivity analyses. The time system used by he OZIPM-4 model is the local daylight saving time (LDT) [14].

5.1 The Methods of Modeling Ozone Formation

The study using the OZIPM-4 model focused on the simulation of the diurnal ozone profile at Hendersonville under different wind fields and other meteorological conditions. At the beginning of each hour, from 6:00 A.M. to 8:00 P.M., an air parcel arrived at Hendersonville. The simulations of ozone formations inside these parcels gave the ozone concentration profile from 6:00 A.M. to 7:00 P.M. Each air parcel was initiated at 6:00 A.M. with chosen initial conditions and picked up the hourly emissions of pollutants as it moved toward the Hendersonville site.

Methodologically, the simulation of ozone formation in a moving air parcel simulated the photo-chemical reactions of pollutants in a Lagrangian Coordinate System. The simulated ozone profile at Hendersonville provided a simple pattern of ozone formation in an Eulerian Coordinate System. A

Lagrangian Coordinate System is defined as a relative coordinate system, where the phenomena of physics or chemistry is described by following the movement of a parcel of mass. An Eulerian Coordinate System is an absolute coordinate system where the phenomena of physics or chemistry are observed as a function of time for any point of the system. The ozone profile in the Eulerian Coordinate System was found by simulating ozone formation of a series of air parcels in the Lagrangian Coordinate System.

5.2 The Preparation Inputs for the OZIPM-4 Model

The study grouped the inputs of the OZIPM-4 model into four categories: meteorological data, wind field, initial and boundary (top and surrounding) conditions, and hourly emissions (kg/sq-km) of NMOC and NOx.

Inputs of Meteorological Information

The required meteorological inputs were: hourly temperature and relative humidity, mixing heights of morning and afternoon and atmospheric pressure. Table 5-1 gives the averages of temperatures, relative humidities and atmospheric pressures of the ten highest ozone days. The mixing heights used were 200 m at 8:00 A.M. and 2500 m at 2:00 P.M. based on data in Table 4-2. The mixing heights of each hour, which is also listed in Table 5-1, were calculated using the OZIPM-4 model by inputting the mixing heights of morning and afternoon. The atmospheric pressure used for the modeling was 29.5 in of Hg. Figure 5-1 shows the curve of hourly mixing

Table 5-1. The Meteorological Data Used by the OZIPM-4 Model

Time (LDT)	Mixing Height(m)	Tem. (K)	Relative Humidity(%)	Humidity ppm	Pressure In. of Hg
1	200	295.2	76.1	19404.0	29.5
2	200	294.5	79.0	19425.6	29.5
3	200	294.3	79.6	19185.8	29.4
4	200	293.9	81.5	19191.6	29.4
5	200	293.5	83.1	19245.8	29.5
6	200	294.3	81.7	19824.7	29.5
7	200	297.1	71.1	20332.6	29.5
8	200	299.7	62.2	20626.0	29.5
9	583	302.1	52.4	19966.7	29.5
10	967	304.3	45.7	19715.2	29.5
11	1350	305.7	41.4	19222.2	29.5
12	1733	306.7	37.5	18289.4	29.5
13	2117	307.2	36.3	18291.2	29.5
14	2500	306.9	38.4	19052.6	29.4
15	2500	307.3	35.7	18036.3	29.4
16	2500	306.7	37.2	18180.5	29.4
17	2500	305.7	40.1	18612.1	29.4
18	2500	304.5	45.1	19570.1	29.4
19	2500	302.7	50.4	19746.6	29.4
20	2040	301.5	53.7	19768.2	29.5
21	1580	300.4	59.7	20632.2	29.5
22	1120	298.9	68.8	21886.1	29.5
23	660	298.0	72.7	21896.0	29.5
24	200	297.0	76.5	21805.8	29.5

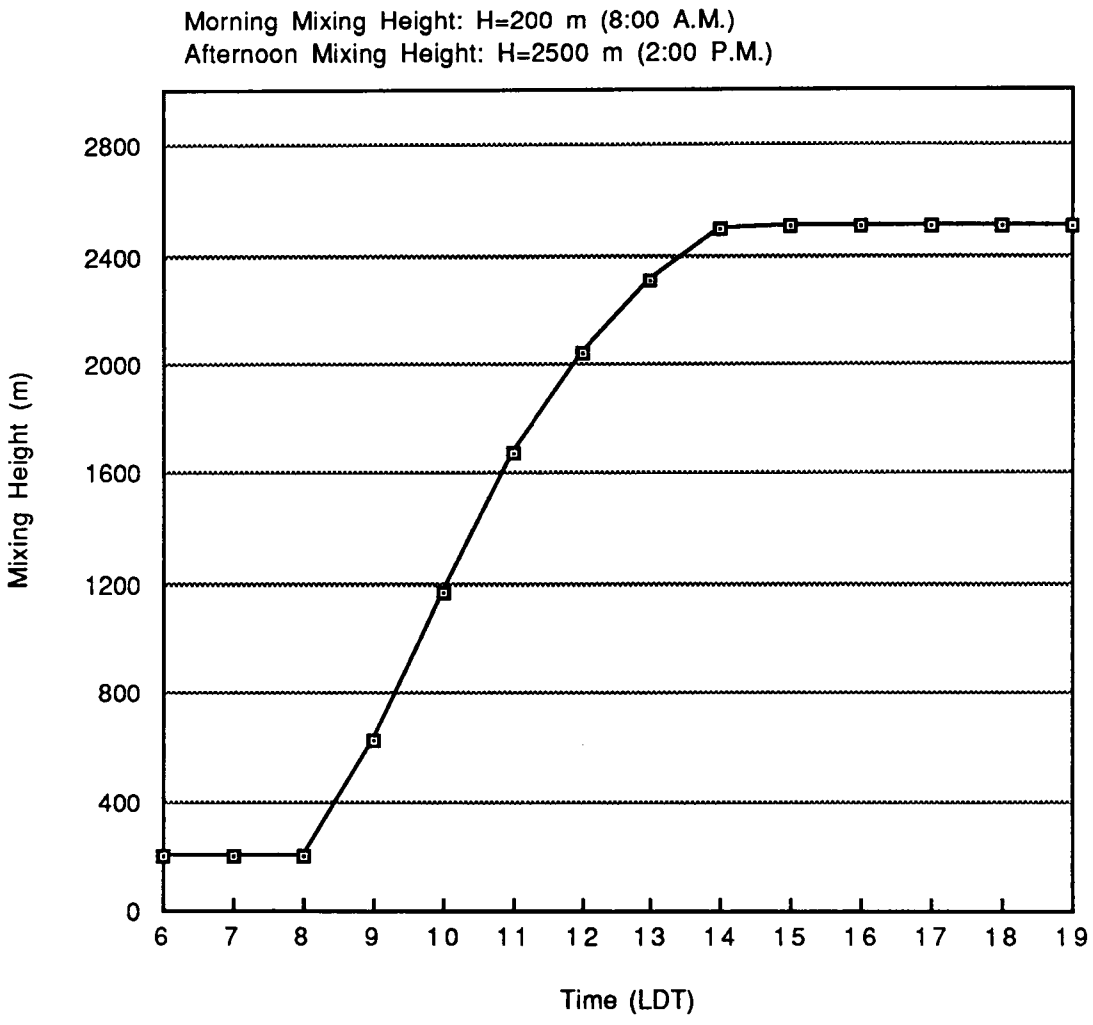


Figure 5-1. The Mixing Height Profile

heights, while Figures 4-2, 4-3 and 4-4 of Section 4 provide the wind speed, temperature, and relative humidity profiles.

The Photochemical Reaction Rates of Ozone Formation

Ozone formation is the result of a series of photochemical reactions which are influenced by the time-variable sunlight intensity. The sunlight intensity is a function of the meteorological conditions as well as the location and date simulated. The speed of NO_2 photolysis is related to solar intensity. Table B-13 (Appendix B) and Figure 5-2 give the hourly NO_2 photolysis reaction coefficients. The date chosen for the simulations was June 21, 1988, which had the longest diurnal time of the entire year. The point of 36.667 latitude and 86.167 longitude was chosen to represent the geographic position of the middle Tennessee area.

The Inputs of Speciated Emissions

For the OZIPM-4 model, the required inputs related to emissions were the hourly emissions (kg/sq-km) of anthropogenic NMOC and NOx. The model also provided an option of choosing the hourly emissions (kg/sq-km) of biogenic VOCs by species. A set of ratios were used to separate OLE, PAR, TOL, XYL, FORM, ALD2, ETH and non-reactive species from total VOCs emissions. A NO_2/NOx ratio was used to separate NO and NO_2 from NOx [14].

The speciation of NMOC and NOx of anthropogenic sources provided the hourly emissions (mole/hr) by chemical species. The results were used to prepare the emission related inputs

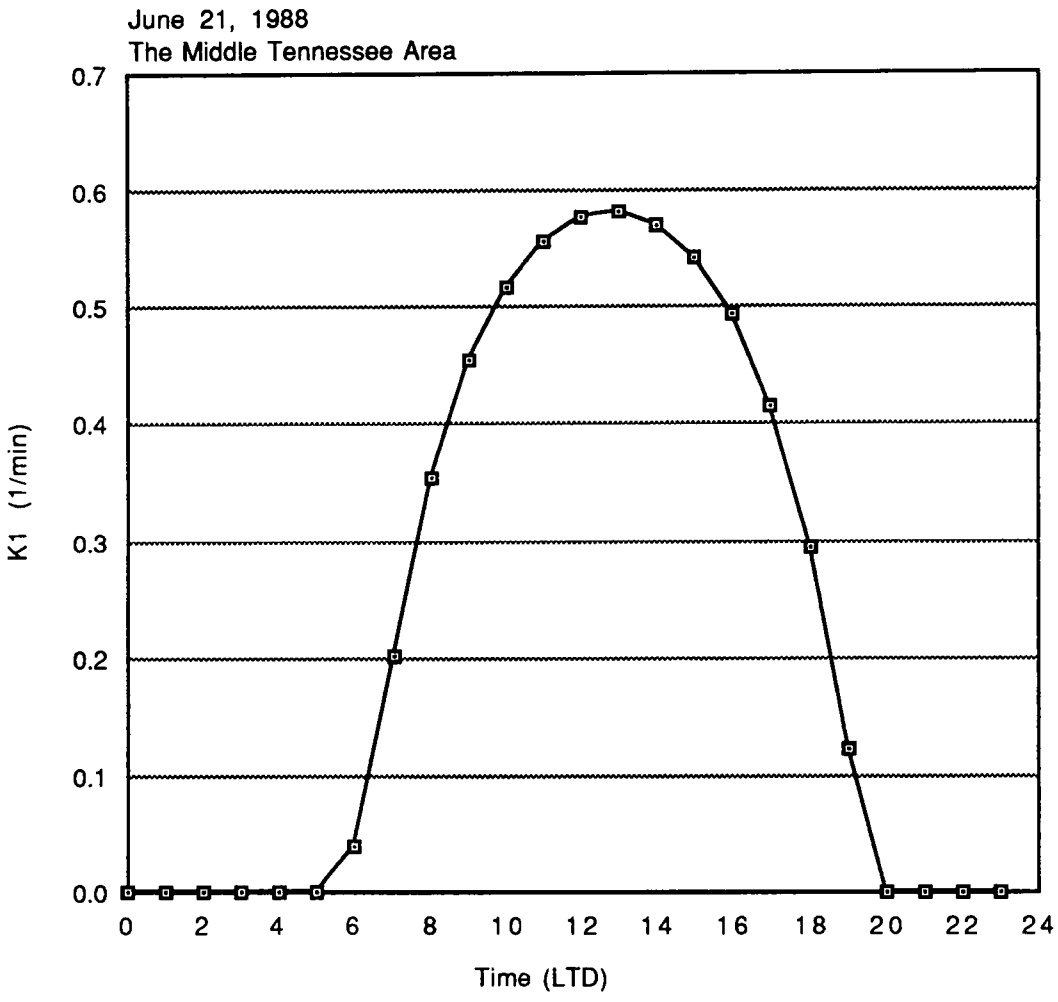


Figure 5-2. The NO2 Photolysis Reaction Rates for Ozone Formation

for the model. If ozone formation of a moving parcel was simulated, the required hourly emissions were chosen as the emissions of the grid, which was the grid passed by the air parcel at the beginning of the hour. Thus, the total hourly emissions (kg/sq-km) were calculated using the speciated emissions from Section 3 and the molecular weight table (Table 3-1). A set of ratios of distributing NMOC and the NO_2/NOx ratio could be calculated, and these ratios were required as inputs of the OZIPM-4 model.

The OZIPM-4 model does not include ISOP as an active anthropogenic NMOC species. However, the speciation results showed that there were ISOP emitted from anthropogenic sources. In order to input the ISOP emissions to the model, the emissions were considered as non-active anthropogenic emissions first and then were added back as biogenic emissions. Thus the input emissions of ISOP, accounted for as biogenic emissions, included the anthropogenic emissions of ISOP and the actual biogenic emissions.

Figures 5-3 and 5-4 show the composition of anthropogenic active NMOC emissions from 6:00 A.M. to 6:00 P.M. for Davidson County and the Nashville metropolitan area. Figures 5-5 and 5-6 provide the temporal allocation of the emitted NMOC and NOx in Davidson County.

The OZIPM-4 model also required the input of biogenic emissions for each grid, the hourly biogenic emissions of ISOP were based on the research of [15] (Table B-13 and Figure 5-7). ISOP was the major species of the emissions of NMOC from biogenic sources.

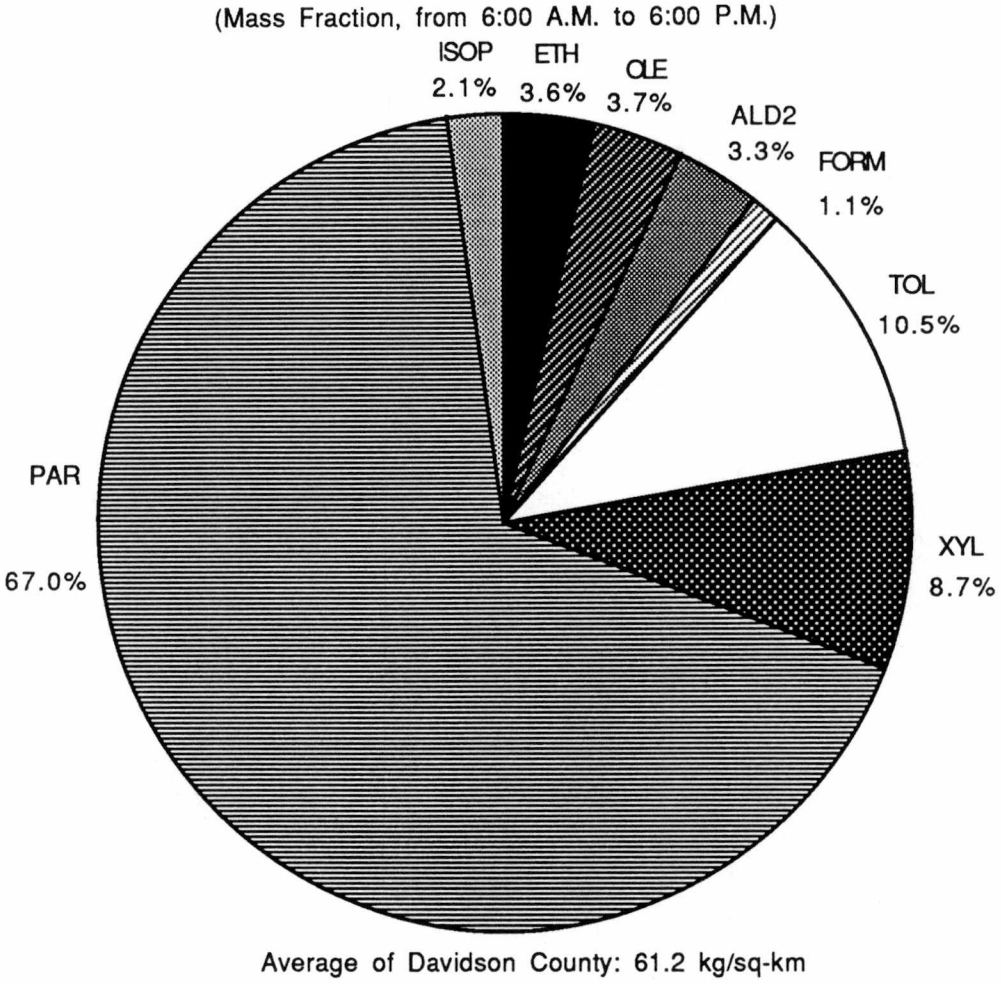


Figure 5-3. The Components of Anthropogenic VOC Emissions (Davidson County)

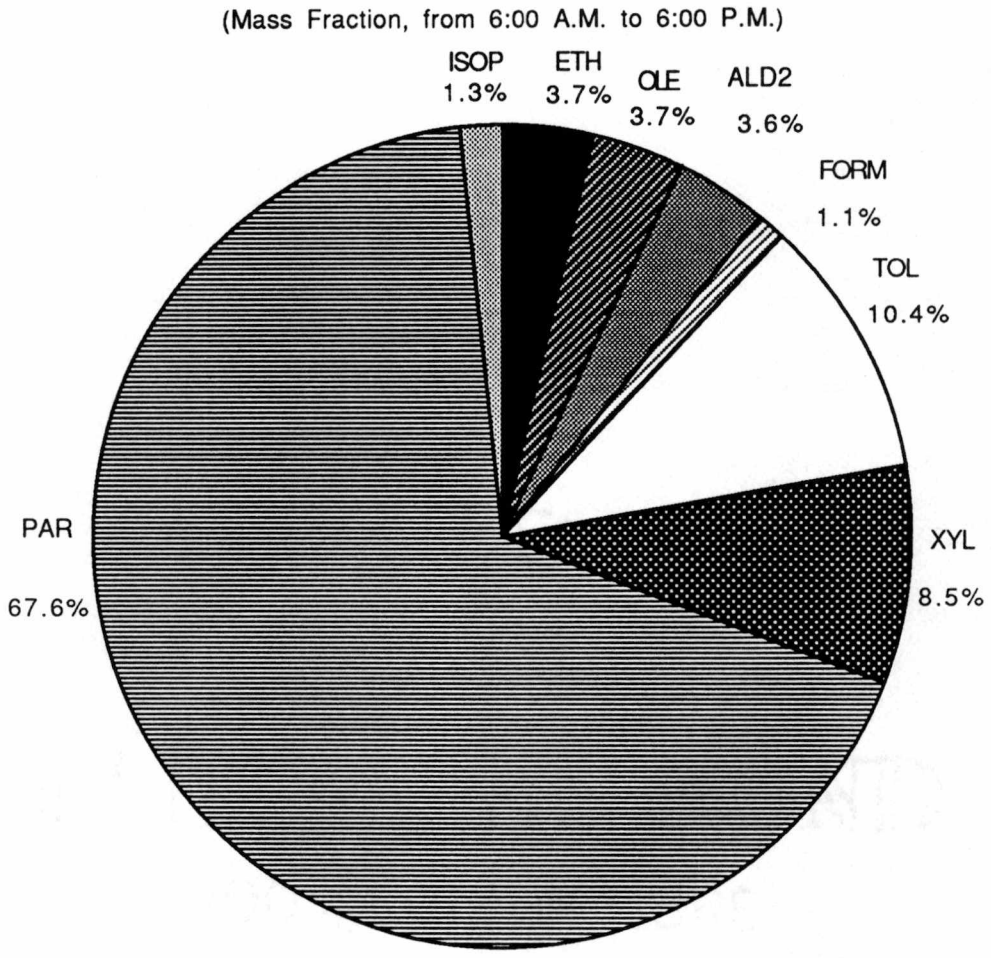


Figure 5-4. The Components of Anthropogenic VOC Emissions (the Nashville Metropolitan Area)

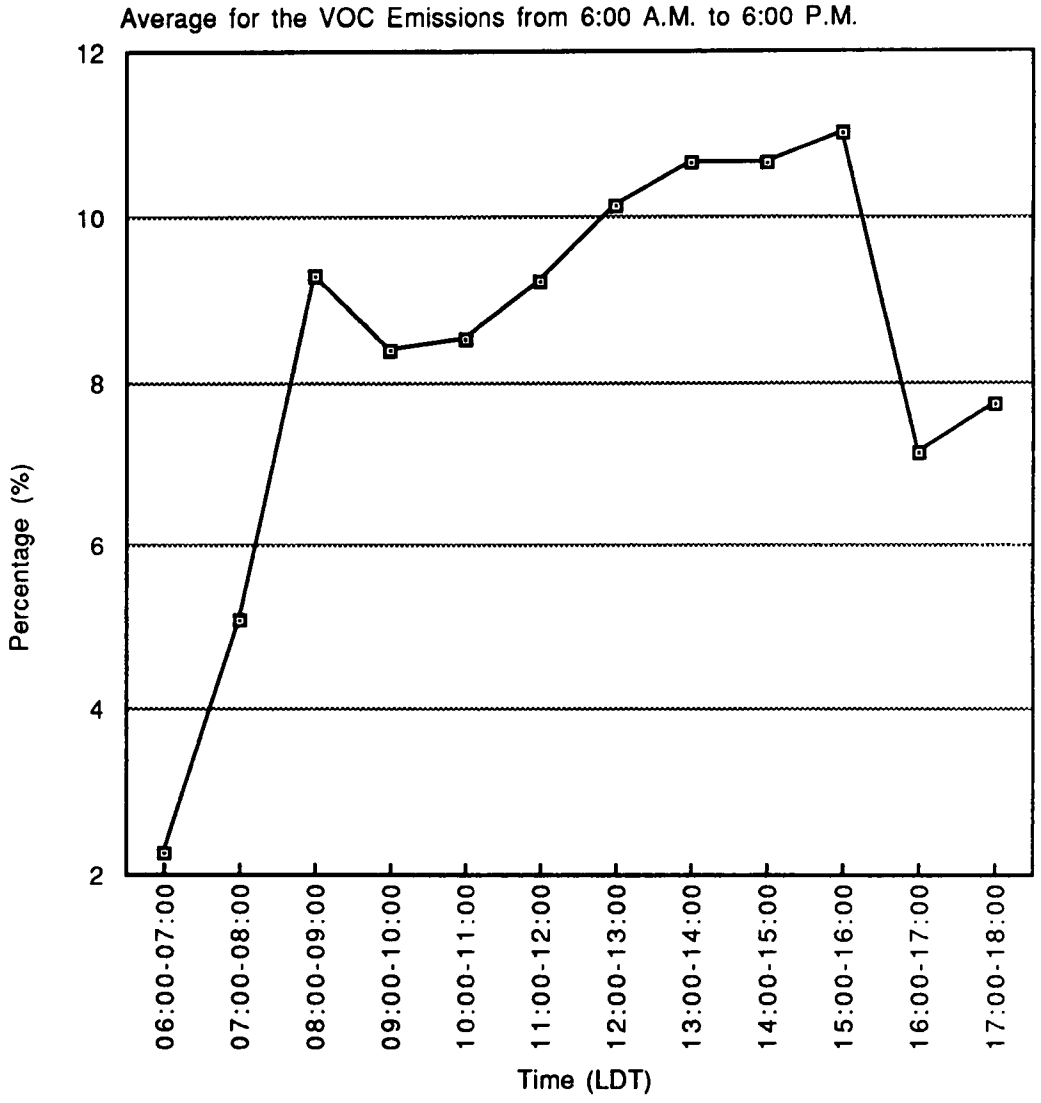


Figure 5-5. The Temporal Allocation of VOC Emissions (Davidson County)

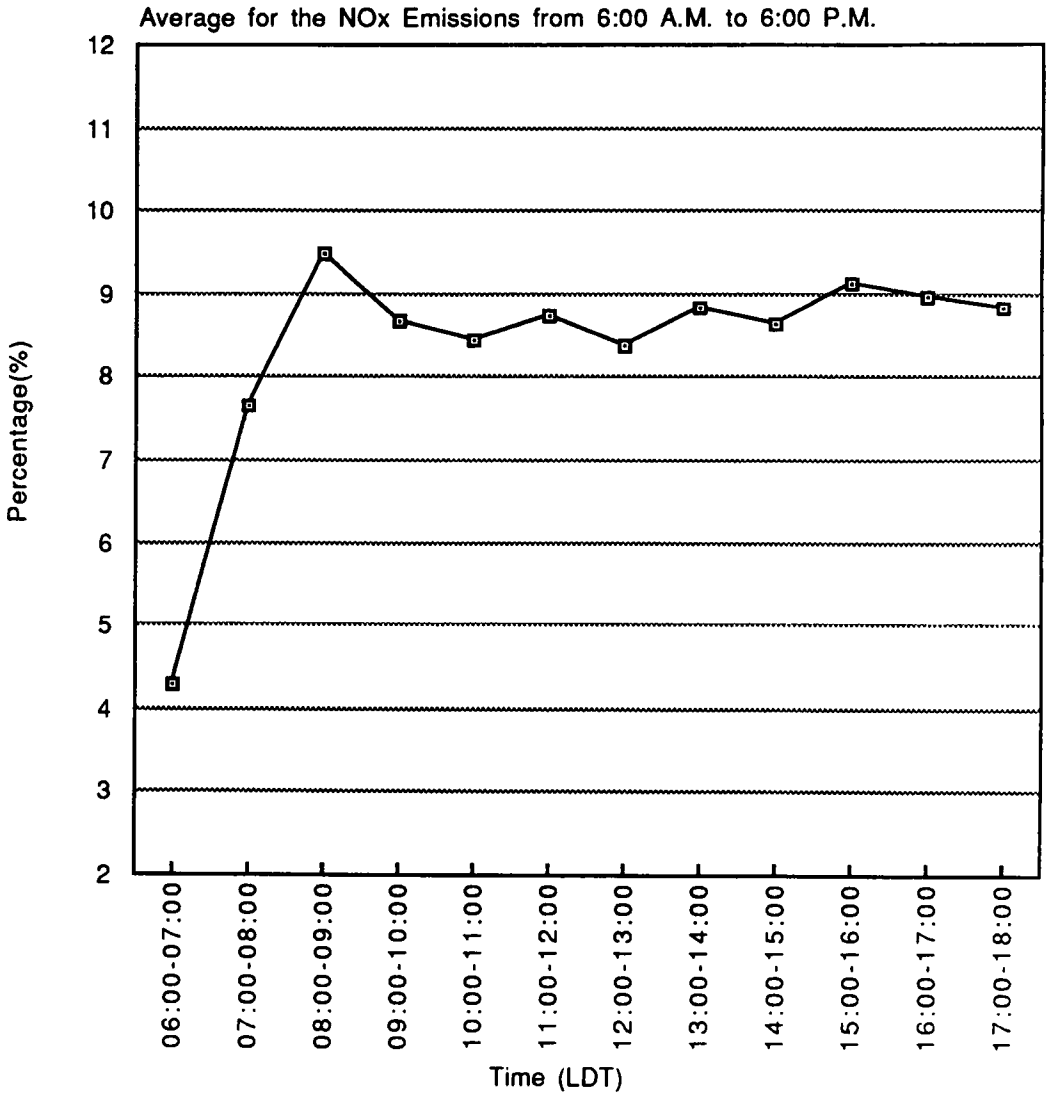


Figure 5-6. The Temporal Allocation of NOx Emissions (Davidson County)

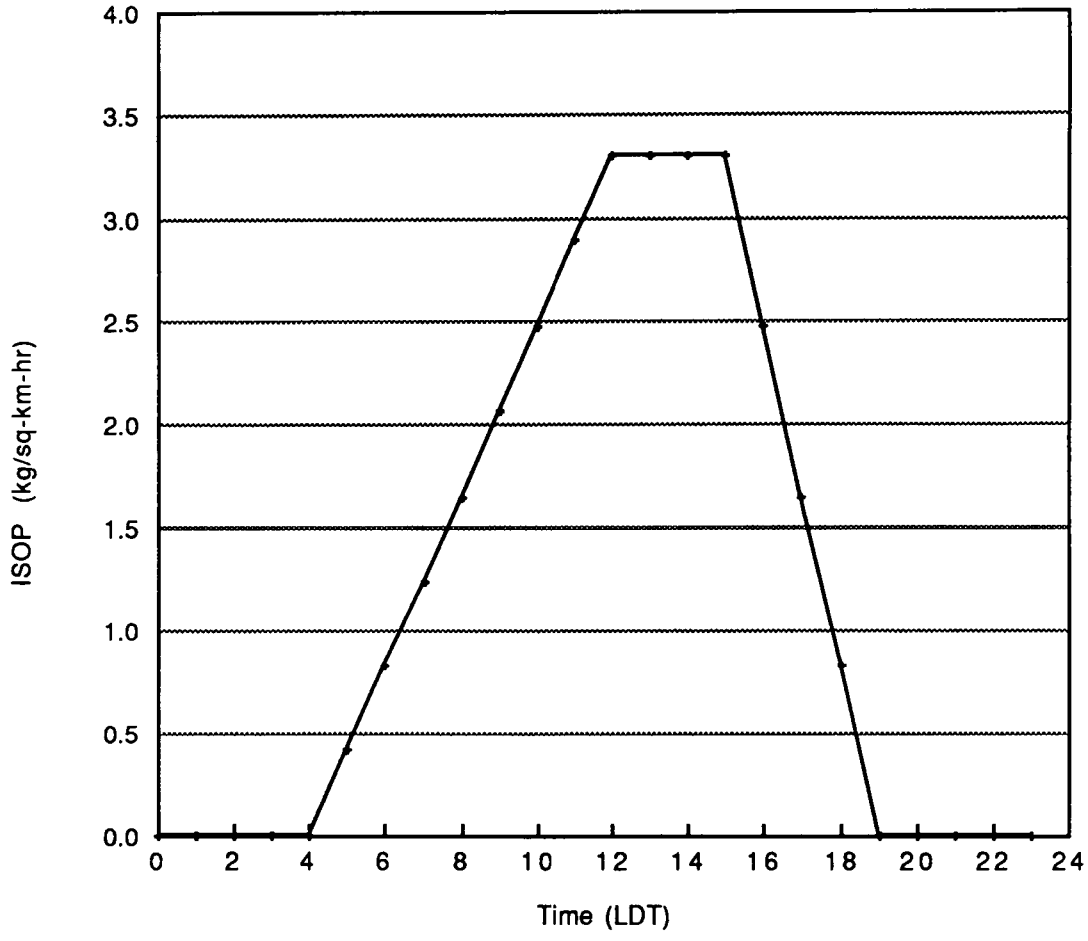


Figure 5-7. The Hourly Biogenic Emissions

Aloft Boundary Conditions and Initial Conditions

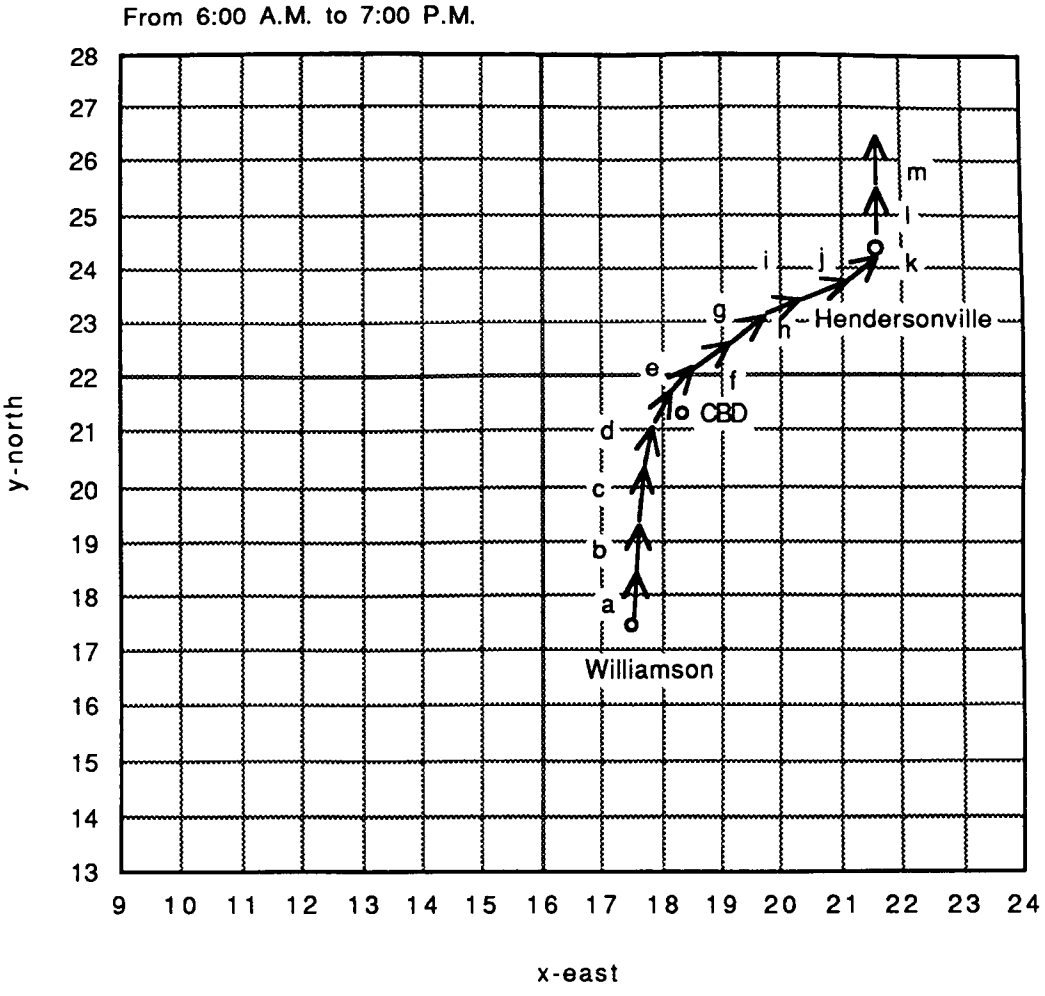
The advection of ozone from aloft can change the amount of ozone inside the simulated parcel. During the early morning hours, the advection happens when the mixing height increases. It has been found that the advection from aloft is an important factor affecting the maximum afternoon ozone levels observed within or downwind from cities [6].

Top boundary conditions used by the OZIPM-4 model included the concentrations of ozone, NMOC and NO_2. They were: 0.04 ppm for ozone, 0.025 for NMOC and 0.001 for NOx. The initial conditions of NMOC and NOx were also required, they were 0.025 ppm for VOCs (NMOC) and 0.001 ppm for NOx.

The Wind Fields

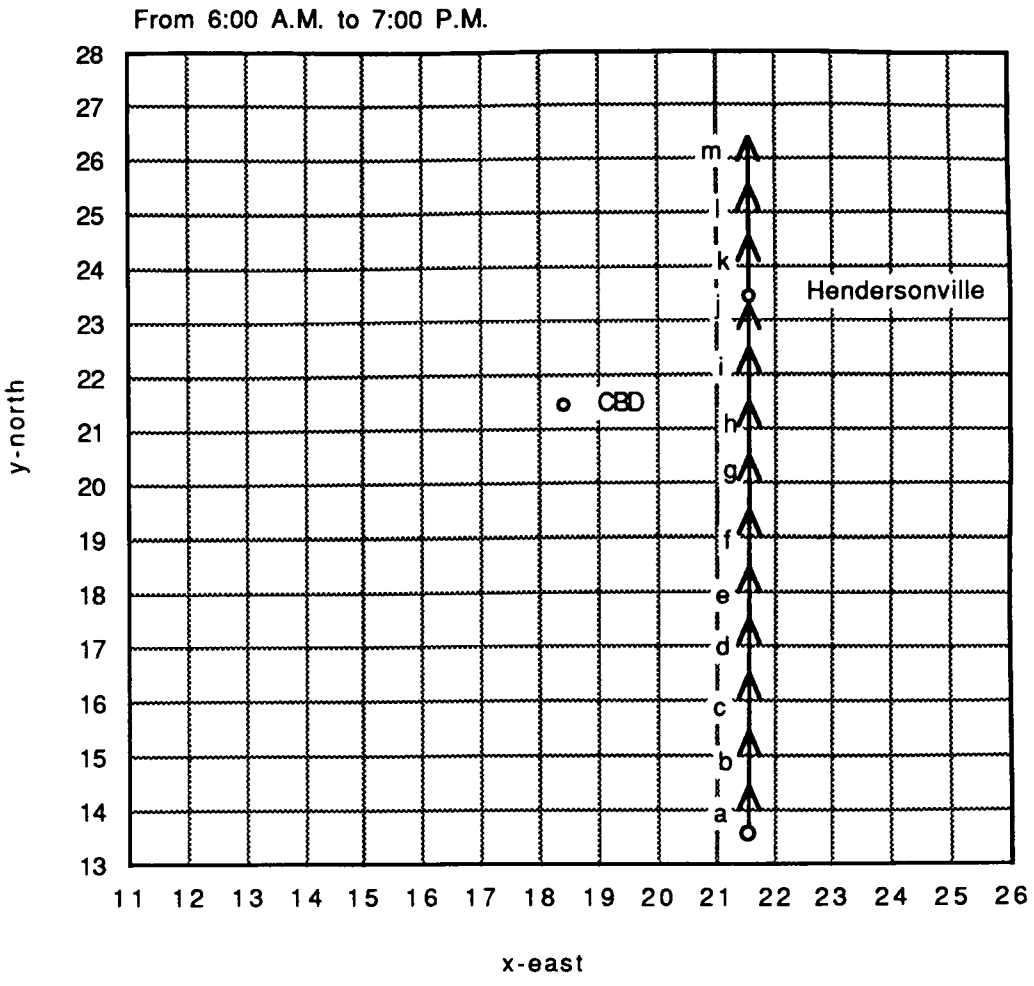
The transport of pollutants was dependent on the wind field chosen. One of the wind fields was a calm wind field, i.e. the wind speeds were assumed to be zero. Under the calm wind field, ozone formation of the Nashville metropolitan area was simulated to reflect the ozone pollution at the extreme meteorological condition. The wind field was called wind field zero.

There were three other wind fields which were used: wind field one, two and three. Wind field one was used to find the ozone concentration profile at Hendersonville. Wind fields two and three were used for sensitivity analyses which will be discussed in Section 6. Figures 5-8, 5-8 and 5-10 give the three wind fields.



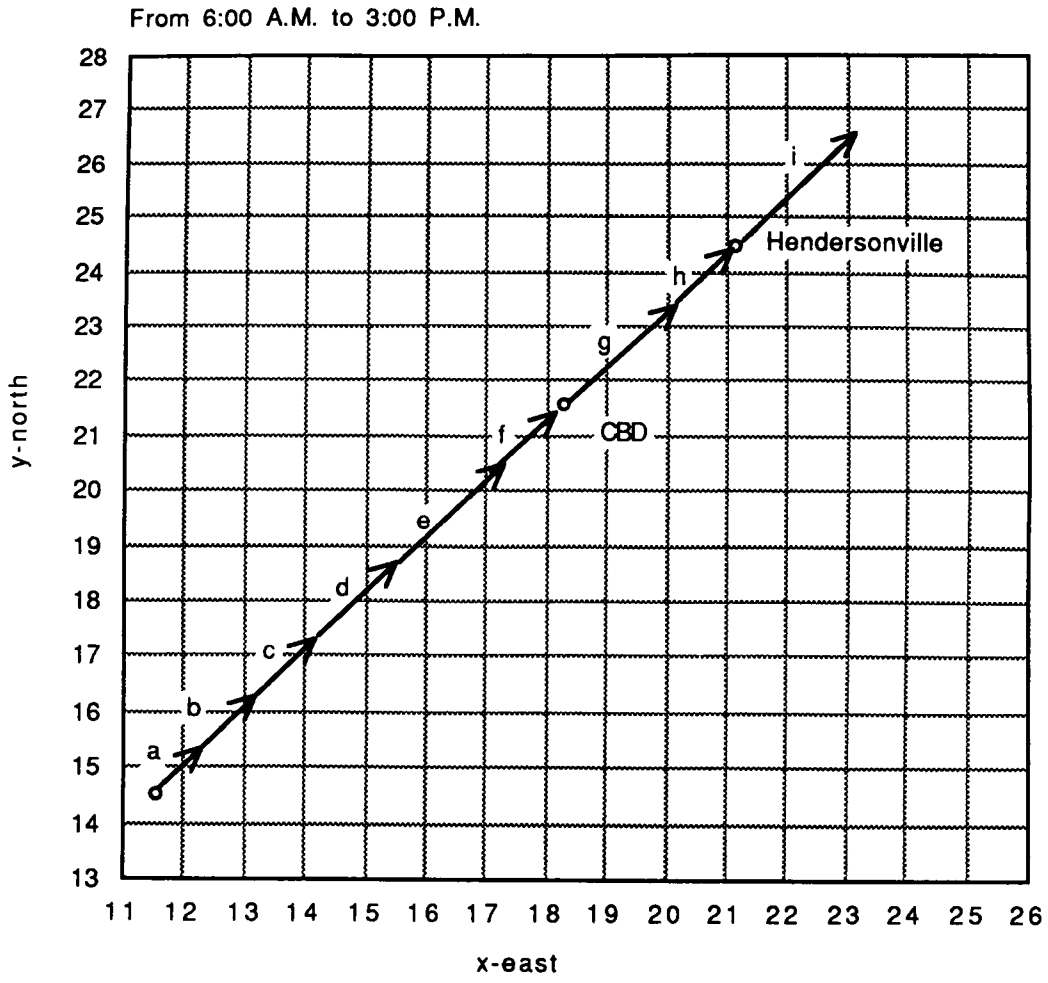
06:00-07:00 -- a
07:00-08:00 -- b
08:00-09:00 -- c
09:00-10:00 -- d
10:00-11:00 -- e
11:00-12:00 -- f
12:00-13:00 -- g
13:00-14:00 -- h
14:00-15:00 -- i
15:00-16:00 -- j
16:00-17:00 -- k
17:00-18:00 -- l
18:00-19:00 -- m

Figure 5-8. Wind Field One



06:00-07:00 -- a
07:00-08:00 -- b
08:00-09:00 -- c
09:00-10:00 -- d
10:00-11:00 -- e
11:00-12:00 -- f
12:00-13:00 -- g
13:00-14:00 -- h
14:00-15:00 -- i
15:00-16:00 -- j
16:00-17:00 -- k
17:00-18:00 -- l
18:00-19:00 -- m

Figure 5-9. Wind Field Two



06:00-07:00 -- a
07:00-08:00 -- b
08:00-09:00 -- c
09:00-10:00 -- d
10:00-11:00 -- e
11:00-12:00 -- f
12:00-13:00 -- g
13:00-14:00 -- h
14:00-15:00 -- i

Figure 5-10. Wind Field Three

5.3 Simulations Using the OZIPM-4 Model

The ozone formations of the metropolitan area and the Hendersonville monitoring site were carried out. In total, there were 25 scenarios of different simulations under different conditions. Table 5-2 lists the scenarios and wind fields.

The Nashville Metropolitan Area

Nine grids, (17,19), (18,19), (19,19), (17,20), (18,20), (19,20), (17,21), (18,21), and (19,21), were used to represent the Nashville metropolitan area.

The ozone formation of the area was simulated under the calm wind field, and an ozone concentration profile from 9:00 A.M. to 8:00 P.M. was found (Figure 5-11).

In order to investigate the relative importance of contributions to unacceptable ozone levels from point, area, mobile, and biogenic sources, ten simulations were carried out under different conditions of pollutant emissions. Letting P, A, M and B represent the emissions from point, area, mobile and biogenic sources, ten combinations of emissions were simulated. They were: PAMB, PMB, PAM, M, PAB, AMB, AB, MB, PB, B. This simulation cases were called scenario 1 to 10 (Table 5-2). The maximum hourly averages of ozone concentration are given in Figure 5-12 for the ten combinations of emissions. Generally, it was found that as the emissions increased, ozone concentrations increased. The peak of hourly average of ozone concentrations was only 0.08 ppm without the emissions from mobile sources. With mobile

Table 5-2. The List of Scenarios And Wind Fields

Scenario	Wind field	Location	Purpose	Note
1	zero	Nashville	PAMB	A fixed air parcel at the Nashville Metropolitan Area
2	zero	Nashville	PAM	A fixed air parcel at the Nashville Metropolitan Area
3	zero	Nashville	AMB	A fixed air parcel at the Nashville Metropolitan Area
4	zero	Nashville	MB	A fixed air parcel at the Nashville Metropolitan Area
5	zero	Nashville	PAM	A fixed air parcel at the Nashville Metropolitan Area
6	zero	Nashville	M	A fixed air parcel at the Nashville Metropolitan Area
7	zero	Nashville	PB	A fixed air parcel at the Nashville Metropolitan Area
8	zero	Nashville	PAB	A fixed air parcel at the Nashville Metropolitan Area
9	zero	Nashville	B	A fixed air parcel at the Nashville Metropolitan Area
10	zero	Nashville	AB	A fixed air parcel at the Nashville Metropolitan Area
11	one	Hendersonville	PAMB	A moving air parcel which arrived at Hendersonville at 17:00
12	one	Hendersonville	PAM	A moving air parcel which arrived at Hendersonville at 17:00
13	one	Hendersonville	AMB	A moving air parcel which arrived at Hendersonville at 17:00
14	one	Hendersonville	MB	A moving air parcel which arrived at Hendersonville at 17:00
15	one	Hendersonville	PAM	A moving air parcel which arrived at Hendersonville at 17:00
16	one	Hendersonville	M	A moving air parcel which arrived at Hendersonville at 17:00
17	one	Hendersonville	PB	A moving air parcel which arrived at Hendersonville at 17:00
18	one	Hendersonville	PAB	A moving air parcel which arrived at Hendersonville at 17:00
19	one	Hendersonville	B	A moving air parcel which arrived at Hendersonville at 17:00
20	one	Hendersonville	AB	
21	one	Hendersonville	The simulation of ozone formation at Hendersonville	The ozone profile at Hendersonville
22	one	Hendersonville	Temperature sensitivity analysis	The ozone profile at Hendersonville
23	two	Hendersonville	Wind field sensitivity analysis	The ozone profile at Hendersonville
24	one	Hendersonville	Aloft ozone conc. sensitivity analysis	The ozone profile at Hendersonville
25	three	Hendersonville	A scenario fits the monitorin data	The ozone profile at Hendersonville

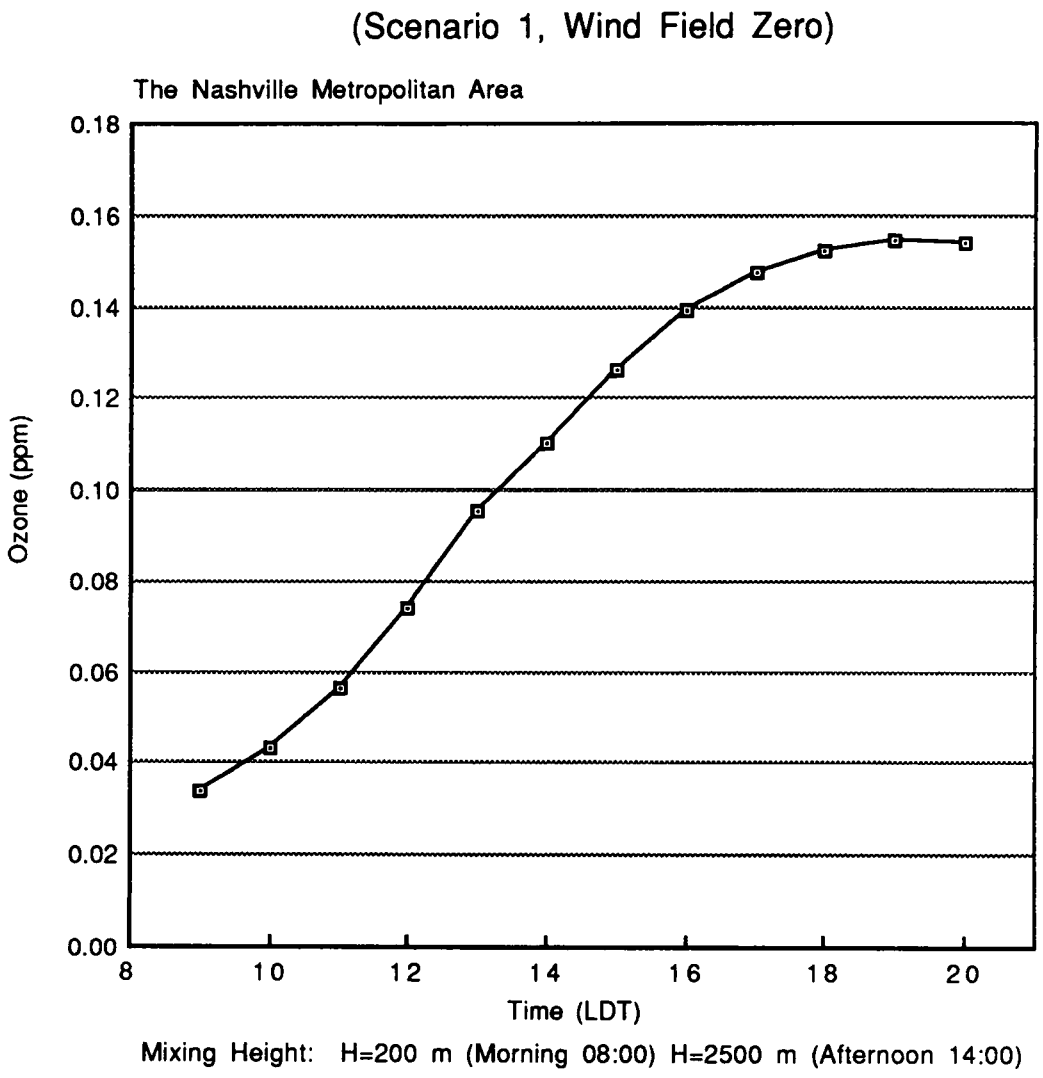


Figure 5-11. Ozone Concentration Profile (Scenario 1)

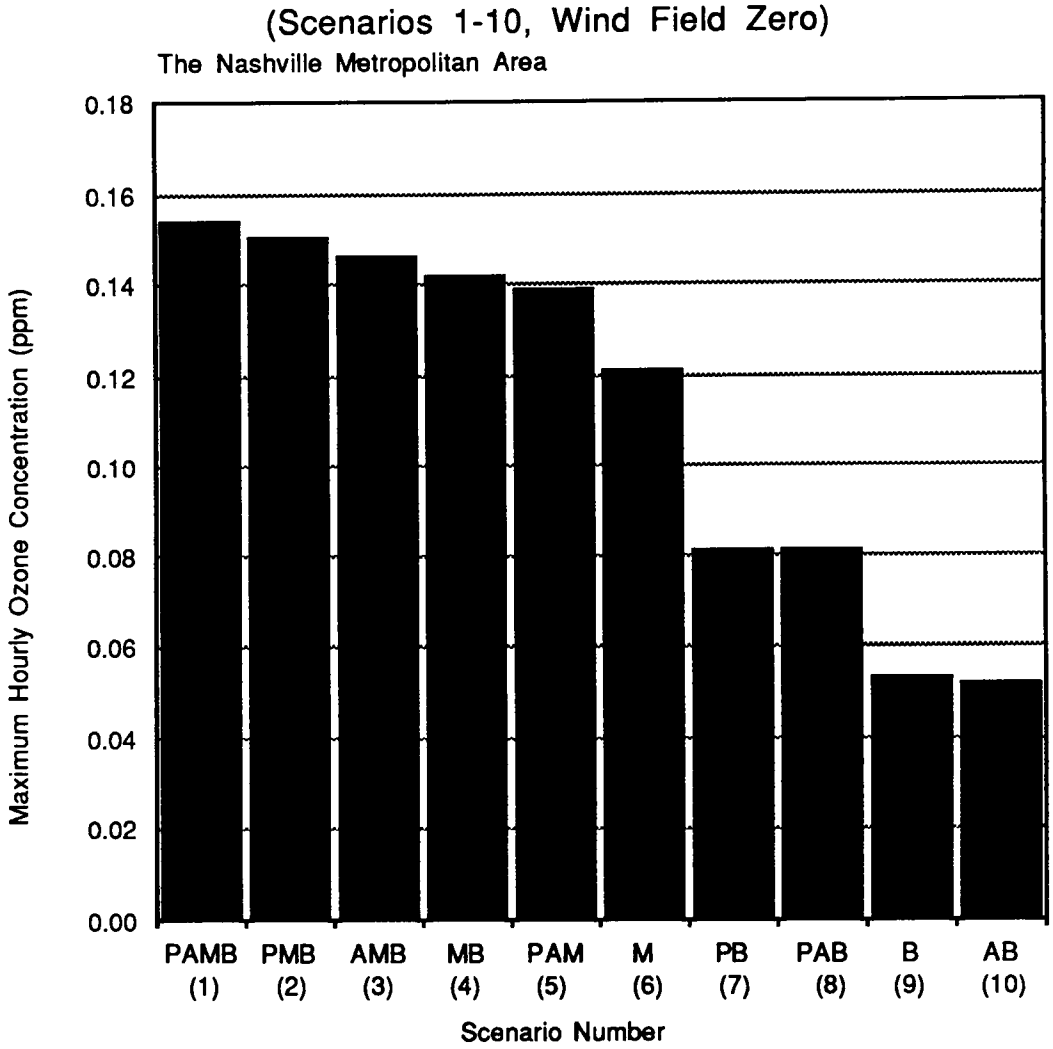


Figure 5-12. The Contributions of Different Emission Categories to Ozone Formation (the Nashville Metropolitan Area, Scenarios 1-10)

sources included, the peak was 0.155 ppm or nearly double the value without mobile sources. Thus the most important contributor for the unacceptable ozone levels was the mobile source category.

Hendersonville

In addition to the scenarios under the calm wind field, there were eleven scenarios under wind field one. Two kinds of simulation results were found by the study. They were: the ozone formation of a moving parcel along a wind trajectory, and the ozone concentration profile at Hendersonville.

A moving air parcel which arrived at Hendersonville at 17:00 was simulated and the results are given in Figure 5-13 (scenarios 11). Examples of input and output files (scenario 11) of the OZIPM-4 could be found in Figures B-1 and B-2. Similarly, the relative importance of contributions to unacceptable ozone levels from point, area, mobile, and biogenic sources was studied by simulating the ozone formations for the ten combinations of emissions. PAMB, PMB, PAM, M, PAB, AMB, AB, MB, PB, B. A moving air parcel which arrived at Hendersonville at 17:00 was used, but it only picked up part of the emissions according to the combination chosen. These simulation cases were called scenario 11 to 20 (Table 5-2). The hourly maximum ozone concentrations for these scenarios were provided in Figure 5-14. The same conclusion achieved was that the most important contributor for the unacceptable ozone levels was the mobile source category. The results of these analyses for the Nashville metropolitan area and Hendersonville were summarized in Table B-14.

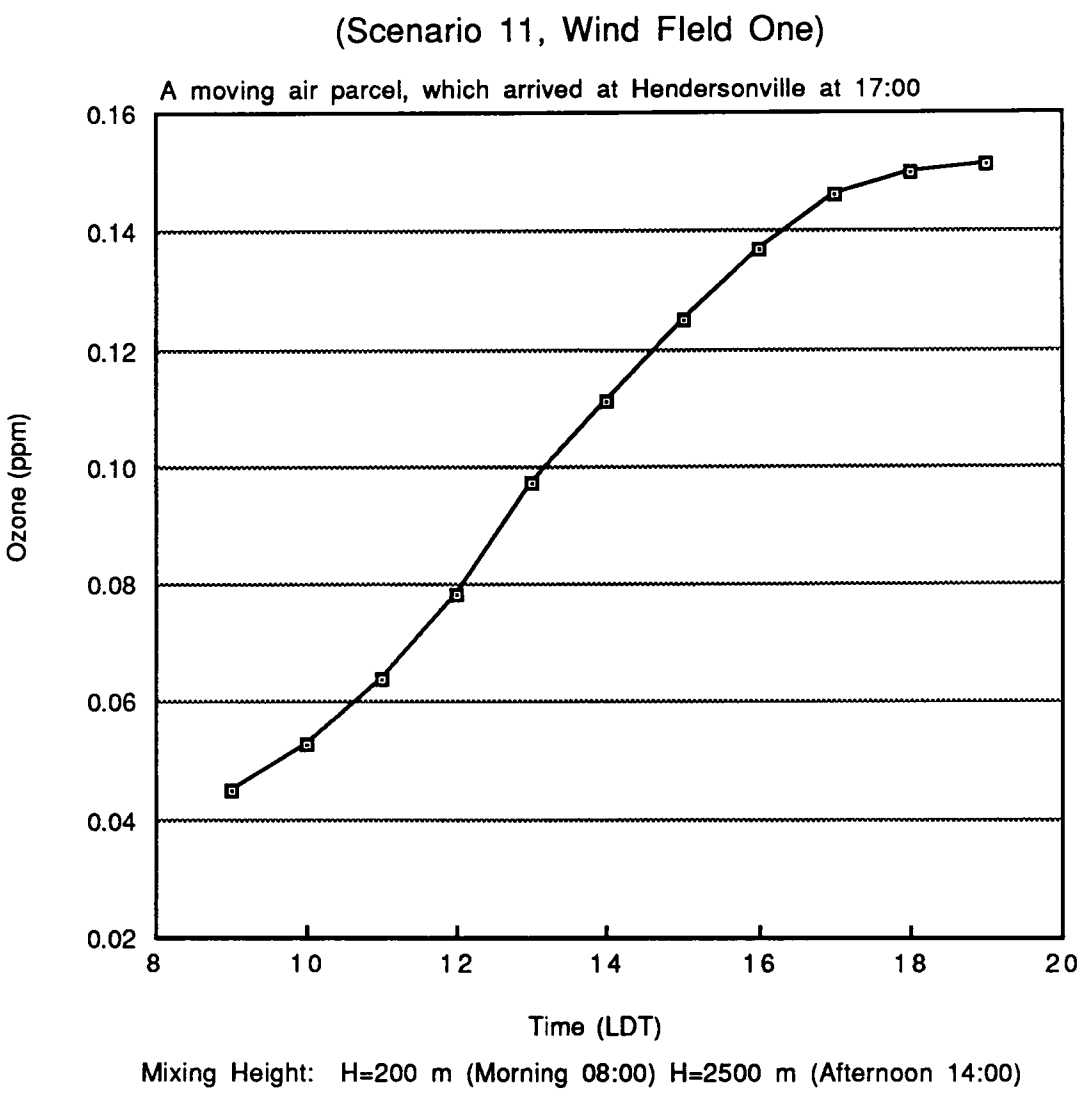


Figure 5-13. Ozone Concentration Profile (Scenario 11)

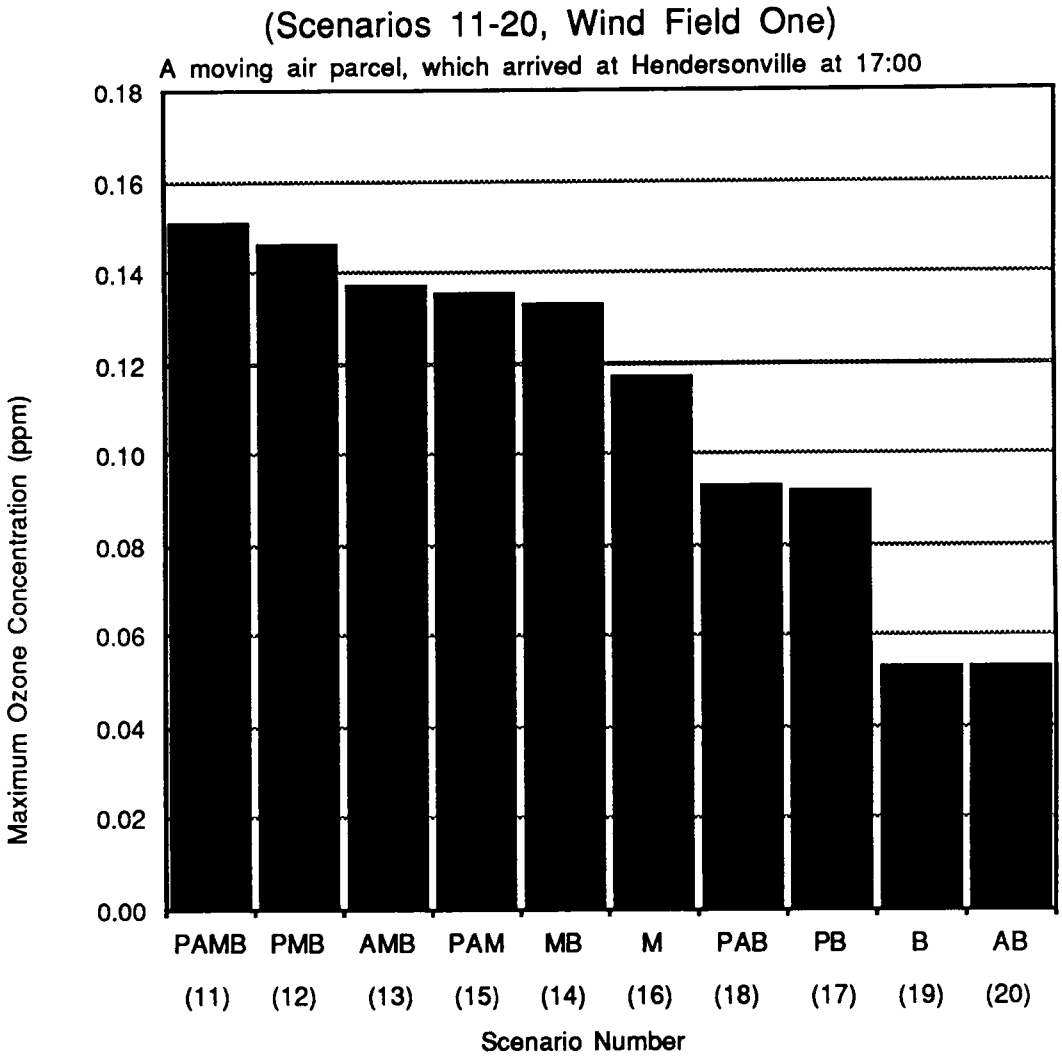


Figure 5-14. The Contributions of Different Emission Categories to Ozone Formation (Hendersonville, Scenarios 11-20)

Scenario 21 provided a simulated ozone profile at Hendersonville. The chosen wind filed was wind field one (Figure 5-8): There were eleven hourly wind trajectories which arrived at Hendersonville at the beginning of each hour from 9:00 A.M. to 8:00 P.M. By simulating ozone formation of the eleven air parcels related to the trajectories, the ozone concentrations were developed. Table 5-3 provides the simulation results of scenarios 11 and 21. Scenario 11 represented the simulation for a moving parcel which arrived at Hendersonville at 17:00. Scenario 21 provided the ozone predicted profile at Hendersonville by simulating the ozone concentrations of eleven different air parcels which arrived at Hendersonville for the hours between 9:00 and 19:00. Figure 5-8 shows the wind field used. Figure 5-15 is the result for scenario 21 showing the concentration of each air parcel as it passed over the site.

A reasonable simulation study should predict the ozone violation and give an explanation of the difference between the simulated results and monitoring data. The simulated ozone concentrations obtained from scenario 21 are superimposed over the contours of the maximum and minimum ozone concentrations of the ten highest ozone violation days and is given in Figure 5-16. The peak ozone concentration of scenario 21 was at 6:00 P.M., and the hourly concentrations provided in scenario 21 during the morning hours were lower than the contour of the minimum ozone concentrations actually observed. Generally speaking, the peak ozone concentrations from the simulation were found around 5:00 P.M. to 7:00 P.M., whereas the measured ozone peak concentrations occurred between 10:00 A.M. and 6:00 P.M., they were earlier than that predicted in scenario 21. Analysis of Table B-9 also indicates that in the early morning hours of 8:00 A.M. or 9:00 P.M., the

Table 5-3. The Simulation of Ozone Formation at Hendersonville

Time	Ozone Conc. (ppm)	
	Scencario 11	Scenario 21
9	0.045	0.042
10	0.053	0.050
11	0.064	0.061
12	0.078	0.079
13	0.097	0.083
14	0.111	0.104
15	0.125	0.109
16	0.137	0.135
17	0.146	0.146
18	0.150	0.150
19	0.151	0.132

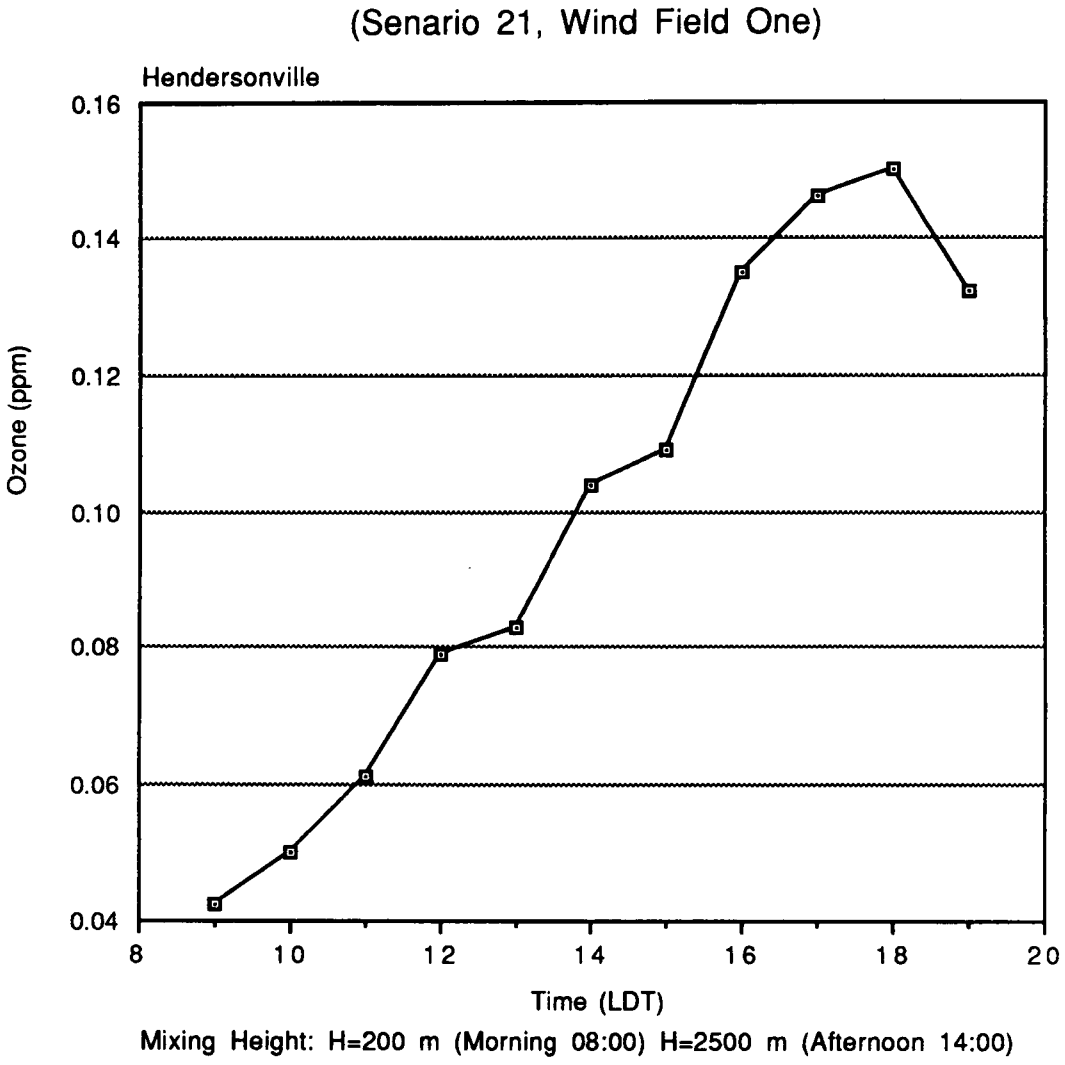
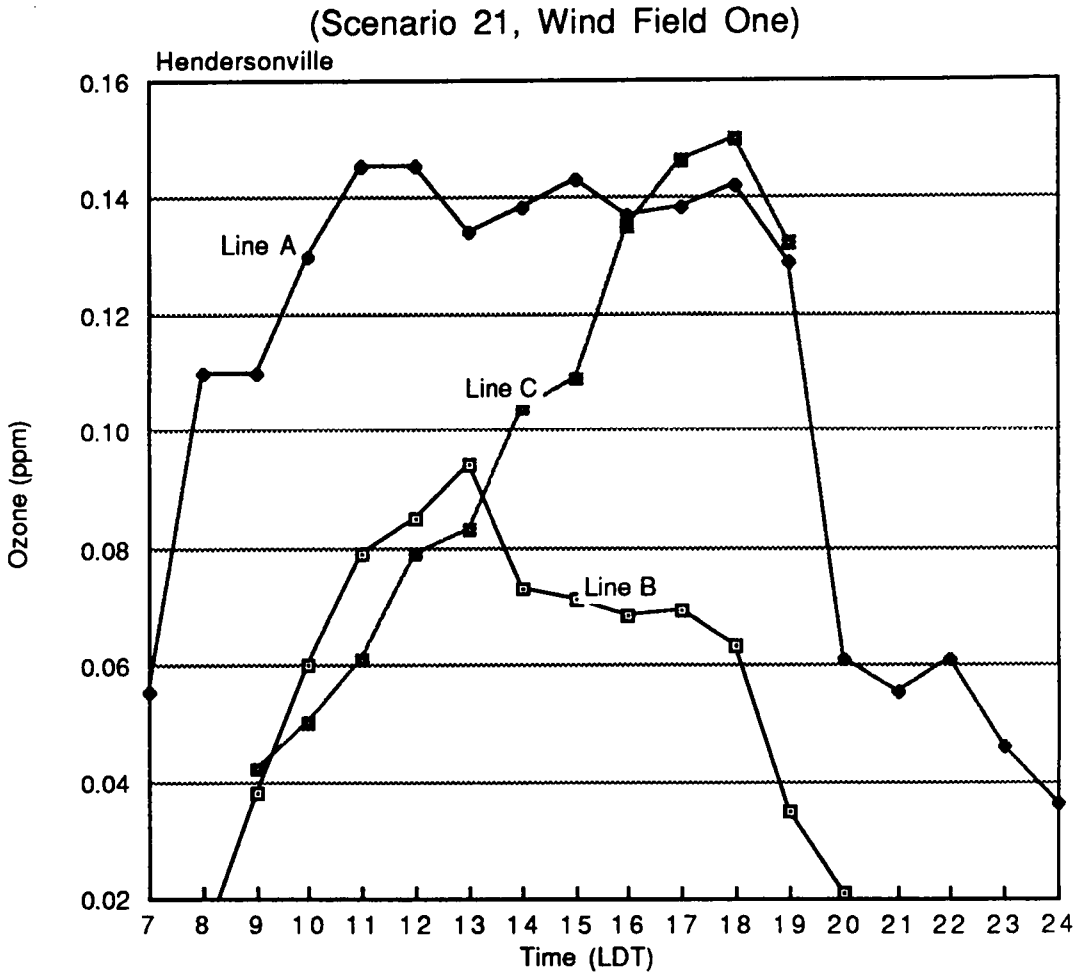


Figure 5-15. Ozone Concentration Profile (Scenario 21)



Line A: Max O3 Conc. from Monitoring Sites
Line B: Min O3 Conc. from Monitoring Sites
Line C: Simulation Result of Scenario 21, Wind Field One
Mixing Height: H=200 m (Morning 08:00) H=2500 m (Afternoon 14:00)

Figure 5-16. Ozone Concentration Profile (Comparison with Monitoring Data, Scenario 21)

ozone concentration can be high depending on the day chosen. The relatively high levels of ozone in the early morning hours were not predicted by the modeling due to the relatively short time period in which sunlight was available. It was hypothesized that the early formation may have been caused by the presence of higher ozone concentrations aloft which may have been brought downward to the ground as the mixing height to increase in the morning hours. This is discussed further in the next section.

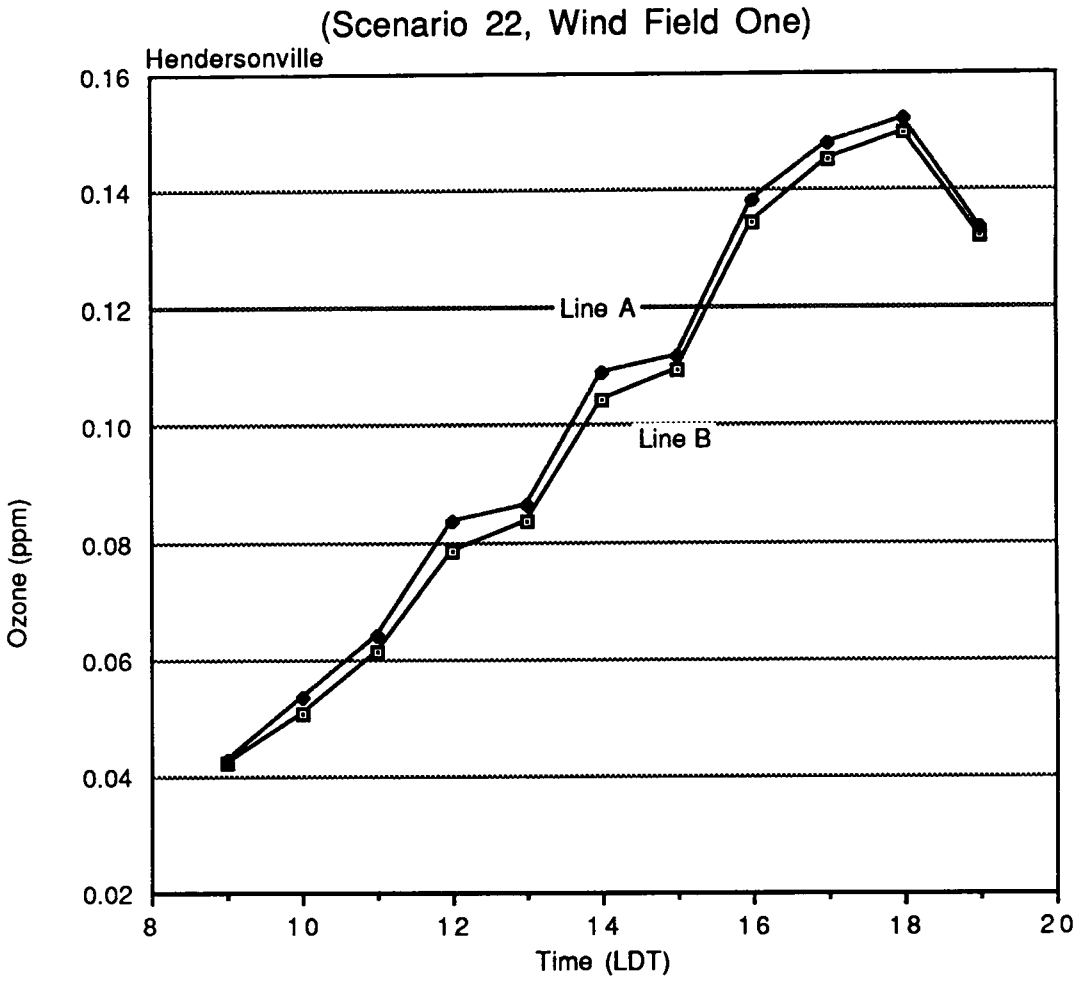
6.0 THE ANALYSIS OF OZONE FORMATION

As pointed out before, ozone formation is a complex photochemical process. The major factors which influence ozone formation include ambient temperature, mixing height, wind field, and aloft ozone concentration. In order to further analyze the ozone formation in the middle Tennessee area, sensitivity analyses were performed.

6.1 Ambient Temperature

The OZIPM-4 model allows the hourly ambient temperature as an input. The chemical kinetic mechanism is temperature dependent. As the ambient temperature rises, the chemical species react faster, leading to an earlier formation of ozone peak and higher ozone concentrations.

In order to focus on the influence of temperature on ozone formation, all inputs except the ambient temperature, were kept the same as the inputs discussed in Section 5. The wind field one was chosen (Figure 5-8). The hourly temperatures used were 3 °C higher than the hourly average temperatures of the ten highest ozone days. It was found that the peak of ozone increased about 3 % because of the increased temperature. Obviously, the higher temperatures worsen the problem of ozone formation even without accounting for the changes in evaporative emissions from the mobile sources (Figure 6-1, scenario 22).



Line A: 3 Degree C Increament of Tem.
Line B: Average Tem. of the Ten Highest Days of Ozone
Mixing Height: H=200 m (Morning 08:00) H=2500 m (Afternoon 14:00)

Figure 6-1. Ozone Concentration Profile (Temperature Sensitivity Analysis, Scenario 22)

6-2 Wind Field

The wind field determined how the pollutants were transported. Unacceptable ozone levels observed at Hendersonville were generally caused by winds which came from southwest to northeast during the summer days (Tables 4-4 and B-9).

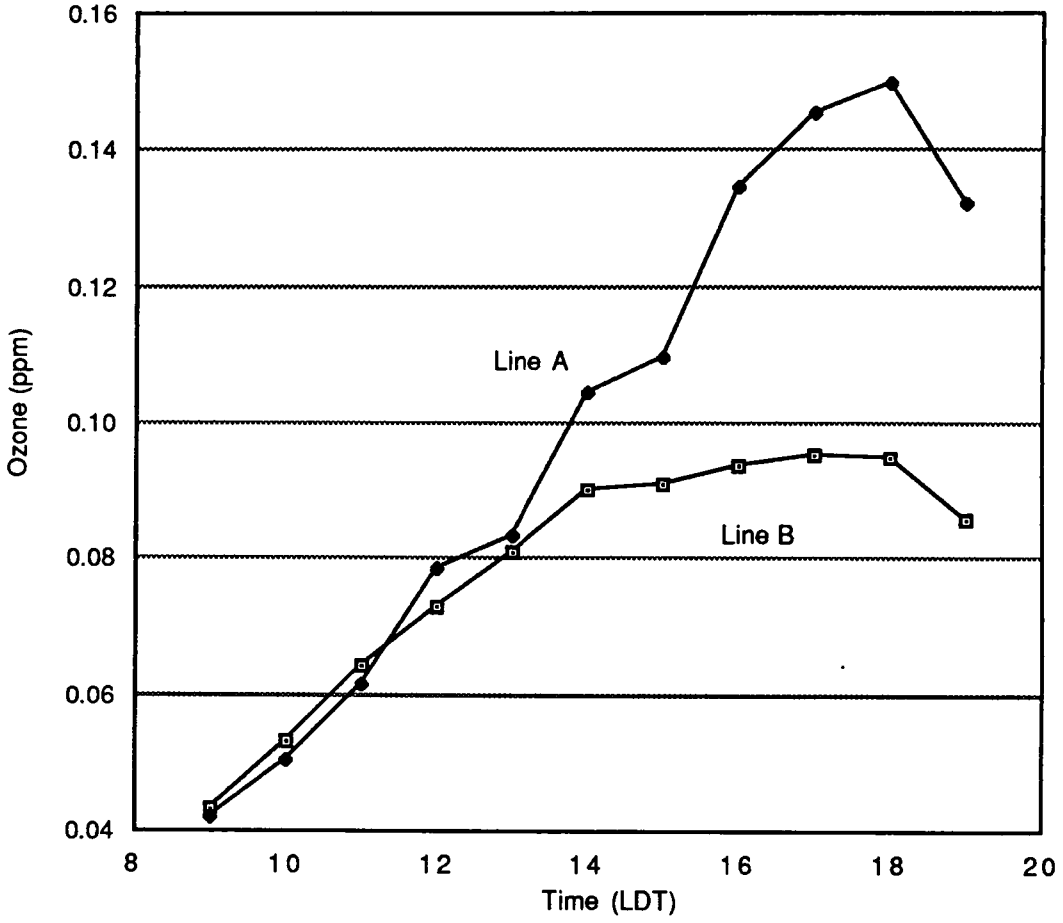
The ozone concentration at the beginning of each hour at Hendersonville was determined by the wind trajectory, along which the moving air parcel traveled. As pointed out in the last section, all eleven hourly parcels were determined by the chosen wind field. A change in the wind trajectory would result in a change in the amounts of pollutants emitted into the simulated parcel because the distribution of the emissions varied both temporally and spatially.

To compare the difference of ozone formation under different wind fields, another wind field, wind field two, was chosen (Figure 5-9). Figure 6-2 gives the results of the simulation under wind field two, which is scenario 23 and compares the results to the previous results from wind field one (scenario 21). While scenario 21 resulted in a predicted exceedance of the standard, scenario 23 predicted significantly less ozone at the Hendersonville site, illustrating the sensitivity to the choice of wind field.

6-3 Aloft Ozone Concentration

The unscavenged ozone aloft has a greater impact than the initial ozone concentration on the maximum afternoon ozone levels within or downwind from the urban area [6]. In

(Scenario 21, Wind Field One & Scenario 23, Winf Field Two)



Line A: Simulation Result of Scenario 21, Wind Field One
Line B: Simulation Result of Scenario 23, Wind Field Two

Figure 6-2. Ozone Concentration Profiles (Wind Field Sensitivity Analysis, Scenarios 21 and 23)

fact, the mixing height can be viewed as the top of a surface-based layer of air which is well-mixed due to mechanical and thermal turbulence. When the mixing height starts to rise in the morning, aloft ozone, NMOC and NO_2 will be entrained to the ground-base layer. An increase in aloft ozone concentration will result in the change of the amount of ozone entrained from the top layer.

An analysis of the effect of ozone aloft was conducted by increasing the aloft ozone concentration to 0.08 ppm. Previously all scenarios had used 0.04 ppm. The wind field used is wind field one (Figure 6-3, Scenario 24). The 0.04 ppm increase in aloft ozone resulted in a 0.02 ppm increase in the ground ozone concentration at the time of maximum ground-level concentration.

6.4 Ozone Formation of Scenario 25

Based on the knowledge of the sensitivity analyses conducted, another scenario of ozone formation was carried out, which fits the monitoring data.

The hourly wind speed of this wind field (wind field three, Figure 5-10, scenario 25) was the hourly average wind speed of the ten highest ozone days. The wind direction was designated from southwest to northeast (Figure 5-10). The aloft ozone concentration was set to 0.08 ppm. The mixing heights in the morning (6:00 A.M.) and afternoon (2:00 P.M.) were 400 m and 2500 m, respectively. In this case, the predicted profile lies within the measured ranges of concentrations (Figure 6-4). The afternoon ozone levels dropped within contours of the measured ozone concentration.

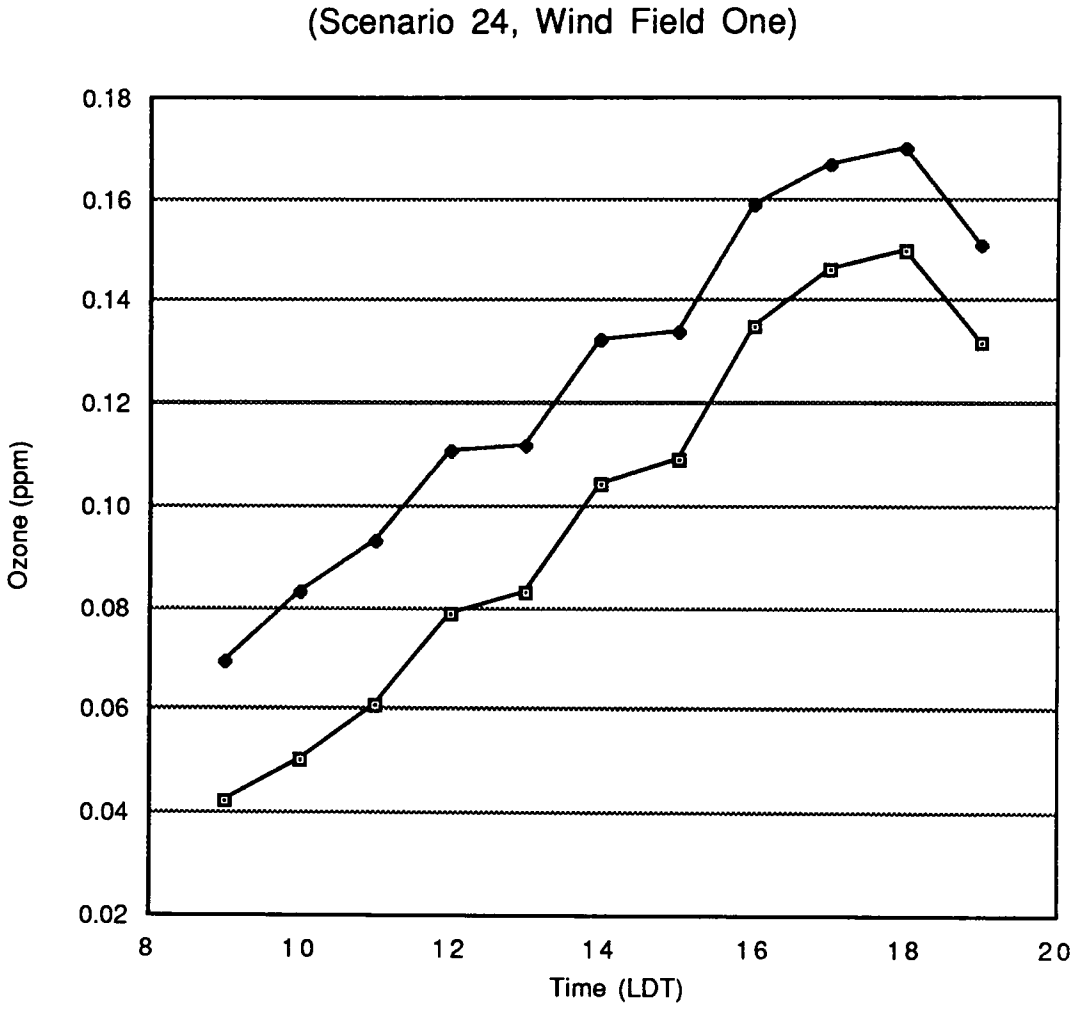
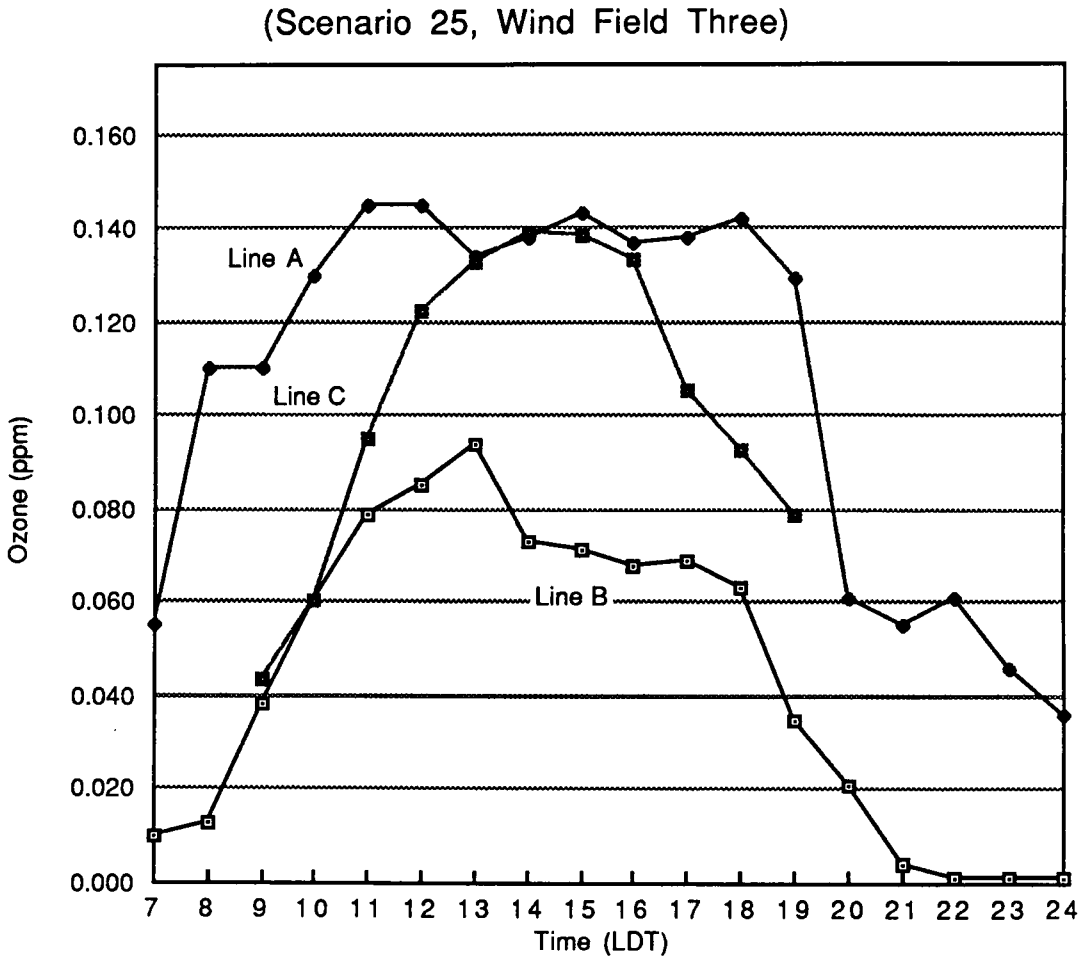


Figure 6-3. Ozone Concentration Profile (Aloft Ozone Conc. Sensitivity Analysis, Scenario 24)



Line A: Max O3 Conc. from Monitoring Site
Line B: Min O3 Conc. from Monitoring Site
Line C: Scenario 24, Wind Field Three, Aloft Ozone Conc. 0.08 ppm

Figure 6-4. Ozone Concentration Profile (Scenario 25)

The hourly wind speeds of wind field three were relative higher than the hourly wind speeds used by wind fields one or two. The higher hourly wind speed resulted in the shorter residence times for the simulated air parcels in the Nashville metropolitan area. The higher ozone aloft would likely occur in a multi-day episode as the previous days ozone concentration becomes trapped aloft as the evening inversion is established. It is hypothesized that the aloft ozone may increase each day during a stable high pressure period resulting in successively more influence each day on ground-level concentration until the weather pattern changes. Additional data are needed to confirm this.

7.0 SIMULATION OF OZONE FORMATION USING THE URBAN AIRSHED MODEL

After finishing the preliminary simulations of ozone formation using the OZIPM-4 model, the Urban AIRSHED model, a more sophisticated photochemical model, was used to to find how the ozone was formed and transported in a three dimensional region mode for the middle Tennessee area. At the end of this section, there is a brief discussion of the advantages and disadvantages of the two models.

7.1 Preparation of Input Files for the Middle Tennessee Area

The Urban AIRSHED model requires 13 input files. They are: AIRQUALITY, BOUNDARY, CHEMPARAM, DIFFBREAK, EMISSIONS, METSCALARS, PTSOURCE, REGIONTOP, SIMCONTROL, TEMPERATUR, TERRAIN, TOPCONC, WIND. Except for certain physical or chemical parameters, the inputs are hourly gridded physical, chemical or emissions variables. These files can be categorized as files related to air quality, meteorology, emissions, chemical reaction parameters or simulation control.

For those files related to air quality, AIRQUALITY provides the information on the air quality of the simulated region at the beginning of the simulated period. BOUNDARY states the air quality of the surrounding boundary excluding the top. TOPCONC provides the air quality of the region top.

For the files related to meteorology, TEMPERATUR contains the hourly temperatures of each surface grid.

DIFFBREAK gives the hourly mixing heights measured from each surface grid. WIND contains the information on two dimensional wind field, the wind speeds in the x direction and in y direction were assigned to each grid. METSCALARS provides all other needed hourly miscellaneous parameters which include NO_2 photolysis coefficient, stability class, water concentration, vertical temperature gradient, and atmospheric pressure.

There are two emissions related files, EMISSIONS and PTSOURCE. EMISSIONS provides the gridded hourly speciated VOCs, NOx and CO emissions from area, mobile and biogenic sources, because it is logical to assume that all these source are ground level sources. PTSOURCE contains the following information on a point source: the location of the source (x,y) in UTM coordinates, (m,n) of grid numbers, stack height, and hourly emissions from the stack.

CHEMPARAM contains the reaction rates of chemical reactions involved in ozone formation. SIMCONTROL is the file which controls the computer simulation process for ozone formation, namely, the information for the simulated period, relative error tolerance, step size of the simulation, etc.

The study area was discussed in Section 2.1. Because of the limitation of computer facilities, the simulated area designed for the middle Tennessee area was smaller than the study area. A three dimensional region was chosen to simulate ozone formations for the middle Tennessee area, and the region was defined by a (20 x 20 x 3) grid system. Vertically, the region was divided into three layers with two of them below the mixing height.

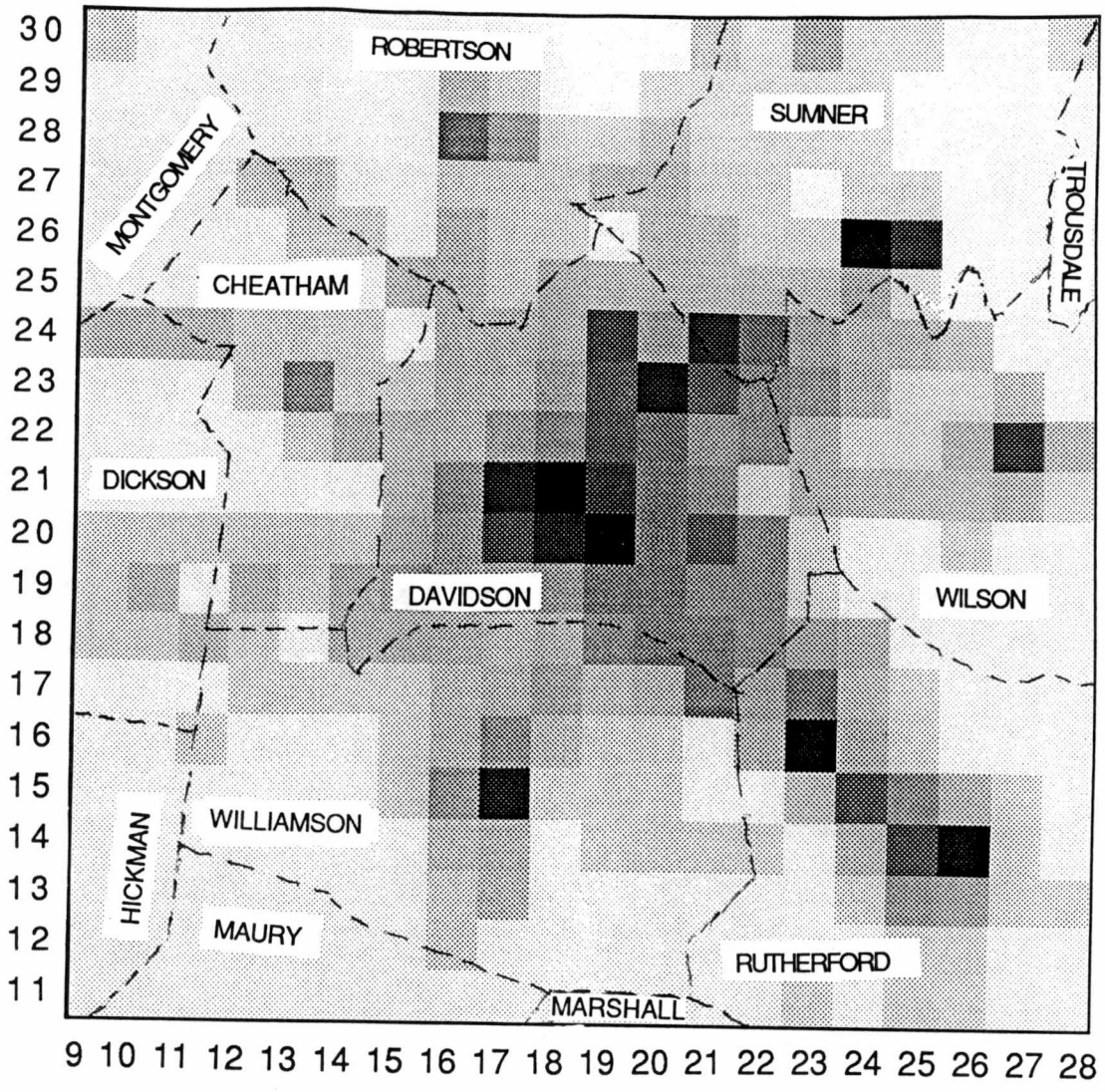
The concentrations of chemical species used by files AIRQULITY, BOUNDARY, and TOPCONC are listed in Table 7-1. For AIRQUALITY, the initial concentrations of chemical species were assigned non-zero values in order to avoid mathematical divergence which could result in failure of the simulation. To simplify the study, boundary conditions were assumed to be homogeneous both temporally and spatially.

The hourly averages of temperatures of the ten highest ozone days (Table 5-1) were used for the TEMPERATUR file to provide the hourly temperatures of the surface layer. DIFFBREAK gives the hourly height of mixing layer. WIND has the information of two dimensional wind field. The wind field used was wind field one (Figure 5-8). METSCALARS provides all other needed hourly miscellaneous parameters which are given on an hourly basis. They are: NO_2 photolysis coefficient, stability class, water concentration, vertical temperature gradient, and atmospheric pressure. The required inputs of meteorological data are given in Section 5 and Appendix B (Table 5-1).

In order to reduce the complexity of emissions related inputs, the emissions from point sources were assumed to be emitted from ground level. Thus only the EMISSIONS file was needed to house the emission data. For each grid, the hourly emissions from point, area, mobile and biogenic sources were summed up as the total emissions for each chemical species. These chemical species were ten VOCs species (OLE, PAR, TOL, XYL, FORM, ALD2, ETH, MEOH, ETOH, ISOP), two NOx species (NO and NO_2) and CO. Figures 7-1 and 7-2 give the distribution of hourly VOCs and NOx emissions from 12:00-13:00.

Table 7-1. The Concentrations Used as Initial, Surrounding and Top Boundary Conditions

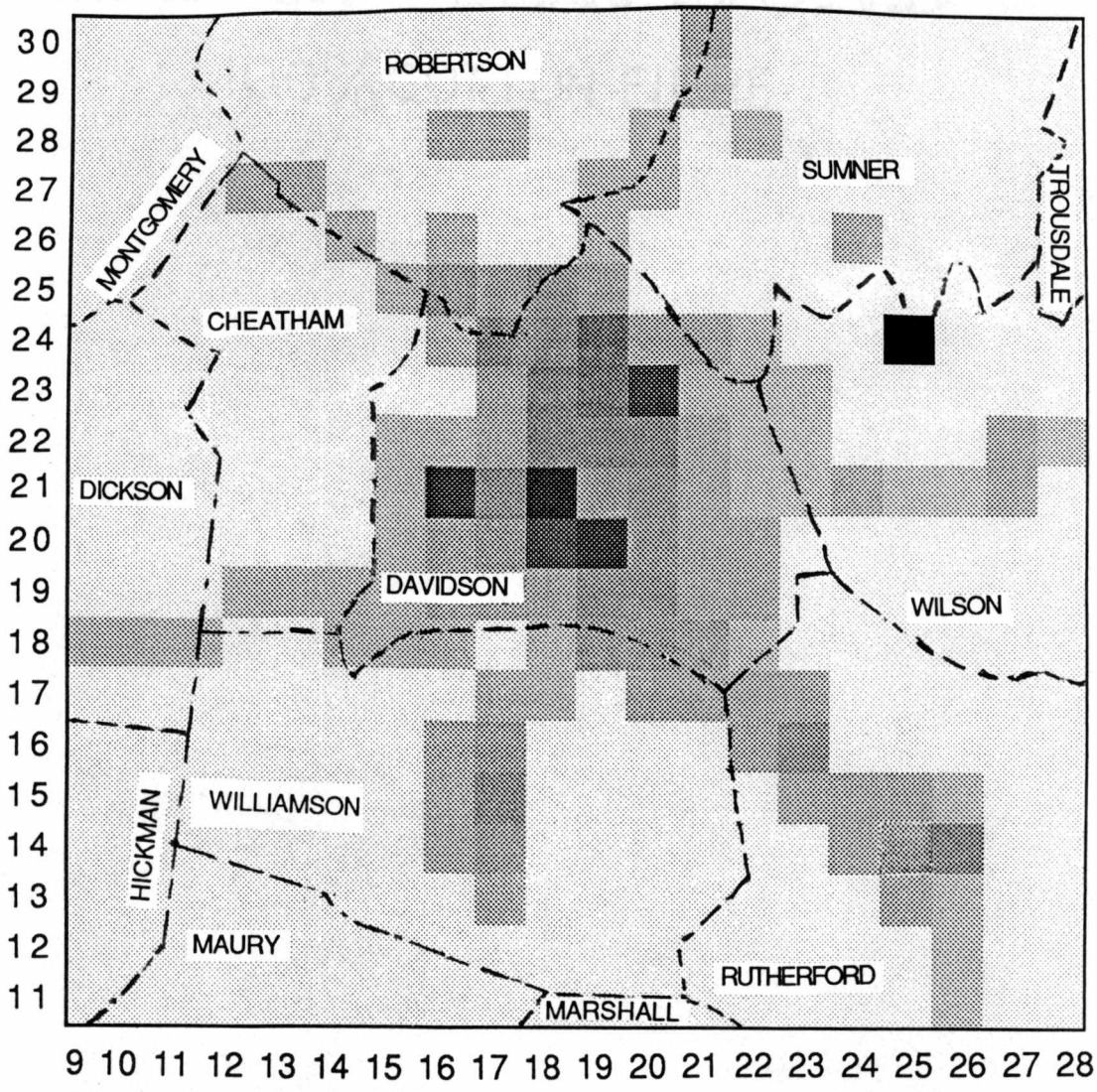
Group	Species	Concentration	Unit
NOx	NO	0.000100	ppm
	NO2	0.000900	ppm
O3	O3	0.040000	ppm
VOCs	OLE	0.000500	ppmc
	PAR	0.012450	ppmc
	TOL	0.001050	ppmc
	XYL	0.000650	ppmc
	FORM	0.001750	ppmc
	ALD2	0.000925	ppmc
	ETH	0.000850	ppmc
CO	CO	0.025000	ppm



Note: CBD is located at grid (18,21)

- 3-4 kg/sq-km
- 4-5 kg/sq-km
- 5-6 kg/sq-km
- 6-7 kg/sq-km
- 7-8 kg/sq-km
- 8-9 kg/sq-km
- 9-10 kg/sq-km
- 10-11 kg/sq-km
- 11-12 kg/sq-km
- 12-13 kg/sq-km
- 13-14 kg/sq-km
- 14-15 kg/sq-km
- 15-16 kg/sq-km
- 16-17 kg/sq-km
- 17-18 kg/sq-km
- 18-19 kg/sq-km
- 19-20 kg/sq-km
- 21-22 kg/sq-km
- 22-23 kg/sq-km
- 31-32 kg/sq-km

Figure 7-1. VOC Emissions (12:00-13:00)



Note: CBD is located at grid (18,21)

0-1 kg/sq-km	7-8 kg/sq-km
1-2 kg/sq-km	8-9 kg/sq-km
2-3 kg/sq-km	10-11 kg/sq-km
3-4 kg/sq-km	11-12 kg/sq-km
4-5 kg/sq-km	24-25 kg/sq-km
5-6 kg/sq-km	42-43 kg/sq-km
6-7 kg/sq-km	83-84 kg/sq-km

Figure 7-2. NOx Emissions (12:00-13:00)

There were 85 chemical reactions adopted by the Urban AIRSHED model. Eleven of them were photochemical reactions. All of the chemical reaction coefficients were stored in the CHEMPARAM file. The simulated date of ozone formation was June 21, 1988. The start and the end times of the simulation were 00:00 and 24:00. A copy of the SIMCONTROL file is given in Figure B-3 which identifies the values of relative error tolerance and step size of the simulation used for the ozone simulation [10,16].

7.2 Simulation of the Urban AIRSHED Model Using the UTK VAX/VMS Main-frame System

The version of the Urban AIRSHED model which was used was downloaded from the Bulletin Board of EPA in North Carolina. By using PCPLUS an IBM-PC software, the model was first copied to an IBM-PC computer, then it was uploaded to the UTK VAX/VMS main-frame system.

Because there were differences among the compilers of different computers, several minor adjustments were made on the main FORTRAN program of the model in order to successfully compile the program on the UTK VAX/VMS system. A 100,000 blocks (one block is 512 kilo-bytes) VAX account was used for the simulation. The main FORTRAN program used about 2,000 blocks. Three sub-directories were built which housed the input files, output files, and the programs of the model.

All of the input files were transformed as binary files because it was required by the model. A batch file SUBMIT.COM was developed for the execution of the program. By submitting

the batch file to the UTK VAX/VMS system from any terminal, the results of the simulation were sent automatically back to the account by the computer. Figure 7-3 lists the files including all the commands needed to run the Urban AIRSHED model on the UTK VAX/VMS system. The simulation of ozone formation consumed about five hours of CPU time.

There were three output file: TRACE.DOC, AIRQUALITY.BIN, and AVERAGE.BIN. TRACE.DOC was the file which recorded the information on the simulation process. AIRQUALITY.BIN contained the instantaneous concentrations of 26 chemical species at the beginning of each hour. AVERAGE.BIN contained the hourly average concentrations of the chemical species simulated. The names of the chemicals are given in Table B-15 (Appendix B). AIRQUALITY.BIN and AVERAGE.BIN were binary files, and were transformed to ASCII files: AIRQUALITY.ASC and AVERAGE.ASC. Each ASCII file used about 20,000 blocks of storage space.

7.3 Preparation of Ozone Contours from the Two Output Files

The results of hourly average and instantaneous ozone concentrations were the most important outputs for the study. For each ground level grid, the simulation provided 24 instantaneous ozone concentrations at the beginning of each hour from 0:00 to 24:00, and the 23 hourly average concentrations from 0:00 to 23:00.

The structures of holding data were the same for both output files. Several smaller FORTRAN programs were written to create 24 files which contained the instantaneous ozone concentrations for the beginning of each hour, and to create 23

```
$ASSIGN [AIRSHED.NEWAIRSHED.INPUT]METSCALARS.BIN        FOR007
$ASSIGN [AIRSHED.NEWAIRSHED.INPUT]SIMCONTROL.BIN        FOR008
$ASSIGN [AIRSHED.NEWAIRSHED.INPUT]CHEMPARAM.BIN         FOR009
$ASSIGN [AIRSHED.NEWAIRSHED.INPUT]AIRQUALITY.BIN        FOR010
$ASSIGN [AIRSHED.NEWAIRSHED.INPUT]BOUNDARY.BIN          FOR011
$ASSIGN [AIRSHED.NEWAIRSHED.INPUT]DIFFBREAK.BIN         FOR012
$ASSIGN [AIRSHED.NEWAIRSHED.INPUT]EMISSIONS.BIN         FOR013
$ASSIGN [AIRSHED.NEWAIRSHED.INPUT]PTSOURCE.BIN          FOR014
$ASSIGN [AIRSHED.NEWAIRSHED.INPUT]TEMPERATUR.BIN        FOR017
$ASSIGN [AIRSHED.NEWAIRSHED.INPUT]TOPCONC.BIN           FOR043
$ASSIGN [AIRSHED.NEWAIRSHED.INPUT]REGIONTOP.BIN         FOR044
$ASSIGN [AIRSHED.NEWAIRSHED.INPUT]TERRAIN.BIN           FOR045
$ASSIGN [AIRSHED.NEWAIRSHED.INPUT]WIND.BIN              FOR046

$ASSIGN [AIRSHED.NEWAIRSHED.OUTPUT]TRACE.DOC            FOR003
$ASSIGN [AIRSHED.NEWAIRSHED.OUTPUT]AIRQUALITY.BIN       FOR042
$ASSIGN [AIRSHED.NEWAIRSHED.OUTPUT]OUTPUT.DOC           FOR047
$ASSIGN [AIRSHED.NEWAIRSHED.OUTPUT]AVERAGE.BIN          FOR041

$RUN SYS$USER3:[AIRSHED.NEWAIRSHED.PROGRAM]UAMZHOU.EXE
```

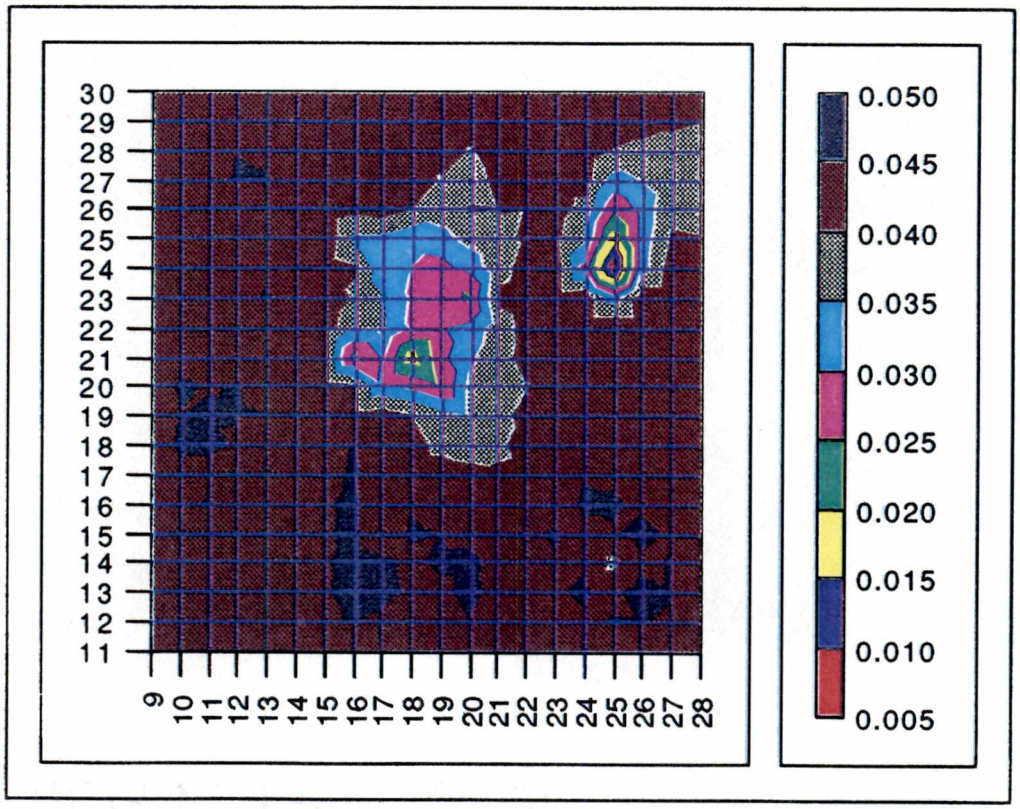
Figure 7-3. The Commands Used to Run the Urban Airshed Model

files which had the information of the hour average ozone concentrations. Downloaded from the UTK VAX/VMS system to an IBM-PC computer, these files were created as LOTUS-123 files. In order to give the ground level ozone contours of the whole simulated area for the hourly average and instantaneous ozone concentrations, a graphic software package was used on a Macintosh computer. The LOTUS-123 files were transformed to Macintosh files by using a software package called Apple-Exchange. Finally, graphics for these files were created using the Wingz software of Macintosh. Two example graphics are given in Figures 7-4 and 7-5.

7.4 The Results of Simulation

Temporally, the unacceptable ozone level was formed in the later afternoon. It reached the maximum concentration at 7:00 P.M. (Figure 7-5). Geographically, the peak ozone was found near Hendersonville (a small town located downwind of the Nashville metropolitan area) rather than downtown Nashville. The hourly average and instantaneous ozone concentration of the region provided a panorama of how the unacceptable ozone was formed and transported. Figures 7-4 and 7-5 give the instantaneous ozone concentrations of the region at 10:00 A.M. and 7:00 P.M. An ozone peak and ozone hole were found in Figure 7-5. The ozone peak was a small area where the ozone levels were between 0.13-0.14 ppm.

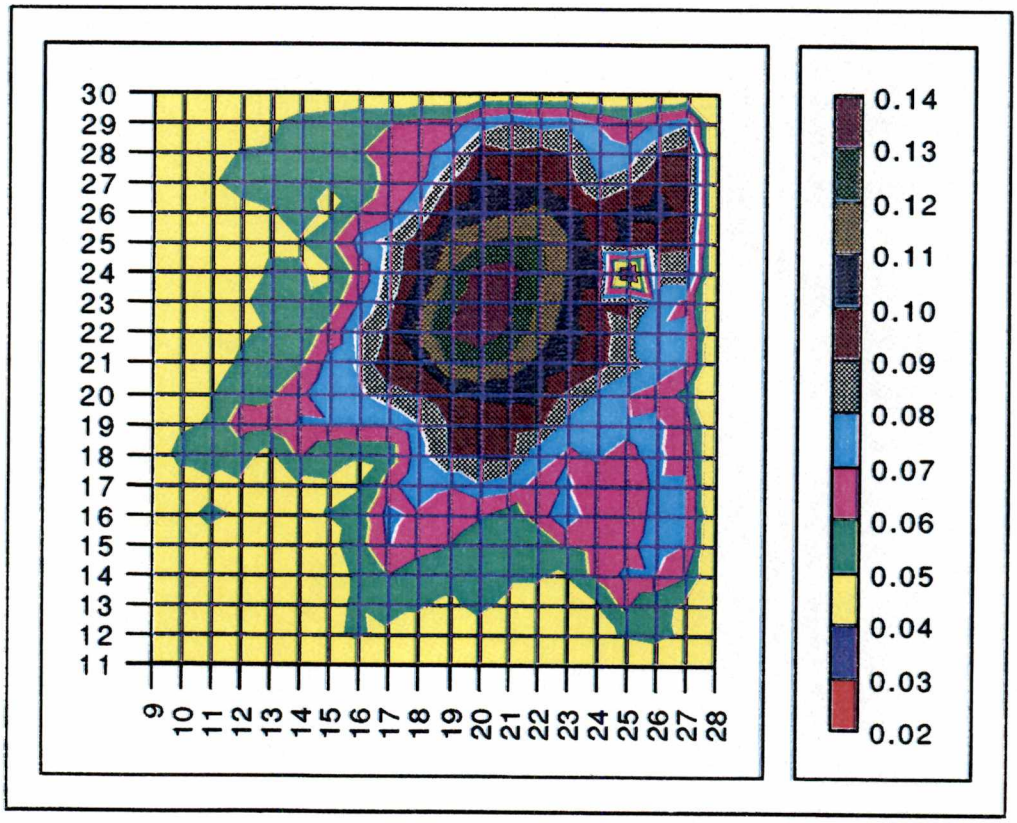
By using the method of wind trajectories, the ozone profile at Hendersonville was given by the OZIPM-4 model. Similarly, the ozone profile could be found from the simulation results of the Urban AIRSHED model. The monitoring station of Hendersonville was located at the grid (24,21). In order to



Note: CBD is located at grid (18,21)

The Middle Tennessee Area

Figure 7-4. Instantaneous Ground Level Ozone Concentration (10:00)



Note: CBD is located at grid (18,21)

The Middle Tennessee Area

Figure 7-5. Instantaneous Ground Level Ozone Concentration (19:00)

compare with the results from the OZIPM-4 model, the ozone profile was found by selecting the instantaneous ozone concentration at the beginning time of each hour (Figure 7-6) of the grid, because the ozone profile from the OZIPM-4 model was the instantaneous ozone concentration of each hour.

Scavenging Effects of NOx Sources

The simulation results showed that there was an ozone hole located at grids (25,24) (see Figures 7-4 and 7-5). In order to compare the ozone formation at the hole (located at grid (25,21) with the ozone formation at the Hendersonville site (located at grid (21,24)), two ozone concentration profiles (Table 7-2) are drawn together in Figure 7-6. The maximum ozone level of grid (25,24) was 0.058 ppm compared to the peak concentration 0.134 of grid (24,21).

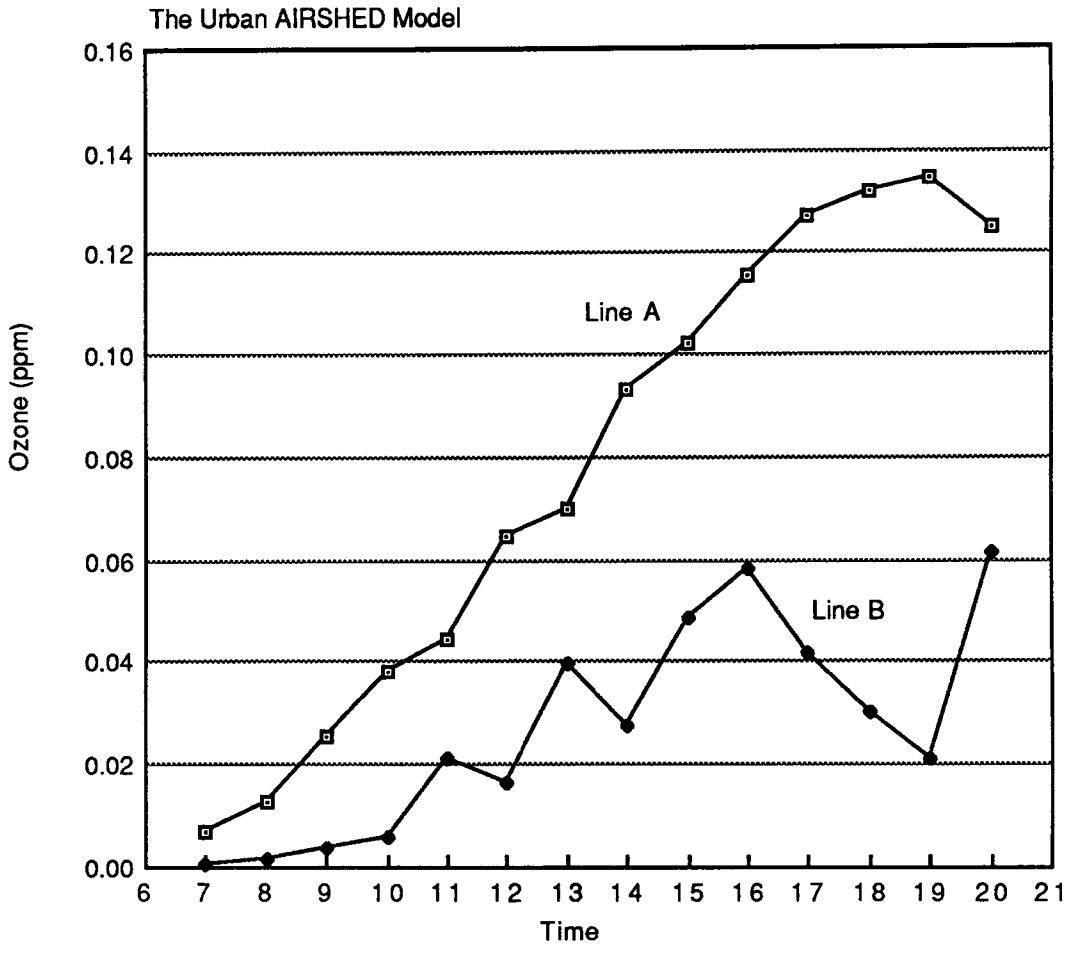
There was a major steam plant in Sumner County, which was a major NOx point source. The location of the steam plant was grid (25,24). As mentioned in Section 1.2, NOx is a scavenger of ozone. The principle of scavenging effect of NOx is given in equation (4) of Section 1.2, that is, ozone reacts with nitrogen oxide to form nitrogen dioxide and oxygen.

7.5 Comparison of the OZIPM-4 Model with the Urban AIRSHED Model

Both the OZIPM-4 model and the Urban AIRSHED model have been used to simulate ozone formations in the middle Tennessee area. A comparison of the simulated results of the two models is very interesting and useful. In addition to

Table 7-2. Some Simulation Results from the Urban AIRSHED Model

Time	Ozone Conc. (ppm)		
	The Urban AIRSHED Model		The OZIPM-4 Model
	Grid(21,24) Hendersonville	Grid(25,24) The Steam Plant	Scenario 21 Hendersonville
7	0.007	0.000	
8	0.013	0.001	
9	0.025	0.004	0.042
10	0.038	0.006	0.050
11	0.045	0.021	0.061
12	0.065	0.016	0.079
13	0.070	0.039	0.083
14	0.093	0.028	0.104
15	0.102	0.049	0.109
16	0.116	0.058	0.135
17	0.127	0.042	0.146
18	0.132	0.030	0.150
19	0.134	0.021	0.132
20	0.125	0.061	



Line A: Ozone profile of grid (24,21), the Hendersonville Air Monitoring Site
Line B: Ozone profile of grid (25,24), a Steam Plant of Sumner County

Figure 7-6. Ozone Concentration Profiles at Hendersonville and the Steam Plant

providing profiles of instantaneous ozone concentration at Hendersonville (as in the OZIPM-4 model), the Urban AIRSHED model gave the hourly average and instantaneous ozone concentrations of each grid of the simulated region. The results from the Urban AIRSHED model provided a general understanding of how ozone was formed and transported.

Both models provided ozone profiles at Hendersonville. The profiles are drawn together in Figure 7-7 in order to compare with each other. The shapes of two curves are similar, but the predicted ozone level by the OZIPM-4 model is a little higher than the ozone level predicted by the Urban AIRSHED model.

Ozone formation is a process resulting from mutual influences of transport, diffusion and chemical reactions of chemical species in ambient air. The OZIPM-4 model considers factors of transport and chemical reactions. By using the wind trajectory to predict ozone level, the transport effect of pollutants was considered, but the influences of diffusion were omitted by the model. The diffusion effect on the ozone formation is considered by the Urban AIRSHED model by using turbulent diffusion coefficients in the model. That is why the predicted ozone levels at Hendersonville from the OZIPM-4 model were slightly higher than the levels predicted from the Urban AIRSHED model.

Methodologically, the OZIPM-4 model was used to provide ozone profiles at Hendersonville by simulating moving air boxes in Lagrangian Coordinate System. On the other hand, the Urban AIRSHED model was used to simulate the ozone formation in Eulerian Coordinate System. The OZIPM-4 model ran on an IBM-PC computer; the Urban AIRSHED model ran on

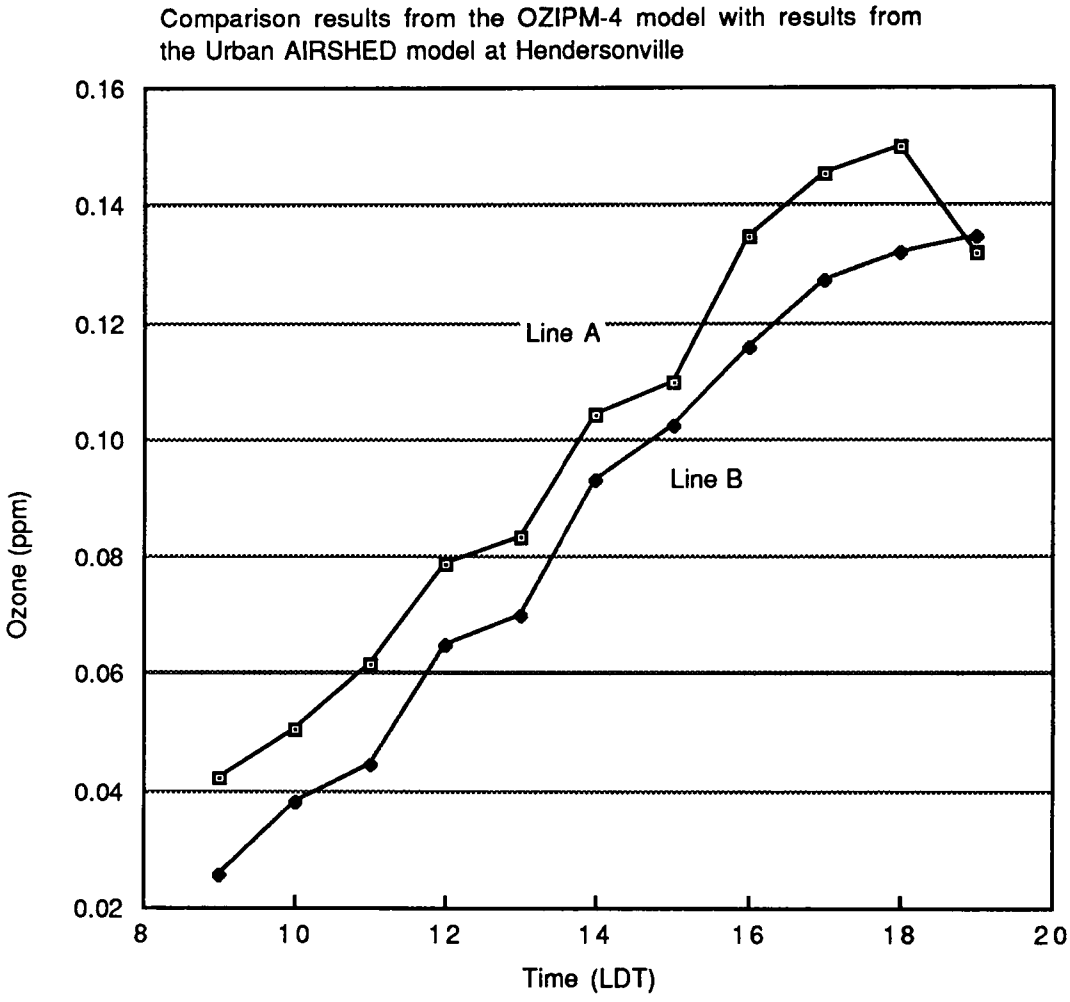


Figure 7-7. The Comparison of Two Models Used

the UTK VAX/VMS mainframe system. For the OZIPM-4 model, it was required to wisely choose a wind trajectory for each hour under a chosen wind field; for the Urban AIRSHED model, it was required to prepare all the emissions for each grid of the entire region.

The comparison of the labor forces needed and the computer facilities required by the two models also provides some idea about advantages and disadvantages of the two models. The OZIPM-4 model was much simpler than the Urban AIRSHED model and the required inputs for the OZIPM-4 model were relatively easier to prepare. On the other side, the Urban AIRSHED model required the emissions data of each grid of the region and the detailed meteorological, boundary and initial conditions. The IBM-PC computer, because of its economic feasibility, is a more accessible machine. The CPU time required by the OZIPM-4 model was short enough to be ignored (90 seconds for a run), whereas the Urban AIRSHED model required about five hours of CPU time on the VAX/VMS system.

8.0 CONCLUSION

For the base year of 1988, the ozone simulations in the middle Tennessee area have been accomplished by using the OZIPM-4 model and the Urban AIRSHED model. The simulation results were shown to be reasonable by comparing the simulated ozone profile with the historical monitoring station data.

Even though, the reasons for unacceptable ozone level formation were complex, the violations observed at Hendersonville were mainly a result of the high level of emissions of VOCs and NOx and the dominant wind direction from southwest to northeast in the summer which placed the station in the path of the plume from a major metropolitan area.

There was a series of interesting results which came from the simulations by using the OZIPM-4 model. The analysis of the ozone formation at downtown Nashville shows the relative contribution of different source categories of emissions to ozone levels. It was found that emissions from the mobile sources had the largest influence on unacceptable ozone level formation both at downtown Nashville and Hendersonville. Mobile sources were the major contributor of VOCs and NOx emissions. Several sensitivity analyses were carried out to help determine the reasons of unacceptable ozone formation. It was found that higher aloft ozone concentration could result in higher and earlier peak ozone formation. Higher diurnal temperatures could also speed up the ozone formation and increase formed ozone concentrations.

The application of the Urban AIRSHED model on the middle Tennessee area provided a panorama of how the pollutants were formed and transported. The hourly instantaneous and average ozone and other 23 chemical concentrations (Table B-15) of the entire region were the outputs of the model. The comparison of the patterns of temporal and spatial VOCs and NOx to the relevant patterns of ozone pollution provided insight into how the ozone peak was formed and moved due to the transport of reactive pollutants. The peak ozone area moved toward the northeast from downtown Nashville and reached its maximum value at 7:00 P.M. at a location near Hendersonville. One of the interesting results was the discovery of an ozone hole due to the scavenging effect of NOx resulting from a steam plant (NOx source). The location of the ozone hole corresponded to the location of the steam plant. However, the steam plant was not an impact at the Hendersonville site under the conditions modeled. Further research is needed to determine the potential impact of such NOx sources under meteorological conditions that would transport this type of plume across the urban area.

One of the highlights of the research was the demonstration of applying the simpler OZIPM-4 model to create ozone profile versus time at Hendersonville. The OZIPM-4 model was a trajectory model, thus chemical reactions and ozone formation were simulated in a Lagrangian Coordinate System. The ozone profile at Hendersonville was provided by choosing a wind trajectory for each hour and predicting the ozone concentration at Hendersonville at the beginning of the hour.

It was of interest to compare these two models. Both of them were used to simulate the ozone formation. The OZIPM-4 model was a simpler and cheaper model. The Urban AIRSHED model was a sophisticated and EPA preferred model. It was found that, at Hendersonville, the ozone concentrations from the OZIPM-4 model were slightly higher than the values from the Urban AIRSHED model. The reason was that the Urban AIRSHED model included movement of pollutants due to transport and diffusion whereas the OZIPM-4 model only considered transport.

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APPENDIXES

APPENDIX A. ALLOCATION OF POPULATION

APPENDIX B. TABLES AND FIGURES

APPENDIX A. ALLOCATION OF POPULATION

A.0 ALLOCATION OF POPULATION

Most categories of the area sources investigated were population-based (Table 3-3). The determination of the gridded emissions from populate-based area sources required the population values of the grids belonging to Davidson and the seven surrounding counties. The U.S. Department of Commerce's 1980 Cencus of Population and Housing [17] provided the population census of Nashville. The basic unit area for the population census was a tract and each county was divided into many tracts.

The preparation of the gridded emissions required the population for each grid in 1988. First the population of 1988 of each county was calculated from the historical population data of the county. The population of each tract of 1988 was then calculated based on the population of 1980 and the population ratio of the tract-related county from 1980 to 1988, the ratio was the population of 1988 divided by the population of 1980. Finally, the population of each grid of 1988 was calculated from the population of the tracts nested by the grid.

A.1 The Population of 1988 of Each County

Table A-1 lists the population of 1980 for all the relevant counties. The population of each county of 1988 was calculated from the historical population of the county. The Tennessee Planning Office published the 1986 and 1987 estimated population for all Tennessee counties. Assuming

Table A-1. The Population Data of Davidson County and the Seven Surrounding Counties

County	1980	1986	1987
Davidson	477811	497800	505900
Cheatham	21616	24800	25800
Dickson	30037	32900	33800
Robertson	37021	40500	41900
Rutherford	84058	102500	107300
Sumner	85790	96700	99600
Williamson	58108	72000	75500
Wilson	56064	63800	66400

that the population of each county was linear increasing from 1986 to 1988, the population of 1988 was determined by the following equation,

$$\text{Pop of 1988} = 2 * (\text{Pop of 1987}) - \text{Pop of 1986} \qquad (12)$$

A.2 The Population of Each Tract for 1988

Because a tract was the basic unit for the population census, the population distribution inside the tract was assumed to be uniform. For each tract, the population of 1980 was found in [17]. An example can be found in Table B-16 (Appendix B). The geographic location of each tract was drawn in the maps of [17]. It was found that there were more census tracts near cities compared with other areas. The detailed tract maps of Nashville metropolitan area of Davidson County and Murfreesboro City of Rutherford County are also provided. For each tract, the population of 1988 was calculated by multiplying the population of 1980 by the population ratio (Table A-1) of the county which the tract was located in.

A.3 The Population of Each Grid in 1988

The calculation of the population of 1988 of each grid was the final also the most difficult step. As defined in Section 2.1, each grid was a (5 x 5 sq-km) square. Generally, a grid was separated into several parts by the tracts which were partially covered by the grid (Figure A-1). The population of the grid was calculated from the population of these tracts.

The method of calculation can be demonstrated by the following example (Figure A-1). A grid was separated by census tract **A**, **B**, **C**, and **D** into four small areas, called **a**, **b**, **c**, and **d**.

The area ratio of **a** to tract **A** could be calculated by dividing the area of **a** by the area of **A.** Similarly, the ratios related to area **B**, **C** and **D** can be found too. If α, β, χ, and δ were used to express the four ratios, then the population of the grid of 1988 was,

$$\text{Population of } (i,j) = \alpha * P1 + \beta * P2 + \chi * P3 + \delta * P4 \qquad (13)$$

Here P1, P2, P3 and P4 were the population of 1988 for the tracts of **A**, **B**, **C**, and **D**.

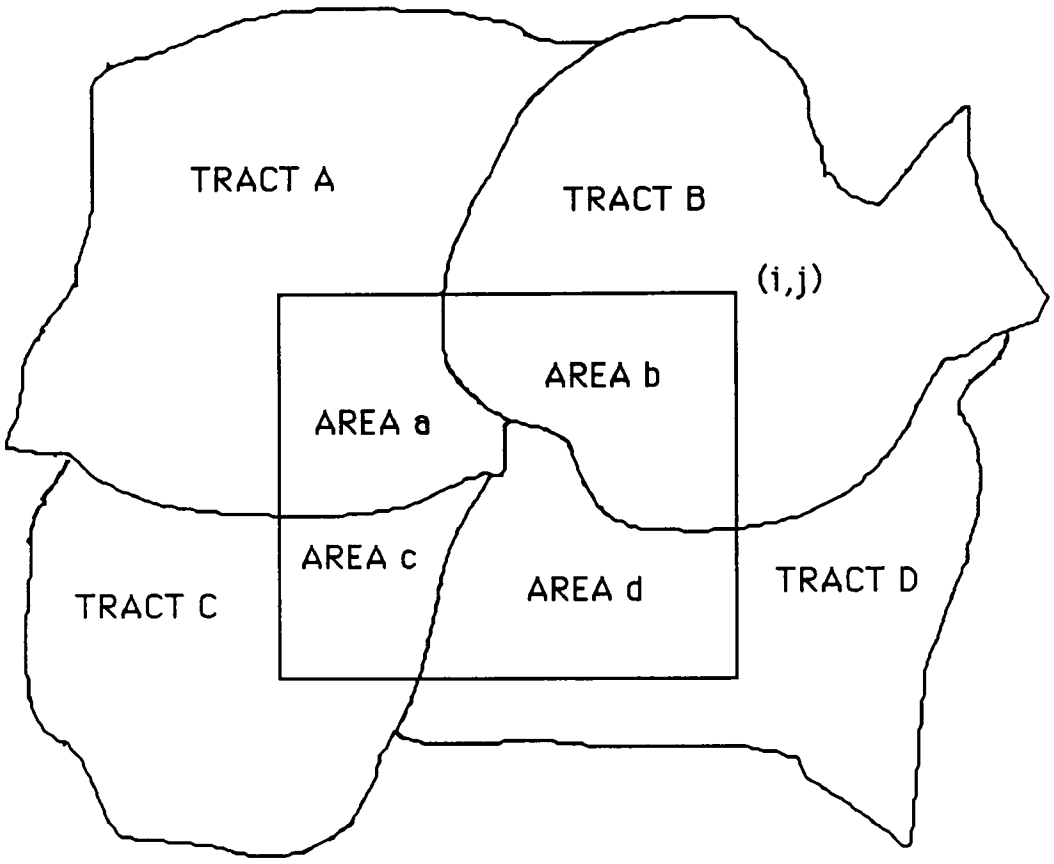


Figure A-1. An Example of Grid And Tracts

APPENDIX B. TABLES AND FIGURES

Table B-1. The Transformation of Coordinate Systems

X-EAST	Y-WEST	UTM-E	UTM-W	LONGITUDE	LATITUDE	TYPE	POP	COUNTY
-5	24	402.00	4015.00	88:05:28	36:16:36	2		
-4	24	407.00	4015.00	88:02:08	36:16:38	2		
-3	24	412.00	4015.00	87:58:47	36:16:40	2		
-2	24	417.00	4015.00	87:55:27	36:16:42	2		
-1	24	422.00	4015.00	87:52:07	36:16:43	2		
0	24	427.00	4015.00	87:48:46	36:16:44	2		
1	24	432.00	4015.00	87:45:26	36:16:46	2		
2	24	437.00	4015.00	87:42:05	36:16:47	2		
3	24	442.00	4015.00	87:38:45	36:16:48	2		
4	24	447.00	4015.00	87:35:24	36:16:49	2		
5	24	452.00	4015.00	87:32:04	36:16:50	1	152	DICKSON
6	24	457.00	4015.00	87:28:44	36:16:51	1	305	DICKSON
7	24	462.00	4015.00	87:25:23	36:16:52	1	275	DICKSON
8	24	467.00	4015.00	87:22:03	36:16:52	1	259	DICKSON
9	24	472.00	4015.00	87:18:42	36:16:53	1	331	DICKSON
10	24	477.00	4015.00	87:15:22	36:16:53	1	494	DICKSON
11	24	482.00	4015.00	87:12:02	36:16:54	1	528	DICKSON
12	24	487.00	4015.00	87:08:41	36:16:54	1	784	CHEATHAM
13	24	492.00	4015.00	87:05:21	36:16:54	1	1814	CHEATHAM
14	24	497.00	4015.00	87:02:00	36:16:54	1	1444	CHEATHAM
15	24	502.00	4015.00	86:58:40	36:16:54	1	815	CHEATHAM
16	24	507.00	4015.00	86:55:19	36:16:54	1	90	DAVIDSON
17	24	512.00	4015.00	86:51:59	36:16:54	1	1870	DAVIDSON
18	24	517.00	4015.00	86:48:39	36:16:54	1	1754	DAVIDSON
19	24	522.00	4015.00	86:45:18	36:16:53	1	5237	DAVIDSON
20	24	527.00	4015.00	86:41:58	36:16:53	1	11805	DAVIDSON
21	24	532.00	4015.00	86:38:37	36:16:52	1	12777	SUMNER
22	24	537.00	4015.00	86:35:17	36:16:52	1	7295	SUMNER
23	24	542.00	4015.00	86:31:56	36:16:51	1	2792	WILSON
24	24	547.00	4015.00	86:28:36	36:16:50	1	1360	WILSON
25	24	552.00	4015.00	86:25:16	36:16:49	1	864	WILSON
26	24	557.00	4015.00	86:21:55	36:16:48	1	567	WILSON
27	24	562.00	4015.00	86:18:35	36:16:47	1	567	WILSON
28	24	567.00	4015.00	86:15:14	36:16:46	1	466	WILSON
29	24	572.00	4015.00	86:11:54	36:16:45	1	524	WILSON
30	24	577.00	4015.00	86:08:34	36:16:43	1	175	WILSON
31	24	582.00	4015.00	86:05:13	36:16:42	2		
32	24	587.00	4015.00	86:01:53	36:16:40	2		
33	24	592.00	4015.00	85:58:32	36:16:39	2		

Table B-2. The VOC Speciation Coefficients for Each Category of Area Sources (the Seven Surrounding Counties)

No	Profile	OLEMOLE	PARMOLE	TOLMOLE	XYLMOLE	FORMMOLE	ALD2MOLE	ETHMOLE	ISOPMOLE
1	1190	0.0008610	0.0263600	0.0025740	0.0031060	0.0000000	0.0002392	0.0000000	0.0000000
2	1190	0.0008610	0.0263600	0.0025740	0.0031060	0.0000000	0.0002392	0.0000000	0.0000000
3	1190	0.0008610	0.0263600	0.0025740	0.0031060	0.0000000	0.0002392	0.0000000	0.0000000
4	1196	0.0000646	0.0090530	0.0000869	0.0000942	0.0000000	0.0000053	0.0000000	0.0000000
5	1196	0.0000646	0.0090530	0.0000869	0.0000942	0.0000000	0.0000053	0.0000000	0.0000000
6	1195	0.0000973	0.0180300	0.0009661	0.0003875	0.0000000	0.0001112	0.0016050	0.0000000
7	1016	0.0012890	0.0460200	0.0017390	0.0002562	0.0000000	0.0002464	0.0000000	0.0000000
8	1194	0.0007864	0.0347200	0.0021380	0.0020840	0.0000000	0.0005941	0.0000000	0.0000000
9	1191	0.0000320	0.0431800	0.0000192	0.0000000	0.0000000	0.0000569	0.0000000	0.0000000
10	76	0.0000000	0.0387700	0.0005427	0.0014130	0.0000000	0.0013160	0.0000000	0.0000000
11	197	0.0000000	0.0189500	0.0000000	0.0000000	0.0001998	0.0000000	0.0000000	0.0080100
12	202	0.0000073	0.0010680	0.0000109	0.0000094	0.0000000	0.0000000	0.0000000	0.0000000
13	9022	0.0015140	0.0165300	0.0000033	0.0000028	0.0000000	0.0000000	0.0033400	0.0000000
14	195	0.0000000	0.0006234	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
15	1185	0.0012680	0.0290600	0.0014450	0.0013530	0.0000000	0.0000000	0.0000000	0.0000000
16	2	0.0000000	0.0351500	0.0000000	0.0000000	0.0162200	0.0000000	0.0000000	0.0000000
17	1	0.0000000	0.0276500	0.0000000	0.0000000	0.0139900	0.0000000	0.0000000	0.0000000
18	195	0.0000000	0.0006234	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
19	3	0.0000000	0.0202200	0.0002171	0.0000000	0.0026640	0.0000000	0.0000000	0.0000000
20	1178	0.0011380	0.0211100	0.0016700	0.0045110	0.0000000	0.0002994	0.0000000	0.0000000
21	2	0.0000000	0.0351500	0.0000000	0.0000000	0.0162200	0.0000000	0.0000000	0.0000000
22	1	0.0000000	0.0276500	0.0000000	0.0000000	0.0139900	0.0000000	0.0000000	0.0000000

Table B-2. (Continued)

No	Profile	OLEMOLE	PARMOLE	TOLMOLE	XYLMOLE	FORMMOLE	ALD2MOLE	ETHMOLE	ISOPMOLE
23	3	0.0000000	0.0202200	0.0002171	0.0000000	0.0026640	0.0000000	0.0000000	0.0000000
24	3	0.0000000	0.0202200	0.0002171	0.0000000	0.0026640	0.0000000	0.0000000	0.0000000
25	1185	0.0012680	0.0290600	0.0014450	0.0013530	0.0000000	0.0000000	0.0000000	0.0000000
26	2	0.0000000	0.0351500	0.0000000	0.0000000	0.0162200	0.0000000	0.0000000	0.0000000
27	1	0.0000000	0.0276500	0.0000000	0.0000000	0.0139900	0.0000000	0.0000000	0.0000000
28	3	0.0000000	0.0202200	0.0002171	0.0000000	0.0026640	0.0000000	0.0000000	0.0000000
29	1201	0.0015280	0.0268500	0.0016970	0.0001366	0.0028670	0.0013380	0.0007970	0.0000000
30	1186	0.0008297	0.0502500	0.0004688	0.0005948	0.0001542	0.0015890	0.0015510	0.0000147
31	1186	0.0008297	0.0502500	0.0004688	0.0005948	0.0001542	0.0015890	0.0015510	0.0000147
32	1201	0.0015280	0.0268500	0.0016970	0.0001366	0.0028670	0.0013380	0.0007970	0.0000000
33	1186	0.0008297	0.0502500	0.0004688	0.0005948	0.0001542	0.0015890	0.0015510	0.0000147
34	1186	0.0008297	0.0502500	0.0004688	0.0005948	0.0001542	0.0015890	0.0015510	0.0000147
35	1186	0.0008297	0.0502500	0.0004688	0.0005948	0.0001542	0.0015890	0.0015510	0.0000147
36	1099	0.0027930	0.0162600	0.0001307	0.0001122	0.0057630	0.0017820	0.0055190	0.0000000
37	122	0.0001188	0.0019650	0.0000000	0.0000000	0.0000000	0.0000000	0.0031020	0.0000000
38	122	0.0001188	0.0019650	0.0000000	0.0000000	0.0000000	0.0000000	0.0031020	0.0000000
39	122	0.0001188	0.0019650	0.0000000	0.0000000	0.0000000	0.0000000	0.0031020	0.0000000
40	307	0.0014590	0.0380200	0.0000000	0.0000000	0.0000000	0.0000000	0.0068130	0.0000000
41	307	0.0014590	0.0380200	0.0000000	0.0000000	0.0000000	0.0000000	0.0068130	0.0000000
42	121	0.0044170	0.0465600	0.0000000	0.0000000	0.0000000	0.0000000	0.0069160	0.0000000
43	121	0.0044170	0.0465600	0.0000000	0.0000000	0.0000000	0.0000000	0.0069160	0.0000000
44	121	0.0044170	0.0465600	0.0000000	0.0000000	0.0000000	0.0000000	0.0069160	0.0000000

Table B-3. The VOC Speciation Coefficients for Rural-Based Area Sources (Day Time)
(the Seven Surrounding Counties)

County	Cheatham	Dickson	Robertson	Rutherford	Sumner	Williamson	Wilson
OLEMOLE	0.0010037	0.0009824	0.0009512	0.0009919	0.0010101	0.0008699	0.0010192
PARMOLE	0.0334677	0.0329597	0.0321069	0.0338453	0.0334039	0.0326830	0.0335362
TOLMOLE	0.0010034	0.0010645	0.0011603	0.0010039	0.0009953	0.0011662	0.0009733
XYLMOLE	0.0005376	0.0005650	0.0006062	0.0005474	0.0005309	0.0006809	0.0005199
FORMMOLE	0.0013774	0.0014690	0.0016148	0.0013649	0.0013696	0.0015677	0.0013384
ALD2MOLE	0.0011260	0.0011776	0.0012540	0.0011549	0.0011095	0.0013310	0.0010873
ETHMOLE	0.0015525	0.0012767	0.0008565	0.0014742	0.0016143	0.0005250	0.0017230
ISOPMOLE	0.0000007	0.0000005	0.0000001	0.0000010	0.0000006	0.0000005	0.0000006

Table B-4. The VOC Speciation Coefficients for Different Groups of Area Sources (the Seven Surrounding Counties)

County	Rural	Aircraft	Railroad	Boat
	Night	24-hr	24-hr	24-hr
OLEMOLE	0.0014590	0.0027930	0.0015280	0.0008297
PARMOLE	0.0380200	0.0162600	0.0268500	0.0502500
TOLMOLE	0.0000000	0.0001307	0.0016970	0.0004688
XYLMOLE	0.0000000	0.0001122	0.0001366	0.0005948
FORMMOLE	0.0000000	0.0057630	0.0028670	0.0001542
ALD2MOLE	0.0000000	0.0017820	0.0013380	0.0015890
ETHMOLE	0.0068130	0.0055190	0.0007970	0.0015510
ISOPMOLE	0.0000000	0.0000000	0.0000000	0.0000147

Table B-5. The Temporal Allocation Coefficients for the Rural-based Emissions

County	VOC		NOx	
	RU1	RU2	RU1	RU2
Cheatham	0.7554	0.2446	0.9827	0.0173
Dickson	0.8060	0.1940	0.9883	0.0117
Robertson	0.8969	0.1031	0.9954	0.0046
Rutherford	0.7752	0.2248	0.9831	0.0169
Sumner	0.7433	0.2567	0.9801	0.0199
Williamson	0.9897	0.0103	0.9996	0.0004
Wilson	0.7251	0.2749	0.9797	0.0203

Table B-6. The VOC Speciation Coefficients for Each Category of Area Sources (Davidson County)

	OLEMOLE	PARMOLE	TOLMOLE	XYLMOLE	FORMMOLE	ALD2MOLE	ETHMOLE	ISOPMOLE
GASOLINE AND CRUDE OIL STORAGE (FIXED ROOF)	0.0000000	0.0536700	0.0001519	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
VOL STROAGE	0.0000000	0.0469700	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
VOL TRANSFER (OTHER)	0.0000000	0.0469700	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
GASOLINE BULK PLANTS	0.0000000	0.0469700	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
SERVICE STATIONS (TANK TRUCK UNLOADING)	0.0008610	0.0263600	0.0025740	0.0031060	0.0000000	0.0002392	0.0000000	0.0000000
SERVICE STATIONS (VEHICLE REFUELING)	0.0009670	0.0599600	0.0001480	0.0000946	0.0000000	0.0026720	0.0000000	0.0000029
SERVICE STATIONS (TANK BREATHING LOSSES)	0.0008610	0.0263600	0.0025740	0.0031060	0.0000000	0.0002392	0.0000000	0.0000000
SERVICE STATIONS (TANK TRUCKS IN TRANSIT)	0.0008610	0.0263600	0.0025740	0.0031060	0.0000000	0.0002392	0.0000000	0.0000000
INORGANIC CHEMICAL MANUFACTURE	0.0019100	0.0255200	0.0005871	0.0003259	0.0006620	0.0011910	0.0011200	0.0000587
PLASTIC PRODUCTS MANUFACTURER	0.0092230	0.0072030	0.0046050	0.0000000	0.0000000	0.0000000	0.0032000	0.0000000
OTHERS	0.0019100	0.0255200	0.0005871	0.0003259	0.0006620	0.0011910	0.0011200	0.0000587
PAPER PRODUCTS	0.0058020	0.0478300	0.0000000	0.0000000	0.0000000	0.0069760	0.0000000	0.0000000
MISCELLANEOUS METAL PRODUCTS	0.0002734	0.0188900	0.0000933	0.0000000	0.0000000	0.0000000	0.0023960	0.0000000
PLASTIC PRODUCTS	0.0080350	0.0449900	0.0012940	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
OTHERS	0.0019100	0.0255200	0.0005871	0.0003259	0.0006620	0.0011910	0.0011200	0.0000587
ARCHITECTRAL COATINGS	0.0012890	0.0460200	0.0017390	0.0002562	0.0000000	0.0002464	0.0000000	0.0000000
AUTO REFINISHING	0.0007864	0.0347200	0.0021380	0.0020840	0.0000000	0.0005941	0.0000000	0.0000000
OTHERS	0.0019100	0.0255200	0.0005871	0.0003259	0.0006620	0.0011910	0.0011200	0.0000587
SOLVENT METAL CLEANING (COLD CLEANERS)	0.0099880	0.0199800	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
DRY CLEANING (PERCHLOROETHYLENE)	0.0000646	0.0090530	0.0000869	0.0000942	0.0000000	0.0000053	0.0000000	0.0000000
ADHESIVES	0.0000000	0.0444000	0.0022030	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
CONSUMER/COMMERCIAL SOLVENT USE	0.0000000	0.0189500	0.0000000	0.0000000	0.0001998	0.0000000	0.0000000	0.0000000

Table B-6. (Continued)

	OLEMOLE	PARMOLE	TOLMOLE	XYLMOLE	FORMMOLE	ALD2MOLE	ETHMOLE	ISOPMOLE
MUNICIPAL WASTE LAND FILLS	0.000007	0.001068	0.000011	0.000009	0.000000	0.000000	0.000000	0.000000
OPEN BURNING (ON-SITE INCINERATION)	0.000119	0.001965	0.000000	0.000000	0.000000	0.000000	0.003102	0.000000
OPEN BURNING (RESIDENTIAL)	0.004417	0.046560	0.000000	0.000000	0.000000	0.000000	0.006916	0.000000
COMMERCIAL/INSTITIONAL	0.000000	0.034330	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
COMMERCIAL BAKERIES	0.000000	0.034330	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
PESTICIDE APPLICATION	0.000000	0.038770	0.000543	0.001413	0.000000	0.001316	0.000000	0.000000
STA. EXTERNAL COMBUSTION (COAL)	0.001268	0.029060	0.001445	0.001353	0.000000	0.000000	0.000000	0.000000
STA. EXTERNAL COMBUSTION (FUEL OIL)	0.000000	0.035150	0.000000	0.000000	0.016220	0.000000	0.000000	0.000000
STA. EXTERNAL COMBUSTION (NATURAL GAS)	0.000000	0.020220	0.000217	0.000000	0.002664	0.000000	0.000000	0.000000
STA. EXTERNAL COMBUSTION (LP GAS)	0.004159	0.032340	0.000000	0.000000	0.002531	0.000000	0.000000	0.000000
STA. EXTERNAL COMBUSTION (FOREST FIRES)	0.001459	0.038020	0.000000	0.000000	0.000000	0.000000	0.006813	0.000000
STA. EXTERNAL COMBUSTION (STRUCTURE FIRES)	0.001459	0.038020	0.000000	0.000000	0.000000	0.000000	0.006813	0.000000
WASTE DISPOSAL COMBUSTION	0.001459	0.038020	0.000000	0.000000	0.000000	0.000000	0.006813	0.000000
OTHER VOC SOURCES	0.001910	0.025520	0.000587	0.000326	0.000662	0.001191	0.001120	0.000059
NON-HIGHWAY VEHICLES (RAIL)	0.001528	0.026850	0.001697	0.000137	0.002867	0.001338	0.000797	0.000000
NON-HIGHWAY VEHICLES (AIRCRAFT)	0.002793	0.016260	0.000131	0.000112	0.005763	0.001782	0.005519	0.000000
NON-HIGHWAY VEHICLES (VESSELS)	0.000830	0.050250	0.000469	0.000595	0.000154	0.001589	0.001551	0.000015
NON-HIGHWAY VEHICLES (OFF-HIGHWAY MOTORCYCLES)	0.005802	0.047830	0.000000	0.000000	0.000000	0.006976	0.000000	0.000000
NON-HIGHWAY VEHICLES (FARM EQUIPMENT)	0.001528	0.026850	0.001697	0.000137	0.002867	0.001338	0.000797	0.000000
NON-HIGHWAY VEHICLES (CONSTRUCTION EQUIPMENT)	0.000830	0.050250	0.000469	0.000595	0.000154	0.001589	0.001551	0.000015
NON-HIGHWAY VEHICLES (INDUSTRIAL EQUIPMENT)	0.000830	0.050250	0.000469	0.000595	0.000154	0.001589	0.001551	0.000015
NON-HIGHWAY VEHICLES (LAWN AND GARDEN EQUIPMENT)	0.001528	0.026850	0.001697	0.000137	0.002867	0.001338	0.000797	0.000000

Table B-7. The VOC Weighted Speciation Coefficients for Davidson County

	Day Time	Night Time
OLEMOLE	0.0015231	0.0018492
PARMOLE	0.0355659	0.0252672
TOLMOLE	0.0006833	0.0011133
XYLMOLE	0.0004400	0.0001160
FORMMOLE	0.0004040	0.0033194
ALD2MOLE	0.0011325	0.0013136
ETHMOLE	0.0005999	0.0026507
ISOPMOLE	0.0000176	0.0000000

Table B-8. The VOCs Weighted Coefficients for Mobile Sources

VOC	1203 LDGV (EXHAUST)	1204 LDGV (EVAP/REFU)	1186 HDDV (ALL)
OLEMOLE	0.0014920	0.0006930	0.0015300
PARMOLE	0.0325000	0.0539800	0.0268500
TOLMOLE	0.0009970	0.0010600	0.0017000
XYLMOLE	0.0012590	0.0005780	0.0001370
FORMMOLE	0.0004990	0.0000000	0.0028700
ALD2MOLE	0.0616200	0.0010400	0.0013400
ETHMOLE	0.0029980	0.0000107	0.0007970
ISOPMOLE	0.0000248	0.0000000	0.0000000

Table B-9. The Ozone Profiles of the Ten Highest Ozone Days

Date	87/08/03	88/06/20	87/08/25	86/08/25	86/06/22	86/07/24	88/06/14	88/07/09	88/08/01	88/05/27	Min.	Max.
1	0.001	0.040	0.007	0.001	0.001	0.050	0.003	0.019	0.002	0.004	0.001	0.050
2	0.001	0.040	0.003	0.001	0.001	0.023	0.006	0.034	0.002	0.004	0.001	0.040
3	0.001	0.035	0.005	0.001	0.001	0.018	0.001	0.017	0.002	0.001	0.001	0.035
4	0.001	0.002	0.011	0.001	0.001	0.010	0.001			0.004	0.001	0.011
5	0.001	0.002	0.010	0.001	0.001	0.003	0.001	0.021	0.006	0.004	0.001	0.021
6	0.001	0.010	0.003	0.001	0.004	0.001	0.001	0.029	0.004	0.006	0.001	0.029
7	0.001	0.055		0.003	0.025	0.006		0.033	0.007		0.001	0.055
8		0.110	0.025	0.013	0.045	0.047	0.021	0.062	0.028	0.022	0.013	0.110
9	0.038	0.110	0.052		0.062	0.072	0.050	0.095	0.052	0.048	0.038	0.110
10		0.130	0.070		0.086	0.095	0.091	0.111	0.060	0.065	0.060	0.130
11	0.110	0.145	0.088		0.111	0.082	0.119	0.120	0.100	0.079	0.079	0.145
12	0.139	0.145	0.112		0.139	0.109	0.121	0.138	0.138	0.085	0.085	0.145
13	0.150	0.115	0.132		0.103	0.125	0.116	0.134	0.132	0.094	0.094	0.134
14	0.130	0.105	0.135	0.073	0.081	0.138	0.124	0.130	0.123	0.104	0.073	0.138
15	0.091	0.110	0.143	0.085	0.071	0.131	0.132	0.123	0.116	0.116	0.071	0.143
16	0.068	0.115	0.135	0.104	0.071	0.100	0.137	0.110	0.103	0.119	0.068	0.137
17	0.075	0.125	0.124	0.129	0.069	0.087	0.138	0.086	0.099	0.125	0.069	0.138
18	0.063	0.110	0.115	0.142	0.069	0.082	0.124	0.083	0.092	0.137	0.063	0.142
19	0.043	0.075	0.035	0.129	0.071	0.072	0.034	0.069	0.075	0.121	0.035	0.129
20	0.034	0.045	0.055	0.061	0.042	0.021	0.044	0.058	0.038	0.070	0.021	0.061
21	0.048	0.030	0.055	0.033	0.004	0.043	0.018	0.055	0.025	0.031	0.004	0.055
22	0.042	0.005	0.056	0.021	0.001	0.057	0.016	0.061	0.021	0.019	0.001	0.061
23	0.026	0.002	0.044	0.012	0.004	0.005	0.001	0.046	0.013	0.012	0.001	0.046
24	0.019	0.015	0.055	0.001	0.001	0.001	0.003	0.036	0.012	0.006	0.001	0.036

Table B-10. The Wind Speeds and Directions of the Ten Highest Ozone Days (km/hr)

Date	87/08/03		88/06/20		87/08/25		86/08/25		86/06/22		86/07/24		88/06/14		88/07/09		88/08/01		88/05/27	
1	7.4	SSW	5.4	S	7.6	SSW	7.6	ENE	5.4	SW	5.4	NE	0.0	C	13.0	W	9.4	S	5.4	S
2	9.3	ESE	0.0	C	0.0	C	5.4	SSE	9.4	WW	7.6	NNE	9.4	S	7.6	W	5.4	S	7.6	S
3	13.0	SSW	0.0	C	0.0	C	5.4	E	9.4	S	5.4	NE	7.6	SSW	11.2	W	5.4	N	0.0	C
4	7.4	S	11.2	N	0.0	C	7.6	NNE	7.6	S	7.6	NE	0.0	C	9.4	WSW	0.0	C	7.6	SSW
5	5.6	S	0.0	C	0.0	C	0.0	C	5.9	SE	0.0	C	0.0	C	7.6	W	0.0	C	0.0	C
6	11.1	S	7.6	S	3.6	E	5.4	SSW	7.6	N	0.0	C	0.0	C	11.2	NW	0.0	C	0.0	C
7	7.4	SSW	13.0	SW	0.0	C	5.4	NE	5.4	ESE	3.6	ESE	0.0	C	9.4	NNW	9.4	SSE	0.0	C
8	9.3	S	11.2	SW	7.6	E	5.4	N	14.8	SSE	5.4	SSE	5.4	WSW	7.6	E	3.6	S	5.4	SSW
9	7.4	W	11.2	NW	7.6	SSE	7.6	SSW	11.2	S	5.4	ESE	11.2	W	9.4	E	5.4	S	7.6	WSW
10	9.3	SSW	7.6	NNE	11.2	SW	5.4	W	13.0	W	7.6	E	5.4	N	11.2	SSE	5.4	SW	5.4	W
11	7.4	SSW	11.2	N	13.0	WSW	14.8	NNW	11.2	WSW	9.4	WNW	9.4	NW	9.4	E	3.6	S	11.2	SW
12	14.8	SW	13.0	SSW	11.2	S	13.0	WSW	7.6	SW	13.0	WNW	7.6	W	7.6	E	7.6	ENE	11.2	WSW
13	5.6	SE	9.4	S	14.8	W	9.4	SE	11.2	WNW	7.6	WSW	5.4	NNW	5.4	NE	11.2	SSW	7.6	NNW
14	16.7	S	9.4	WSW	14.8	W	7.6	NE	14.8	W	7.6	S	13.0	W	7.6	W	9.4	SE	9.4	SW
15	20.4	WNW	11.2	NNE	11.2	NNE	9.4	SE	13.0	NNW	18.4	W	8.3	NNW	13.0	SW	5.4	NNE	0.0	C
16	14.8	W	13.0	SSE	11	WSW	14.8	SSE	13.0	NNW	14.8	WSW	9.4	NE	37.1	SSE	5.4	W	7.6	SE
17	13.0	WNW	13.0	S	14.8	SW	13.0	S	18.4	W	9.4	NNE	5.4	E	29.5	SSW	0.0	C	11.2	SE
18	11.1	W	11.2	WSW	9.4	SW	11.2	SSW	13.0	WSW	13.0	NNE	13.0	NW	18.4	N	13.0	ENE	9.4	S
19	16.7	W	11.2	SW	7.6	SW	7.6	SW	11.2	SW	5.4	NE	13.0	WNW	11.2	NW	9.4	E	7.6	NW
20	20.4	NNW	9.4	SW	9.4	E	5.4	S	7.6	W	5.4	WSW	13.0	NW	16.6	W	9.4	SW	9.4	NNW
21	9.3	NE	7.6	SW	9.4	ESE	7.6	S	9.4	WSW	13.0	SSW	9.4	NW	11.2	WNW	0.0	C	0.0	C
22	14.8	S	9.4	S	7.6	E	9.4	E	7.6	WSW	11.2	S	5.4	N	11.2	S	14.8	W	7.6	SW
23	9.3	SW	7.6	S	7.6	ESE	7.6	S	13.0	S	11.2	SSW	7.6	WNW	9.4	S	9.4	WSW	9.4	SSW
24	11.1	NW	9.4	S	5.4	E	5.4	S	13.0	S	9.4	E	5.4	WSW	9.4	S	9.4	WNW	9.4	SSW

Table B-11. The Temperature Profiles of the Ten Highest Ozone Days

Date	87/08/03		88/06/20		87/08/25		86/08/25		86/06/22		86/07/24		88/06/14		88/07/09		88/08/01		88/05/27	
	F	K	F	K	F	K	F	K	F	K	F	K	F	K	F	K	F	K	F	K
1	78	299.0	75	297.0	67	292.6	69	293.7	75	297.0	78	298.7	65	291.5	83	301.5	74	296.5	52	284.3
2	77	298.0	75	297.0	68	293.2	67	292.6	71	294.0	77	298.2	64	290.9	81	300.4	75	297.0	50	283.2
3	76	298.0	74	296.5	67	292.6	66	292.0	72	295.4	76	297.6	65	291.5	79	299.3	74	296.5	51	283.7
4	76	298.0	72	295.4	66	292.0	66	292.0	70	294.3	75	297.0	67	292.6	78	298.7	74	296.5	49	282.6
5	76	298.0	72	295.4	64	290.9	65	291.5	70	294.3	75	297.0	66	292.0	77	298.2	73	295.9	49	282.6
6	76	298.0	74	296.5	66	292.0	65	291.5	72	295.4	75	297.0	69	293.7	79	299.3	74	296.5	51	283.7
7	80	300.0	80	299.8	71	294.8	69	293.7	76	297.6	79	299.3	74	296.5	83	301.5	78	298.7	61	289.3
8	83	301.0	85	302.6	73	295.9	74	296.5	82	300.9	84	302.0	80	299.8	87	303.7	83	301.5	66	292.0
9	88	304.0	87	303.7	81	300.4	80	299.8	85	302.6	88	304.3	83	301.5	91	305.9	86	303.2	72	295.4
10	91	306.0	91	305.9	85	302.6	84	302.0	87	303.7	94	307.6	89	304.8	96	308.7	89	304.8	75	297.0
11	93	307.0	93	307.0	89	304.8	86	303.2	91	305.9	94	307.6	90	305.4	99	310.4	92	306.5	78	298.7
12	97	309.0	94	307.6	91	305.9	87	303.7	94	307.6	96	308.7	92	306.5	99	310.4	94	307.6	79	299.3
13	97	309.0	94	307.6	92	306.5	89	304.8	92	306.5	98	309.8	92	306.5	103	312.6	94	307.6	81	300.4
14	86	303.0	94	307.6	94	307.6	90	305.4	93	307.0	99	310.4	93	307.0	102	312.0	95	308.2	82	300.9
15	89	305.0	93	307.0	95	308.2	91	305.9	93	307.0	98	309.8	94	307.6	102	312.0	97	309.3	82	300.9
16	91	306.0	93	307.0	95	308.2	90	305.4	91	305.9	98	309.8	95	308.2	91	305.9	97	309.3	82	300.9
17	94	308.0	89	304.8	94	307.6	89	304.8	92	306.5	96	308.7	92	306.5	81	300.4	96	308.7	81	300.4
18	93	307.0	90	305.4	91	305.9	85	302.6	90	305.4	94	307.6	90	305.4	76	297.6	95	308.2	80	299.8
19	89	305.0	85	302.6	89	304.8	83	301.5	83	301.5	91	305.9	87	303.7	78	298.7	90	305.4	76	297.6
20	86	303.0	83	301.5	83	301.5	82	300.9	82	300.9	90	305.4	84	302.0	79	299.3	87	303.7	74	296.5
21	82	301.0	82	300.9	82	300.9	77	298.2	82	300.9	87	303.7	82	300.9	76	297.6	88	304.3	72	295.4
22	82	301.0	76	297.6	82	300.9	75	297.0	80	299.8	84	302.0	81	300.4	75	297.0	85	302.6	64	290.9
23	82	301.0	76	297.6	80	299.8	77	298.2	74	296.5	82	300.9	78	298.7	74	296.5	83	301.5	61	289.3
24	81	300.0	72	295.4	79	299.3	75	297.0	73	295.9	81	300.4	76	297.6	72	295.4	83	301.5	58	287.6

Table B-12. The Humidity Profiles of the Ten Highest Ozone Days

Date	87/08/03		88/06/20		87/08/25		86/08/25		86/06/22		86/07/24		88/06/14		88/07/09		88/08/01		88/05/27	
	%	ppm	%	ppm	%	ppm	%	ppm	%	ppm	%	ppm	%	ppm	%	ppm	%	ppm	%	ppm
1	90	29994	69	20392	75	17026	65	15961	87	26024	71	23435	81	17029	47	18412	90	26111	86	11411
2	90	28928	69	20392	70	16482	75	17140	93	24289	73	23567	84	17029	53	19068	90	26953	93	11411
3	90	28160	70	20392	73	16482	84	18412	90	24371	76	23567	81	17029	56	19068	90	26024	86	10989
4	90	28160	73	19698	78	17083	81	17809	97	24371	78	23567	75	17029	60	19764	93	26852	89	10581
5	87	27061	76	20392	81	16482	81	17140	100	25161	78	23435	78	16970	60	19068	97	26852	93	10989
6	90	28066	71	20392	81	18351	87	18351	97	26024	81	24327	70	16970	58	19764	93	26852	89	11373
7	79	28066	60	21126	70	18289	75	20392	84	26024	74	25079	61	17641	49	19068	87	28736	72	13208
8	74	28928	48	19633	68	18947	71	21126	67	25077	65	26025	51	17641	43	19068	74	28736	61	13208
9	65	29994	40	17691	53	18947	60	21126	49	24289	57	26025	41	15801	38	19068	65	27786	48	12722
10	60	29994	38	19004	45	18289	53	21878	49	26024	46	25079	35	16372	32	18412	59	27786	40	11808
11	54	28928	33	17750	41	18947	51	21126	47	23489	38	21121	32	15231	30	19068	52	26852	36	11808
12	48	28928	31	17083	38	19004	48	19698	37	20392	37	21947	29	14687	27	17134	49	26852	31	10581
13	43	26248	31	17083	37	19904	42	19698	41	21126	35	21947	31	15855	24	17200	46	25077	33	11851
14	75	32144	30	16482	36	19692	41	19764	38	20392	33	21197	28	14738	24	16595	48	26953	31	11411
15	63	30094	32	17083	33	19004	41	21197	33	17809	35	21947	26	14209	24	16595	42	25167	28	10581
16	56	28161	33	17809	35	19692	43	19764	42	21197	35	21947	25	14209	34	17200	39	23567	30	11411
17	53	29305	42	19764	34	19004	43	21947	40	21197	39	22710	26	13202	56	20461	40	23567	32	11851
18	54	29305	39	19068	38	19004	53	19764	42	20461	43	23567	32	15283	74	22710	43	24371	33	11851
19	59	28161	46	19068	40	10094	53	21197	60	23567	47	23567	36	15855	74	24371	52	25167	37	11411
20	63	27061	49	19004	54	21126	56	21126	62	23567	48	23567	41	16427	69	23567	59	26111	36	10581
21	69	26248	51	19004	58	21874	76	24289	64	24371	55	24371	44	16427	79	24371	61	26953	40	10989
22	72	27061	69	21126	58	21874	84	25077	69	24371	63	25161	49	17691	82	24371	72	29836	70	14253
23	72	27061	69	21126	64	23489	76	24289	87	25161	65	24371	56	18287	84	24371	77	29836	77	14253
24	74	27061	79	21126	67	23489	81	24289	87	24371	67	24371	60	18287	90	24371	77	29836	83	13743

Table B-13. The NO2 Photolysis Rates, Biogenic Emissions and Average Wind Speeds

Time (hour)	Reaction Rate for NO2 Photolysis (K1) (1/min)	Biogenic Emissions(ISOP) (kg/sq-km-hr)	Wind Speed (m/s)
1	0.0000	0.00	2.1
2	0.0000	0.00	1.9
3	0.0000	0.00	1.8
4	0.0000	0.00	1.8
5	0.0000	0.42	0.6
6	0.0390	0.83	1.4
7	0.2016	1.24	1.7
8	0.3545	1.65	2.3
9	0.4535	2.06	2.6
10	0.5180	2.48	2.5
11	0.5570	2.89	3.1
12	0.5772	3.30	3.3
13	0.5815	3.30	2.7
14	0.5701	3.30	3.4
15	0.5422	3.30	3.4
16	0.4927	2.48	4.3
17	0.4140	1.65	3.9
18	0.2944	0.83	3.8
19	0.1225	0.00	3.1
20	0.0000	0.00	3.3
21	0.0000	0.00	2.4
22	0.0000	0.00	3.0
23	0.0000	0.00	2.8
24	0.0000	0.00	2.7

Table B-14. The Contributions of Different Emission Categories to Ozone Formation

Combination	The Nashville Metropolitan Area		Hendersonville	
	Scenario	Ozone (ppm)	Scenario	Ozone (ppm)
PAMB	1	0.154	11	0.151
PMB	2	0.150	12	0.146
AMB	3	0.146	13	0.137
MB	4	0.142	14	0.133
PAM	5	0.139	15	0.135
M	6	0.121	16	0.117
PB	7	0.081	17	0.092
PAB	8	0.081	18	0.093
B	9	0.053	19	0.053
AB	10	0.052	20	0.053

Table B-15. The Chemicals Simulated by the Urban AIRSHED Model

No.	Chemical
1	NO
2	NO2
3	O3
4	OLE
5	PAR
6	TOL
7	XYL
8	FORM
9	ALD2
10	ETH
11	CRES
12	MGLY
13	OPEN
14	PNA
15	NXOY
16	PAN
17	CO
18	HONO
19	H2O2
20	HNO3
21	MEOH
22	ETOH
23	ISOP
24	CLBR

Table B-16. The Population data of Tracts of the Middle Tennessee Area (Extract)

TRACTS	1980	1988	County
131	2209	2376	Davidson
132	7052	7586	Davidson
133	5076	5460	Davidson
134	4572	4918	Davidson
135	2830	3044	Davidson
136	8162	8780	Davidson
137	5712	6145	Davidson
138	2216	2384	Davidson
139	2306	2481	Davidson
140	3094	3328	Davidson
141	570	613	Davidson
142	3294	3544	Davidson
143	2989	3215	Davidson
144	3335	3588	Davidson
145	795	855	Davidson
146	1248	1343	Davidson
147	219	236	Davidson
148	4072	4380	Davidson
149	1301	1400	Davidson
150	2918	3139	Davidson
151	4756	5116	Davidson
152	3032	3262	Davidson
153	4027	4332	Davidson
154	13670	14705	Davidson
155	6778	7291	Davidson
156.01	5253	5651	Davidson
156.02	12598	13552	Davidson
156.03	10197	10969	Davidson
157	2834	3049	Davidson
158	9070	9757	Davidson

Scenario 11 Wind Field One

```
TITL
SOURCE
PLAC        36.667   86.167      5.    1988.      6.      21.
Nashville-Hendersonville
TIME         0600.    2000.
DILU          200.    2500.    0800.    1400.      0.
TEMP           13.    293.5    294.3    297.1    299.7    302.1
    304.3    305.7    306.7    307.2    306.9    307.3    306.7
    305.7    304.5
WATE           13.     29.5
     83.1     71.1     62.2     52.4     45.7     41.4     37.5
     36.3     38.4     35.7     37.2     40.1     45.1     50.4
TRAN          0.04     0.04    0.025    0.025   0.0009   0.0009
MASS          -13.    0.025    0.001     200.
   0.3219   0.0286   4.0471   7.9014   13.082   25.791   5.8956
   10.178   9.3899   16.699   0.2752       0.       0.
   0.4399   0.0160   2.4692   7.7981   5.9865   25.522   5.0306
   6.1614   7.0082   10.897   0.1160       0.       0.
REAC           8.     0.10
   0.0319   0.0377   0.0378   0.0048   0.1187   0.0857   0.6644
                0.019
BIOG          -13.       1.     200.
ISOP           0.      0.0      0.0       0.       0.       0.
                      68.12
     0.83     1.24    2.074     2.28     2.70     3.11     3.52
     3.52     3.52     3.52     2.48     1.65     0.83
SPEC           5.
O3      NO2      PAR      FORM     CO
CALC         0.025    0.001       1.      60.       0.
```

Figure B-1. An Example Input File for the OZIPM-4 Model

```
                    Scenario 11          Wind Field One

PHOTOLYTIC RATE CONSTANTS CALCULATED FOR

        Nashville-Hendersonville

LATITUDE    36.667

LONGITUDE   86.167

TIME ZONE   5.0

DATE        6    21   1988

TIME        600  TO   2000    LOCAL DAYLIGHT TIME

DILUTION DETERMINED FROM THE FOLLOWING

INVERSION HEIGHTS    INITIAL  200.    FINAL    2500.

TIMING               START    800.    STOP     1400.

MIXING HEIGHTS (AT THE BEGINNING OF EACH HOUR)

TIME      800    900    1000   1100   1200   1300   1400
HEIGHT    200.0  200.0  200.0  627.8  1165.5 1669.6 2042.7

TEMPERATURE (AT THE BEGINNING OF EACH HOUR)

HOUR      0      1      2      3      4      5      6      7      8      9
          10     11     12     13
TEMP      293.5  294.3  297.1  299.7  302.1  304.3  305.7  306.7  307.2  306.9
          307.3  306.7  305.7  304.5

RELATIVE HUMIDITY (AT THE BEGINNING OF EACH HOUR)

HOUR      0      1      2      3      4      5      6      7      8      9
          10     11     12     13

RH (%)    83.1   71.1   62.2   52.4   45.7   41.4   37.5   36.3   38.4   35.7
          37.2   40.1   45.1   50.4

WATER CONCENTRATIONS (AT THE BEGINNING OF EACH HOUR)

HOUR      0      1      2      3      4      5      6      7      8      9
          10     11     12     13

PPM       19784. 17761. 18338. 17953. 17931. 18348. 17937. 18325. 19912. 18217.
          19393. 20244. 21573. 22583.
PRESSURE  29.50 INCHES OF HG

REACTIVITY
EMISSIONS      ETH FRACTION .032  OLE FRACTION .038  ALD2 FRACTION .038
EMISSIONS      FORM FRACTION .005  TOL FRACTION .119  XYL FRACTION .086
EMISSIONS      PAR FRACTION .664  NR FRACTION .019
SURFACE LAYER  ETH FRACTION .034  OLE FRACTION .020  ALD2 FRACTION .037
SURFACE LAYER  FORM FRACTION .070  TOL FRACTION .042  XYL FRACTION .026
SURFACE LAYER  PAR FRACTION .498  NR FRACTION .273
ALOFT          ETH FRACTION .034  OLE FRACTION .020  ALD2 FRACTION .037
ALOFT          FORM FRACTION .070  TOL FRACTION .042  XYL FRACTION .026
ALOFT          PAR FRACTION .498  NR FRACTION .273
NO2/NOX        .100
```

Figure B-2. An Example Output File (Extract) from the OZIPM-4 Model

```
SIMCONTROL
0  0  96173    0. 96173   24.
Simulation of the Nashville Metropolitan Area                    96173 0.0000000E+01     96173 0.2400000E+02
F  T  T  F  T  T  F
0.5000000E+00 0.1000000E+01 0.1000000E+00         20 0.1000000E-07         20
0.1000000E-02 0.1000000E-01 0.1000000E+01 0.1000000E+01         1         1         1         1         0         0
```

Figure B-3. An Example SIMCONTROL File Used for the Simulation of Ozone Formation in 1988

VITA

Mr. Nianjun Zhou was born in Harbin, Heilongjiang Province, China on October 26, 1962. He was educated in Yixin, Jiangsu Province, China from 1968 to 1972 as a primary school student and educated in Harbin from 1972 to 1978 as a middle school student, and graduated from the No.124 Middle School of Harbin in July, 1978. From 1978 to 1982, he studied as a undergraduate student majoring in Electronic Engineering at Beijing University, Beijing, China. He continued his studies as a graduate student and earned his Master of Science Degree in July 1985 majoring in Systems Sciences. From 1985 to 1988, he worked as a teaching and research assistant at first, and later as a lecturer at Beijing University. He was sent by the National Environmental Protection Agency of China and Beijing University to the University of Tennessee at Knoxville in August 1988 as an exchange student. At present he is completing the thesis for Master of Science Degree in Environmental Engineering.