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Analysis of ozone data trends as an effect of meteorology and development of forecasting models for predicting hourly ozone concentrations and exceedances for Dayton, OH, using MM5 real-time forecasts

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Analysis of Ozone Data Trends as an Effect of Meteorology and Development of Forecasting Models for Predicting Hourly Ozone Concentrations and Exceedances for Dayton, OH, Using MM5 Real–Time Forecasts

by

Raga Smitha Kalapati

Submitted as partial fulfillment of the requirements for

Master of Science degree in Civil Engineering

Ashok Kumar.

Advisor: Dr. Ashok Kumar

Graduate School

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An Abstract of

Analysis of Ozone Data Trends as an Effect of Meteorology and Development of Forecasting Models for Predicting Hourly Ozone Concentrations and Exceedances for Dayton, OH, Using MM5 Real-Time Forecasts

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The objective of this research was to develop and evaluate models for predicting hourly ozone concentrations, ozone exceedances and hourly air quality index (AQI) in Dayton, OH. As the hourly ozone concentrations are closely related to the meteorological conditions, three variables- temperature, wind speed, and dew point temperature- were chosen for this study. The ozone data were extracted from the EPA's AIRS database for the period 1996-2003. The meteorological data was taken from the National Climatic Data Center (NCDC) for the same period.

An analysis of variations in hourly ozone concentrations and ozone episode occurrences was carried out for the period Apr.-Oct. for the years 1996-1999. Also, analysis of the long-term trends in annual means of ozone concentrations, temperature, wind speed, and dew point temperature was performed using the same data set. Based on this analysis, the ozone data was divided into pre-summer (Apr.-Jul.) and post-summer (Aug.-Oct.) seasons, to account for seasonal variations, and each season was further divided into three regimes, namely, stable period (hours: 1-8), ascent period (hours: 9-16), and descent period (hours: 17-24). The KZ filter technique was used to reduce the scatter in the time series, and models were developed for the three regimes for each season by regression, using the corresponding independent parameter values.

A total of twelve models were developed to predict ozone concentrations for pre-summer and post-summer periods. Six models considered temperature, wind speed, and dew point temperature as the independent variables (three-parameter models), and the other six considered temperature and wind speed as variables (two-parameter models). Also, three models each for pre-summer and post-summer season were developed for predicting the ozone exceedances. The performance of the models was evaluated in three ways:

a) Initial evaluation (or validation) of the models was conducted using 2002 data.

b) The effectiveness of these models was further evaluated using available MM5 (a mesoscale meteorological forecasting model) real-time forecasts from the Ohio State University for the months of Aug.-Oct., 2003.

c) Finally, the performance of the three-parameter models was compared with that of the two-parameter models. All the evaluations were made using statistical evaluation parameters discussed later.

The study shows that the forecasts of hourly ozone concentrations made by the models based on KZ filters are reliable only to a limited extent. However, the models performed well in predicting AQI values reported by the EPA. Also, the three-parameter models performed better in predicting the peak concentrations when compared to the two-parameter models.

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Nomenclature

Symbol	Units	Description
C_p	ppb	Predicted ozone concentration
C_o	ppb	Observed ozone concentration
C_p	ppb	Average predicted ozone concentration
C_o	ppb	Average observed ozone concentration
cld	Dimensionless	Cloud Cover
CO	-	Carbon monoxide
D_{kz}	^0F	Filtered Dew point Temperature
dsp	meters/second	Wind Speed
D(t)	^0F	Dew point Temperature at time t
m	Dimensionless	Final low pass filter
N_r	Dimensionless	Number of forecasts in uncertainty level r
O_{kz}	ppb	Filtered hourly ozone concentration
O(t)	ppb	Ozone concentration at time t
p	Dimensionless	Number of passes
PM-2.5	-	Particulate matter with size less than 2.5 μ
PM-10	-	Particulate matter with size less than 10 μ
prep	inches	Precipitation
rhu	(%)	Relative humidity
SO_2	-	Sulfur dioxide
Td	^0F	Dew point temperature

T_{kz}	^0F	Filtered surface temperature
$T(t)$	^0F	Surface temperature at time t
W_{kz}	mph	Filtered wind speed
$W(t)$	mph	Wind speed at time t
Y_i	Dimensionless	Each iteration of moving average

Chapter 1

Introduction

1.1 Overview

Ozone is considered to be one of the most important noxious air pollutants in view of its concentrations and its effects on human health. It is one of the six common air pollutants that have been identified by the U.S Environmental Protection Agency (EPA) to cause adverse effects to public health and environment. It is linked to a wide range of health impacts, including respiratory distress, resulting in increased emergency hospital visits, hospital admissions and even premature deaths. Elevated levels above the national standard (0.085 ppm) may cause lung and respiratory disorders. Recent scientific evidence indicates that there is no lower threshold for the health effects of ground-level ozone. Due to its dependence on weather conditions, ozone is typically a summer-time pollutant and a chief component of summer-time smog.

High concentrations of ozone occur during the summer months i.e. from May through September (often termed as 'ozone season') in the northern hemisphere. These high concentration episodes are now proclaimed as "Ozone Action Days" (OADs) by many urban areas.

The photochemical processes leading to ozone formation in the atmosphere are complex and nonlinear. Ozone is a secondary component and is created by chemical reactions between its precursors which include nitrogen oxides (NOx) and volatile organic compounds (VOCs). Emissions from industrial facilities and electric utilities, motor vehicle exhaust, gasoline vapors, and chemical solvents are some of the major sources of NOx and VOCs. In the presence of sunlight (ultra-violet radiation) and suitable meteorological conditions, the precursors react photochemically to produce ozone.

1.2 Objective

Accurate O_3 forecasts can be useful tools for air pollution control officials and public health officials in preventing the detrimental health effects of this pollutant through emergency air pollution control actions and public health warnings. Research in the development of ozone forecasting models for urban areas around the world has been continuous over the last two decades. Efforts have been made to forecast ground-level ozone based on various meteorological parameters such as temperature, wind speed, relative humidity, background and previous ozone concentrations, and ozone precursor (volatile organic compounds and oxides of nitrogen) levels. Use of so many predictors for forecasting ozone necessitates the development of parallel forecasting models for each of them, ultimately making the process too complicated and unrealistic.

The objective of this study was to develop simple ozone forecasting models to predict hourly maximum ozone concentration and air quality index for the next hour for Dayton, Ohio, using the Kolmogorov – Zurbenko (KZ) filtering technique and regression analysis. The KZ filter technique was used to reduce the scatter in ozone data, and regression analysis was used to develop the models following the method approached by Kumar et al. (2000). The dataset for the years 1996-1999 was used for the development of the models. Temperature, wind speed, and dew point temperature were chosen as independent variables. The variations in ozone concentrations, ozone episode occurrences, and long-term trends in annual means of ozone concentrations, temperature, wind speed, and dew point temperature were analyzed for the period of 1996-1999.

The ozone concentrations were correlated to hourly temperature, wind speed and dew point temperature. The models obtained were three-parameter models. The efficiency of these models was compared to the two-parameter models which were obtained using temperature and wind speed as independent variables. Separate models for accounting for peak ozone concentrations were developed.

The data for the year 2002 was used for the validation of the models. The forecasting ability of the models was further analyzed using MM5 (a mesoscale meteorological forecasting model) real-time forecasts for temperature, wind speed, and dew point temperature for the year 2003. These evaluations using real-time forecasts are generally not reported by researchers for air quality predictions.

All the evaluations and comparisons are based on statistical parameters, such as fractional bias (FB), normalized mean square error (NMSE), factor of two (Fa_2), and forecasting skill (FC) discussed later.

Chapter 2

Literature Review

2.1 Ground-Level Ozone

Ozone is a tri-atomic molecule that is photochemically (with the direct interaction from sunlight) produced in the troposphere through a series of chemical reactions involving the ozone precursors. Precursors are the raw chemical ingredients that are oxides of nitrogen (NOx), and volatile organic compounds (VOCs). The simple form of the ozone formation reaction is given as follows:

VOC + NOx + Heat +Sunlight →Ground Level Ozone 2.1

Motor vehicle exhaust and industrial emissions, gasoline vapors, and chemical solvents are some of the major sources of NOx and VOCs that help to form ozone. NOx is emitted from motor vehicles, power plants, and other sources of combustion. VOCs are emitted from a variety of sources such as motor vehicles, chemical plants, refineries, factories, consumer and commercial products, and other industrial sources.

The concentration of ozone in ambient air is dependent on various meteorological parameters that play a crucial role in ozone pollution. These include the following:

- Solar radiation
- Temperature
- Wind speed
- Dew point temperature
- Relative humidity
- Cloud cover
- Wind direction
- Pressure gradients

Ozone pollution is the periodic increase in the concentration of ozone in the ambient air, the natural air that surrounds us. It is mainly a daytime problem especially during summer months because warm temperatures play a role in its formation. When temperatures are high, sunshine is strong, and winds are weak, ozone can accumulate to unhealthy levels.

At elevated levels, ozone is known to damage human lungs and vegetation. It also plays a significant role in fashioning climate change.

Physical and chemical properties of ozone are listed in Table 2.1.

Table 2.1 Properties of Ozone

Attribute	Properties
Name	Ozone; also called trioxygen and triatomic oxygen
Physical description	Colorless to blue gas; pungent odor; nonflammable; powerful oxidizer; unstable – may decompose spontaneously and violently to oxygen; reactive – may react violently with combustible materials and reducing agents; potentially explosive
Chemical formula	O_3
Molecular weight	48.0
Boiling point Freezing point	-169° F at 1 atm -315° F
Density	1.62 g/cm³ at -320° F
Relative density referenced to air	1.66
Vapor pressure	20 mm Hg at -250° F
Solubility in water	0.001% by weight at 32° F

Source: National Institute of Occupational Safety and Health
The Physical and Theoretical Chemistry Laboratory, Oxford University

2.2 Health Effects and Other Impacts of Ground Level Ozone

Roughly one out of every three people in the United States is at a higher risk of experiencing problems from ground-level ozone (EPA, 2004). Exposure to ground level ozone aggravates asthma, damages the lining of the lungs, and makes breathing more difficult. It can also worsen bronchitis, heart disease, emphysema, asthma, and reduce lung capacity. Ozone is a particular threat to people who already have respiratory problems. When ozone levels are high, more people with asthma have attacks that require medical attention or the use of additional medication. The reason for this is that ozone makes people more sensitive to allergens, which are the most common triggers for asthma attacks.

Ozone affects plants in several ways. It interferes with the ability of plants to produce and store food, making them more susceptible to disease, insects, other pollutants, harsh weather, and other environmental stresses. Ozone can adversely impact ecological functions such as water movement, mineral nutrient cycling, and habitats for various animal and plant species.

Man-made materials like rubber, textile dyes, fibers, and paints can also be affected by the strong oxidizing properties of ozone. Materials may be weakened or damaged, become brittle and crack, and fade more quickly due to exposure to ozone.

2.3 Ozone Regulations

The adverse effects of ozone have led the EPA to list ozone as one of the six ‘criteria pollutants’. The EPA uses the criteria pollutants as indicators of air quality, and has established for each of them a maximum concentration, above which, known or anticipated adverse effects on human health and environment may occur. When the pollutant levels in an area have caused a violation of a particular standard, the area is classified as "non-attainment" for that pollutant. The EPA then imposes federal regulations on pollutant emissions, and designates a time period in which the area must again attain the standard. These threshold concentrations are called National Ambient Air Quality Standards (NAAQS).

The NAAQS criteria designated to protect human health with an adequate margin of safety are called the primary standards, while those to protect the environment are called secondary standards.

Table 2.2 shows the current NAAQS for ozone.

Table 2.2 Current National Ambient Air Quality Standards for Ozone

Standard Type	Standard
1-hour Average, Primary and Secondary	0.125 ppm (246 $\mu g/m^3$)
8-hour Average, Primary and Secondary	0.085 ppm (167 $\mu g/m^3$)

On April 30, 1971, the EPA first promulgated the primary and secondary NAAQS for photochemical oxidants under section 109 of the Clean Air Act (CAA, 1971). These standards were set at an hourly average of 0.08 ppm total photochemical oxidant, not to be exceeded more than 1 hour/year.

In July 1997, the EPA published revisions to the ozone standard, setting it at 0.08 ppm for an 8-hour average. The new standard is based on averaging air quality measurements over 8-hour blocks of time, instead of the 1-hour blocks of time required by the current standard. To attain this standard, the 3-year average of the fourth-highest daily maximum 8-hour average of continuous ambient air monitoring data over each year must not exceed 0.08 ppm. Eight-hour averaging is more consistent with the health information that prompted the EPA to propose revisions to the standard. However, based on its inability to implement the more stringent 8-hour standard due to extensive litigation, the EPA reinstated the 1-hour standard again on July 20, 2000. On November 13, 2002, the EPA and nine other environmental groups agreed upon a schedule for the agency to promulgate air quality designations for the 8-hour ozone NAAQS.

Among its most recent actions the EPA promulgated air quality designations for the 8-hour Ozone NAAQS on April 15, 2004, in which it released a list of 474 counties nationwide that are either partially or entirely in non-attainment under new health standards for ground-level ozone.

2.4 Air Quality Index

The Air Quality Index (AQI) is a uniform system developed by the EPA to enable the public to determine whether air quality levels in a particular location are good, moderate, unhealthful, or worse. EPA and local officials use the AQI to provide the public with simple information on local air quality, the health concerns for different levels of air pollution, and how they can protect their health when pollutants reach unhealthy levels. Table 2.3 shows the AQI for ozone. The higher the AQI value, the greater the level of air pollution, and the greater the health concern. For example, an AQI value of 50 represents good air quality with little potential to affect public health, while an AQI value over 300 represents hazardous air quality.

Table 2.3: Air Quality Index (AQI) of Ozone

Index Values	Levels of Health Concern	Cautionary Statements
0-50	Good	None
51-100*	Moderate	Unusually sensitive people should consider reducing prolonged or heavy exertion outdoors.
101-150	Unhealthy for Sensitive Groups	Active children and adults, and people with lung disease, such as asthma, should reduce prolonged or heavy exertion outdoors.
151-200	Unhealthy	Active children and adults, and people with lung disease, such as asthma, should avoid prolonged or heavy exertion outdoors. Everyone else, especially children, should reduce prolonged or heavy exertion outdoors.
201-300	Very Unhealthy	Active children and adults, and people with lung disease, such as asthma, should avoid all outdoor exertion. Everyone else, especially children, should avoid prolonged or heavy exertion outdoors.
301-500	Hazardous	Everyone should avoid all physical activity outdoors.

* Generally, an AQI of 100 for ozone corresponds to an ozone level of 0.08 parts per million (averaged over 8 hours).

Source: U. S. EPA, http://www.epa.gov/airnow/aqibroch/aqi.html

2.5 Ozone in Montgomery County

Table 2.4 summarizes the criteria pollutant concentrations in the year 2002 for Montgomery County. The pollutant's NAAQS, highest recorded concentration, second highest recorded concentration, number of exceedances, and the number of monitoring stations are given in this table. Table 2.5 provides an overview of the most important sources of criteria air pollution, including the precursor emissions of ozone (NOx and VOC's) for Montgomery County for the year 1999. This table shows the significance of mobile sources in ozone production. Table 2.6 indicates the percentage of days in the year 2002 when the air quality was good, moderate or unhealthful based on the AQI scale discussed in the previous section. As seen in the table about 50% of the days did not have good air quality in Montgomery County.

Table 2.4: Summary of Pollutant Concentration for Montgomery County, 2002

Pollutant	NAAQS Standards	Highest Recorded Concentration	Second Highest Recorded Concentration	Number of NAAQS Exceedances	Stations
CO,1-hr average	35 ppm	3.7 ppm	3.4 ppm	0	2
8-hr average	9 ppm	2.1 ppm	1.8 ppm	0	2
Ozone,1-hr average	0.125 ppm	0.12 ppm	0.117 ppm	0	1
8-hr average	0.085 ppm	0.1 ppm	0.097 ppm	16	1
PM-2.5, 24-hr average	65 µg/ m3	55 µg/ m3	51 µg/ m3	0	5
Annual AM	15 µg/ m3	18.4 µg/ m3	17.5 µg/ m3	5	5
PM-10, 24-hr average	150 µg/ m3	49 µg/ m3	49 µg/ m3	0	2
Annual AM	50 µg/ m3	24 µg/ m3	18 µg/ m3	0	2
SO2, 24-hr average	0.14 ppm	.021 ppm	.02 ppm	0	1
Annual AM	0.03 ppm	0.004 ppm	0 ppm	0	1

Table 2.5: Summary of Emissions of Criteria Air Pollutants for Montgomery County for the Year 1999

Source Type	Carbon Monoxide (Tons)	Nitrogen Oxides (Tons)	PM-2.5 (Tons)	PM-10 (Tons)	Sulfur Dioxide (Tons)	Volatile Organic Compounds (Tons)
Mobile Sources	161,112	22,863	2,546	8,117	1,626	14,680
Area Sources	4,522	170	1,742	6,103	1,518	12,803
Point Sources	849	4,413	1,224	1,569	9,029	3,705
All Sources	166,483	27,446	5,512	15,788	12,172	31,189

Table 2.6: AQI Values for Montgomery County for the Year 2002

Air Quality Index:	
Percentage of days with good air quality:	50
Percentage of days with moderate air quality:	43
Percentage of days with unhealthful air quality for sensitive populations:	6
Percentage of days with unhealthful air quality:	0
Maximum AQI level in 2002	161
Median AQI level in 2002	50
90th Percentile AQI level in 2002	90

2.6 Air Quality Forecasting

Air quality forecasts play an important role in forming regulations, ensuring public health safety, establishing standards and enforcing protective measures (EPA, 1992). According to Ojha et al. (2002), availability of reliable and accurate forecasts serves in a variety of ways:

- Fulfills the need for public information
- Helps in preventing exposure to air pollutants
- Helps regulators, industries, and public to take appropriate corrective measures
- Increases general awareness towards air quality issues

The major steps in developing a forecasting model are:

1. Understanding the nature of the pollutant: This helps in addressing questions such as how the pollutant is formed, when the pollutant is formed and how the local weather affects this pollutant.

2. Performing literature review: Thorough literature review is required to help in addressing questions such as how to determine the factors that affect pollutant concentrations, how to fill in missing data, which model to use and what are the acceptable evaluation techniques and parameters to be employed.

3. Developing predictive equations: After getting a better understanding of the pollutant, a forecasting model should be developed. A variety of techniques are available for this purpose.

4. Evaluating the forecasting model: The forecasting model is based on observations and predictive equations. In order to develop a reliable and accurate forecasting model, it is essential that the weather and air quality monitoring data be free from errors and up-to-date. The developed model needs to be evaluated for its performance and accuracy.

2.7 Ozone Forecasting Methods and their Comparison

This section presents the most common methods used to forecast ozone concentrations. The methods are listed as follows:

- Persistence
- Climatology
- Criteria
- CART (Classification and Regression Tree)
- Regression
- Artificial Neural Networks
- 3-D Air Quality Models
- Phenomenological/Intuition Method

The description, development, operation and limitations of each method are given in Table 2.7.

Table 2.7: Comparison of Ozone Forecasting Methods

	Persistence	**Climatology**	**Criteria**	**CART**	**Regression**	**Neural Networks**	**3-D Air Quality Models**	**Phenomenological/Intuition Method**
Development Effort	Low	Low/ Moderate	Low/ Moderate	Moderate	Moderate	Moderate/High	Very High	High
Accuracy	Low	Low	Moderate	Moderate/ High	Moderate/ High	Moderate/High	Moderate/ High	High
Method Description	Today's (or yesterday's) observed pollutant concentration is tomorrow's forecasted pollutant concentration.	Historical frequency of pollutant events help guide and bound pollutant forecast.	When parameters that influence pollution are forecasted to reach a pre-determined level (criteria), high pollutant concentrations are forecasted.	A decision Tree predicts pollutant concentration based on values of various meteorological and air quality parameters.	A regression equation predicts pollutant concentrations using observed and forecasted meteorological and air quality variables.	A non-linear set of equations and weighting factors predicts pollutant concentrations using observed and forecasted meteorological and air quality variables.	A prognostic modeling system simulates the physical and chemical processes that lead to the formation and accumulation of air pollutants.	A person synthesizes meteorological and air quality information, including pollutant concentration predictions from other methods to produce a final air quality forecast.
Data needs	Yesterday's air quality data.	None	Observed and forecasted upper-air and surface meteorological and air quality data.	Observed and forecasted upper-air and surface meteorological and air quality data.	Observed and forecasted upper-air and surface meteorological and air quality data.	Observed and forecasted upper-air and surface meteorological and air quality data.	Prognostic gridded meteorological fields, gridded emissions, and boundary conditions.	Observed and forecasted meteorological data and charts and observed air quality data.

Strengths	Works well in areas that have several continuous days of high pollutant and low pollutant concentrations.	Helps guide and bound forecasts derived from other methods.	Quick, used to get initial idea" about forecast conditions.	Automatically differentiates between days with similar pollutant concentrations.	Commonly used and easy to operate. Produces generally good forecasts. develop.	Allows for non-linear relationships to	Predicts pollutant concentrations in areas that are not monitored. Helps in understanding pollutant processes including transport issues.	Helps temper the predictions from other methods with common sense and experience. Typically has the highest accuracy.
Potential Limitations	Doesn't predict the beginning or end of an episode; low accuracy.	Not a stand-alone method.	Is not well suited to forecast exact concentrations.	Requires a modest amount of expertise to develop.	Doesn't accurately Predict extreme concentrations.	Doesn't accurately predict extreme concentrations. 50% more effort to develop than regression with only slight improvement in forecast accuracy.	Expensive and difficult to develop. Accuracy of air quality predictions depend on accuracy of meteorological and emissions predictions.	Prediction may be biased from one forecaster to another.

Note: Based on the information provided on the EPA site. http://www.epa.gov/airnow/aq_forecasting_guidance-1016.pdf

2.8 Overview of the Studies in Ozone Forecasting

Different techniques have been adopted to forecast ozone concentrations for many cities worldwide. The basis of the models range from analyzing trends in ground level ozone to simple regression models to far more complex urban air-shed models and fuzzy-logic-based models.

Forecasting models for ozone concentrations could be based on deterministic equations derived from theories related to physical and chemical processes in the atmosphere (Seinfeld 1986). Stochastic models based on regression methods that include past values of ozone, ozone precursor, and meteorological conditions as inputs have been widely employed as an alternative to deterministic models in order to forecast the ozone concentrations. In early regression models, a linear specification was often adopted (Milionis and Davies 1994, Ryan 1995). Some examples report results from nonlinear multiple regression (Cobourn and Hubbard 1999), artificial neural networks (Comrie 1997, Prybutok, Yi and Mitchell 2000), additive models (Niu 1996, Davis and Speckman 1999), CART models (Burrows, Benjamin, Beauchamp, Lord, Mc-Collor and Thomson 1995) and even fuzzy-logic-based models (Jorquera, Perez, Cipriano, Espejo, Letelier and Acuna 1998). Most of the recent research studies on ozone forecasting, such as Cobourn and Hubbard (1999), Lissens et al. (2000), Spellman (1999), Bernard et al. (1998), Chang and Cardeline (2000), used both linear and non-linear methods, or their combinations, and different meteorological parameters, that ultimately succeeded in predicting daily maximum ozone concentrations.

Time series models were used extensively in the 1970s and 1980s; most of them were univariate models, and usually their performance was not good enough to develop environmental warning systems (Myrabo et al., 1976; Aron and Aron, 1978; McCollister and Wilson, 1975; Pryor et al., 1981, Simpson and Leyton, 1983).

There was an early attempt to apply the Kalman filter methodology (Desalu et al., 1974), but it was not tested with real data nor was it used for air pollution forecasts.

In the early 1990s, Young et al. (1991) introduced a comprehensive framework for analyzing time series of environmental data. They advocated an approach in which seasonal and trend components are decomposed into quasi-orthogonal components (the so-called 'unobserved component time series model') by applying forward recursive Kalman filters and the backward recursive fixed interval smoothing (FIS) algorithm to estimate the joint trend and seasonal models. Schlink et al. (1997) and Ng and Yan (1998) have reported applications of this methodology to air quality forecasts.

Flaum et al. (1996) employed the Kolmogorov-Zurbenko filter to moderate the influence of meteorological fluctuations on ambient ozone levels. The authors employed the $KZ_{29,\ 3}$ filter to the logarithm of the maximum daily ozone concentration and two meteorological variables.

A method for moderating the influence of meteorological fluctuations on ambient ozone levels was also presented. This method is an expansion of the techniques presented by Rao et al. (1992), Rao and Zurbenko (1994) and Rao et al. (1995). The authors investigated techniques to simultaneously moderate the effects of two meteorological variables from the ozone time series. The effects of different meteorological variables that affect ambient ozone concentrations were examined. To this end the correlation between several meteorological variables and ozone concentrations were determined. The results indicated that inclusion of two meteorological variables strengthens the relationship between ozone and meteorological effects. The combination of temperature and dew point temperature improves the ability to filter out the influence of meteorology on ambient ozone concentrations. Further, removing the effects of the above two variables on ozone concentrations reduces the variance of the meteorologically independent ozone time series. It was also reported that the ozone trends studied at several other locations in the eastern United States by this method were not significantly different from those presented earlier, in which only one meteorological variable (surface temperature) has been considered as a surrogate for meteorological conditions that affect ozone.

Kumar et al. (2000) used the KZ filter to develop a forecasting model for predicting the maximum ozone concentration for non-attainment areas of Ohio. Ojha et al. (2002) compared the KZ regression technique and artificial neural networks by predicting hourly ozone concentrations for Cincinnati, Ohio. Ghose (2003) used the same comparison for Columbus, Ohio. Studies show that the KZ filtering techniques has been successfully applied for predicting ozone concentrations in Ohio.

A similar approach was used for this study. Of many possible parameters that influence the ozone concentrations, temperature, wind speed, and dew point temperature are chosen in this research.

2.9 Summary of Literature Review

- NOx and VOCs are mainly responsible for the formation of ozone, but meteorology plays a crucial role in the reaction phenomenon.
- Accurate next hour forecasts are useful in preventing the detrimental health effects of ozone through emergency air pollution control actions and public health warnings.
- There are numerous methods available for forecasting ozone levels. Depending upon the desired results, an appropriate technique is adopted.
- The most common method adopted is regression analysis.

- Most of the recent research studies on ozone forecasting used various methods or their combinations and different meteorological parameters for predicting ozone concentrations.
- The primary objective of the researchers has been to develop a forecasting model to predict the maximum ozone concentration.
- There has been limited work in the area of developing models to predict the ozone concentration for the next hour.
- Only a few studies focused on fair comparisons among forecasting methods, especially when real-world data is analyzed.

Some forecasting systems operating in European countries have the ability to predict the hourly ozone concentrations. This study develops simple forecasting systems that can be used by local agencies for predicting hourly ozone concentrations.

Temperature was the automatic choice because of its direct impact on the ozone concentrations. Wind speed and dew point temperature were also incorporated to enhance the model performance.

Chapter 3

Database Development

3.1 Ozone Data

The ozone concentrations in the state of Ohio are monitored between the months of April through October every year. The hourly ozone concentration measurements were obtained from the EPA's Aerometric Information Retrieval System (AIRS) database. Detailed information of the monitoring site is given in Table 3.1. The data was obtained from this station for the time period 1995-2003. Table 3.2 gives an example of the original format of the data.

Table 3.1: Details of the Ozone Monitoring Station in Dayton, OH

Station ID	39-113-0019
City	Dayton
County	Montgomery
Monitor type	SLAMS
Site address	2100 Timber Lane
Land use	Suburban

Table 3.2: Original Format of the Ozone Data

```
RD|I|39|035|0034|44201|1|1|008|019|20030730|14:00|45|||||||||||||||
RD|I|39|035|0034|44201|1|1|008|019|20030730|15:00|43|||||||||||||||
RD|I|39|035|0034|44201|1|1|008|019|20030730|16:00|46|||||||||||||||
RD|I|39|035|0034|44201|1|1|008|019|20030730|17:00|49|||||||||||||||
RD|I|39|035|0034|44201|1|1|008|019|20030730|18:00|48|||||||||||||||
RD|I|39|035|0034|44201|1|1|008|019|20030730|19:00|34|||||||||||||||
RD|I|39|035|0034|44201|1|1|008|019|20030730|20:00|17|||||||||||||||
```

3.2 Meteorological Data

In this research temperature, wind speed and dew point temperature were considered as variables for the development of the model. This data for a selected station (see Table 3.3 for station details) was obtained from the National Climatic Data Center (NCDC) on a CD-ROM for the time period 1995-2002. The original format of the data obtained from NCDC is given in Table 3.4.

Table 3.3: Details of the Station Monitoring Meteorological Data in Dayton, OH

Station ID	724290
Station Name	Dayton International Airport
City	Dayton
County	Montgomery
Cooperative station number	338598
WBAN number	93815

Table 3.4: Original Format of the Meteorological Data

```
USAF  WBAN YR--MODAHRMN DIR SPD GUS CLG SKC L M H  VSB WW WW
WW W TEMP DEWP    SLP   ALT    STP MAX MIN PCP01 PCP06 PCP24 PCPXX
SD
724290 93815 200201010000 280   7 *** 722 CLR 0 0 0 10.0 ** ** ** *   19    8 1023.0
30.16  985.0 *** ***  0.00 ***** ***** ***** **
724290 93815 200201010054 270   6 *** 722 CLR * * * 10.0 00 ** ** *   16    8 1023.2
30.16 ****** *** ***  0.00 ***** ***** ***** **
724290 93815 200201010154 260   6 *** 722 CLR * * * 10.0 00 ** ** *   15    7 1023.4
30.17 ****** *** ***  0.00 ***** ***** ***** **
724290 93815 200201010254 250   7 *** 722 CLR * * * 10.0 00 ** ** *   13    2 1023.2
30.16 ****** *** ***  0.00 ***** ***** ***** **
```

3.3 Pre-processing of Data

The ozone data obtained from the EPA was disordered formatted files and required a lot of processing to get it into the desired format. The files were exported to an MS Access database, where the data was sorted in separate tables by year in the chronological order with the help of built in queries. Each table had the details of monitoring site, year being monitored, month, day and the hour of the day (at which the ozone concentration was monitored). An example of the formatted data table is shown Table 3.5.

Table 3.5: Formatted Ozone Data

Transaction Description	Action Code	State Code	County Code	City Code	Pollutant Code	YYYYMMDD	Hour	Ozone Concentration (ppb)
RD	I	39	113	0019	44201	19950401	00:00	18
RD	I	39	113	0019	44201	19950401	01:00	21
RD	I	39	113	0019	44201	19950401	02:00	20
RD	I	39	113	0019	44201	19950401	03:00	20
RD	I	39	113	0019	44201	19950401	04:00	18
RD	I	39	113	0019	44201	19950401	05:00	15
RD	I	39	113	0019	44201	19950401	06:00	8
RD	I	39	113	0019	44201	19950401	07:00	4
RD	I	39	113	0019	44201	19950401	08:00	11

The meteorological data obtained from the NCDC were also text files and were formatted by importing them into an MS Access database. The data was then converted into the desired format in separate tables for each year. An example of the final form of the table is as shown below:

Table 3.6: Formatted Meteorological Data

Station	Call	YYYYMMDDHRMIN	Wind Speed (mph)	Temperature (^{0}F)	Dew point (^{0}F)
724290	DAY	199504010000	6	37	33
724290	DAY	199504010100	4	37	32
724290	DAY	199504010200	0	37	32
724290	DAY	199504010300	6	37	32
724290	DAY	199504010400	7	36	32
724290	DAY	199504010500	6	36	31
724290	DAY	199504010600	7	35	32
724290	DAY	199504010700	7	35	32
724290	DAY	199504010800	6	34	32

3.4 Missing Values

Equipment defects or failure can cause problems of missing and erroneous data. They can be periods of data missing completely at random or missing at random. These periods of missing data invalidate the assumption of equally spaced observations. A method to overcome this limitation is to develop schemes for interpolating the missing values.

The method used to fill the missing data could affect the ability of a model to forecast in two ways:

1) Structural change: When the produced data have different dynamic properties, the structure of the fitted model could differ from the actual model.

2) Bias in model parameters: When the interpolation method of filling is used, the interpolated values do not cause the structure of the model to change, but do in fact cause the values of the model's parameters to change.

Both structural changes in the model and the bias in the model's parameters could cause the resulting time series model to produce inaccurate forecasts.

Linear interpolation through averaging of two adjacent bracketing values has been frequently employed to replace missing values in air pollution data (Aramburu, 1983). This technique can be used with a measure of confidence by professionals who are confronted with the task of filling missing data for air pollution data (Terry et al. 1986). In this study, the method of linear interpolation was adopted for filling the missing data.

Table 3.7 below shows the number and percentage of missing values in ozone concentration, temperature, wind speed, and dew point temperature in the model development period, Apr.1996 –Oct.1999 and the evaluation period Apr. – Oct., 2002.

Table 3.7: Number and Percentage of Missing Values in the Period Apr. 1996- Oct.1999 and Apr. 2002-Oct.2002

Year Apr.-Oct.	Total Data Points	Ozone (ppb)		Temperature (^{0}F)		Wind Speed (mps)		Dew Point Temperature (^{0}F)	
		Missing	% Missing	Missing	% Missing	Missing	% Missing	Missing	% Missing
1996	5136	106	2.06	226	4.40	226	4.40	226	4.40
1997	5136	32	0.62	47	0.91	47	0.91	47	0.91
1998	5136	26	0.50	63	1.22	63	1.22	63	1.22
1999	5136	18	0.35	46	0.89	46	0.89	46	0.89
2002	5136	26	0.50	8	0.15	8	0.15	8	0.15

Finally, once the missing values are filled, the ozone data and the meteorological data are stored together in a single table according to the year as shown below:

Table 3.8: Final Format of the Ozone and Meteorological Data

Date	Time	Raw Oz	Temp	WS	Dew Pt
19960401	00:00	35	50.0	19.0	47
19960401	01:00	29	47.0	18.0	46
19960401	02:00	31	46.0	21.0	44
19960401	03:00	31	44.0	29.0	41
19960401	04:00	32	42.0	28.0	40
19960401	05:00	33	41.0	24.0	39
19960401	06:00	33	40.0	26.0	39
19960401	07:00	33	39.0	24.0	37
19960401	08:00	35	35.0	28.0	34
19960401	09:00	34	34.0	25.0	33

3.5 Forecasted Data

The MM5 real time forecasted data for temperature, wind speed, and dew point temperature were required for the model analysis. The data were extracted from the Polarmet web site maintained by the Polar Research Group at Ohio State University (Bromwich, 2003). The model predicts meteorological parameter values for every three hours. The forecasted data for the year 2003 was available only for the months of August to October for the city of Dayton. This data was modified to a desired format and used for model evaluation. Table 3.9 gives an example of the original format of the extracted data.

Table 3.9: Original Format of the MM5 Forecasted Meteorological Data

station name,	time,	T(F),	Td(F),	slp,	rhu(%),	dd(dgr),	dsp(mps),	cld,	prep
Dayton,OH	0	79.22	66.05	1013.01	62.53	36.26	3.83	0.85	0.00
Dayton,OH	3	77.08	66.35	1014.26	67.94	27.47	9.26	0.96	0.00
Dayton,OH	6	74.58	65.91	1015.89	72.76	27.71	8.63	0.99	1.06
Dayton,OH	9	73.28	66.43	1016.08	77.54	41.55	8.29	0.99	0.71
Dayton,OH	12	72.50	66.23	1016.39	79.07	38.99	8.11	1.00	0.07
Dayton,OH	15	75.38	63.29	1016.51	64.44	41.16	6.35	1.00	0.51
Dayton,OH	18	77.76	62.76	1015.85	58.28	14.57	6.54	1.00	2.02
Dayton,OH	21	80.69	60.68	1015.29	48.96	358.89	7.54	1.00	0.95
Dayton,OH	24	80.58	62.44	1015.11	52.38	33.79	7.84	1.00	0.01

Chapter 4

Data Analysis

Knowledge of spatial and temporal variations of ozone is crucial for developing improved models of predicting ozone patterns and establishing effective strategies to reduce the amount of ambient ozone. A comprehensive analysis of the variations in hourly ozone concentrations, ozone episode occurrences, and long-term trends in annual means of ozone concentrations, temperature, wind speed, and dew point temperature was performed for the period Apr.-Oct. for the years 1996-1999. The results are discussed in this chapter.

4.1 Annual Trends in Hourly Ozone Concentrations

Figure 4.1 statistically summarizes the annual averages of hourly ozone concentrations in the study region from 1996-1999 using box plots, in which the percentiles (5^{th}, 10^{th}, 25^{th}, 50th, 75th, 90th, and 95^{th}), means, and maxima are indicated. The figure shows that all the maxima values exceeded the standard of 85 ppb and the 95^{th} percentiles were found below 85 ppb for all the years.

Table 4.1 shows that the annual mean and 50th -95th percentiles of the hourly ozone concentrations over the period of interest exhibit decreasing trends (-0.2%/yr) with the average values in the range of 30-35 ppb.

Similar studies in Montreal (1994), Korea (1999), three sites near Lake Michigan (1998) and sites in the northeastern United States (1995) exhibited declining trends of ozone during the recent decades.

Figure 4.1:

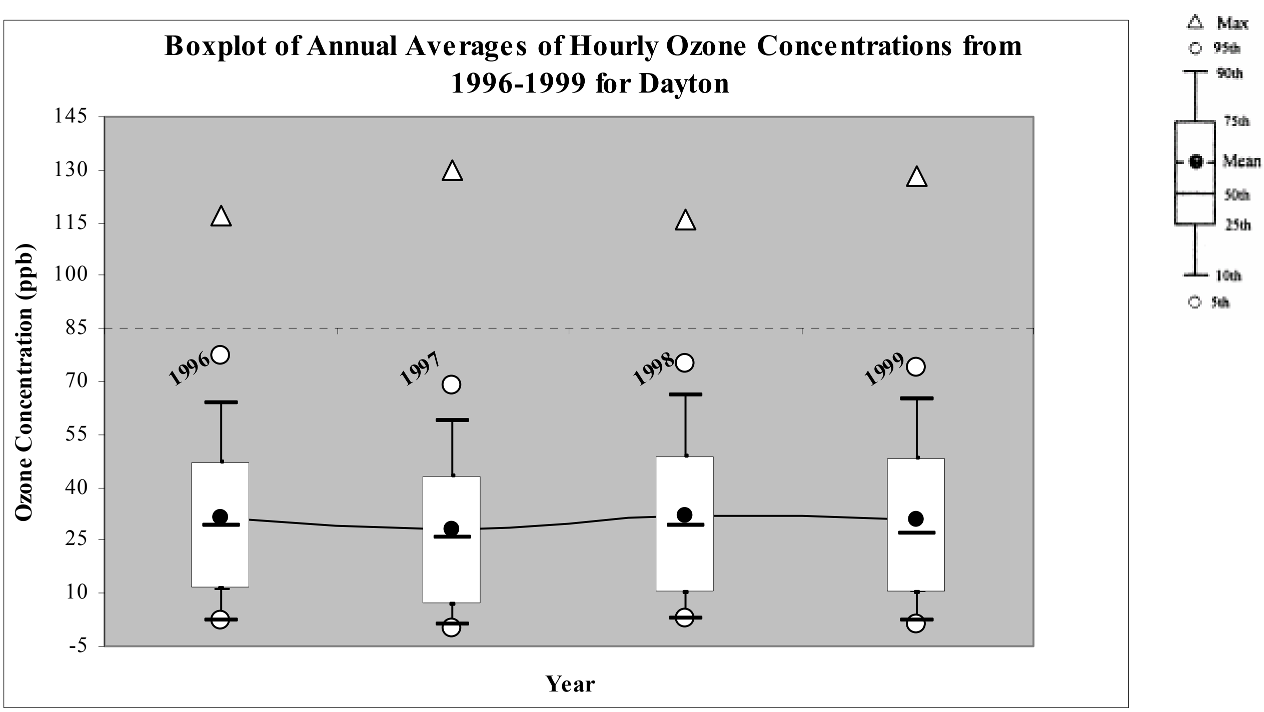


Table 4.1: Change in Annual Means and Percentiles of Hourly Ozone Concentrations in the City of Dayton, 1996-1999

Mean	Percentile			
	50th	75th	90th	95th
-0.20	-1.63	0.81	0.81	-2.45

4.2 Long-term Trends in the Annual Means of Hourly Ozone Concentrations, Temperature, Wind Speed, and Dew Point Temperature

The long-term trends in the annual means of hourly ozone concentrations, temperature, wind speed, and dew point temperature from 1996-1999 are presented in the Figure 4.2 The trend lines, obtained by the least square regression method, are indicated by dotted lines for all the variables. The corresponding slopes are given in Table 4.2. The negative and positive values indicate decreasing trends of ozone, wind speed, and dew point temperature and increasing trend of temperature respectively. This can also be observed in Figure 4.2.

Figure 4.2:

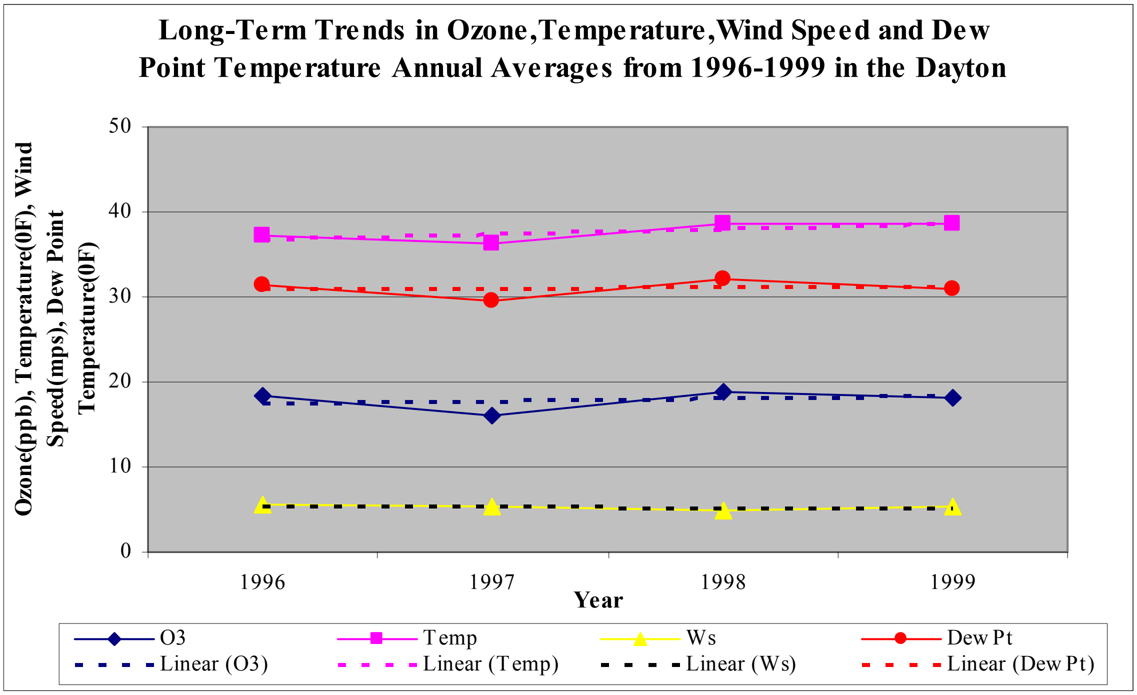


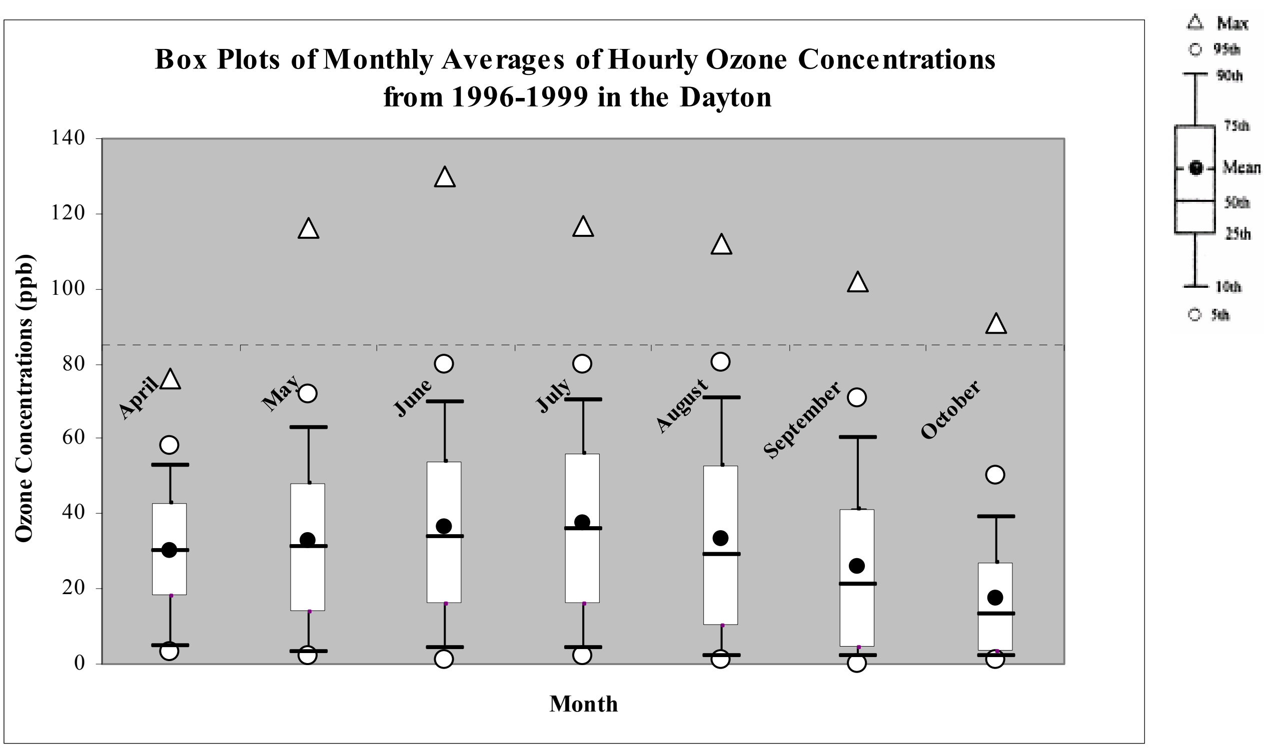
Table 4.2: Slopes of the Trend Lines of Ozone, Temperature, Wind Speed, and Dew Point Temperature from 1996-1999

Parameter	Slope
Ozone	-0.023
Temperature	0.358
Wind Speed	-0.032
Dew point Temperature	-0.122

4.3 Seasonal Trends in Hourly Ozone Concentrations

The monthly averages of hourly ozone concentrations are summarized in Figure 4.3. The figure shows that all of the maxima exceed the standard value of 85 ppb, except for the month of April. A study in eastern Canada (1994), which considered seasonal variations in monthly means of the ozone concentrations of the urban and rural sites, concluded that the site under considerable anthropogenic influence recorded the highest concentrations from Jul. to Aug. (summer months). Similar results were obtained in this study. The monthly means of hourly ozone concentrations exhibit maximum variation in the summer months (May.–Aug.).

Figure 4.3

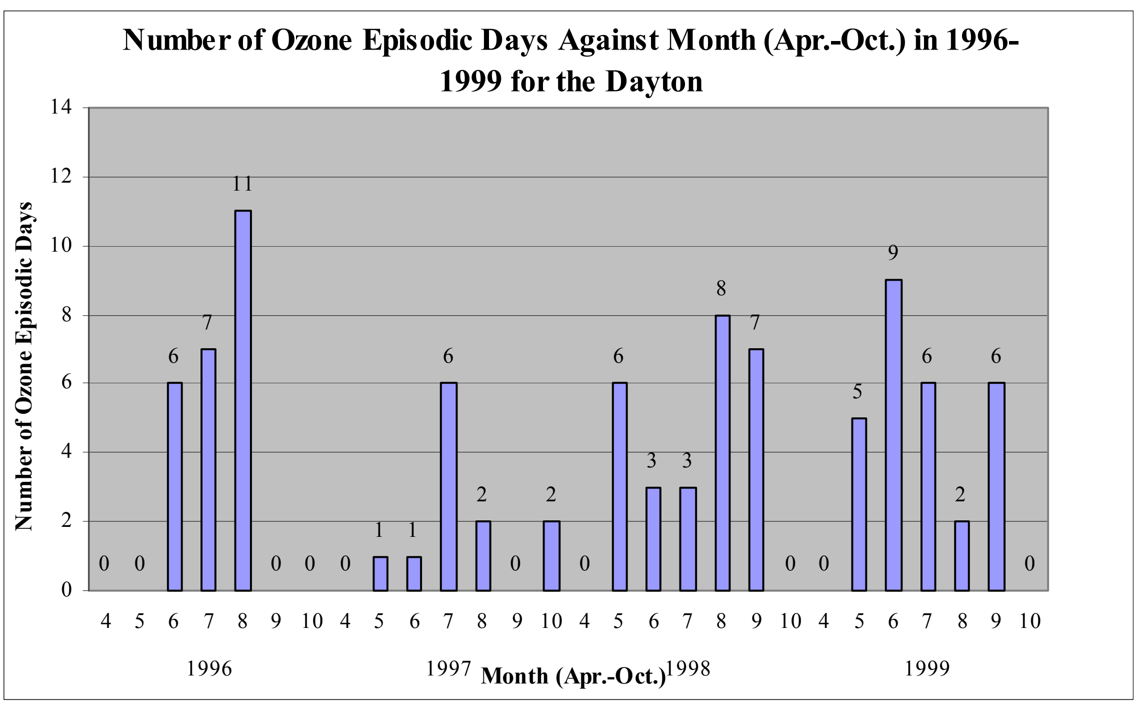


4.4 Ozone Episodes

The number of monthly ozone episodic days shown in Figure 4.4 indicates that the maximum exceedance occur during the months of June to August for all the years. Late May and early September were also found to be potential in the years 1998 and 1999. Over a 4-year period of around 736 days (Apr. to Oct.), 91 episodic days were found. That is, on an average, one day in a week was episodic in the years 1996-1999.

Conversely, in a study carried out in Taiwan (2004), which analyzed the meteorological effects on high ozone episodes, it was seen that the ozone episodes occurred most often in autumn and least frequently in summer.

Figure 4.4



4.5 Meteorological Effects on Ozone Episodes

Figures 4.5, 4.6, and 4.7 plot the hourly ozone concentrations that exceeded 85 ppb with the corresponding meteorological parameter values. High values of temperature (70-90 ^{0}F), dew point temperature (50-70 ^{0}F) and low wind speeds (<8 mps) were found during these days in all the years. Hence, it is clear from the figures that meteorological conditions play an important role in the occurrence of ozone exceedances.

Figure 4.5

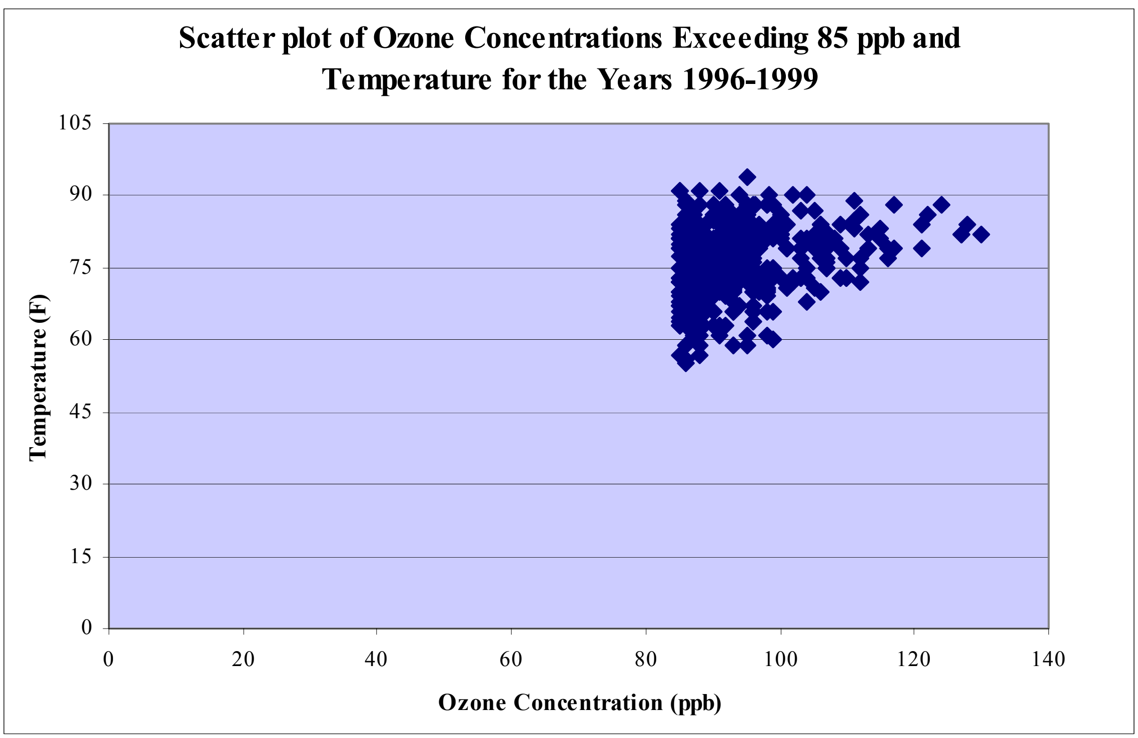


Figure 4.6

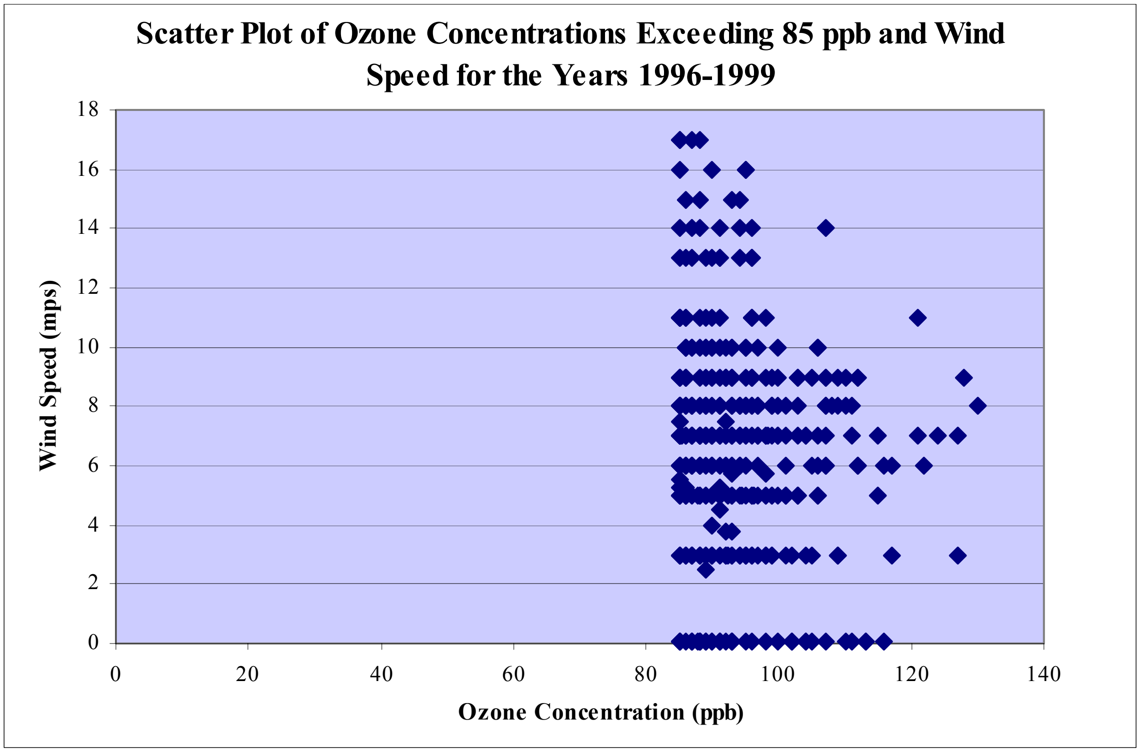
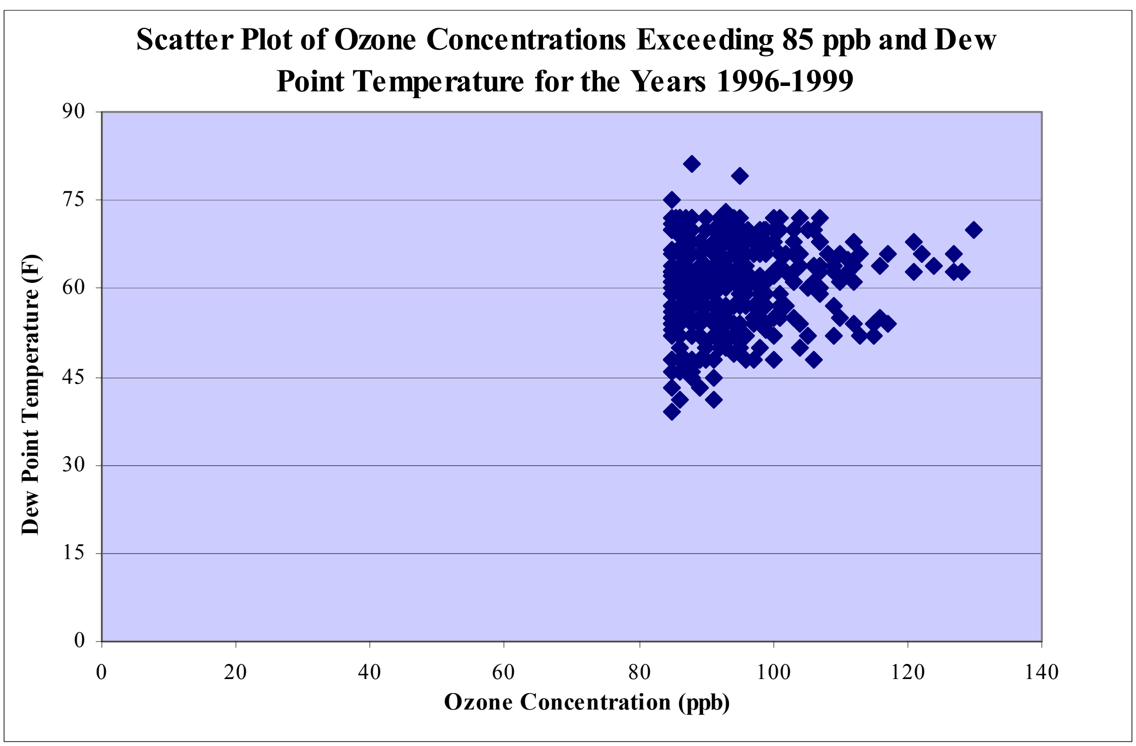


Figure 4.7



4.6 Conclusions From Data Analysis

The variations in ambient hourly ozone concentrations in the city of Dayton were analyzed for the period 1996-1999. The following conclusions were drawn from the analysis:

- Most of the annual and monthly means of the maxima exceeded 85 ppb.
- All of the 95th percentiles of annual and monthly means were below 85 ppb.
- The long-term trends in the annual means depict decreasing trends of ozone, wind speed, and dew point temperature and an increasing trend of temperature.
- The seasonal pattern of surface hourly ozone concentrations showed maximum variation during the summer months (May.-Aug.).
- Ozone episodes occurred on days with high temperatures and dew point temperatures and low wind speeds, which are typical in the months of Jun.-Aug.

From the analysis, it can be concluded that one out of seven days exceeded the ozone standard. The air quality in Dayton is a serious issue and, hence, accurate predictions are needed in order to take precautionary measures to avoid ozone episodic days. The following chapter discusses the development of a model to forecast the hourly ozone concentrations for the city of Dayton.

Chapter 5

Methodology

This section deals with the development of the model and statistical evaluation. Considering the different methods discussed in section 2.6, the regression method was chosen for this study, as it is easy to develop and operate. This method has been well documented and widely used in various disciplines. It has been successfully used for ozone forecasting in many parts of the country.

5.1 KZ Filtering Technique

The models were developed using the KZ filtering technique coupled with regression analysis. This technique, developed by Rao and Zurbenko (1995), is a statistical method of moderating the influence of meteorology on surface ozone concentrations. In this study the temperature, wind speed, and dew point temperature were used as independent variables and KZ filter was used to reduce the fluctuations. According to this method, time series of the log of the ozone concentration (Oz) can be represented by the following equation:

$$X(t) = e(t) + S(t) + W(t) = \text{Baseline}(t) + W(t) \tag{5.1}$$

where:

X (t) = Original ozone concentration time series

e (t) = Long-term trend component

S (t) = Seasonal variation

W (t) = Short-term variation, and

t is the time.

The baseline is separated from the short-term variation using the Kolmogorov-Zurbenko ($KZ_{m,\ p}$) filter. The $KZ_{m,\ p}$ is a low-pass filter produced by repeated iterations of a simple moving average (Zurbenko, 1991). Each iteration of the moving average Y_i is defined as follows:

$$Y_i = (1/m)\sum_{j=-k}^{k} X_{i+j} \tag{5.2}$$

where,

m = 2k +1.

The Y_i becomes the input for the second pass, and the process continues accordingly. Determination of the final low-pass filter (specifying "m" and the number of passes "p") is an iterative process in which the user determines if the white noise (short-term variation) has been removed. The output time series, Y_t, is the low frequency part of X_t denoted as:

$$Y_t = KZ_{m,\,p}(X_t) \tag{5.3}$$

Y_t contains both the long-term trend and seasonal effects.

Based on the above theory, simple forecasting models to predict the hourly ozone concentrations for different seasons in the city of Dayton, Ohio have been developed in this study.

5.2 Model Development

A total of twelve models were developed in this study. Six models used temperature, wind speed, and dew point temperature as independent parameters (here after referred to as three-parameter models). The other six considered temperature and wind speed as independent variables (here after referred to as two-parameter models). Initially the entire dataset (Apr.-Oct.) was considered for the model development and it was seen that the seasonal variations were not accounted for. Based on the analysis performed on the ozone data in chapter 4, it was seen that the seasonal patterns of the hourly ozone concentrations show maximum variation during the summer months. Hence, the dataset was divided into two groups namely pre-summer (Apr.-Jul.) and post-summer (Aug.-Oct.). It was noticed that this classification did not improve the model performance, as the hourly concentrations varied over a wide range. Hence, following the method adopted by Kim (2003), it was determined to split each day into three regimes. According to this study, the observed concentrations against hour in a day, shows that the first 8-hours of the day is the stable period of the ozone levels, the second 8-hours is the ascent period, and the remaining 8-hours is the descent period.

A similar trend was observed with the data considered in this study. (An example is shown in Figure 5.1.) The ozone data for pre-summer and post-summer was divided into three regimes, namely, hours: 1-8, hours: 9-16 and hours: 17-24. A more or less uniform dataset was obtained from this classification. KZ filter technique was used to reduce the scatter in the time series, and three models each for pre-summer and post-summer were developed. Following this method the two-parameter models were developed for both of the seasons. An overview of the developed models is given in Table 5.1.

Figure 5.1

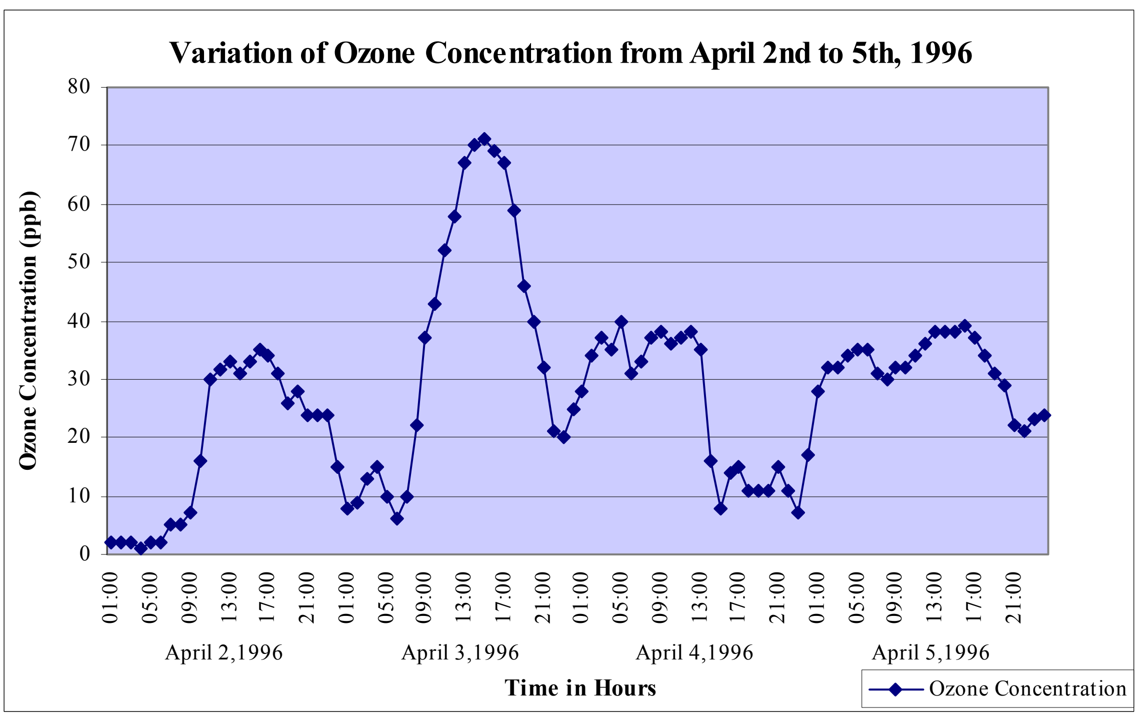


Table 5.1: Summary of the Models Developed

Season	Hour of the day	Years of Data Considered	Variables Involved	Number of Models
Pre-Summer	1-8, 9-16, 17-24	1996-1999	Temperature, Wind Speed, Dew point Temperature	3
			Temperature, Wind Speed	3
Post-Summer	1-8, 9-16, 17-24	1996-1999	Temperature, Wind Speed, Dew point Temperature	3
			Temperature, Wind Speed	3

Overview of the KZ model

The development of the model involved two steps:

1) Application of the KZ filter

The ozone and the meteorological data stored in MS Access were imported into MS Excel spreadsheet and separated by year. The data was separated by year because the ozone data between November and March (both inclusive) is not monitored, and hence treated as missing data. Also, the records with zero values of ozone concentrations and the corresponding independent parameter values were deleted. The natural logarithm of ozone concentration is calculated. Different combinations of $KZ_{m,p}$ filters were studied by dividing the data set into three regimes (Hr:1-8, 9-16 and 17-24) for pre-summer (Apr.-Jul.) and post-summer (Aug.-Oct.).

Different values of ‘m’ (sample size) and ‘p’ (number of iterations) were investigated. The values of ‘m’ studied were 50, 100, 200, 275 and 300 depending on the number of data points. The values of ‘p’ investigated were 1, 2, and 3.

Linear regression of the filtered natural logarithm of the ozone concentration as a function of the filtered temperature, filtered wind speed, and filtered dew point temperature was performed for each of the filters separately to obtain the coefficient of determination, R^2.

The optimal $KZ_{m,\ p}$ filter was chosen by examining coefficients of determination. Tables 5.2, 5.3, 5.4, and 5.5 list the values of R^2 obtained for pre-summer and post-summer for both three-parameter and two-parameter models. Since the ideal value for R^2 is 1, the filters which provided the best values were chosen for the model development (also highlighted in these tables). It is observed that it cannot be ascertained that increasing the number of iterations (i.e., ‘p’) will improve the value of R^2. Rao et al. (1995) have used the (365, 3) filter for developing a noise-free temperature independent time series for a site located in New Haven, CT.

Table 5.2: Coefficient of Determination for Different Combinations of KZ Filters for Pre-summer (Apr.-Jul.), Three-parameter Model

Hour: 1-8		Hour: 9-16		Hour: 17-24	
Type of Filter	**R^2**	**Type of Filter**	**R^2**	**Type of Filter**	**R^2**
100,1	0.42	100,1	0.69	100,1	0.41
100,2	0.38	100,2	0.73	100,2	0.45
100,3	0.36	100,3	0.76	100,3	0.48
200,1	0.31	200,1	0.76	200,1	0.44
200,2	0.36	200,2	0.83	200,2	0.46
200,3	0.32	200,3	0.88	200,3	0.47
275,1	0.31	275,1	0.82	275,1	0.39
275,2	0.32	275,2	0.89	275,2	0.31

Table 5.3: Coefficient of Determination for Different Combinations of KZ Filters for Post-summer (Aug.-Oct.), Three-parameter Model

Hour: 1-8		Hour: 9-16		Hour: 17-24	
Type of Filter	**R^2**	**Type of Filter**	**R^2**	**Type of Filter**	**R^2**
50,1	0.54	50,1	0.79	50,1	0.80
50,2	0.55	50,2	0.77	50,2	0.84
50,3	0.56	50,3	0.76	50,3	0.85
100,1	0.61	100,1	0.84	100,1	0.87
100,2	0.66	100,2	0.83	100,2	0.91
100,3	0.64	100,3	0.84	100,3	0.92
200,1	0.71	200,1	0.86	200,1	0.93
200,2	0.75	200,2	0.90	200,2	0.95
275,1	0.76	275,1	0.89	275,1	0.95
300,1	0.76	300,1	0.91	300,1	0.96

Table 5.4: Coefficient of Determination for Different Combinations of KZ Filters for Pre-summer (Apr.-Jul.), Two-parameter Model

Hour: 1-8		Hour: 9-16		Hour: 17-24	
Type of Filter	R^2	Type of Filter	R^2	Type of Filter	R^2
100,1	0.38	100,1	0.52	100,1	0.33
100,2	0.33	100,2	0.57	100,2	0.37
100,3	0.29	100,3	0.59	100,3	0.41
200,1	0.23	200,1	0.62	200,1	0.37
200,2	0.22	200,2	0.68	200,2	0.44
200,3	0.18	200,3	0.72	200,3	0.45
275,1	0.15	275,1	0.69	275,1	0.35
275,2	0.11	275,2	0.75	275,2	0.37
275,3	0.09	275,3	0.86	275,3	0.34

Table 5.5: Coefficient of Determination for Different Combinations of KZ Filters for Post-summer (Aug.-Oct.), Two-parameter Model

Hour: 1-8		Hour: 9-16		Hour: 17-24	
Type of Filter	R^2	Type of Filter	R^2	Type of Filter	R^2
50,1	0.52	50,1	0.69	50,1	0.74
50,2	0.53	50,2	0.67	50,2	0.77
50,3	0.53	50,3	0.65	50,3	0.79
100,1	0.57	100,1	0.77	100,1	0.80
100,2	0.58	100,2	0.76	100,2	0.82
100,3	0.55	100,3	0.77	100,3	0.83
200,1	0.60	200,1	0.82	200,1	0.85
200,2	0.56	200,2	0.86	200,2	0.86
275,1	0.62	275,1	0.87	275,1	0.87
300,1	0.61	300,1	0.88	300,1	0.88

2) Development of the Model

With the KZ filter chosen, a linear regression of the filtered natural log of ozone concentration [$O_{KZ}(t)$] on filtered temperature [$T_{KZ}(t)$], filtered wind speed [$W_{KZ}(t)$], and filtered dew point temperature [$D_{KZ}(t)$] was performed with the dataset. Three-parameter and two-parameter models were developed for the periods Apr.-Jul. and Aug.-Oct. Each model was evaluated by comparing the model with an independent dataset collected from that site. The relation between the independent variables and the dependent parameter can be expressed in the following linear equation:

$$O\kappa z(t) = aT\kappa z(t) + bW\kappa z(t) + cD\kappa z(t) + d + \varepsilon(t) \tag{5.4}$$

where,

$O_{kz}(t)$ is the filtered natural logarithm of the hourly ozone concentration for the chosen KZ filter,

$T_{kz}(t)$ is the filtered hourly temperature for the chosen KZ filter,

$W_{kz}(t)$ is the filtered hourly wind speed for the chosen KZ filter,

D_{kz}(t) is the filtered hourly dew point temperature for the chosen KZ filter,

a is the coefficient of $T_{kz}(t)$,

b is the coefficient of $W_{kz}(t)$,

c is the coefficient of D_{kz}(t),

d is the regression constant, and

$\varepsilon(t)$ is the residual and represents the variation in ozone concentrations attributable to factors other than temperature, wind speed and dew point temperature.

Excluding the residual, the relationship between the variables in the above equation may be expressed as in Equation 5.5

$$O\kappa z(t) = aT\kappa z(t) + bW\kappa z(t) + cD\kappa z(t) + d \tag{5.5}$$

Three other equations were developed using the dataset. Equation 5.6 is a relationship between the filtered temperature and the raw temperature. This relationship was obtained by linear regression using $T_{kz(m,p)}$ as the dependent variable.

$$T_{KZ\,(m,p)}(t) = a_1T(t)+c_1 \tag{5.6}$$

where,

$T_{kz(m,p)}\,(t)$ is the filtered temperature for the chosen KZ filter,

$T(t)$ is the hourly temperature,

$a_1(t)$ is the coefficient of the hourly temperature, and

c_1 is the constant.

Equation 5.7 is a relationship between the filtered wind speed and the raw wind speed. This relationship was obtained by linear regression using $W_{kz(m,\,p)}$ as the dependent variable.

$$W_{KZ(m,p)}\,(t)=a_2W(t)+c_2 \tag{5.7}$$

where,

$W_{kz(m,p)}\,(t)$ is the filtered hourly wind speed for the chosen KZ filter,

$W(t)$ is the hourly wind speed,

$a_2(t)$ is the coefficient of the hourly wind speed, and

c_2 is the regression constant.

Equation 5.8 is the relationship between filtered dew point temperature and raw dew point temperature. This relationship was obtained by linear regression using $D_{kz(m,p)}$ as the dependent variable.

$$D_{KZ(m,p)}\,(t)=a_3D(t)+c_3 \tag{5.8}$$

where,

$D_{kz(m,p)}$ (t) is the filtered hourly dew point temperature for the chosen KZ filter,

$D(t)$ is the raw hourly dew point temperature,

$a_3(t)$ is the coefficient of raw hourly dew point temperature, and

$c_3(t)$ is the regression constant.

Finally, Equation 5.9 is the relationship between the natural log of the ozone concentration and the filtered natural log of the ozone concentration. This relationship was obtained by linear regression using $O_{kz(m,p)}$ as the predictor variable.

$$\ln O(t) = a_4O_{KZ(m,p)}(t)+c_4 \tag{5.9}$$

where ,

$O_{kz(m,p)}$ is the filtered natural logarithm of the hourly ozone concentration for the chosen KZ filter,

$O(t)$ is the hourly ozone concentration,

a_4 is the coefficient of the filtered natural logarithm of the hourly ozone concentration for the chosen KZ filter, and

c_4 is the regression constant.

By substituting Equations 5.6, 5.7 and 5.8 in Equation 5.4, and the resultant expression in Equation 5.9, the natural logarithm of hourly ozone concentration may be expressed as a function of hourly temperature, wind speed, and dew point temperature. This relationship, expressed in Equation 5.10, is essentially the final forecasting model.

$$\ln O(t) = A * T(t) + B * W(t) + C * D(t) + E \tag{5.10}$$

where ,

O(t) is the hourly ozone concentration,

T(t) is the hourly temperature and *A* is coefficient of *T(t),*

W(t) is the hourly wind speed and *B* is coefficient of *W(t),*

D(t) is the hourly dew point temperature and C is the coefficient of D(t),

E is the regression constant

These models were developed using the time-series data between 1996 and 1999 (both inclusive) for Dayton, Ohio. The models were then validated by predicting the ozone concentrations for year the 2002, and comparing against the observed concentration for the same period. The final form of the model equation is shown in Chapter 6.

5.3 Model Evaluation

Model evaluation is performed to explore the forecast performance of the developed models. Research work done during the 1980's and 1990's led to the development of the following performance measures to evaluate the air quality models. The US EPA has developed some guidelines in order to validate and calibrate models in a comprehensive manner.

Gudivaka and Kumar (1990) worked on statistics relevant to model evaluation and have applied them to heavy gas models. Another study, Kumar et al. (1993) employed statistical tools to evaluate the prediction of lower flammability distances. Other evaluation studies, (Patel and Kumar, 1998, and Kumar et al., 1999) clearly indicate that fractional bias (FB), normalized mean square error (NMSE), and factor of "2' (Fa_2) are three important statistical parameters to evaluate model performance.

The model evaluation parameters along with the forecasting skill are discussed in detail as follows:

1) Coefficient of Determination (R^2)

R^2 is a measure of the correlation between the dependent and independent variables in a regression analysis. It is calculated as the square of the correlation coefficient, r, and varies between 0 and 1. An ideal model would have an R^2 of 1.

2) Fractional Bias (FB)

Thel bias is normalized to make it non-dimensionless. this fractional bias (FB) varies between +2 and -2 and has an ideal value of zero for an ideal model. It is written in symbolic form as:

$$FB = 2*(\overline{Co} - \overline{Cp}) / (\overline{Co} + \overline{Cp}) \qquad (5.11)$$

3) Normalized Mean Square Error (NMSE)

This statistic emphasizes the scatter in the entire data set and is known as Normalized Mean Square Error (NMSE). The normalization by the product Cp*Co assures that the NMSE will not be biased towards models that over predict or under predict. Smaller values of NMSE denote better model performance. The expression for the NMSE is given by:

$$NMSE = \overline{(Cp - Co)^2} / \overline{(CoCp)} \qquad (5.12)$$

4) Factor of x (Fa_X)

The factor of two (Fa_X) is defined as the percentage of the predictions within a factor of 'x' of the observed values. The ideal value for the factor of 'x' should be 1 (100%).

Fa_X = Fraction of data which $(1/x) <= C_p/C_o <= x$ (5.13)

In the present study the value of 'x' was considered '2'.

5) Forecasting Skill

Another indicator of performance of a forecasting model is forecasting skill (FC). Chenevez and Jensen (2001) proposed an indicator for calculating the performance of a model while making peak forecasts. This indicator is being used for the evaluation of performance of the forecasting systems currently operating in Denmark.

They have defined forecasting skill (FC) of a model as:

$FC = 100*N_r/N$ (5.14)

where,

N_r is the number of forecast hits inside an uncertainty interval r, and

N is the total number of forecasts.

An ideal model will have both the FB and NMSE equal to zero and Fa_2 value equal to one (Table 5.6). Such models are very difficult to develop in reality owing to many unaccounted reasons and errors.

Table 5.6: Evaluation Parameters for a Perfect Model

R^2	1.0
FB	0
NMSE	0
Fa_2	1.0
FC	100%

R^2 values of the models were not calculated as it is considered unreliable in judging the performance of a forecasting model. Studies have revealed that that R^2 is useful in explaining the fluctuations in data, but not completely reliable in indicating the accuracy of model perfections. Thus, a model with an R^2 value of '0' may not be a completely bad forecast and an R^2 value of'1' does not necessarily represent a perfect model. The U.S.EPA's "Protocol for Determining the Best Performing Model" (EPA, 1992) suggests that R^2 should be used for the primary screening of the available models. It states FB, and NMSE are the most important statistical parameters (rather than R^2) for model evaluation studies.

Hence, in this study R^2 was used only to fit a model and not to check for the model performance.

Evaluation of the models developed in this study was done in three different ways:

1. The models were validated using the data for the year 2002. Observed temperature, wind speed, dew point temperature and ozone concentrations were used. The dataset for the year 2002 was separated into pre-summer and post-summer, and each period was again divided into three sets based on the hour of the day. The predicted ozone values for each hour of each set were obtained using observed meteorological parameter values. These predicted ozone concentration values, obtained by using the corresponding model, were compared against observed values, using the statistical parameters. As the observed meteorological parameter values were used, this does not lead to a perfect evaluation. However, the evaluation gives us a good idea of the performance of the model, if perfect forecasted meteorological variable values were available.

2. MM5 real-time meteorological forecasts were used for the second evaluation. In practice, the actual data is not available unless monitored, and hence the forecasts are carried out using the predicted values for independent parameters. As this data was available only for the months of Aug.-Oct. 2003, the predicted values were obtained only for that period using the corresponding model. The performance of this model was checked using the observed ozone data for 2003.

The evaluation will also reflect the meteorological forecasting ability of the MM5 model.

3. The models developed using temperature and wind speed as variables (two-parameter models) were evaluated for 2002 using observed data and for 2003 using MM5 data in the similar manner as discussed in step 1 & 2.These two-parameter models were then compared with the three-parameter models using evaluation parameters.

The models were also checked for their performance in predicting hourly AQI values, and the results were plotted for the observed and predicted values for the models.

Chapter 6

Results and Discussion

The final forecasting model equations and their evaluations are provided in this chapter. The application of the model evaluation techniques and the calculation of specific performance parameters based on air quality evaluation studies are also presented.

6.1 Models Developed

The final model equation obtained for predicting ozone concentration, is in the form

$$\ln (Oz) = (A*T) + (B*W) + (C*D) + E \qquad (6.1)$$

where,

T = hourly temperature in ^oF,

W = hourly wind speed in mph,

D = hourly dew point temperature in ^oF,

Oz = hourly ozone concentration in ppb,

A = coefficient of temperature T,

B = coefficient of wind speed W,

C = coefficient of dew point temperature D,

E = regression constant.

Tables 6.1 and 6.2 summarize the coefficients of the three-parameter and two-parameter models developed for pre-summer and post-summer seasons.

The values of coefficients for temperature from the tables indicate that the KZ model has shown a positive relationship between the hourly ozone concentrations and hourly temperature for pre-summer and post-summer seasons.

The co-efficient of wind speed was negative for hr: 9-16 models for pre-summer, indicating a negligible effect of wind speed during this period in which high concentrations of ozone occur. During other periods (hr: 1-8, 17-24), wind speed has shown more significance on the ozone concentration than temperature.

The wind speed was seen to have more impact on ozone concentrations than temperature during all periods of post-summer. This may be due to the presence of low temperatures in the post-summer season. It has been reported in the literature that wind plays a very complex role in the transport of ozone and ozone pre-cursors in and out of an area, and the ozone-wind relationship depends on the historical data at a specific site (Hubbard and Cobourn, 1998).

A clear idea of how the dew point temperature affects the ozone concentrations could not be found from the values obtained. However, in most cases it was seen to have less impact on ozone concentrations than temperature and wind speed. Moreover, during morning times (hr: 1-8), dew point temperature was noticed to have more impact than temperature for both pre-summer and post-summer. A detailed examination of the predicted results indicates that the peak values were predicted well qualitatively by including dew point temperature as a variable.

Table 6.1: Summary of Coefficients of the KZ Regression Models Developed for Pre-summer: Apr.-Jul.

Type of Model	Hour of the Day	Coefficient of Temperature (A)	Coefficient of Wind Speed (B)	Coefficient of Dew point Temperature (C)	Regression Constant (E)
Three-parameter Model	1-8	-0.008	0.132	0.037	0.82
	9-16	0.049	-0.071	-0.038	3.535
	17-24	0.040	0.042	-0.015	1.132
Two-parameter Model	1-8	0.014	0.128	-	0.609
	9-16	0.010	-0.117	-	4.231
	17-24	0.025	0.043	-	0.931

Table 6.2: Summary of Coefficients of the KZ Regression Models Developed for Post-summer: Aug.-Oct.

Type of Model	Hour of the Day	Coefficient of Temperature (A)	Coefficient of Wind Speed (B)	Coefficient of Dew point Temperature (C)	Regression Constant (E)
Three-parameter Model	1-8	0.015	0.095	0.026	-0.829
	9-16	0.069	0.102	-0.018	-0.496
	17-24	0.037	0.139	0.027	-2.869
Two-parameter Model	1-8	0.031	0.054	-	-0.349
	9-16	0.056	0.117	-	-0.640
	17-24	0.052	0.079	-	-1.940

As discussed earlier, the KZ filter is used to reduce the scatter in the raw data. The effect of the KZ filter application on the raw time series data is depicted in Figures A.1-A.4 of Appendix A. The reduction in the fluctuation is clearly demonstrated by these figures.

The hourly ozone concentrations for the year 2002 were predicted for the three-parameter models using the observed temperature, wind speed, and dew point temperature values, and were evaluated against the observed concentrations. Also, the models were evaluated using real-time forecasted meteorological data (MM5 data) for the year 2003, and were compared against observed values for the same period. For Dayton, the forecasted data was available only for the months of Aug. to Oct., 2003. This data was used for the evaluation of the models.

Similarly, the two-parameter models were evaluated, and their performance was compared with three-parameter models.

6.2 Models Developed for Pre-summer (Apr.-Jul.)

The hourly concentrations for Apr.-Jul., 2002 were predicted. The model evaluation parameters discussed in Section 5.3 were calculated and the results are summarized in the Table 6.3 for pre-summer. Appendix B provides the figures that plot observed and predicted concentrations. The results of these statistical analyses meet the criteria specified by Kumar et al. (1993) for an acceptable air quality model. NMSE and Fa_2 are close to the ideal values (zero). Forecasting skill, FC, was less than 50 percent for all the models and needs further improvement. It can be seen that all the FB values were negative, indicating the tendency of the model to over-predict, which is also apparent from Figures B.1-B.3. As a further attempt to examine the usefulness of the models, AQI generated from the observed concentrations and predicted concentrations were compared. It can be seen from Table 6.4 for pre-summer that the models are acceptable in predicting ranges rather than discrete values, and extreme values in particular. It was noticed that the models are predicting most of the values in the 41-80 ppb range.

The results of statistical analysis and AQI forecasting of the two-parameter model for the year 2002 are also given in Tables 6.3 and 6.4 respectively. NMSE and Fa_2 were close to ideal values. The 9-16 hour model seemed to over-predict, but the other models were under-predicting. This is evident from the values of FB in Table 6.3 and Figures B.4-B.6. The models meet the requirements of an acceptable air quality model, but, unlike the three-parameter models, these models were unable to predict most of the peak concentrations. It is noticed that considering dew point temperature, as an additional variable, accounted for the majority of the peak values, although the models tend to over-predict most of the time.

6.3 Models Developed for Post-Summer (Aug.-Oct.)

A similar evaluation was performed for post-summer. The figures are given in Appendix C. The performance characteristics for the year 2002 are provided in Table 6.3 for post-summer. All the values obtained were close to the ideal values. Again, negative FB values were obtained, indicating the over-predicting tendency of the models, which can be seen from Figures C.1-C.3. A better forecasting ability of the models was seen except for the 9-16 hour model, which needs improvement. The AQI forecasting for post-summer, as seen in Table 6.4, shows a tendency of the models to over-predict AQI most of the time. This is generally acceptable in declaring an ozone action day for avoiding non-attainment status of an area.

The result of the evaluation of the two-parameter model (refer to summary Tables 6.3 and 6.4) shows that 1-8 hour and 17-24 hour models were under-predicting (Figures C.4-C.6). Although the statistical parameter values were close for three-parameter and two-parameter models, the three-parameter models performed better in predicting the peak concentrations.

The results of the evaluation of the models for Aug.-Oct., 2003 using MM5 forecasted data for temperature, wind speed, and dew point temperature are also given in the summary tables. The forecasting skill of the models improved when forecasted data was used. Theoretically, forecasted data may or may not improve the forecasting ability of a model. All the models over-predicted most of the values, which can be concluded from the negative FB values (also see Figures C.7-C.9). AQI forecasting, as seen in Table 6.4, shows that the results are in the acceptable range. The observed and the predicted values were fairly close.

The results of the two-parameter models as seen in the summary tables and Figures C.10-C.11 show that the 9-16 hour model did not predict well when the forecasted data was used. The rest of the models were under-predicting.

The three-parameter models performed well in predicting most of the peak concentrations. Previous studies on the forecasting (Kumar et al 2000, Ghose 2003, Tandale 2004), which considered temperature and wind speed or temperature alone, failed to simulate most of the peak concentrations. Considering dew-point temperature as an additional parameter improved the performance of the model in predicting these values.

Table 6.3: Summary of Results for Pre-summer and Post-summer

Type of Model	Hour of the Day	Evaluation Parameters			
Pre-summer (Apr.-Jul.)					
		FB	NMSE	Fa_2	FC
Three-parameter Model	1-8	-0.46	0.194	0.61	44.32
	9-16	-0.17	0.028	0.89	47.69
	17-24	-0.17	0.029	0.75	42.58
Two-parameter Model	1-8	0.40	0.149	0.85	61.9
	9-16	-0.06	0.003	0.88	35.2
	17-24	0.34	0.111	0.86	35.9
Post-summer (Aug.-Oct)					
Type of Model	**Hour of the Day**	**FB**	**NMSE**	**Fa_2**	**FC**
Three-parameter Model	1-8	-0.04	0.001	0.57	81.42
	9-16	-0.01	0.0001	0.88	37.50
	17-24	-0.06	0.002	0.68	58.96
Two-parameter Model	1-8	0.31	0.081	0.64	80.60
	9-16	-0.17	0.023	0.82	37.22
	17-24	0.22	0.032	0.71	59.09
Post-summer (Aug.-Oct.) Using MM5 Data					
Type of Model	**Hour of the Day**	**FB**	**NMSE**	**Fa_2**	**FC**
Three-parameter Model	1-8	-0.25	0.045	0.44	74.45
	9-16	-0.23	0.051	0.83	64.13
	17-24	-0.23	0.041	0.58	45.45
Two-parameter Model	1-8	-0.09	0.007	0.43	79.34
	9-16	-0.84	0.749	0.49	17.02
	17-24	0.69	0.439	0.75	48.72

Table 6.4: AQI Forecasting for Pre-summer and Post-summer

Pre-summer (Apr.-Jul)								
Type of Model	AQI	Corresponding Ozone (ppb)	Hr: 1-8		Hr: 9-16		Hr: 17-24	
			Obs.	Pre.	Obs.	Pre.	Obs.	Pre.
Three-parameter Model	0-50	0-40	93%	74%	31%	24%	59%	42%
	51-100	41-80	7%	24%	62%	58%	38%	57%
	101-150	81-120	0%	2%	7%	14%	3%	1%
	151-200	121-160	0 %	0 %	0 %	4 %	0 %	0 %
Two-parameter Model	0-50	0-40	93%	99%	31%	39%	59%	93%
	51-100	41-80	7%	1%	62%	47%	38%	7%
	101-150	81-120	0%	0%	7%	10%	3%	0%
	151-200	121-160	0 %	0 %	0 %	4 %	0 %	0 %
Post-summer (Aug.-Oct.)								
Type of Model	AQI	Corresponding Ozone (ppb)	Hr: 1-8		Hr: 9-16		Hr: 17-24	
			Obs.	Pre.	Obs.	Pre.	Obs.	Pre.
Three-parameter Model	0-50	0-40	99%	100%	48%	49%	79%	79%
	51-100	41-80	1%	0 %	42%	37%	19%	18%
	101-150	81-120	0 %	0 %	10%	13%	2%	3%
	151-200	121-160	0 %	0 %	0 %	1 %	0 %	0 %
Two-parameter Model	0-50	0-40	99%	100%	48%	41%	79%	92%
	51-100	41-80	1%	0 %	42%	36%	19%	8%
	101-150	81-120	0 %	0 %	10%	21%	2%	0%
	151-200	121-160	0 %	0 %	0 %	2 %	0 %	0 %
Post-summer (Aug.-Oct.) Using MM5 Data								
Type of Model	AQI	Corresponding Ozone (ppb)	Hr: 1-8		Hr: 9-16		Hr: 17-24	
			Obs.	Pre.	Obs.	Pre.	Obs.	Pre.
Three-parameter Model (Using MM5 Data)	0-50	0-40	99%	99%	52%	36%	87%	84%
	51-100	41-80	1%	1 %	46%	48%	12%	14%
	101-150	81-120	0 %	0 %	2%	16%	1%	2%
	151-200	121-160	0 %	0 %	0 %	0%	0 %	0 %
	201-300	161-240	0 %	0 %	0 %	0%	0 %	0 %
	301-500	241-400	0 %	0 %	0 %	0%	0 %	0 %
Two-parameter Model (Using MM5 Data)	0-50	0-40	99%	100%	52%	15%	87%	100%
	51-100	41-80	1%	0%	46%	26%	12%	0%
	101-150	81-120	0 %	0 %	2%	28%	1%	0%
	151-200	121-160	0 %	0 %	0 %	16%	0 %	0 %
	201-300	161-240	0 %	0 %	0 %	10%	0 %	0 %
	301-500	241-400	0 %	0 %	0 %	5%	0 %	0 %

Chapter 7

Exceedance Model

Accurate prediction of the ozone episodic days is required for implementing precautionary measures so as to avoid ozone threats. From the previous chapter, it was seen that the three-parameter model performed well in predicting most of the peak concentrations, but the forecasting ability to predict peaks within ± 10 ppb of the observed values was found to be low (40-50%). Therefore, models to accurately predict peak concentrations were developed for pre-summer and post-summer seasons by examining all the observed values of ozone concentrations above 85 ppb.

7.1 Model Development

The ozone exceedances (> 85ppb) during the years 1996-1999 and the corresponding values of temperature, wind speed, and dew point temperature were extracted and stored in the separate table. The data was divided into pre-summer and post-summer seasons, and each season was further separated based on hour of the day (Hr: 1-8, 9-16, and 17-24). The number of ozone exceedances during the first eight hours of the day (Hr: 1-8) is usually low because of low pre-cursor emissions and low temperatures. Only 0.02% of the total values were found in this period for pre-summer and post-summer seasons in the years 1996-1999. Therefore, models were developed only for Hr: 9-16 and Hr: 17-24 periods. Linear regression of the natural logarithm of the ozone concentrations and three variables was performed, and four models- two for both pre-summer and post-summer- were developed. An overview of the developed models is shown in the Table 7.1.

Table 7.1: Summary of the Models Developed

Season	Hour of the day	Years of Data Considered	Variables Involved	Number of Models
Pre-Summer	9-16, 17-24	1996-1999	Temperature, Wind Speed, Dew point Temperature	2
Post-Summer	9-16, 17-24	1996-1999	Temperature, Wind Speed, Dew point Temperature	2

The models were evaluated for the year 2002. The ozone exceedances in the year 2002 were extracted, and the corresponding meteorological variables were obtained. This data was divided into pre-summer and post-summer seasons. The observed meteorological data and the appropriate models were used to predict the ozone concentrations. These predictions were compared with the observed ozone data for the year 2002.

The performance of the model was studied using the evaluation parameters NMSE, FB, and Fa_2. The forecasting ability of the models to predict the peaks within ± 10 ppb of observed values was also found.

7.2 Results and Discussion

The final model is of the form discussed in Equation 6.1:

$$\ln (Oz) = (A*T) + (B*W) + (C*D) + E \tag{6.1}$$

where,

T = hourly temperature in ^{o}F,

W = hourly wind speed in mph,

D = hourly dew point temperature in ^{o}F,

Oz = hourly ozone concentration in ppb,

A = coefficient of temperature T,

B = coefficient of wind speed W,

C = coefficient of dew point temperature D, and

E = regression constant.

The coefficients of the models are given in Table 7.2 for pre-summer and post-summer seasons.

The evaluation parameters of the model predictions for the year 2002 are summarized in the Table 7.3 for both pre-summer and post-summer seasons.

Table 7.2: Summary of Coefficients of the Exceedance Models for Pre-summer and Post-summer

Pre-summer (Apr.-Jul.)				
Hour of the Day	Coefficient of Temperature (A)	Coefficient of Wind Speed (B)	Coefficient of Dew point Temperature (C)	Regression Constant (E)
1-8	-	-	-	-
9-16	4.079	0.006	-0.002	-0.002
17-24	4.244	0.004	-0.011	-0.001
Post-summer (Aug.-Oct)				
Hour of the Day	**Coefficient of Temperature (A)**	**Coefficient of Wind Speed (B)**	**Coefficient of Dew point Temperature (C)**	**Regression Constant (E)**
1-8	-	-	-	-
9-16	4.369	0.002	-0.0006	0.0002
17-24	4.116	0.004	-0.008	0.0017

Table 7.3: Evaluation Parameters for the Exceedance Models for Pre-summer and Post-summer

Pre-summer (Apr.-Jul.)				
Hour of the Day	Evaluation Parameters			
	FB	NMSE	Fa_2	FC
1-8	-	-	-	-
9-16	-0.48	0.002	1.0	89
17-24	0.25	0.001	1.0	100
Post-summer (Aug.-Oct)				
Hour of the Day	**Evaluation Parameters**			
	FB	**NMSE**	**Fa_2**	**FC**
1-8	-	-	-	-
9-16	0.39	0.001	1.0	82
17-24	0.38	0.001	1.0	82

The temperature was seen to have a strong positive relation with the peak ozone concentration, which is evident from the values of coefficients of temperature in Table 7.2. The wind speed and dew point temperatures have shown a negligible effect on ozone concentrations. The values of NMSE, FB and Fa_2, as seen in the Table 7.3, are close to ideal values and hence meet the requirements of an acceptable air quality model. The forecasting ability of the models for pre-summer was found to be more than 85% and for post-summer it was more than 80%. An increase of approximately 40-60% of the forecasting ability was observed when compared to that of the general three-parameter model described in the previous Chapter.

The model can be used to predict ozone episodes when a possibility of occurrence of high pre-cursor emissions coupled with high temperatures ($> 70^0$F) is forecasted.

Chapter 8

Conclusions

The first part of this study presents the development and evaluation of simple forecasting models using the KZ regression approach for predicting hourly ozone concentrations for Dayton, Ohio, considering temperature, wind speed, and dew point temperature as independent variables. The performances of the developed models meet the general criteria specified by Patel and Kumar (1998) for air quality models. The forecasting skills (FC= ± 10 ppb of observed concentration) of the models were found to be low. The models accounted for most of the peak concentrations. Further analysis of forecasted data indicates that predicted AQI indices are either close to observed values or higher than the observed values. This prediction serves well for public use.

The following conclusions can be drawn from this part of the study:

1. The predictions made by the models are reliable only to a limited extent.
2. The analysis of the raw ozone and meteorological data was helpful in assessing the variations and relations between the parameters.

3. High temperature (70-90 ^{0}F) and dew point temperatures (50-70 ^{0}F), and low wind speeds (<8 mps) were found to be responsible for an ozone episode. However, temperature was a critical parameter influencing its occurrence.

4. Developing different models for the three regimes (Hr: 1-8, 9-16, 17-24) provided more accurate predictions and also helped in accounting for most of the peak concentrations.

5. The three-parameter models showed an over-predicting tendency, and thus performed well in predicting peak concentrations. The two-parameter models were under-predicting in most cases.

6. The KZ model has shown a positive relationship between the ozone concentration and the temperature for all the models. This is in accordance with most previous studies on forecasting of ozone with temperature.

7. The wind speed was seen to have a negligible effect in 9-16th hour during pre-summer in which high concentrations of ozone occur. However, wind speed had a more significant impact than temperature for all other periods of pre-summer (Hr: 1-8, 17-24) and during post-summer.

8. The dew point temperature was noticed to have more impact than temperature during 1-8th hour for both pre-summer and post-summer. Inclusion of dew point temperature improved the ability to predict high ozone concentrations.

The second part of the study focused on developing exceedance models using linear regression analysis. The exceedance models developed for predicting peak concentrations performed well with a forecasting ability (within ±10ppb) in the range of 80-100%, and can be used to forecast an ozone episode when the predicted temperature is more than 70^0F.

In summary, it is suggested to use three parameter models along with the ozone exceedance models to predict hourly ozone concentrations for Dayton area.

8.1 Scope for Future Work

In this research, the performance of the model considering dew point temperature as an independent variable along with temperature and wind speed was studied. The models showed a tendency to over-predict the observed ozone concentrations most of the time. There are many other meteorological variables like wind direction, relative humidity, cloud cover that can be explored for improving forecasting models for ozone. Similarly, other methods of forecasting - such as artificial neural networks, non-linear multiple regression, time-series forecasting, and fuzzy-logic based- can also be employed to develop models which can effectively forecast the ozone concentrations.

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APPENDIX A- Observed and KZ Filtered Figures

Figure A.1

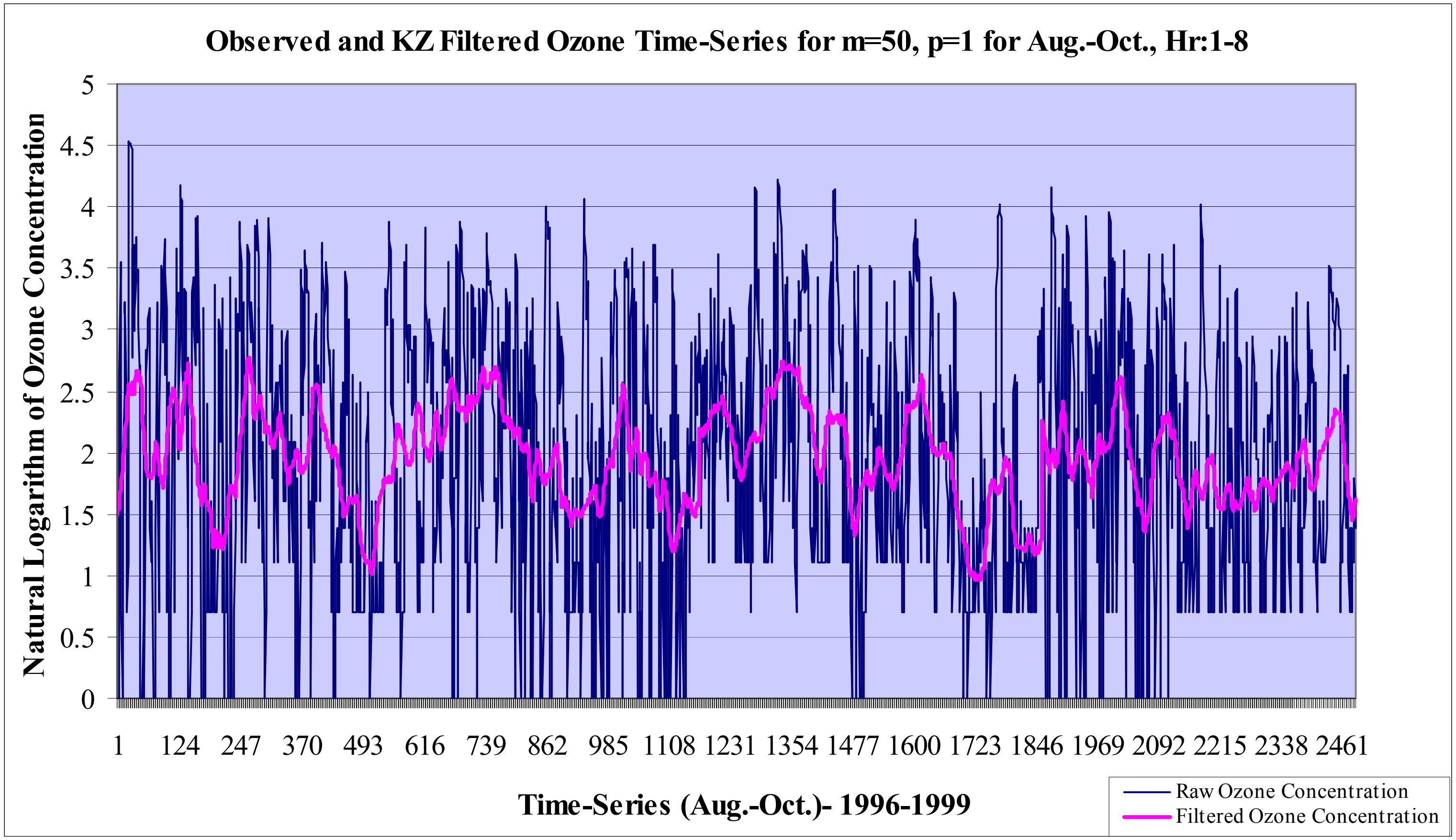
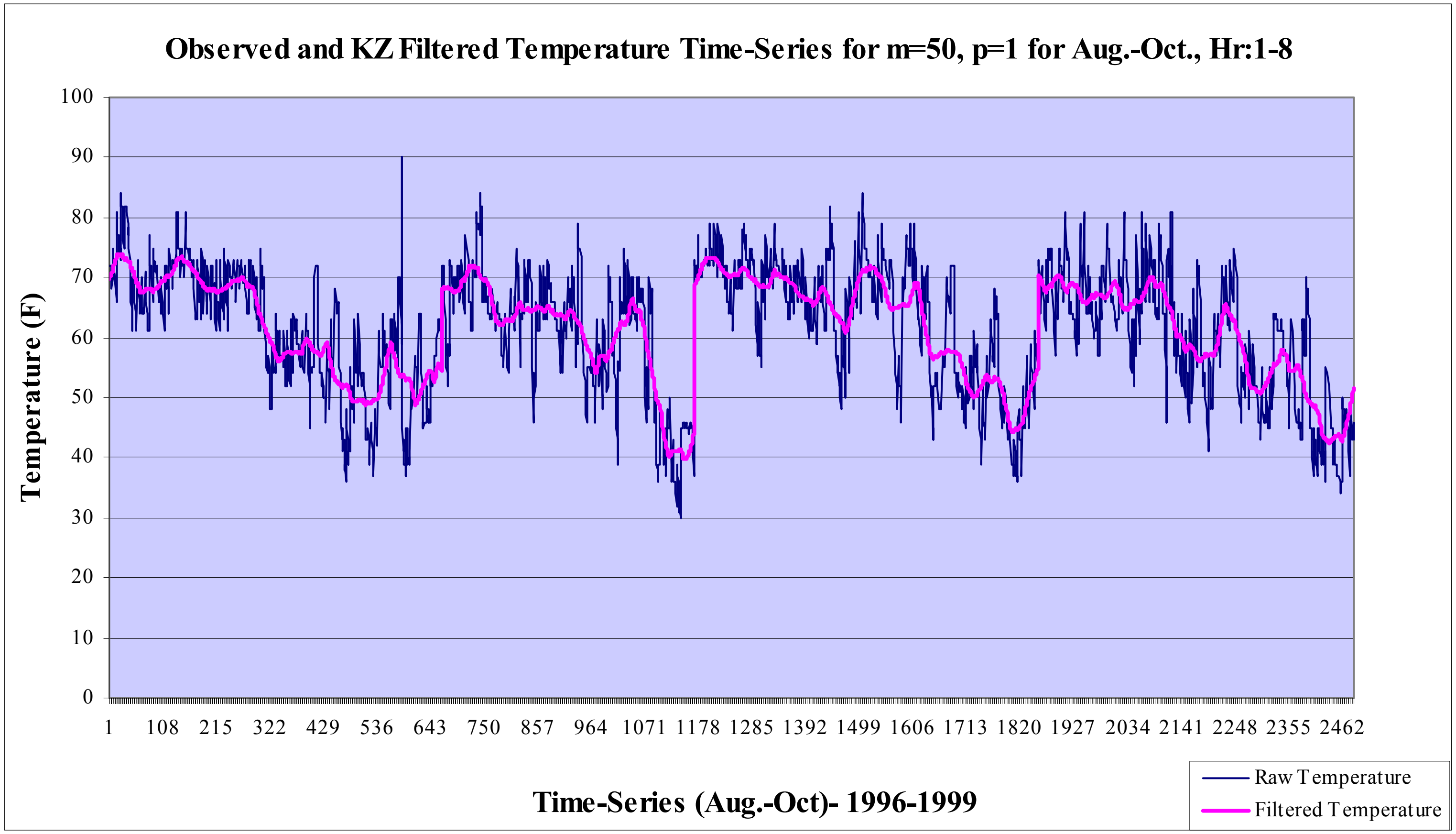
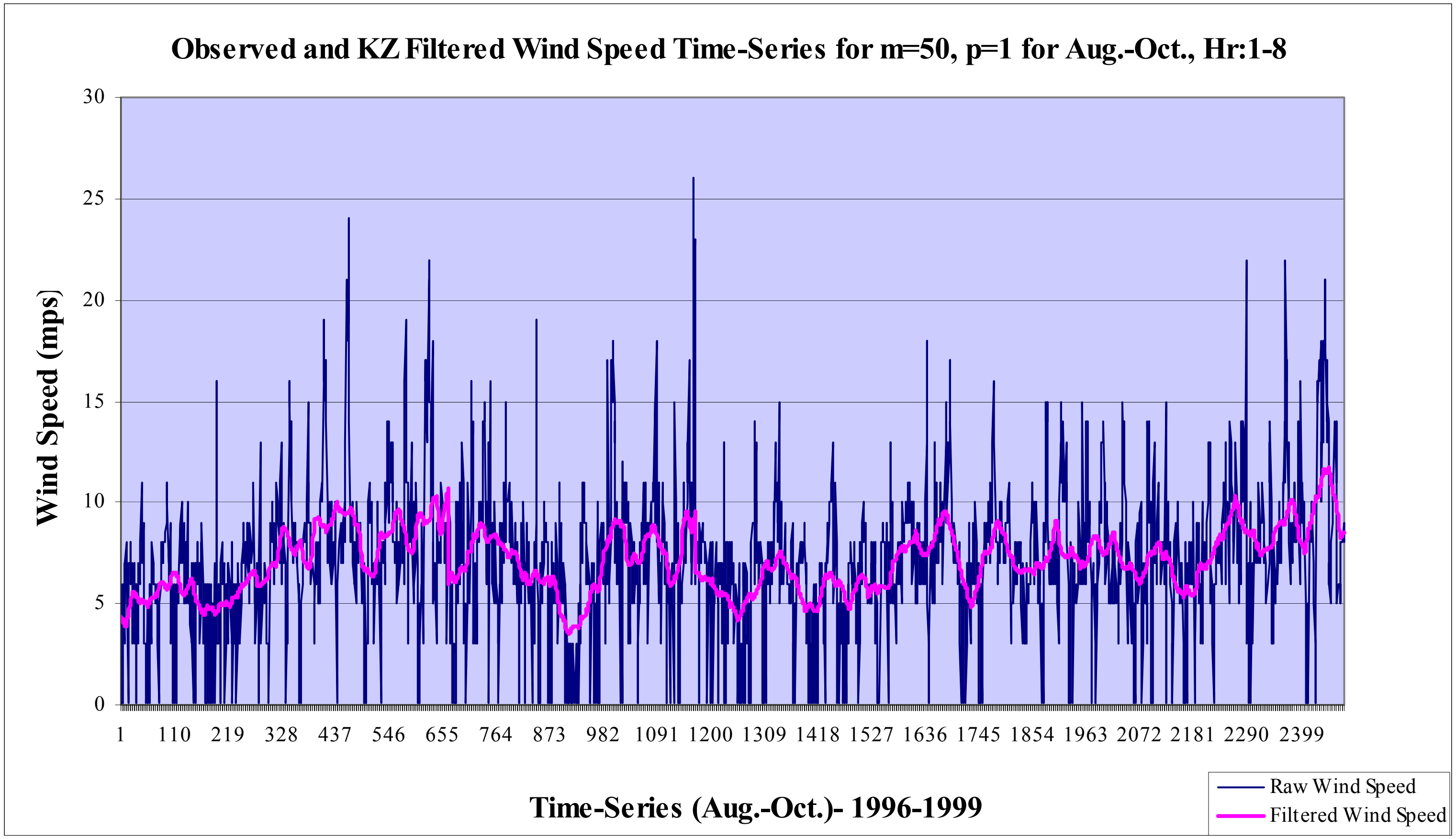

Observed and KZ Filtered Ozone Time-Series for m=50, p=1 for Aug.-Oct., Hr:1-8
Natural Logarithm of Ozone Concentration
5
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
1 124 247 370 493 616 739 862 985 1108 1231 1354 1477 1600 1723 1846 1969 2092 2215 2338 2461
Time-Series (Aug.-Oct.)- 1996-1999
Raw Ozone Concentration
Filtered Ozone Concentration

Figure A.2



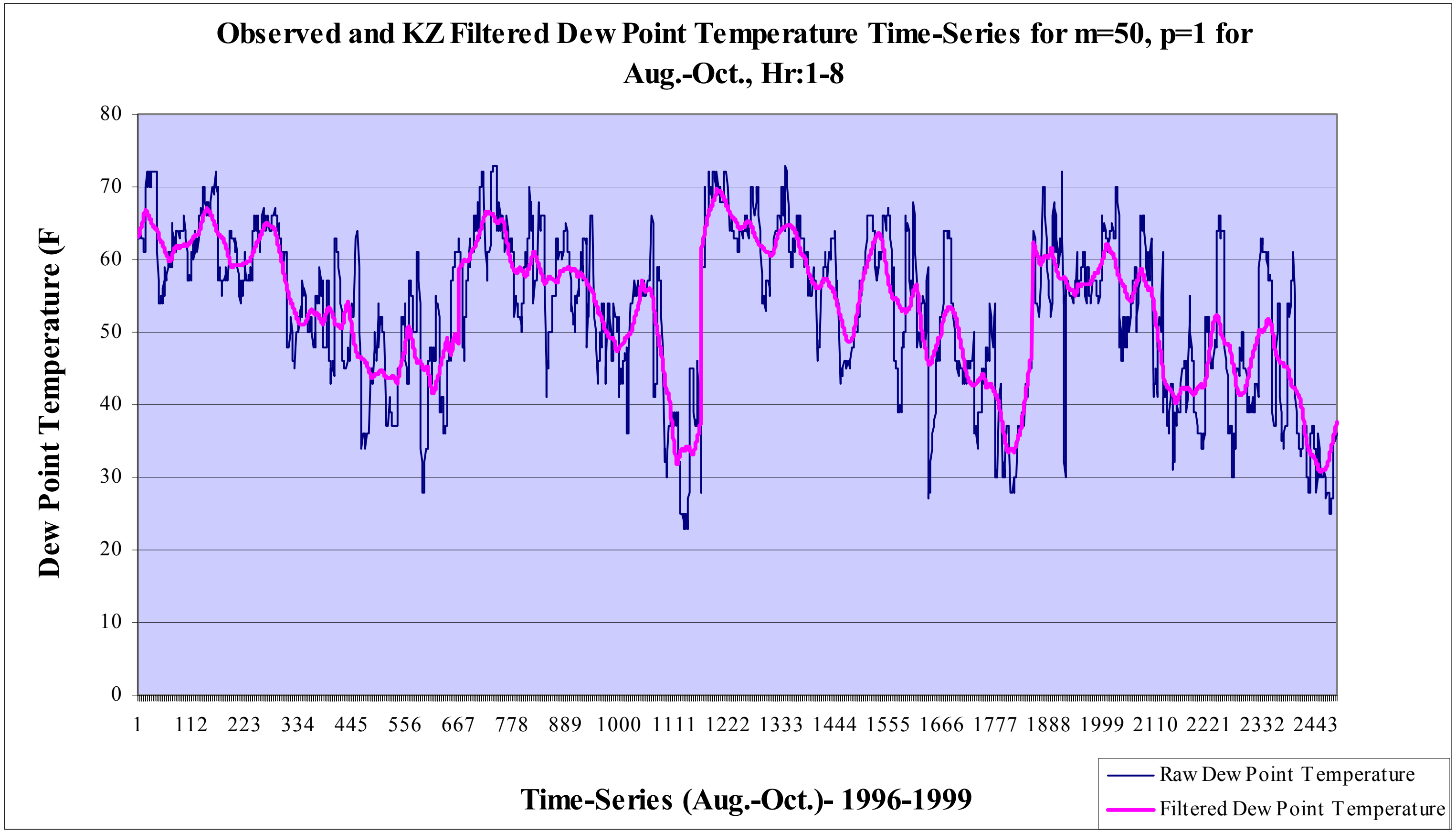
Observed and KZ Filtered Temperature Time-Series for m=50, p=1 for Aug.-Oct., Hr:1-8
100
90
80
70
60
50
40
30
20
10
0
Temperature (F)
1 108 215 322 429 536 643 750 857 964 1071 1178 1285 1392 1499 1606 1713 1820 1927 2034 2141 2248 2355 2462
Time-Series (Aug.-Oct)- 1996-1999
Raw Temperature
Filtered Temperature

Figure A.3



Observed and KZ Filtered Wind Speed Time-Series for m=50, p=1 for Aug.-Oct., Hr:1-8
Wind Speed (mps)
30
25
20
15
10
5
0
1 110 219 328 437 546 655 764 873 982 1091 1200 1309 1418 1527 1636 1745 1854 1963 2072 2181 2290 2399
Time-Series (Aug.-Oct.)- 1996-1999
Raw Wind Speed
Filtered Wind Speed

Figure A.4



Observed and KZ Filtered Dew Point Temperature Time-Series for m=50, p=1 for Aug.-Oct., Hr:1-8
Dew Point Temperature (F
80
70
60
50
40
30
20
10
0
1
112
223
334
445
556
667
778
889
1000
1111
1222
1333
1444
1555
1666
1777
1888
1999
2110
2221
2332
2443
Time-Series (Aug.-Oct.)- 1996-1999
Raw Dew Point Temperature
Filtered Dew Point Temperature

APPENDIX B- Figures for Pre-summer (Apr.-Jul.)

Three-Parameter Models

Figure B .1

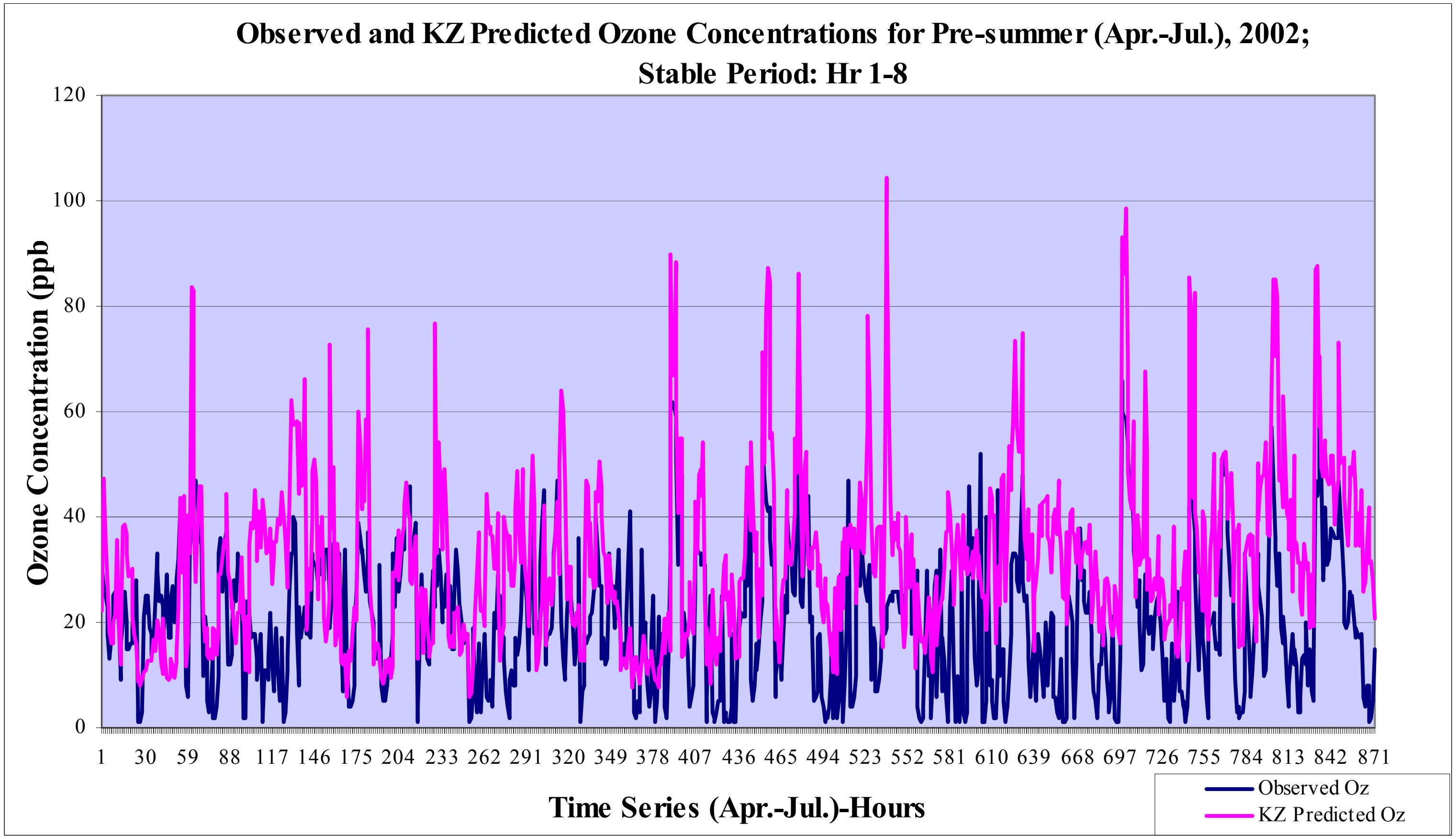
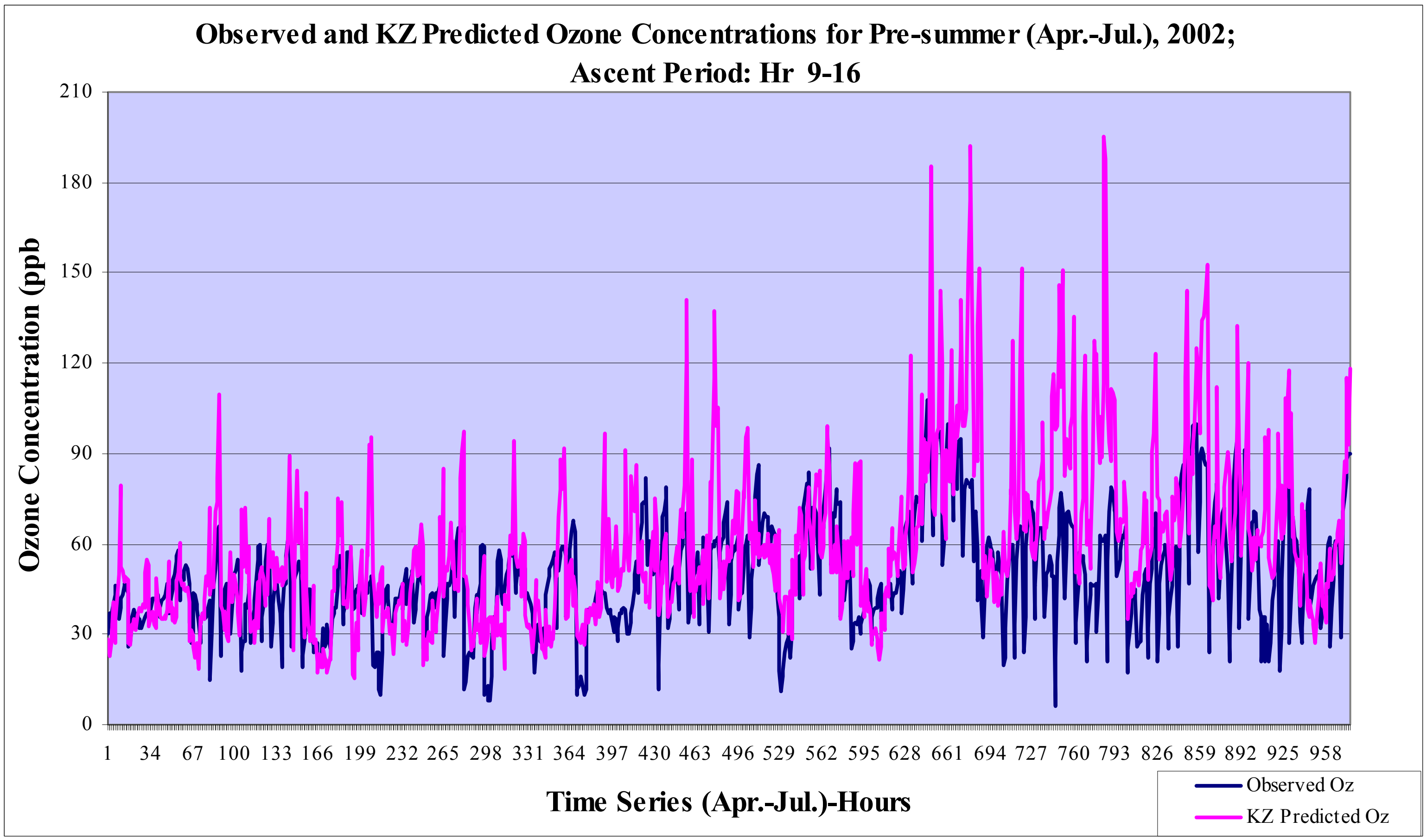
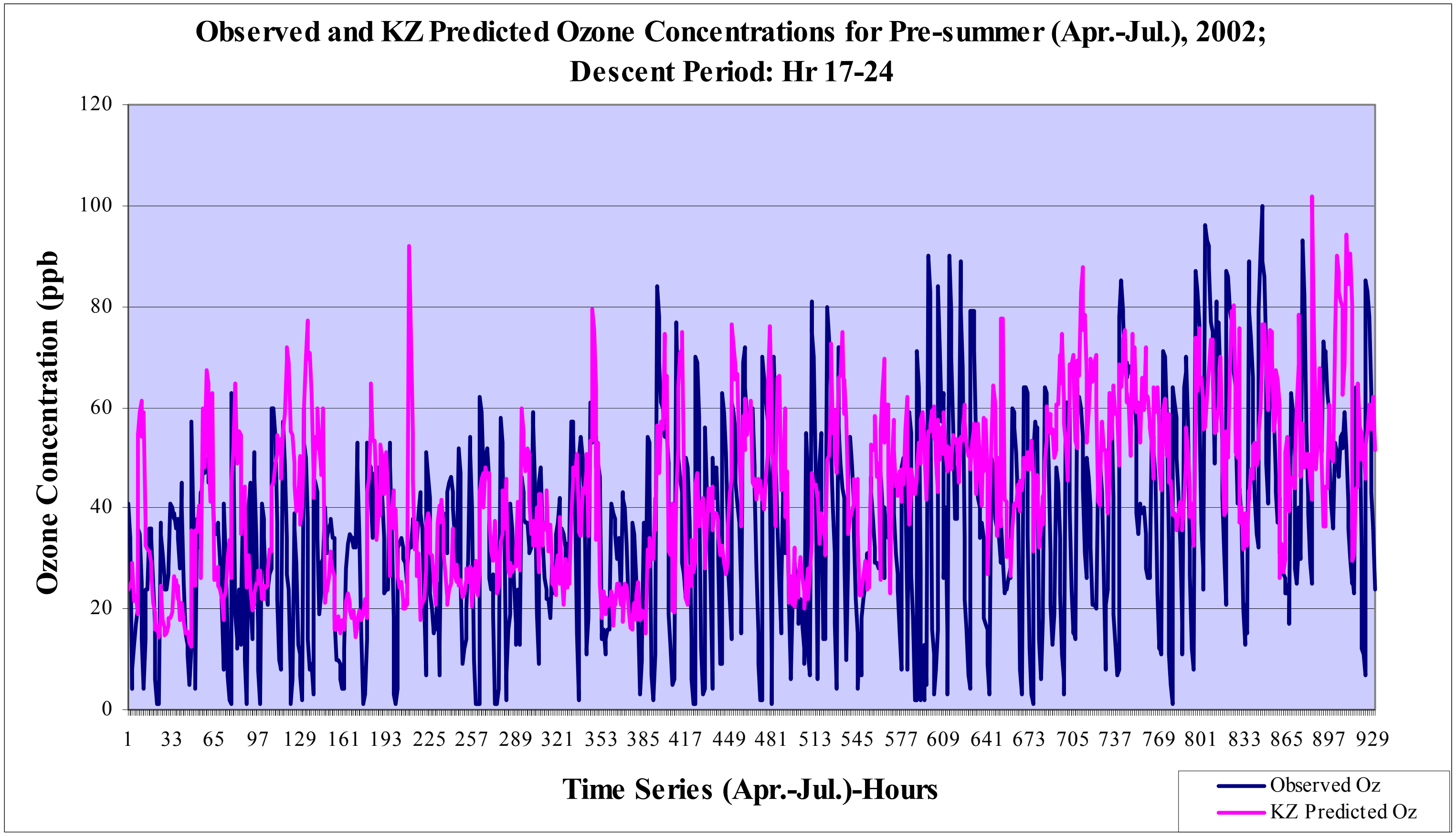


Figure B.2



Observed and KZ Predicted Ozone Concentrations for Pre-summer (Apr.-Jul.), 2002;
Ascent Period: Hr 9-16
Ozone Concentration (ppb
210
180
150
120
90
60
30
0
1 34 67 100 133 166 199 232 265 298 331 364 397 430 463 496 529 562 595 628 661 694 727 760 793 826 859 892 925 958
Time Series (Apr.-Jul.)-Hours
Observed Oz
KZ Predicted Oz

Figure B.3



Observed and KZ Predicted Ozone Concentrations for Pre-summer (Apr.-Jul.), 2002;
Descent Period: Hr 17-24
Ozone Concentration (ppb
0
20
40
60
80
100
120
1 33 65 97 129 161 193 225 257 289 321 353 385 417 449 481 513 545 577 609 641 673 705 737 769 801 833 865 897 929
Time Series (Apr.-Jul.)-Hours
Observed Oz
KZ Predicted Oz

Two-Parameter Models

Figure B.4

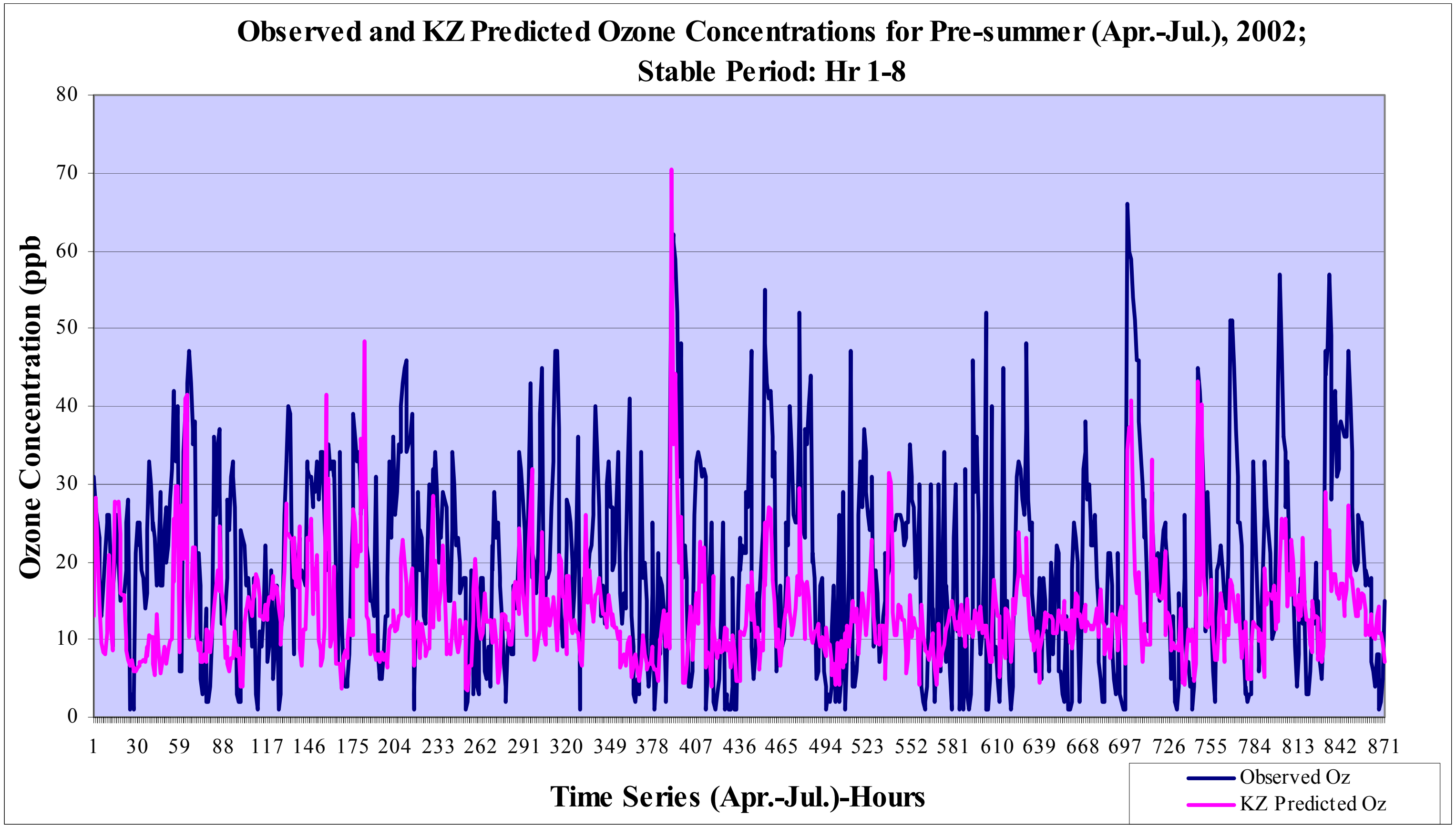


Figure B.5

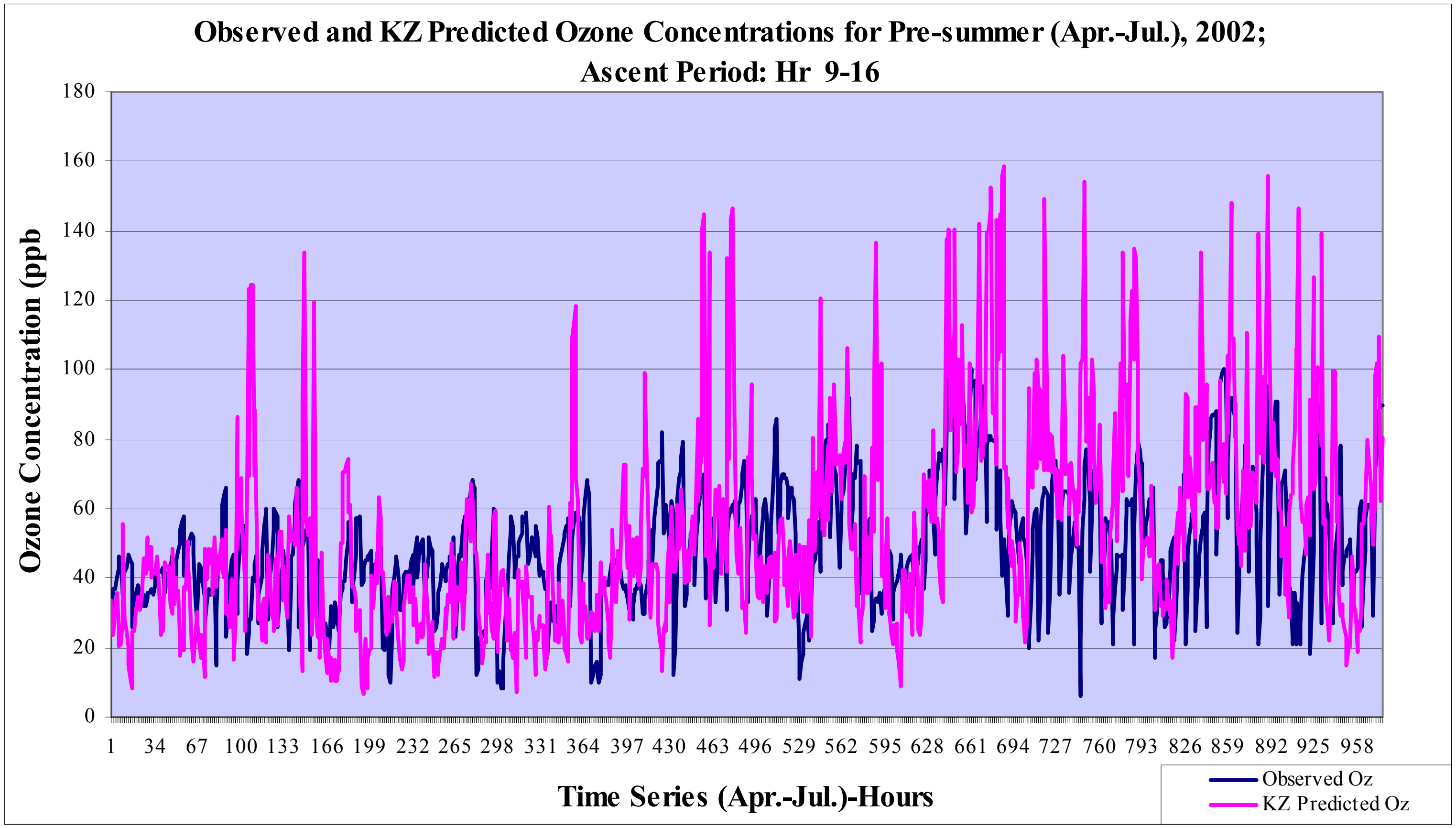
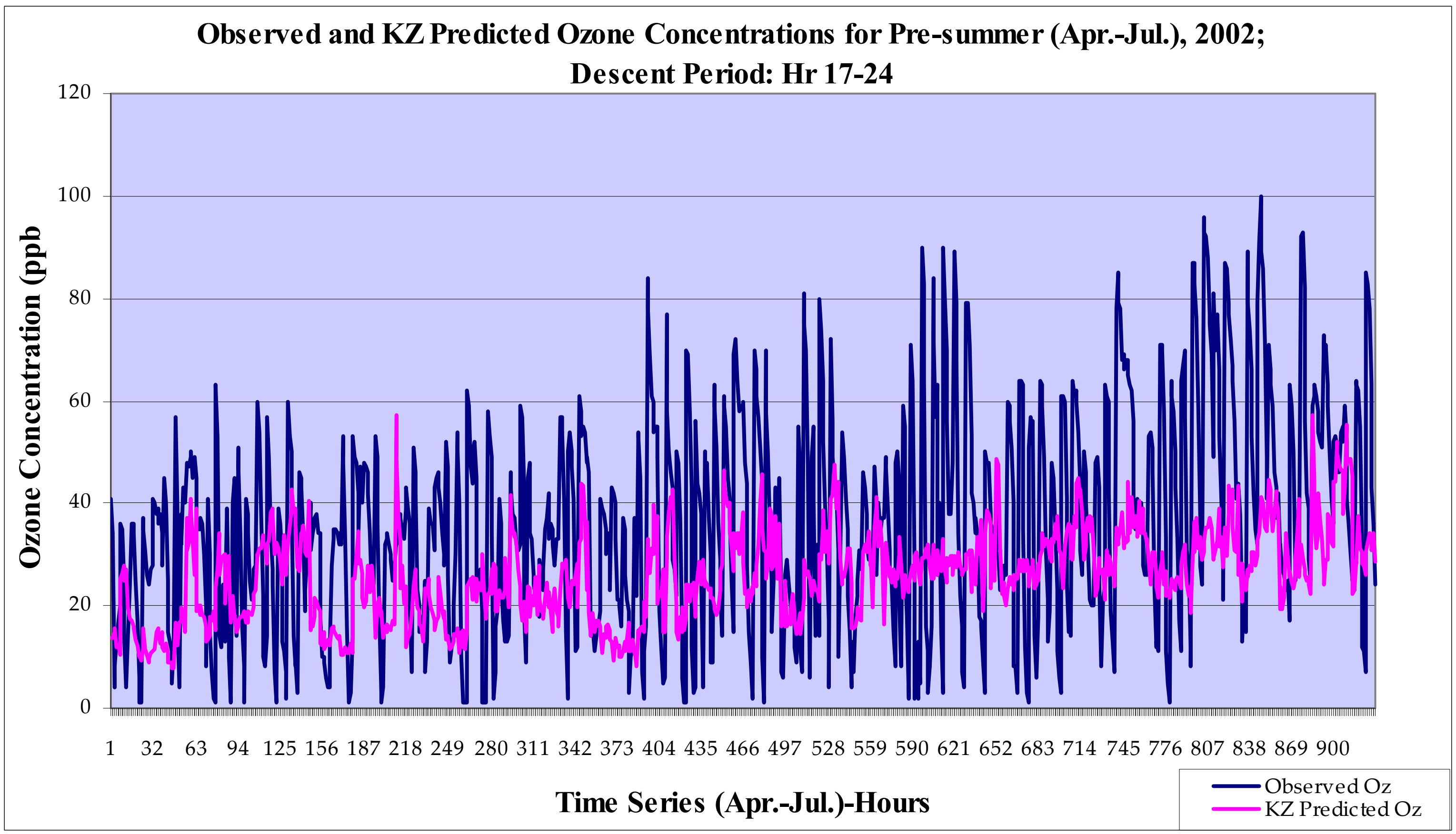

Observed and KZ Predicted Ozone Concentrations for Pre-summer (Apr.-Jul.), 2002;
Ascent Period: Hr 9-16
Ozone Concentration (ppb
0
20
40
60
80
100
120
140
160
180
1 34 67 100 133 166 199 232 265 298 331 364 397 430 463 496 529 562 595 628 661 694 727 760 793 826 859 892 925 958
Time Series (Apr.-Jul.)-Hours
Observed Oz
KZ Predicted Oz

Figure B.6



Observed and KZ Predicted Ozone Concentrations for Pre-summer (Apr.-Jul.), 2002;
Descent Period: Hr 17-24
Ozone Concentration (ppb
120
100
80
60
40
20
0
1 32 63 94 125 156 187 218 249 280 311 342 373 404 435 466 497 528 559 590 621 652 683 714 745 776 807 838 869 900
Time Series (Apr.-Jul.)-Hours
Observed Oz
KZ Predicted Oz

APPENDIX C- Figures for Post-summer (Aug.-Oct.)

Three-Parameter Models

Figure C.1

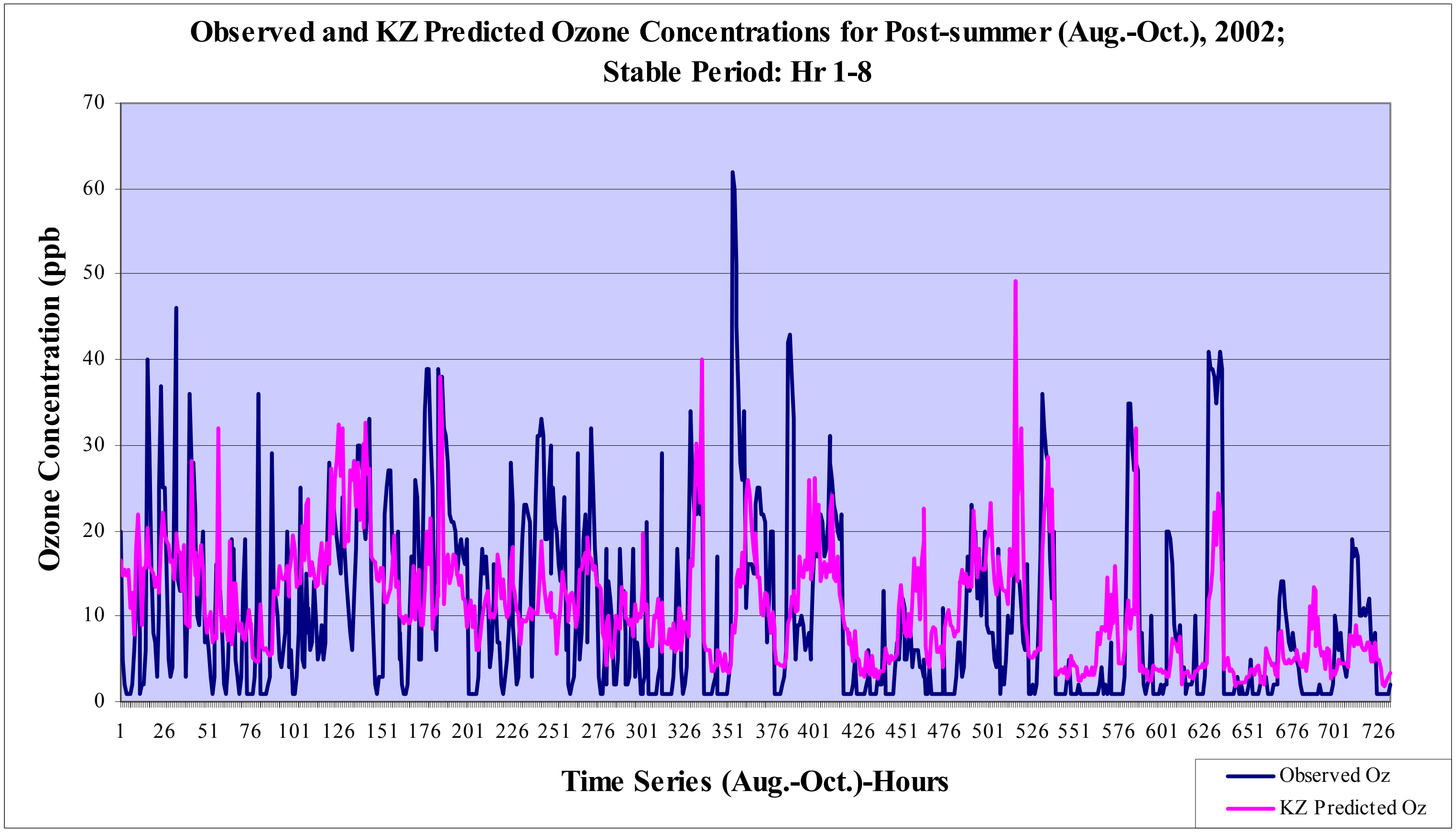
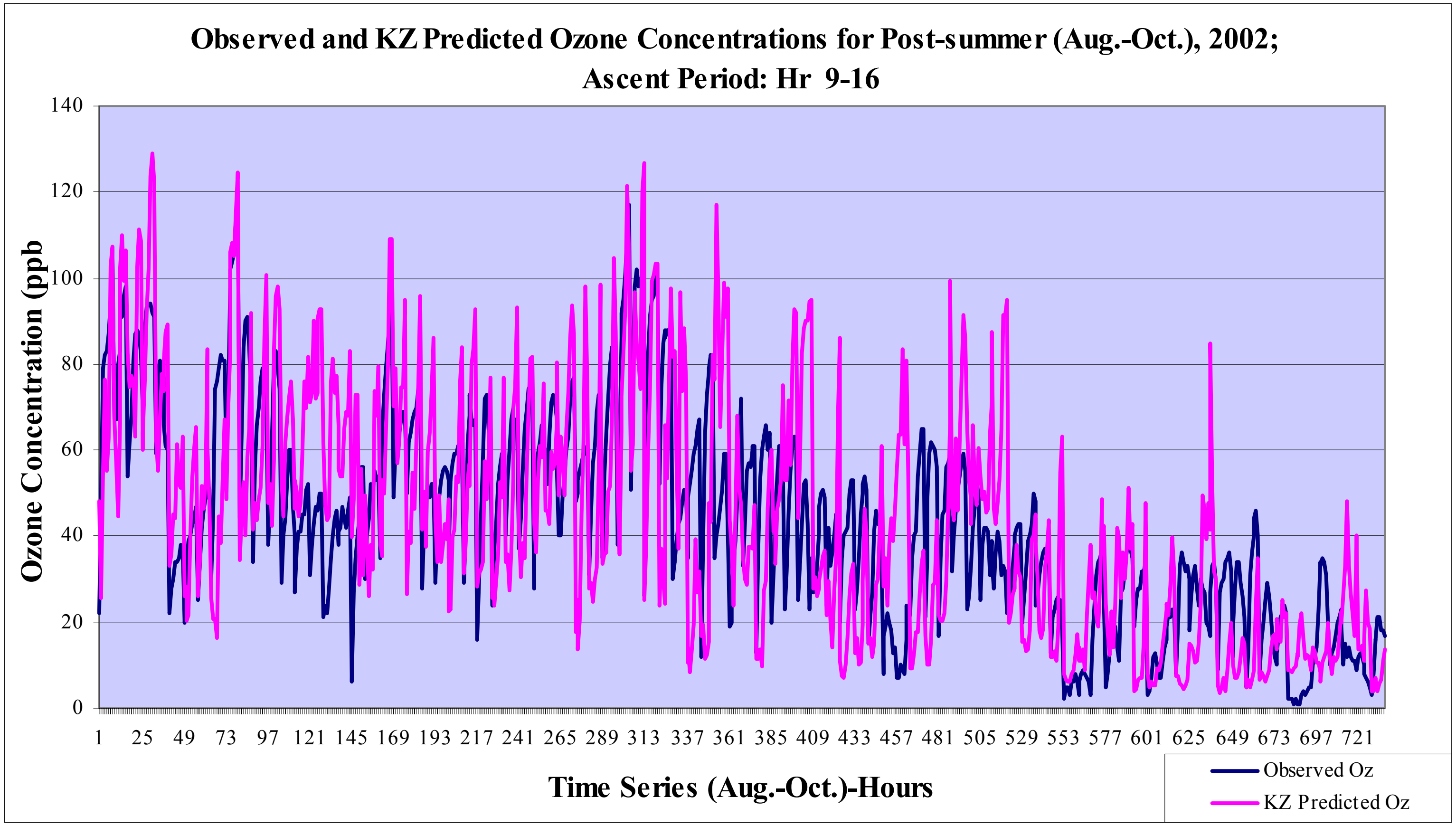
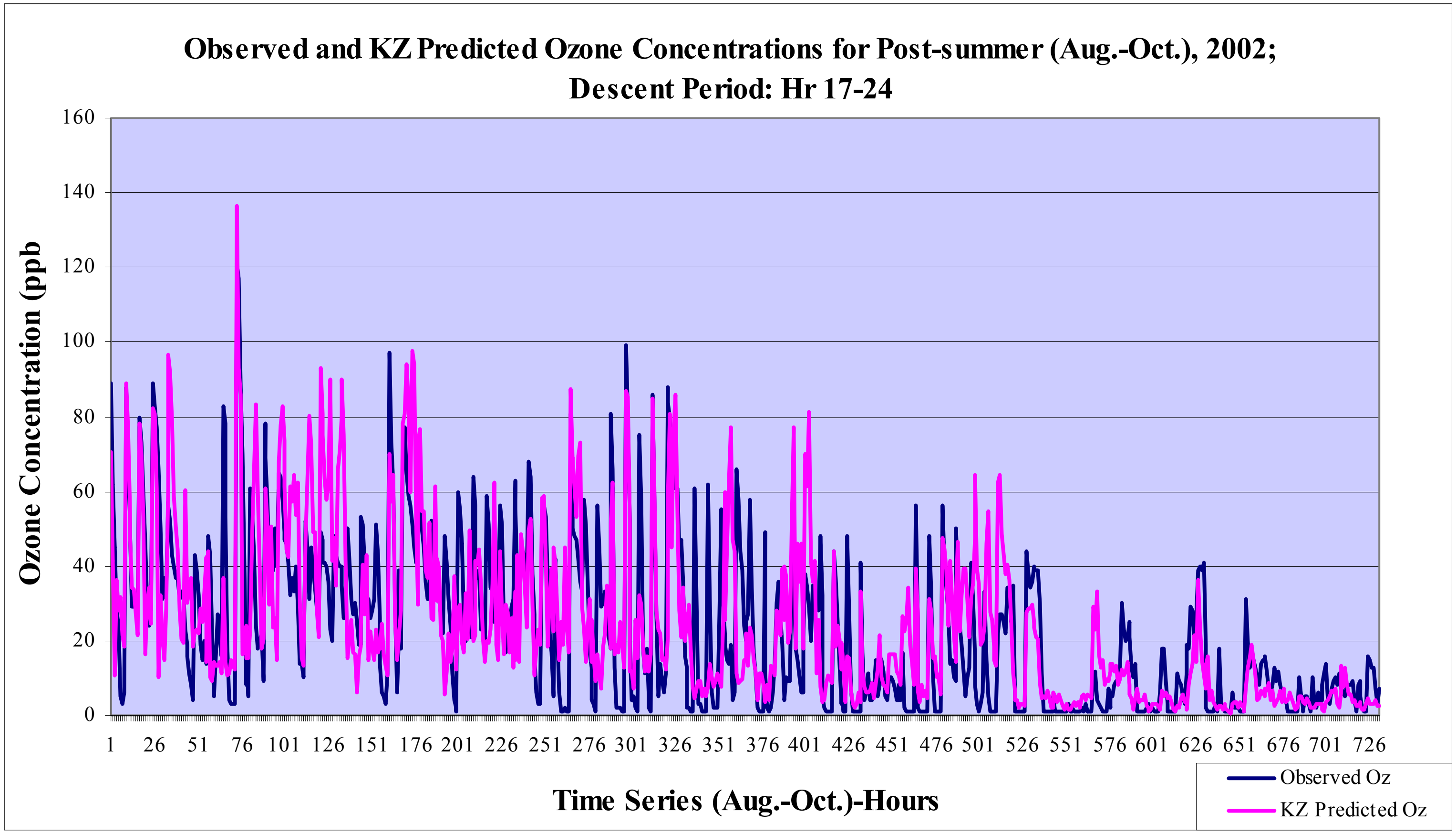


Figure C.2



Observed and KZ Predicted Ozone Concentrations for Post-summer (Aug.-Oct.), 2002;
Ascent Period: Hr 9-16
Ozone Concentration (ppb
0
20
40
60
80
100
120
140
1
25
49
73
97
121
145
169
193
217
241
265
289
313
337
361
385
409
433
457
481
505
529
553
577
601
625
649
673
697
721
Time Series (Aug.-Oct.)-Hours
Observed Oz
KZ Predicted Oz

Figure C.3



Observed and KZ Predicted Ozone Concentrations for Post-summer (Aug.-Oct.), 2002;
Descent Period: Hr 17-24
Ozone Concentration (ppb
160
140
120
100
80
60
40
20
0
1
26
51
76
101
126
151
176
201
226
251
276
301
326
351
376
401
426
451
476
501
526
551
576
601
626
651
676
701
726
Time Series (Aug.-Oct.)-Hours
Observed Oz
KZ Predicted Oz

Two-Parameter Models

Figure C.4

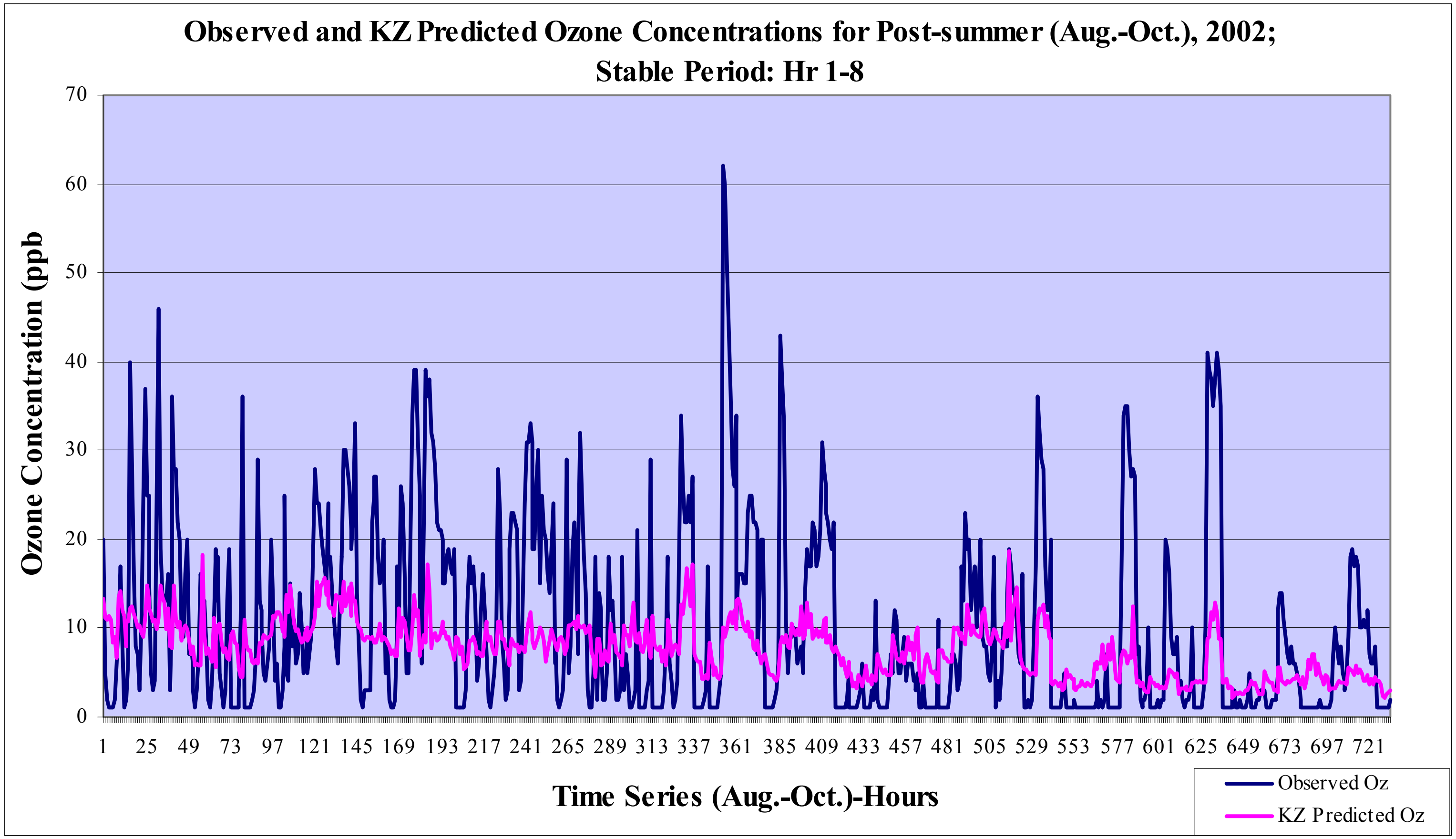
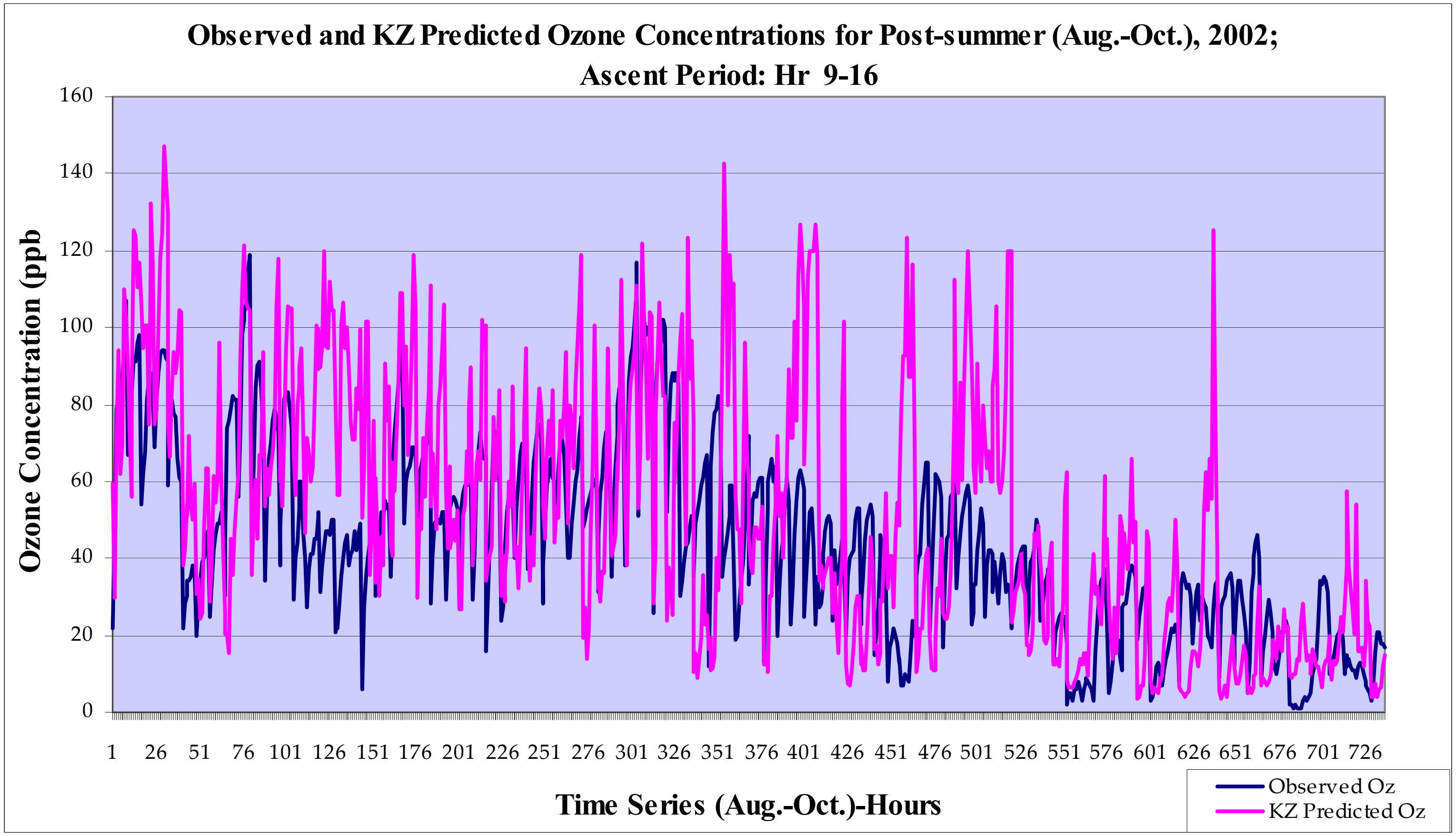
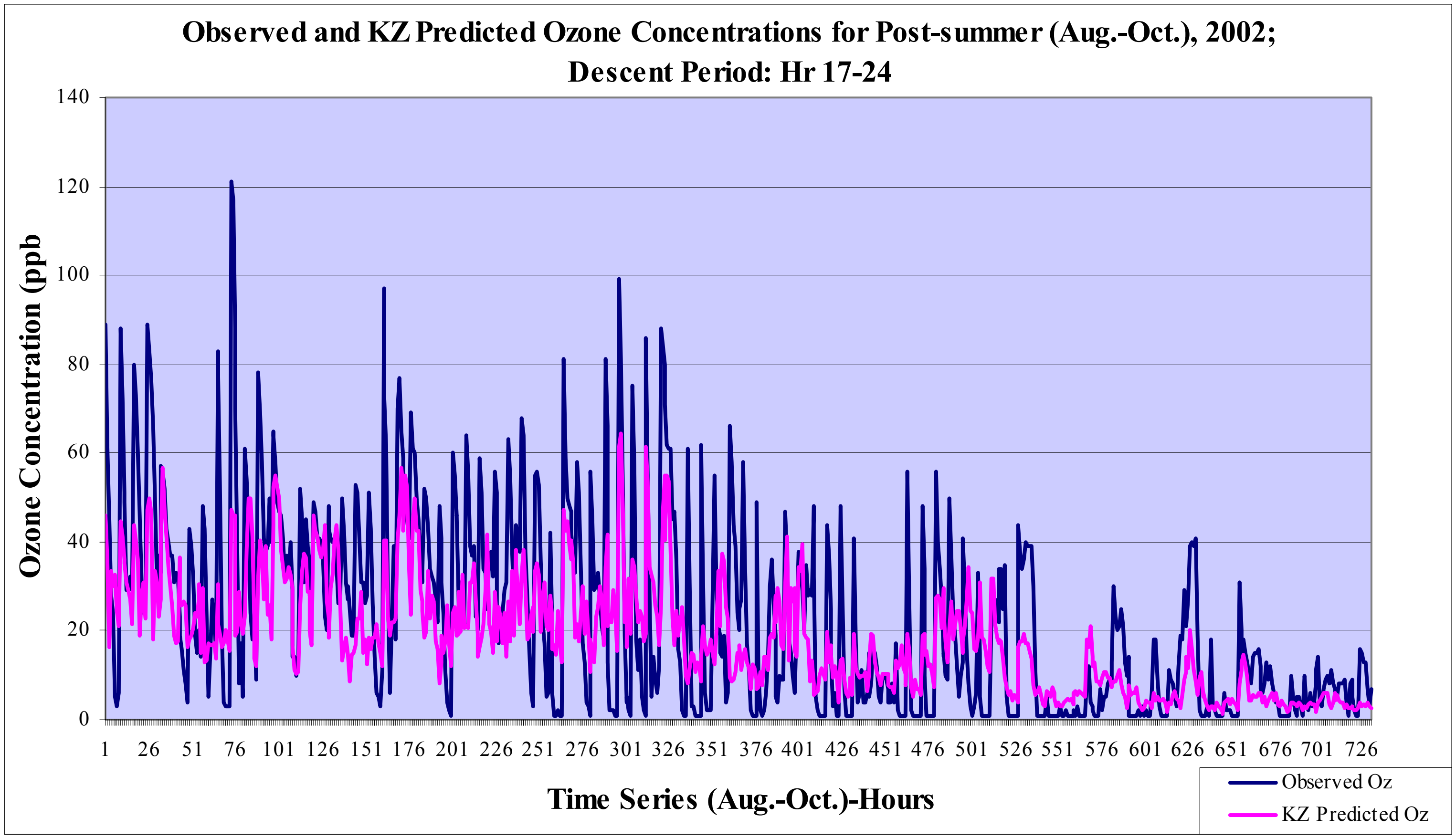


Figure C.5



Observed and KZ Predicted Ozone Concentrations for Post-summer (Aug.-Oct.), 2002;
Ascent Period: Hr 9-16
Ozone Concentration (ppb
160
140
120
100
80
60
40
20
0
1 26 51 76 101 126 151 176 201 226 251 276 301 326 351 376 401 426 451 476 501 526 551 576 601 626 651 676 701 726
Time Series (Aug.-Oct.)-Hours
Observed Oz
KZ Predicted Oz

Figure C.6


Observed and KZ Predicted Ozone Concentrations for Post-summer (Aug.-Oct.), 2002;
Descent Period: Hr 17-24
Ozone Concentration (ppb
140
120
100
80
60
40
20
0
1 26 51 76 101 126 151 176 201 226 251 276 301 326 351 376 401 426 451 476 501 526 551 576 601 626 651 676 701 726
Time Series (Aug.-Oct.)-Hours
Observed Oz
KZ Predicted Oz

Three-Parameter Models

Figure C.7

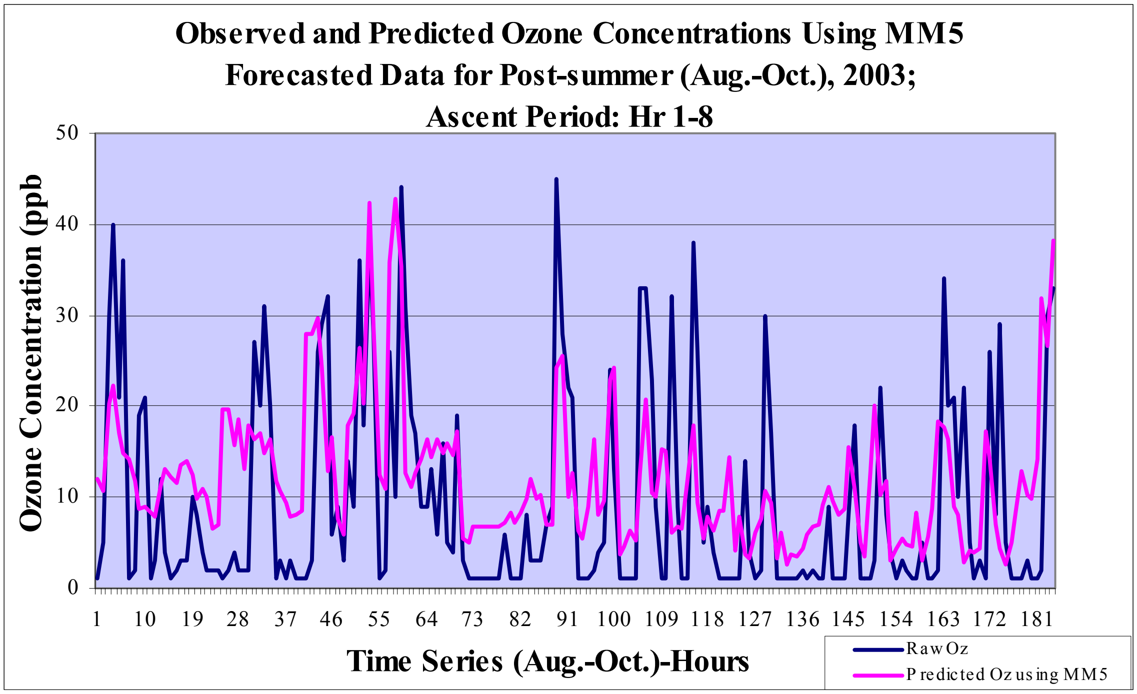


Figure C.8

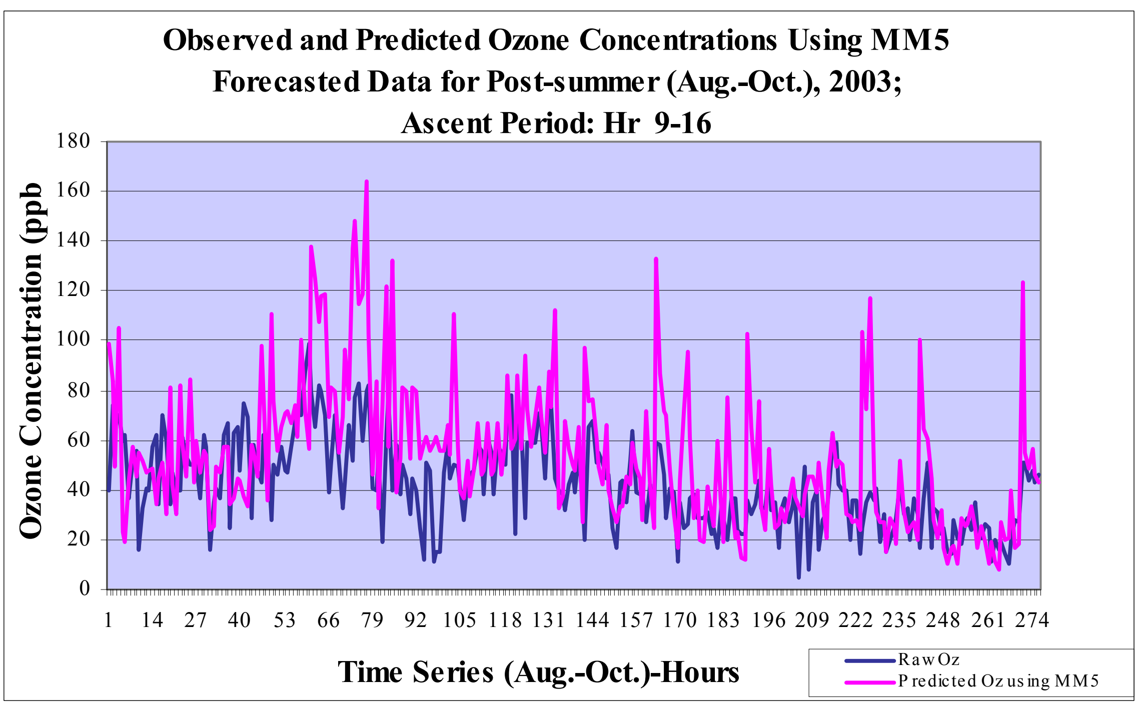
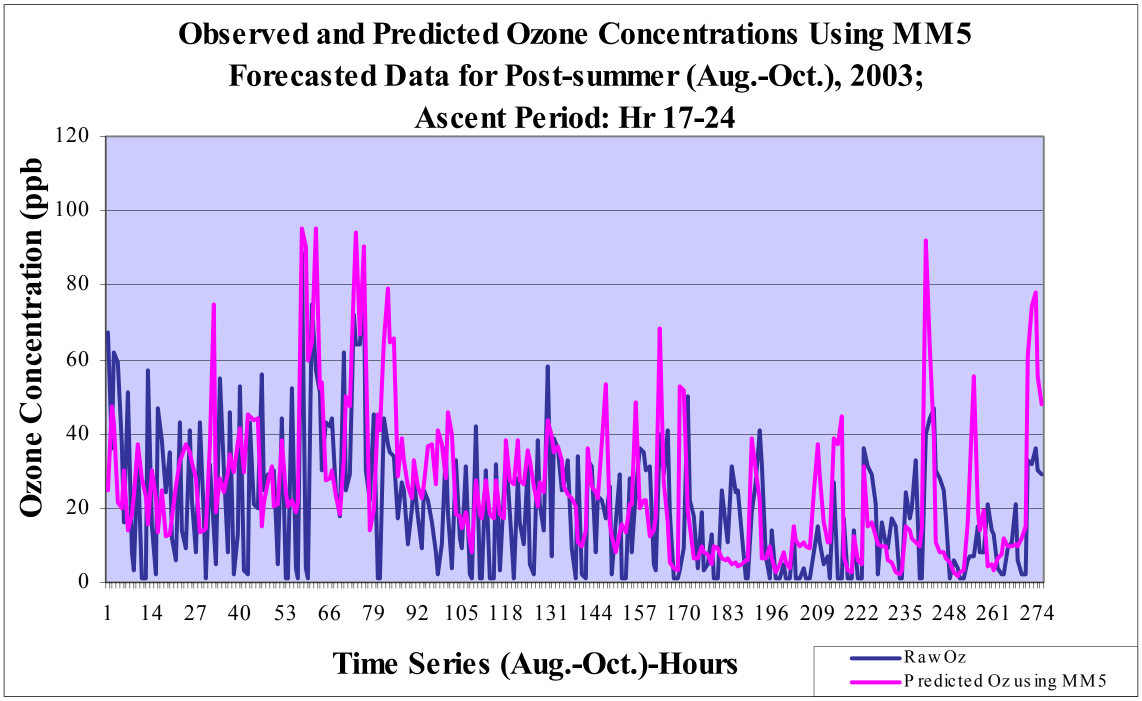


Figure C.9



Two-Parameter Models

Figure C.10

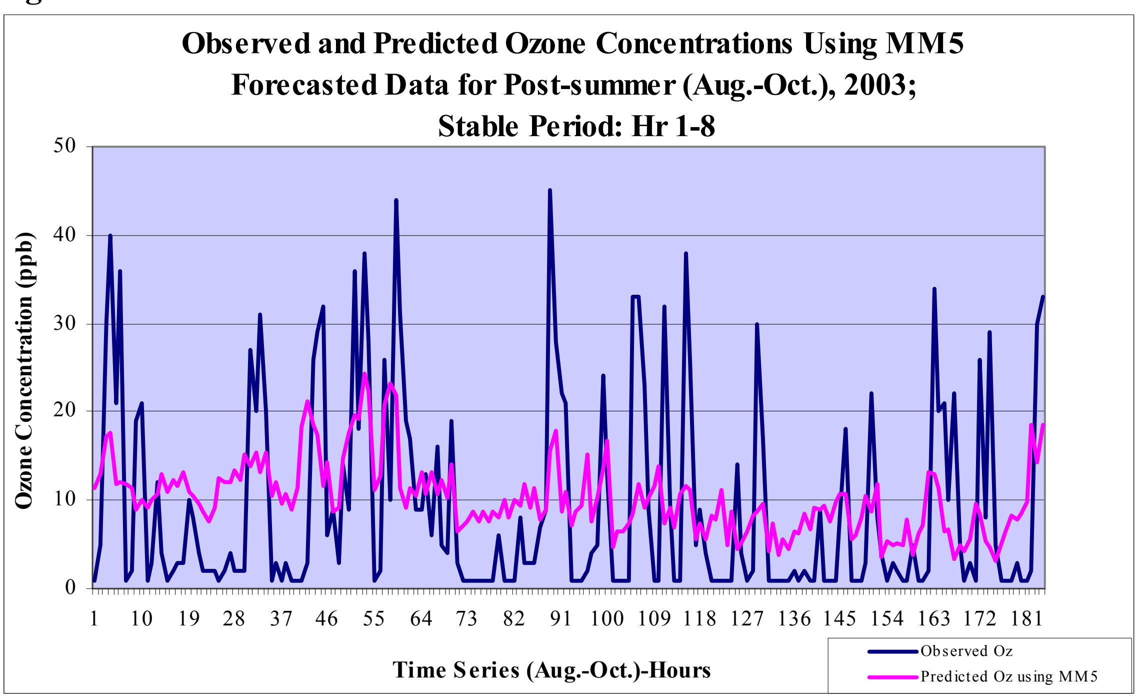


Figure C.11

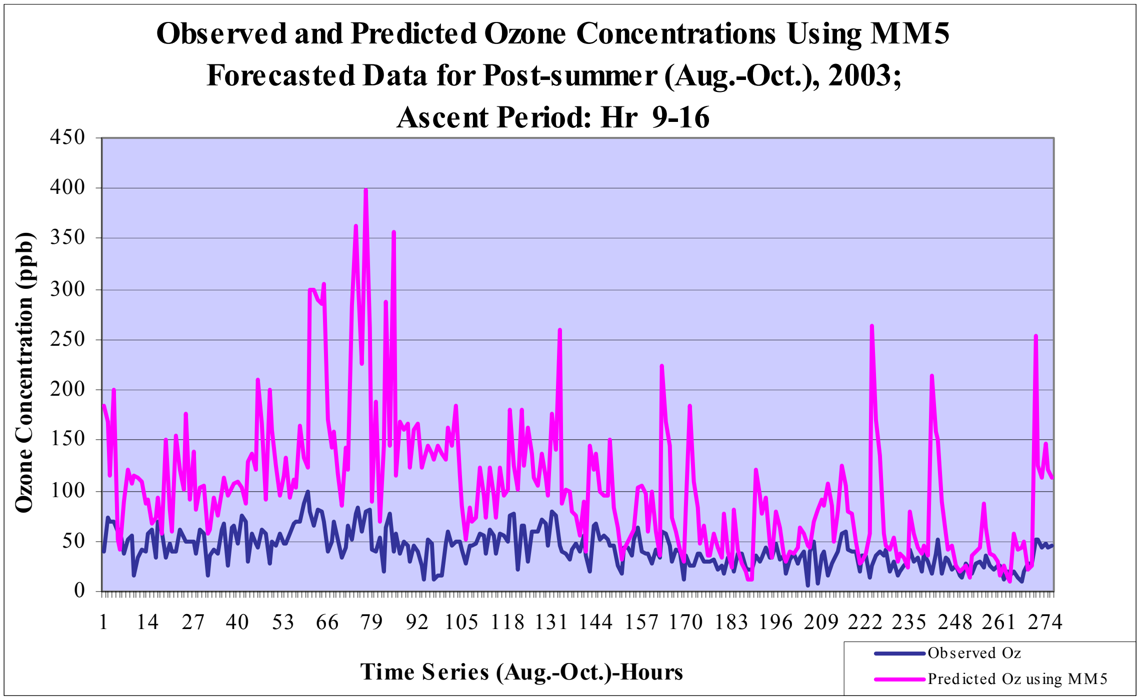


Figure C.12