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Evaluation of the AERMOD model and examination of required length of meteorological data for computing concentrations in urban areas

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The University of Toledo

A Thesis

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Anand Masuraha

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The University of Toledo

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THE DEGREE OF Master of Science in Civil Engineering

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An Abstract of

Evaluation of the AERMOD Model and Examination of Required Length of Meteorological Data for Computing Concentrations in Urban Areas

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The AERMOD and CALPUFF are current EPA's refined models for regulatory use. This study evaluates the performance of both the models in a multiple source urban environment using mercury emission inventories and monitoring data for eight monitoring stations for the year 1990 to 1992. The mercury concentrations were evaluated for general applications as well as regulatory applications for long-term averaging time (quarterly and annual) periods. The evaluation of general applications of the model was based on the qualitative and quantitative analysis. Qualitative model performance was assessed on visual comparison of observed and predicted concentrations of mercury, whereas quantitative model evaluations were assessed on the numerical values of seven statistical parameters. Regulatory applications of the model were evaluated from robust highest concentration (RHC) statistic and Q-Q plots.

The visual comparison and statistical analysis of AERMOD and CALPUFF predicted concentrations with observed concentrations yielded a satisfactory performance and met the criteria for a reasonable model for few statistical parameters in predicting annual and quarterly average concentrations for the multi-source region for general applications. Summary of 95% confidence limits on normalized mean square error (NMSE), fractional bias (FB), geometric mean variance (VG) and geometric mean bias (MG) for each model indicated that the statistics were not significantly different from zero for FB and correlation of r. Confidence limits analysis also showed that the prediction by AERMOD and CALPUFF were not significantly different from each other for multiple stacks in urban areas.

The regulation application results (Q-Q plots and ratios of predicted & observed RHC values) supported the use of the AERMOD and CALPUFF models for annual averaging time.

AERMOD and CALPUFF were further studied to determine the minimum required length of meteorological data. The current recommended contiguous time period of meteorological data by the USEPA for dispersion modeling in permit reviews is 5 years. This study is an attempt to verify the minimum-required-run-length of meteorological data for long-term as well short-term averaging periods. The set of multiple years of meteorological data were used to describe under-predicted periods in long-term (annual & quarterly) and short-term (1-hr, 3-hr, 8-hr, and 24-hr) impacts. Results were obtained for two pollutants (mercury and sulfur dioxide) using the above mentioned regulatory models (AERMOD and CALPUFF). The multiple year run analysis was done by calculating the number of under-predicted periods and by varying the running time interval of meteorological data (i.e., 5-years, 10-years, 15-years, 20-years and 25-years) using the AERMOD and CALPUFF models. The results show that EPA's recommended time length (5-years) is only sufficient for obtaining conservative predictions of concentration for annual averaging time period. For all other time periods, there is still a need to go beyond the regulatory application. Also, 5-year time length is insufficient for obtaining results closer to observed values and varies with different averaging time periods.

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NOMENCLATURE

Symbol	Units	Description
C_o	μg/m^3	Observed Concentrations
C_p	μg/m^3	Predicted Concentrations
$\overline{C_O}$	μg/m^3	Average of Observed Concentrations
$\overline{C_P}$	μg/m^3	Average of Predicted Concentrations
D_i	m	Diameter of Stacks Forming Superstack
D_s	m	Diameter of the Superstack
h_i	m	Height of Stacks Forming Superstack
h_s	m	Height of the the Superstack
Q_i	g/s	Pollutant Emission Rate of Stacks
Q_s	g/s	Pollutant Emission Rate of the Superstack
X_i	m	X-Coordinate of Stacks Forming Superstack
X_s	m	X-Coordinate of Superstack
Y_i	m	Y-Coordinate of Stacks Forming Superstack
Y_s	m	Y-Coordinate of Superstack
σ_{Co}	m	Standard Deviation of Observed Concentration
σ_{Cp}	m	Standard Deviation of Predicted Concentration

Chapter 1

INTRODUCTION

1.1 OVERVIEW

Air pollution control is a vivid example of human struggle against the environment and the successes and failure of supposed human "progress". Glaring effects of such uncontrolled repeated abuse and degradation are the discharge of noxious, toxic and/or even lethal pollutants under the aegis of production, progress, and modernization into a fast deteriorating atmosphere. Results of such exploitation -- innumerable pollution caused tragic incidents termed "episodes", -- include the Bhopal gas tragedy; the Mexico city episode; the New York city episodes of 1953, 1963 and 1966; Meuse valley episode and the London episodes in the 1950s and 1960s. Air pollution is ubiquitous, smoke, haze, dust, mist, foul-smelling and corrosive gases, and toxic compounds are present nearly everywhere, even in the remote, pristine wildness. But, it has become a serious problem only during the last 200 years when growing population and industrialization produced vast quantities of contaminants. In addition to short-term episodic effects, atmospheric pollutants are known to generate long-term effects, which are, however, difficult to forecast. Also predictions of bad air pollution warn of dire consequences like potential global warming, increased acid rain and smog phenomenon, and increased risk of lung and skin cancer due to toxic releases and ozone layer depletion.

Air pollution is not only an emission problem; it is also a weather-related condition or phenomenon and, as such should be considered one of the weather hazards. In fact, air pollution turns out to be by far the worst weather hazard if one compares the average estimated number of lives lost per year in the United States due to air pollution, 15000, with the about 750 deaths per year due to all other major weather hazards combined (Mills et. al, 2005).

Air pollution problems have three main components:

1. emission sources that produce air pollutants;
2. the atmosphere in which transport, diffusion, chemical transformations, and removal processes occur; and
3. receptors near the ground that respond to trace amount of air pollution reaching them.

The last decade has been characterized by a growing interest in long-range air pollution transport phenomena and global effects. First in northern Europe and then in eastern North America, it has been shown that large emissions of primary pollutants, such as mercury (Hg), undergo chemical transformations in the atmosphere. These transformations generate new chemical hundreds or thousands of kilometers downwind species known as “secondary” pollutants, such as the methyl mercury. The secondary species are responsible for new adverse effects, such as acid deposition (or, as commonly and improperly called in the media, acid rain).

Atmospheric mercury and ozone depletion events have been observed in the High Arctic during polar sunrise. Although the mechanisms remain enigmatic, bromine radicals have been identified as potential oxidizers—contributing significantly to the destruction of the ozone in the polar stratosphere and, in their reactive form, playing a key role in mercury oxidation and boundary-layer ozone depletion. (Tarasick et al., 2002)

On a large scale, pollutants affect meteorological parameters. Physical and chemical processes and socio-economic impacts link the six key environmental components (climate change, variability, smog, acidification, stratospheric ozone depletion, and hazardous air pollutants e.g., mercury and long-range transport of atmospheric pollutants). These are not mutually exclusive issues. For example, science has linked emissions from energy production and use to acid rain, smog, climate change and mercury in the environment. Stratospheric ozone depletion influences climate change and vice versa.

Several countries in the world have established air pollution laws and regulations and have implemented air quality and/or emission standards. The United States of America (U.S.), in particular, has developed a large and complex body of air quality laws directed towards the goals of progressive air quality improvement in those regions characterized by unhealthy concentration levels and environmental preservation in regions with clean air. Moreover, the U.S. regulations have incorporated the use of several air quality diffusion models as official regulatory tools.

State and federal regulatory agencies often require a dispersion modeling analysis as part of a permit application. Because of regulatory agencies' reliance on air dispersion models to estimate ambient air impacts, these models are designed to be conservative to ensure the protection of public health and welfare. However, these models tend to be extremely over conservative in predicting worst-case impacts. Accordingly, model selection in an air dispersion modeling analysis can be critical in being able to demonstrate compliance with applicable state and federal ambient air quality standards. In addition to their inherent conservatism, models vary significantly in their treatments of phenomena that often occur at facilities, such as building downwash and cavity effects.

Increasing regulatory requirements mandated by every revision of the Clean Air Act have caused a proliferation of dispersion modeling for permitting and other regulatory work. In such circumstances, selection of accurate, complex, and more refined models is not an easy job. The modeling scenarios are based on the dispersion of a gaseous pollutant from multiple stacks in urban areas located in the northeast U.S. Because this case is based on a specific situation, the results represented a realistic modeling trend in the current environmental dispersion modeling scenario. Therefore, this study first compared and evaluated the performances of two EPA regulatory models, namely AERMOD & CALPUFF, to analyze the predictability and reliability of these models for mercury release. Based on the model evaluation results, AERMOD and CALPUFF were used for obtaining the required meteorological-length-run period for different averaging time.

1.2 BACKGROUND

1.2.1 AERMOD

AERMOD uses a Gaussian and a bi-Gaussian approach in its dispersion model (US EPA, 2002). For convective conditions, AERMOD relies on a skewed probability density function to characterize the vertical distribution. In its simplest form, the Gaussian model assumes that the pollutant does not undergo chemical reactions or other removal processes in traveling away from the source. As the plume grows, pollutants reaching the ground or the top of the mixing height are reflected back toward the plume centerline. Industrial Source Complex (ISC) is a Gaussian plume model and is widely used to access pollution concentration and/or deposition flux on receptor. AERMOD differs from ISC in that it uses current planetary boundary layer (PBL) theory to determine the dispersion parameters σy and σz instead of depending on Pasquill–Gifford–Turner stability curves (US EPA, 2002). AERMOD uses different algorithms based on the dominant meteorological characteristics of the area over which the predictions are to be made (stable or convective). AERMOD generates daily, monthly as well as annual concentrations of pollutants for the ambient air. The model handles a variety of pollutant sources in a wide variety of settings such as rural and urban as well as flat and complex terrain. AERMOD models a system with three separate components (Figure 1.1):

- AERMOD (Aermic Dispersion Model)
- AERMAP (AERMOD Terrain Preprocessor)
- AERMET (AERMOD Meteorological Preprocessor)

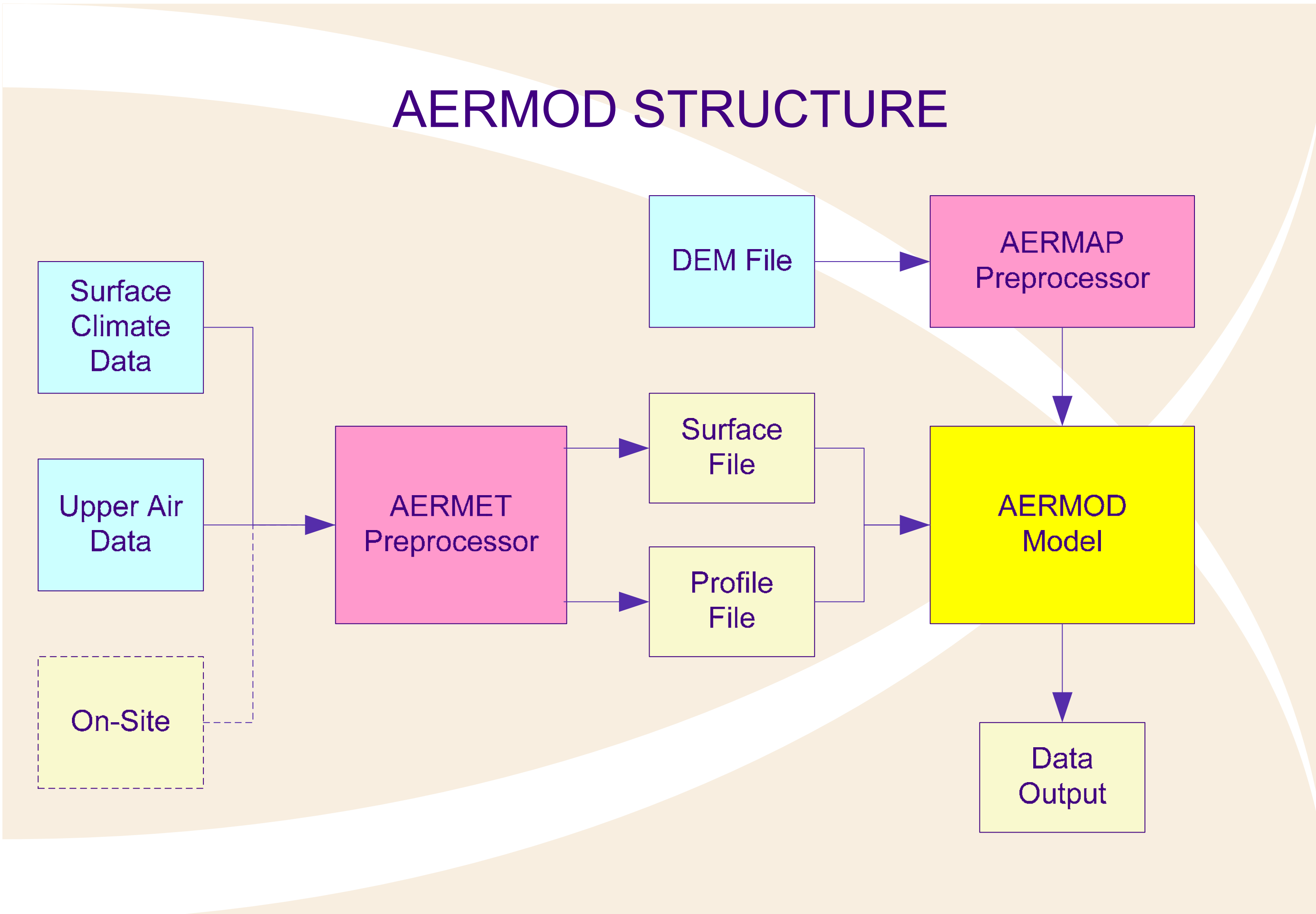

Figure 1.1: Systematic dataflow structure of EPA's AERMOD Model

1.2.2 CALPUFF

CALPUFF is an advanced non-steady-state and Lagrangian puff dispersion model, meteorological and air quality modeling system developed and distributed by Earth Tech, Inc. CALPUFF is a transport and dispersion model that advects "puffs" of material emitted from the model sources, simulating dispersion and transformation processes along the way. It includes algorithms for sub-grid scale effects (such as terrain impingement), as well as, longer range effects (such as pollutant removal due to wet scavenging and dry deposition, chemical transformation, and visibility effects of particulate matter concentrations). The main components of CALPUFF (Figure 1.2) are CALMET (a diagnostic 3-dimensional meteorological model), CALPUFF (an air quality dispersion model), and CALPOST (a post processing package). In addition to these components, there are numerous other processors that may be used to prepare geophysical (land use and terrain) data in many standard formats, meteorological data (surface, upper air, precipitation, and buoy data), and interfaces to other models such as the Penn State/NCAR Mesoscale Model (MM5), the National Centers for Environmental Prediction (NCEP) Eta model and the RAMS meteorological model. CALMET is a meteorological model that develops hourly wind and temperature fields on a three-dimensional gridded modeling domain. Associated two-dimensional fields such as mixing height, surface characteristics, and dispersion properties are also included in the file produced by CALMET.

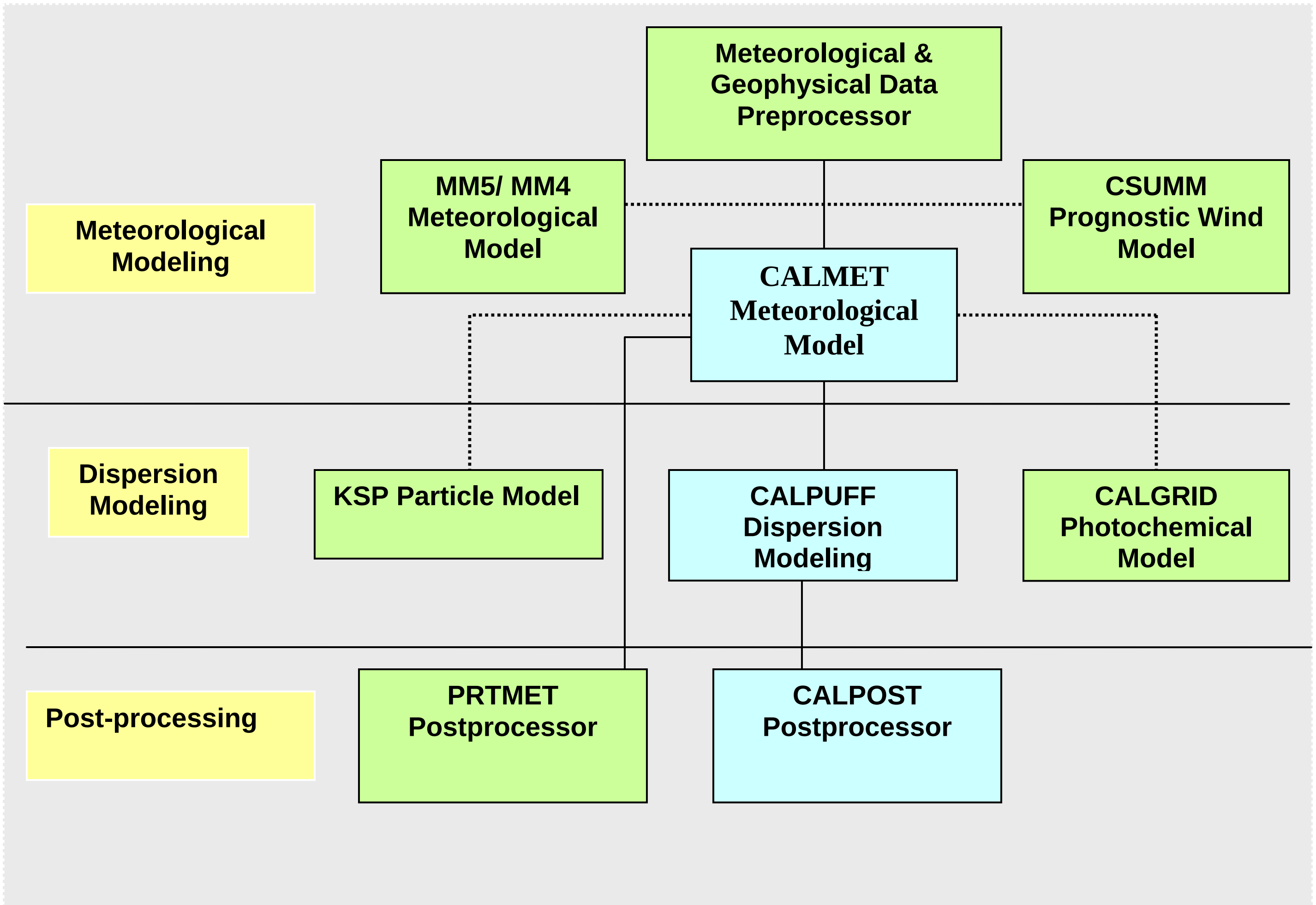

Figure 1.2: Systematic dataflow structure of EPA's CALPUFF Model

Table 1.1 shows the basic structural difference between AERMOD and CALPUFF dispersion models.

Table 1.1: Comparison of AERMOD and CALPUFF

AERMOD	CALPUFF
Steady-state Gaussian plume dispersion model	Non-steady-state Lagrangian puff dispersion model
Simulates transport and dispersion from multiple points, area, or volume sources based on an up-to-date characterization of the atmospheric boundary layer	Simulates the effects of time and space-varying meteorological conditions on pollution transport, transformation and removal
Short range transport model	Long range transport model
Emissions are continuous	Emissions can be continuous or instantaneous
The modeling system consists of one main component AERMOD and two pre-processors: AERMET and AERMAP	The modeling system consists of three components: CALMET, CALPUFF and CALPOST
AERMET is a simple meteorological model	CALMET is a diagnostic 3-dimensional meteorological model
No such pre-processors	Numerous pre-processors to prepare geophysical data, meteorological data
Accounts for building wake effects (i.e., plume downwash)	Contains algorithms for near-source effects such as building downwash, transitional plume rise, partial plume penetration, subgrid scale terrain interactions as well as longer range effects such as pollutant removal, chemical transformation, vertical wind shear, overwater transport and coastal interaction effects
No such fields are produced	Produces 3-D gridded fields of temperature, turbulence, mixing heights, velocity vectors
The model is applicable to primary pollutants and continuous releases of toxic and hazardous waste pollutants	CALPUFF allows for the estimation of both primary and secondary pollutant concentrations

1.2.3 Literature Review on Model Evaluation

Dispersion modeling is an acceptable technique for analyzing the impact of emissions from industrial sources in the US. The United States Environmental Protection Agency (EPA) has developed guidelines on the air quality models (EPA, 2005) and procedures on model evaluation (EPA, 2002). Numerous studies have been conducted to evaluate the performance of regulatory models such as AERMOD and CALPUFF.

Cimorelli et al. (2005) described the AERMOD model and its performance. The paper includes AERMOD's characterization of the boundary layer with computation of the Monin–Obukhov length, surface friction velocity, surface roughness length, sensible heat flux, convective scaling velocity, and both the shear- and convection-driven mixing heights. Perry et al. (2005) described the performance of AERMOD against 17 field study databases for release from several single stacks. The studies included sites with flat and complex terrain, urban and rural conditions, and elevated and surface releases with and without building wake effects. The evaluation measures were focused on those that are relevant to regulatory applications, that is, emphasis on the ability of the model to simulate the upper end of the concentration distributions. AERMOD estimates have been compared with those of other applied models, including ISCST3 (U.S. Environmental Protection Agency 1995), the Hybrid Plume Dispersion Model (HPDM) (Hanna and Paine 1989), the Rough Terrain Diffusion Model (RTDM) (Paine and Egan 1987), and the Complex Terrain Dispersion Model Plus Algorithms for Unstable Situations (CTDMPLUS) (Perry 1992). Of the 17 databases that were considered, 10 were designed to collect data for overall model performance where building wakes were not an issue, while the remaining 7 were specifically focused on building influences. Two pollutants

(SO_2 and SF_6) were used for this study. Of the 17 databases considered, seven emphasized near-field concentrations resulting from building wake effects. Four of the no-wake studies involved short-term, intensive measurements with extensive sampler arrays, while six included long-term, continuous sampling at more limited locations. Robust highest concentration (RHC) results were performed for 1-hr, 3-hr, 24-hr and annual averaging time with Q-Q plots. In model-to-model comparison AERMOD performance was clearly superior to that of ISCST3.

Paine et al. (1998) conducted a model evaluation for AERMOD for several single stacks dispersion. The developmental evaluation was conducted during the model formulation and initial testing used five data sets. A subsequent "independent" evaluation initially involved the three data sets, each with one full year of data for a limited number of fixed SO_2 monitoring sites in the vicinity of an electric utility source. After initial evaluation results for these three data bases were examined by a peer review panel, AERMOD was examined for two other independent data sets of complex terrain dispersion algorithms. This was because of concern about an apparent tendency toward under-prediction by AERMOD for one of the independent databases and complex terrain features. Evaluation statistics were presented in quantile-quantile (Q-Q) plots, residual plots, and robust highest concentration results. These results show that AERMOD is nearly unbiased, on average, across all averaging times. Annual average statistics are less reliable because background concentrations, which are removed from the measured values in many cases, are uncertain and approach the value of the source-caused impact. For all averaging times in general and in most cases, AERMOD's model performance was better than that of ISCST3. As a result of the superior technical formulation of

AERMOD and its better evaluation performance relative to ISCST3, the AERMIC committee concluded that AERMOD can be justified as a replacement for ISCST3 for regulatory modeling applications.

EPA (2002) conducted a peer review on AERMOD for single stack dispersion. The AERMOD consequence analysis was evaluated using two different land classifications (urban and rural), all three types of sources (point, volume and area) in three types of terrain (flat, simple and complex). There were 24 flat terrain point source combinations (6 stack heights, 2 met sites, 2 land classifications); 8 simple terrain point source combinations (2 stack heights, 2 met sites, 2 land classifications); 8 volume source combinations (2 stack heights, 2 met sites , 2 land classifications); 4 area source combinations (1 release height, 2 met sites, 2 land classifications); and 32 point source combination for the complex terrain (2 stack heights, 2 buoyancy types [medium and high], 2 distances to the hills, 4 hill types). In summary, the peer review committee believed that AERMOD incorporates some of the best features of the other models and performed better than other models.

Peter et al. (1999) performed a comparison of AERMOD versus ISCST3 and CTDMPLUS (Complex Terrain Dispersion Model) for several single stacks dispersion. The two sites (Pittsburgh, PA representative of an urban eastern site; and Oklahoma City, OK representative of a southwestern plains site) were selected for this study. Data for the year 1964 were used at Pittsburgh and data for the year 1984 were used at Oklahoma City. Results were compared for short-term (1-hr, 3-hr, and 24-hr) as well as for long-term (annual) averaging time for three types of sources (point, area, and volume). Results showed that the flat and complex terrain models produced similar concentration estimates over all the averaging times but with the differences growing larger as the averaging time increased. However, for certain situations, the differences in the AERMOD predictions were higher or lower than ISCST3 predictions by up to a factor of 3 or more, but in almost every case, the AERMOD concentration predictions were the closest to the air quality measurements, and, on average, showed a slight over-prediction tendency.

Ramakrishnan et al. (2001) compared the results for AERMOD, AEMOD-PRIME, ISC3, and ISC-Prime for short term (1-hr and 3-hr) and long term averaging periods. In comparing model performance for complex terrain scenarios, AERMOD and AERMOD-PRIME results for longer term averaging periods were dramatically lower than ISC3 and ISC-PRIME results. Also AERMOD and AERMOD-PRIME results for shorter term averaging periods can be higher and/or lower than ISCST3 and ISC-PRIME results depending on the land use parameters. A similar study was performed (Tarde and Westbrook, 2001) with AERMOD-PRIME, ISCST-PRIME, and ISCST3 for PM10 emissions for high-2nd high 24-hour averaging period. Results for AERMOD were again found better than the other models.

Laffoon et al. (2004) evaluated the behavior of AERMOD in comparison to ISC, compared the use of onsite meteorological data to the National Weather Service data, and the sensitivity of AERMOD to changes in input land use parameters without the use of observed concentration. They advised the use of the proper Land Use/Land Classification parameter to properly characterize the surrounding terrain and, in particular, surface roughness in order to avoid over- or under-predicting concentrations. Radonjic et al. (2001) analyzed three case studies for AERMOD and ISCST3. The first case study examined the difference in the concentrations of gaseous emissions predicted by

AERMOD and ISCST3 arising from the difference in the wind speed recorded with two methods: on-site meteorological data representing hour by averages and by Automated Surface Observing Stations (ASOS) which simulate airport meteorological stations (the hourly surface aviation observations prepared by National Weather Surface observers). Both data sets were used as inputs in the AERMOD and ISCST3 dispersion models. Three types of stacks (low, medium and high) were tested using 1-hr, 24-hr and annual periods from the same station. In the second case study, the performance of the AERMOD and ISCST3 models was evaluated relative to wind speed variability for both the hourly average and ASOS (airport) observations. The third case study, related to meteorological monitoring, examined data from a two level meteorological tower (recording data at 10 m and 50 m). Results showed that the use of meteorological data sets with lower recorded wind speeds can result in higher predicted air concentrations with both AERMOD and ISCST3. Also the use of hourly average data (only wind speed and direction) can result in higher predictions of downwind concentrations, for both AERMOD and ISCST3. The study didn't use observed concentration for different receptors.

The AERMOD evaluation study by Kumar et al. (2006) focused on comparing the computed ambient air concentrations of sulfur dioxide (SO_2) for 1-hr, 3-hr, and 24-hr averaging periods using the emission inventory data for Lucas County, Ohio, for the year 1990 with the observed concentration. The estimated concentrations in this study were classified based on the stability parameter, Monin-Obukhov length (L), for the two monitoring stations located in the area. The data were divided into two atmospheric stability classes (stable and convective case) as used in the AERMOD model. These categories were further grouped into five sub categories based on the value of L to learn about fine details of model performance. The study concluded that the performance of the AERMOD model did not meet the general criteria specified by Kumar et al. (1993) for air quality models for the 1-hr and 3-hr averaging periods. However, the model showed a better performance for the 24-hr concentrations as compared to the 1-hr and 3-hr averaging periods. Results showed that the AERMOD model had a tendency to under-predict in all the cases, thus showing that the multi-source regions were far more complex than single stack evaluations. The study also incorporated a comparative analysis of predicted SO_2 concentration using different land use types to analyze the model performance, which may be significantly affected by the values of the surface roughness, albedo, and Bowen ratio in certain cases. The study recommended that future work should focus on the correct role of land use parameters in predicting concentrations at the monitors and finding ways to quantify errors due to other factors.

The study by Bhardwaj et al. (2006) and Kumar et al. (2006) focused on finding the suitable guidelines for the input of surface characteristics that helps to obtain predictions close to the observed values for short-term averaging time. The land use parameters were calculated by two different methods. One was by analyzing the correct area of land cover type within a circular area extending approximately three kilometers, and the second was by calculating the weighted average of characteristics by surface area within a 30-degree sector in 12-pie shaped sectors within the three kilometer circle with the meteorological station (Toledo Airport) as the center. They found that the predicted results are closest to the observed values when the meteorological input is obtained using the twelve sectors' land use parameter values around three kilometers at the meteorological site. This study also focused on three realistic scenarios of population (population around the major sources, population which is intermediate of city population and the population around major sources, and the overall population of the city of Toledo) on the AERMOD. The population of the city of Toledo was taken from the US census. The concentrations predicted from these three cases were compared with the observed concentrations. The study analyzed the 1st and 2nd highest concentration values for 1-hr, 3-hr, and 24-hr averaging periods. The study showed that the variation in the input of population had very little impact on the 99.5 percentile value for 1-hr and 3-hr averaging time periods. This implies that if the regulations are based on these percentile values, the population is not a critical parameter for running the AERMOD model.

EPA (1998) conducted a distance sensitivity analysis on CALPUFF. An idealized source was assumed and the study was performed for three years (1988-1990) using the source rings established at 50, 100, 125, 150, 175, and 200 km from the spine. Results were obtained for SO_2, NO_2, PM_{10} for 3-hr, 24-hr and annual averaging time periods. Results showed that CALPUFF is best suited for long term dispersion modeling. EPA study (1998a) on the CALPUFF dispersion model evaluated the observed tracer concentrations from a short-term field experiment (the Great Plains experiment) near Norman, Oklahoma in July 1980. Several tracers were released for a short duration (3-4 hours) and six resulting plume concentrations were recorded at an array of monitors downwind from the source. For the Great Plains experiment, arcs of monitors were located 100 and 600 kilometers from the source. They concluded that model improvement can be made by better representing the wind field. The use of multiple layers seems to improve results substantially.

Walker et al. (2002) compared the results of three atmospheric dispersion models (ISCST3, AERMOD, and CALPUFF) at a natural gas plant in southwestern Nova Scotia for NOx predictions. No observed concentrations were used in the study to compare predicted concentrations. The analysis became more complex with time, and the models reflected this, beginning with ISC, and moving through AERMOD and finally to CALPUFF. Results showed there is a need to go beyond ISC and AERMOD in order to simulate transformations, deposition, and longer-range transport. They have also come to appreciate the public presentation quality of the results achieved in the CALPUFF phase of the work. US EPA (1998) performed a comparison between CALPUFF and ISC3 for steady state (screening) and variable meteorological conditions. Steady state modeling was performed for point source, area source and volume source with statistical parameter fractional bias (FB), where variable meteorological modeling was performed for 3-hr, 24-hr and annual periods. The results showed CALPUFF performed better than ISC3.

An analysis has also been performed using CALPUFF for the year 1992 where the high to low ratio has been computed at each source location for two runs in which one uses the MM5 wind fields and the other uses NWS data only. The MM5 wind fields for this analysis were produced by the United States Park Service. These fields are at an 80 kilometer resolution. In this analysis the run with the MM5 wind fields has utilized measured surface observations and precipitation data because of concerns regarding possible bias in surface predictions of important parameters by the MM5 model. Therefore, the primary difference in the meteorological fields produced by the two runs is in the upper air wind fields. The intent of this analysis is to examine consistency between results obtained with either method of wind field production (Riley, 2002). Not much of the studies have been found on multiple year dispersion modeling using EPA's regulatory models.

1.2.4 Literature Review on Length of Meteorological Data

In the Federal Register Guideline on Air Quality Models (US EPA, 2003), section 9.3.1 is devoted to the required length to sufficiently record meteorological data for air quality dispersion modeling in permit reviews. The recommended contiguous time period of meteorological data for dispersion modeling is 5 years. This multiple year time frame is required because of the variation in any one year of average transport events and other meteorological variables that affect modeled pollutant impacts. The decision to require 5 years of data is a compromise based on the practical feasibility of performing air quality impact evaluations and the original full recommendations on this issue, which were for up to 10 years of meteorology. Per USEPA guidance, 5 years of hourly meteorological data are used. Values of wind speed and direction, temperature, atmospheric stability, and mixing height are determined for each of the 43,824 hours within the data set. The dispersion model computes concentrations for every grid point from every emission point on every hour (U.S. EPA Guideline revised, 2003).

1.3 CONCLUSION FOR LITERATURE REVIEW ON MODEL PERFORMANCE

Almost all of the AERMOD model evaluations except that of Kumar et al. (2006) reported in the literature are for single sources. This study expands the work of Kumar et al. (2006) for multiple sources and is different in the following ways:

- It employs a different urban area (i.e., Southeast Michigan).
- It uses a different pollutant (i.e., mercury).

- It touches on long-term predictions (quarterly and annual) as opposed to daily and hourly predictions.
- It incorporates the suggestions of using 12-pie shaped sectors on land use parameters as described Kumar et al. (2006) and Bhardwaj et al. (2006).

CALPUFF was incorporated in this study to see if the use of CALPUFF provides better results than AERMOD because of the use of the concept of superimposing puffs to compute ground level concentration. Therefore in this study, performance of two of EPA's regulatory models AERMOD (version 4.8.6) and CALPUFF (version 1.5) was evaluated for mercury emission. It is hoped that the evaluation of AERMOD & CALPUFF will give us new insights for their use in urban areas.

1.4 OBJECTIVE OF THIS STUDY

- Comparison and evaluation among five EPA's Air quality models: AERMOD, CALPUFF, ISCST2, ISCLT2, and SCREEN2 for a multiple source urban area for long-term averaging periods. The results for the last three models are taken from the work of Patel and Kumar (1998).
- To perform the sensitivity analysis in AERMOD for urban population option for a multiple source urban area for long-term averaging periods.

- To standardize the minimum required run-length of meteorological data for:
  - Long-term averaging Time Periods
    - Annual averaging time period;
    - Quarterly averaging time period.
  - Short-term averaging Time Periods
    - 1-hr averaging time period;
    - 3-hr averaging time period;
    - 8-hr averaging time period;
    - 24-hr averaging time period.

For this purpose AERMOD and CALPUFF were run for two pollutants, mercury and sulfur dioxide. Mercury data were taken for Wayne County, Michigan (Patel and Kumar, 1998) whereas sulfur dioxide data were taken for Lucas County, Ohio (Bhardwaj master thesis, 2005). Both the pollutant databases were easily available from the previous works.

Chapter 2

DATA BASE

Emission inventories are important tools to describe the emission situation and eventually to manage air quality. It is necessary to have an accurate and high quality description of the emission sources in terms of quantity and dynamic behavior for air quality modeling. Air quality models require comprehensive information on emission sources and emission fluxes in the area under consideration. Information of the stacks that significantly cause the pollutant concentration at the monitoring station is very important to run the model.

2.1 MERCURY EMISSION INVENTORY

The study used the mercury database given by Patel and Kumar (1998). The following write up was taken from their work. Mercury emissions from various combustion and industrial sources pose a serious problem in Southeast (SE) Michigan. Air borne mercury is deposited in the water that affect to the Detroit River and downstream two Great Lakes water (Sills, 1992, and Fischer, 1993). There are approximately 1500 incinerators and numerous other stationary sources contributing mercury to the air that impacts the Great Lakes basin. It is very difficult to estimate the impact of combined all sources on average ambient air mercury concentration. However, major sources of mercury can be identified from the National Acid Precipitation Assessment Program database (NAPAP). The 1985 NAPAP data were used to identify sources and amounts of mercury emissions. According to this data, there were 18 stacks considered as major sources of mercury emission in SE Michigan. These stacks released approximately 3 tons of mercury, or approximately 92% of total yearly mercury emissions out of 3.25 tons total, accordingly to the NAPAP data for the area under study. Other ambient air sources of mercury were municipal incinerators, municipal power plants, and steel companies. The impacts of these minor sources only accounted for another 7 to 8% of mercury emissions were assumed to be insignificant for modeling. Also, possible sources from Canada were not included because of long distances between source locations and air monitoring stations.

The detailed emission inventories of all the selected stacks in SE Michigan for 1990, 1991, and 1992 consist of yearly emission rates of all 18 sources, the source ID, and their locations in Universal Transverse Mercator (UTM) coordinates, and stack parameters which include stack height, stack diameter, stack velocity, and stack exit temperature, where all stacks are considered as point sources. Table 2.1 shows the detail of the chosen stack for years 1990, 1991, and 1992. The data were recorded from the eight monitoring stations locations in Wayne County, Michigan. Table 2.2 shows the addresses of eight chosen monitoring stations and UTM coordinates. Figure 2.1, shows the location of stacks and air monitoring stations in UTM coordinates. Table 2.3 and Figure 2.2 show direct or shortest distances between each monitoring station and stack in SE Michigan. Table 2.4 shows observed quarterly average and annual average concentration of mercury for year 1990, 1991, and 1992.

Table 2.1: Stack Parameters for Mercury in Southeast Michigan

Stack-Parameter, Emissions and location information for Year 1990, 1991 & 1992 in Southeast Michigan													
Stack Description													
ID No.	Height (m)	Dia.(m)	UTM Coordinate (m)		Velocity (m/s)			Temperature (K)			Mercury emission (g/s)		
			Easting	Northing	1990	1991	1992	1990	1991	1992	1990	1991	1992
1	103.20	2.59	3322331	4692994	20.46	20.46	24.96	434.67	434.67	394.11	1.36E-02	3.32E-02	2.03E-02
2	117.35	3.73	309964	4690270	45.15	45.15	45.15	420.78	420.78	420.78	2.68E-08	1.49E-07	3.97E-08
3	129.54	3.91	309934	4690290	48.75	48.75	48.75	433.00	433.00	433.00	5.44E-03	3.89E-03	3.04E-03
4	170.39	4.42	321973	4662374	42.69	42.69	42.69	433.00	433.00	433.00	1.41E-05	6.11E-06	1.78E-06
5	171.60	4.88	322073	4662694	42.70	42.70	42.70	410.78	410.78	410.78	8.98E-06	1.29E-06	1.52E-06
6	245.37	8.53	307723	4637074	39.04	39.04	39.04	405.22	405.22	405.22	2.55E-02	2.57E-02	1.32E-02
7	245.37	8.53	307603	4637014	39.04	39.04	39.04	402.44	402.44	402.44	2.57E-02	2.62E-02	1.42E-02
8	245.37	8.53	307653	4637094	39.04	39.04	39.04	405.22	405.22	405.22	4.62E-06	1.29E-06	1.03E-06
9	245.37	8.53	307653	4637094	39.04	39.04	39.04	405.22	405.22	405.22	1.15E-04	8.87E-05	4.18E-05
10	201.17	7.77	377519	4737146	27.47	27.47	27.47	416.33	416.33	416.33	1.55E-02	1.50E-02	6.67E-06
11	201.17	7.77	377429	4737176	27.47	27.47	27.47	416.33	416.33	416.33	1.57E-02	1.54E-02	6.19E-06
12	88.39	1.37	377429	4737036	22.75	22.75	22.75	588.56	588.56	588.56	1.23E-05	1.23E-05	5.32E-05
13	182.58	4.06	379247	4735668	27.39	27.39	27.39	438.56	438.56	438.56	3.29E-03	2.66E-03	2.89E-09
14	182.58	4.06	379251	4735668	27.39	27.39	27.39	438.56	438.56	438.56	3.00E-03	2.27E-03	4.80E-09
15	182.58	4.06	379247	4735664	27.39	27.39	27.39	438.56	438.56	438.56	3.23E-03	2.85E-03	3.89E-07
16	182.58	4.06	379251	4735664	27.39	27.39	27.39	438.56	438.56	438.56	3.36E-03	3.09E-03	4.51E-07
17	129.54	4.04	379289	4735930	39.96	39.96	39.96	421.89	421.89	421.89	4.78E-06	5.53E-06	5.98E-06
18	182.58	4.98	379319	4735987	42.74	42.74	42.74	425.78	425.78	425.78	6.72E-06	1.97E-06	4.22E-06

Table 2.2: Air Monitoring Stations in Southeast Michigan

Air Monitoring Station's		UTM Coordinate for Air Monitoring Stations	
Sr. No.	Address	X* (m)	Y* (m)
1	Osborn H.S. 11600 E. 7 Mile Detroit	3355129	4699766
2	MC Michael Middle School 6050 Linwood Detroit	327331	4691544
3	Southwestern H.S. 6921 W. Fort Detroit	310464	4693620
4	Stoepel Park 1 14800 Evergreen Detroit	331236	4688936
5	GM Poletown, Poletown Plant 2500 East Grand Blvd. Detroit	327956	4692350
6	Kettering H.S. 6101 Van Dyke Detroit	333767	4694506
7	Salina Middle School 2842 Wyoming Dearborn	322793	4686248
8	Grosse Ile 24975 West River Rd. Grosse Ile	322873	4665994

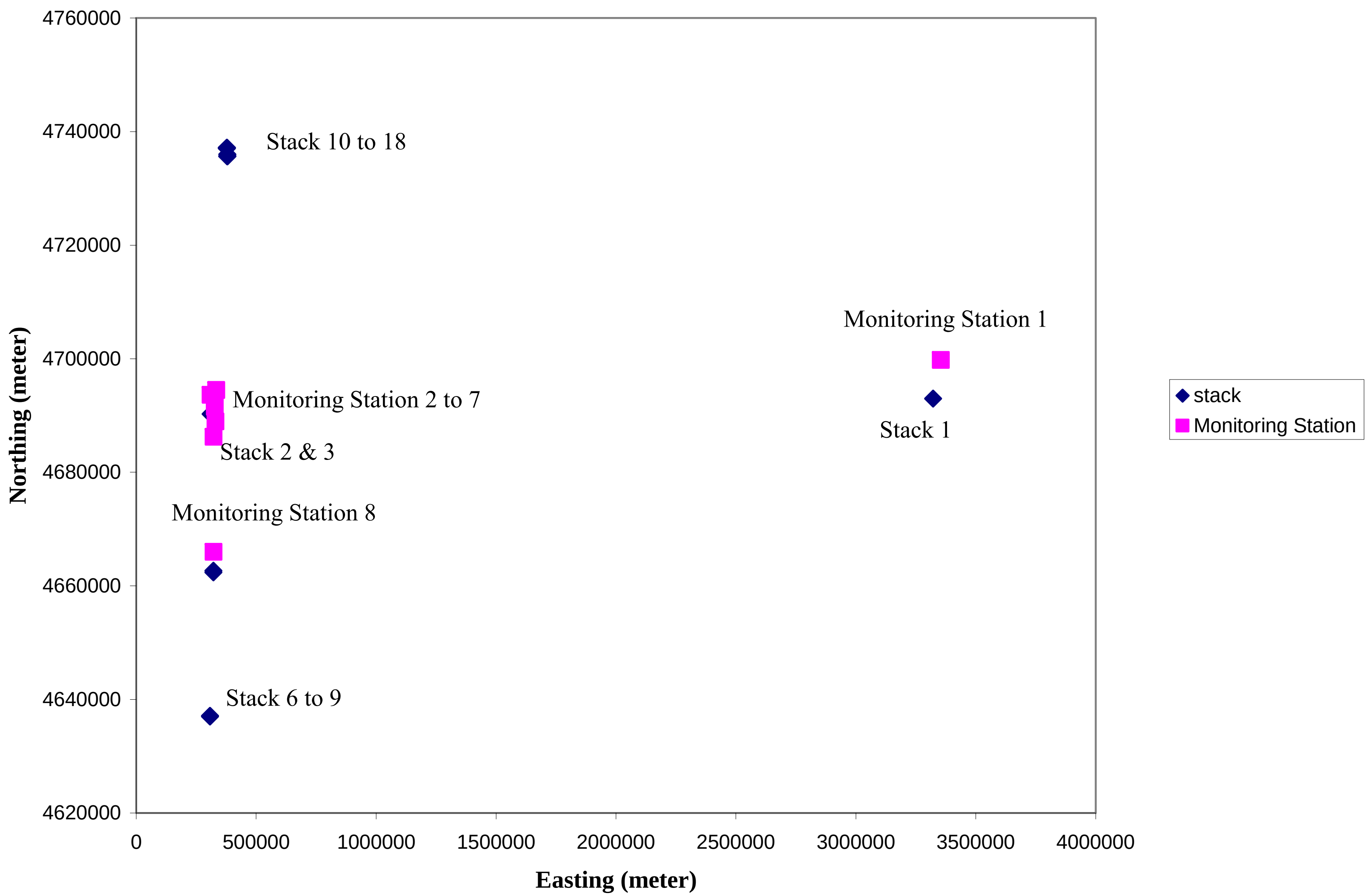

Figure 2.1: Location of Stacks & Air Monitoring Stations in UTM Coordinates in Southeast Michigan

Table 2.3: Shortest or Direct distance between each Air Monitoring Station and Stack in Southeast Michigan

Stack No.	Air Monitoring Station Number and Distance From Stack (m)							
	01	**04**	**05**	**06**	**29**	**30**	**33**	**35**
1	7245	5110	9425	16426	771	2030	11661	26431
2	19698	9371	3387	16815	12705	14449	4841	14048
3	19695	9356	3372	16782	12701	14449	4807	14055
4	37332	27011	21080	30589	30394	32006	20703	3730
5	36999	26676	20745	30283	30060	31674	20372	3396
6	66318	55686	49886	56670	59344	61012	48948	32648
7	66426	55788	49991	56752	59451	61121	49047	32757
8	66332	55695	49897	56664	59357	61027	48954	32663
9	66332	55695	49897	56664	59357	61027	48954	32663
10	56517	67853	72634	74047	63268	61248	74850	88569
11	56469	67806	72592	73989	63223	61204	74804	88534
12	56377	67713	72493	73912	63127	61107	74709	88427
13	56880	68189	72852	74704	63555	61512	75151	88586
14	56883	68192	72855	74708	63558	61515	75154	88588
15	56878	68186	72849	74702	63553	61509	75148	88538
16	56881	68189	72852	74705	63556	61512	75151	88585
17	57078	68390	73062	74878	63760	61718	75354	88809
18	57138	68449	73123	74934	63820	61778	75415	88872

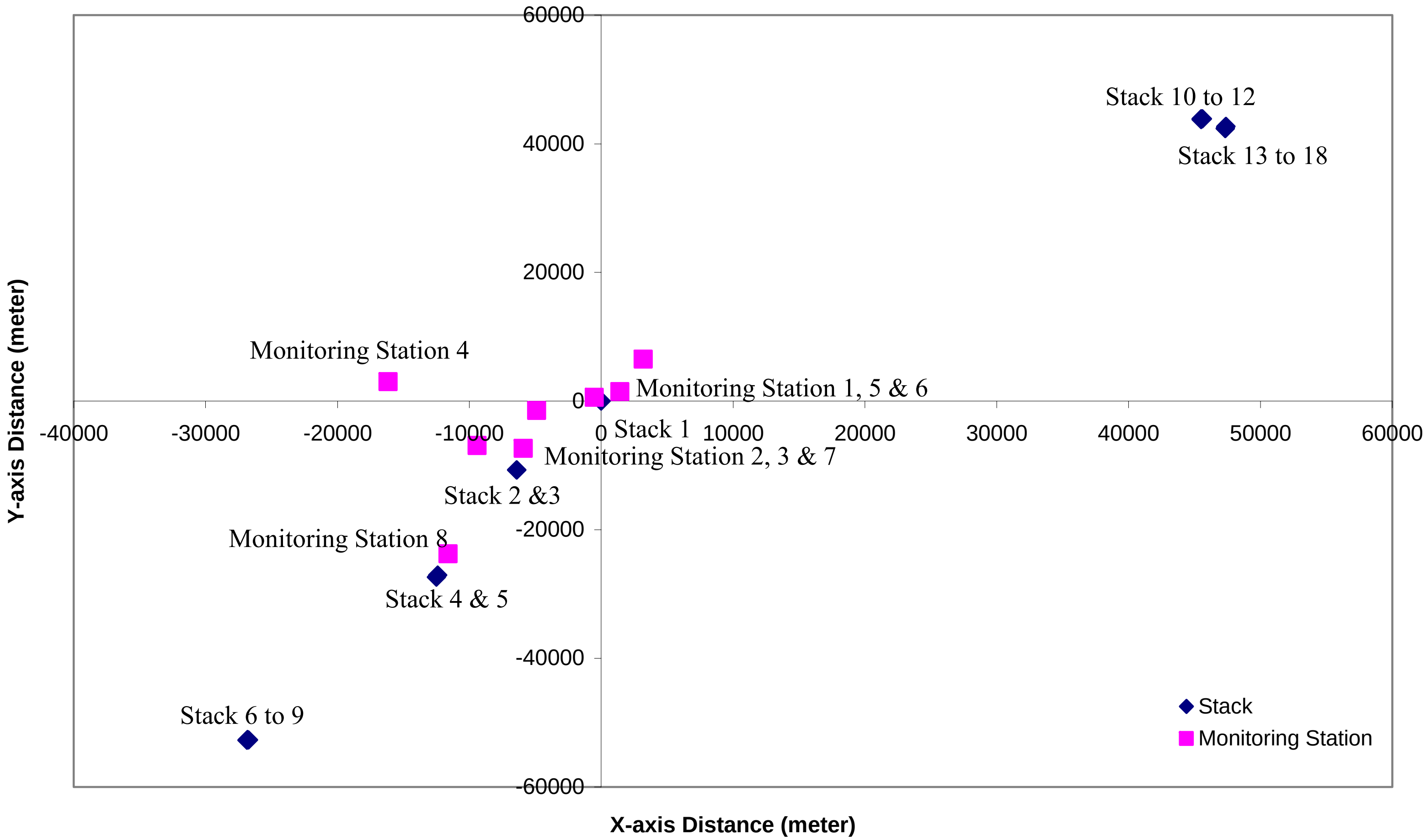

Figure 2.2: Shortest or Direct Distance between Each Air Monitoring Station and Stack in Southeast Michigan

Table 2.4: Observed Quarterly and Annual Average Concentration of Mercury ($\mu g/m^3$) for year 1990, 1991, and 1992 in Southeast Michigan

Sr. No.	Averaging Time	Observed Concentration of Mercury in µg/m3 in Wayne County		
		1990 Report	1991 Report	1991 Report
1	1st Quarter	0.00032	0.00020	0.00019
	2nd Quarter	0.00020	0.00010	0.00051
	3rd Quarter	0.00011	0.00030	0.00045
	4th Quarter	0.00010	0.00040	0.00022
	Annual	0.00018	0.00025	0.00034
2	1st Quarter	0.00022	0.00030	0.00022
	2nd Quarter	0.00029	0.00020	0.00033
	3rd Quarter	0.00024	0.00030	0.00035
	4th Quarter	0.00006	0.00020	0.00012
	Annual	0.00020	0.00025	0.00026
3	1st Quarter	0.00034	0.00030	0.00031
	2nd Quarter	0.00260	0.00030	0.00053
	3rd Quarter	0.00023	0.00030	0.00037
	4th Quarter	0.00009	0.00030	0.00024
	Annual	0.00023	0.00030	0.00036
4	1st Quarter	0.00028	0.00010	0.00034
	2nd Quarter	0.00022	0.00020	0.00031
	3rd Quarter	0.00017	0.00020	0.00024
	4th Quarter	0.00022	0.00020	0.00018
	Annual	0.00022	0.00018	0.00027
5	1st Quarter	0.00025	0.00020	0.00037
	2nd Quarter	0.00018	0.00030	0.00031
	3rd Quarter	0.00021	0.00030	0.00027
	4th Quarter	0.00020	0.00040	0.00032
	Annual	0.00021	0.00030	0.00032
6	1st Quarter	0.00028	0.00030	0.00028
	2nd Quarter	0.00020	0.00050	0.00033
	3rd Quarter	0.00026	0.00020	0.00029
	4th Quarter	0.00016	0.00060	0.00030
	Annual	0.00023	0.00040	0.00030
7	1st Quarter	0.00021	0.00040	0.00032
	2nd Quarter	0.00033	0.00030	0.00047
	3rd Quarter	0.00020	0.00030	0.00029
	4th Quarter	0.00006	0.00030	0.00030
	Annual	0.00020	0.00033	0.00035
8	1st Quarter	0.00032	0.00020	0.00071
	2nd Quarter	0.00017	0.00020	0.00033
	3rd Quarter	0.00026	0.00030	0.00029
	4th Quarter	0.00015	0.00030	0.00016
	Annual	0.00023	0.00025	0.00037

2.2 SULFER DIOXIDE (SO2) EMISSION INVENTORY

The study was used the sulfur dioxide database given by Bhardwaj, Master Thesis (2005). The following write up was taken from their work. A detailed emission inventory for Lucas County was obtained from the Department of Public Utilities, City of Toledo, Ohio for all sources emitting (SO2). The inventory obtained, has complete details of point source for years 1990, 1991 and 1992 for all sources emitting Sulfur Dioxide (SO2). The emission data contained the measurement from stack monitors for three years. The point source report consisted information on facility, stack/discharge and air pollutant emissions. The information on facility includes the UTM (Universal Transverse Mercator) coordinates and the UTM zone in which the stack is situated. The information on the stack includes the stack parameters such as height, diameter, temperature, and flow rate. The information on air pollutant emissions includes the uncontrolled, actual and allowable annual emissions of pollutants. Lucas County has about 123 stacks that emit sulfur dioxide. The emissions from the stacks range from 1 ton/year to 6655 tons/year. For the analysis, stacks were classified into three groups based on the amount of emission emitted per year.

2.2.1 Stacks Classification for Year 1990

The first group consists of 16 stacks which cause about 96.0 percent of the pollutant emissions and each of the individual stacks annual emission rate is greater than 210 tons. The second group consists of 28 stacks causing 3.7 percent of the pollutant emissions and each of the individual stack's annual emissions rate is greater than 5 tons but less than 210 tons. The third group consists of 79 stacks causing 0.24 percent of the pollutant emissions and each of the individual stacks annual emission rate is less than 5 tons. The second and third groups of stacks are modeled as super stacks. The properties of main stacks and super stacks are summarized in the Tables 2.5 and 2.8 respectively.

2.2.2 Stacks Classification for Year 1991

The first group consists of 15 stacks that cause about 95.79% of the pollutant emissions and each of the individual stacks annual emission rate is greater than 200 tons. The second group consists of 40 stacks causing 3.90% of the pollutant emissions and each of the individual stack's annual emissions rate is greater than 10 tons but less than 200 tons. The third group consists of 68 stacks causing 0.31% of the pollutant emissions and each of the individual stacks annual emission rate is less than 10 tons. The second and third groups of stacks are modeled as super stacks. The properties of main stacks and super stacks are summarized in the Tables 2.6 and 2.9 respectively.

2.2.3 Stacks Classification for Year 1992

The first group consists of 16 stacks that cause about 96.71% of the pollutant emissions and each of the individual stacks annual emission rate is greater than 200 tons. The second group consists of 37 stacks causing 3.12% of the pollutant emissions and each of the individual stack's annual emissions rate is greater than 10 tons but less than 200 tons. The third group consists of 70 stacks causing 0.17 percent of the pollutant emissions and each of the individual stacks annual emission rate is less than 10 tons. The second and third groups of stacks are modeled as super stacks. The properties of main stacks and super stacks are summarized in the Tables 2.7 and 2.10 respectively.

2.2.4 Monitoring Data

The ambient air monitoring data are the source of the observed concentrations of sulfur dioxide in the proposed study. The data were recorded from the two monitoring locations in the study area for the period of 1990, 1991, and 1992. The data has been obtained from the US EPA's air quality system. The monitoring data consist of hourly observed values at the above two monitoring stations for three years and details of geographical location of the monitoring sites. The two monitoring stations in the Lucas County are located at 26 Main Street and 600 Collins Park. The UTM coordinates of the two monitoring stations are (289304, 4613488) and (293889, 4615115).

Table 2.5: Ohio EPA emission inventory system point source report for sulfur dioxide for the year 1990

No	Stacks Information	Height (Ft)	Diameter (Ft)	Temperature (Deg. F)	Flow rate (cf/min)	Horizontal UTM (Km)	Vertical UTM (Km)	Emission (Tons/Year)
1	BP Oil Company: Flare Stack & Burner Tip M.W. Kellog	343	0.5	3000	-	295.7	4616.8	260
2	BP Oil Company: 55000 BPD UOP FCC Unit with new B & W Co. Boiler	250	11	400	130619	295.7	4616.8	1659.84
3	Sun Refining: Babcock & Wilcox Heater	100	9.5	390	100000	291.7	4611.8	1099.31
4	Sun Refining: Fluid Catalytic Cracking Unit	249	9.7	450	186844	291.4	4611.8	2238.6
5	Sun Refining: Amine Class Sulfur Recovery Plant	150	3.5	1200	16700	291.4	4611.8	553.92
6	Toledo Coke Corporation: Battery Coke Ovens and Auxiliaries	200	7.5	200	-	292.8	4616.1	259.85
7	Toledo Edison Co: Acme Station: 802 MM BTU/Hr B & W Coal Fired Boiler W/ESP ACME #16 Boiler	246	11	327	295000	290.5	4614.3	668.39
8	Toledo Edison Co: Acme Station: 649 MM BTU/Hr B & W Coal Fired Boiler W/ESP ACME #91 Boiler	298	22	352	133300	290.5	4614.3	554.01
9	Toledo Edison Co: Acme Station: 649 MM BTU/Hr B & W Coal Fired Boiler W/ESP ACME #92 Boiler	298	22	352	133300	290.5	4614.3	461.02
10	Toledo Edison Co: Bayshore Station: Babcock & Wilcox Custom Built Boiler	469	23	300	467000	297.1	4618.3	5065.3
11	Toledo Edison Co: Bayshore Station: Babcock & Wilcox Custom Built Boiler	469	23	300	490000	297.1	4618.3	6642.24
12	Toledo Edison Co: Bayshore Station: Babcock & Wilcox Custom Built Boiler	469	23	300	467000	297.1	4618.3	6655.51
13	Toledo Edison Co: Bayshore Station: Babcock & Wilcox Custom Built Boiler	469	23	300	710000	297.1	4618.3	8225.43
14	Coulton Chemical Corp: Contact Type Sulfuric Acid Plant	120	4	100	25000	295.6	4617.1	294.25
15	LOF CO Rossford plant: Float Glass Melting Furnace	252	8	1310	155300	287.9	4610.3	307.64
16	LOF CO Rossford plant: Float Glass Melting Furnace	212	8	1200	179000	287.9	4610.3	210.35

Table 2.6: Ohio EPA emission inventory system point source report for sulfur dioxide for the year 1991

No	Stacks Information	Height (Ft)	Diameter (Ft)	Temperature (Deg. F)	Flow rate (cf/min)	Horizontal UTM (Km)	Vertical UTM (Km)	Emission (Tons/Year)
1	BP Oil Company: Flare Stack & Burner Tip M.W. Kellog	343	0.5	3000	-	295.7	4616.8	1509
2	BP Oil Company: 55000 BPD UOP FCC Unit with new B & W Co. Boiler	250	11	400	130619	295.7	4616.8	1659.84
3	Sun Refining: Babcock & Wilcox Heater	100	9.5	390	100000	291.7	4611.8	659.02
4	Sun Refining: Fluid Catalytic Cracking Unit	249	9.7	450	186844	291.4	4611.8	2238.6
5	Sun Refining: Amine Class Sulfur Recovery Plant	150	3.5	1200	16700	291.4	4611.8	553.92
6	Toledo Coke Corporation: Battery Coke Ovens and Auxiliaries	200	7.5	200	-	292.8	4616.1	259.85
7	Toledo Edison Co: Acme Station: 802 MM BTU/Hr B & W Coal Fired Boiler W/ESP ACME #16 Boiler	246	11	327	295000	290.5	4614.3	397.96
8	Toledo Edison Co: Acme Station: 649 MM BTU/Hr B & W Coal Fired Boiler W/ESP ACME #91 Boiler	298	22	352	133300	290.5	4614.3	431.68
9	Toledo Edison Co: Acme Station: 649 MM BTU/Hr B & W Coal Fired Boiler W/ESP ACME #92 Boiler	298	22	352	133300	290.5	4614.3	331.04
10	Toledo Edison Co: Bay shore Station: Babcock & Wilcox Custom Built Boiler	469	23	300	467000	297.1	4618.3	5822.67
11	Toledo Edison Co: Bay shore Station: Babcock & Wilcox Custom Built Boiler	469	23	300	490000	297.1	4618.3	5213.87
12	Toledo Edison Co: Bay shore Station: Babcock & Wilcox Custom Built Boiler	469	23	300	467000	297.1	4618.3	6255.02
13	Toledo Edison Co: Bay shore Station: Babcock & Wilcox Custom Built Boiler	469	23	300	710000	297.1	4618.3	7275.41
14	Coulton Chemical Corp: Contact Type Sulfuric Acid Plant	120	4	100	25000	295.6	4617.1	294.25
15	LOF CO Rossford plant: Float Melting Furnace	252	8	1310	155300	287.9	4610.3	263.64

Table 2.7: Ohio EPA emission inventory system point source report for sulfur dioxide for the year 1992

No	Stacks Information	Height (Ft)	Diameter (Ft)	Temperature (Deg. F)	Flow rate (cf/min)	Horizontal UTM (Km)	Vertical UTM (Km)	Emission (Tons/Year)
1	BP Oil Company: Flare Stack & Burner Tip M.W. Kellog	343	0.5	3000	-	295.7	4616.8	1509
2	BP Oil Company: 55000 BPD UOP FCC Unit with new B & W Co. Boiler	250	11	400	130619	295.7	4616.8	1659.84
3	Sun Refining: Babcock & Wilcox Heater	100	9.5	390	100000	291.7	4611.8	688.41
4	Sun Refining: Fluid Catalytic Cracking Unit	249	9.7	450	186844	291.4	4611.8	2238.6
5	Sun Refining: Amine Class Sulfur Recovery Plant	150	3.5	1200	16700	291.4	4611.8	553.92
6	Toledo Coke Corporation: Battery Coke Ovens and Auxiliaries	200	7.5	200	-	292.8	4616.1	259.85
7	Toledo Edison Co: Acme Station: 802 MM BTU/Hr B & W Coal Fired Boiler W/ESP ACME #16 Boiler	246	11	327	295000	290.5	4614.3	397.96
8	Toledo Edison Co: Acme Station: 649 MM BTU/Hr B & W Coal Fired Boiler W/ESP ACME #91 Boiler	298	22	352	133300	290.5	4614.3	425.07
9	Toledo Edison Co: Acme Station: 649 MM BTU/Hr B & W Coal Fired Boiler W/ESP ACME #92 Boiler	298	22	352	133300	290.5	4614.3	331.04
10	Toledo Edison Co: Bay shore Station: Babcock & Wilcox Custom Built Boiler	469	23	300	467000	297.1	4618.3	5443.99
11	Toledo Edison Co: Bayshore Station: Babcock & Wilcox Custom Built Boiler	469	23	300	490000	297.1	4618.3	5213.87
12	Toledo Edison Co: Bayshore Station: Babcock & Wilcox Custom Built Boiler	469	23	300	467000	297.1	4618.3	6455.55
13	Toledo Edison Co: Bayshore Station: Babcock & Wilcox Custom Built Boiler	469	23	300	710000	297.1	4618.3	7750.42
14	Coulton Chemical Corp: Contact Type Sulfuric Acid Plant	120	4	100	25000	295.6	4617.1	294.25
15	LOF CO Rossford plant: Float Glass Melting Furnace	252	8	1310	155300	287.9	4610.3	257.09
16	LOF CO Rossford plant: Float Glass Melting Furnace	212	8	1200	179000	287.9	4610.3	210.37

Table 2.8: Properties of super stacks for 1990

No.	Stack No	Height (m)	Temp (K)	Diameter (m)	Flow rate M^3/S	Exit Velocity (m/s)	Emission g/sec	Horizontal (Km)	Vertical (Km)	Description of the Source
1.	SS002	39.99	547.00	2.90	1300.58	7.02	2.71	290.7	4614.5	Superstack 1 for SO2 emission
2.	SS001	32.76	544.10	2.00	407.95	9.54	42.97	289.1	4614.3	Superstack 2 for SO2 emission

Table 2.9: Properties of super stacks for 1991

No.	Stack No	Height (m)	Temp (K)	Diameter (m)	Flow rate M^3/S	Exit Velocity (m/s)	Emission g/sec	Horizontal (Km)	Vertical (Km)	Description of the Source
1.	SS003	37.30	555.24	3.03	1353.625	7.37	3.05	289.2954	4612.938	Superstack 1 for SO2 emission
2.	SS004	33.11	617.026	1.93	108.462	13.06	38.89	289.0679	4613.458	Superstack 2 for SO2 emission

Table 2.10: Properties of super stacks for 1992

No.	Stack No	Height (m)	Temp (K)	Diameter (m)	Flow rate M^3/S	Exit Velocity (m/s)	Emission g/sec	Horizontal (Km)	Vertical (Km)	Description of the Source
1.	SS005	43.37	540.737	2.97	1197.284	7.20	1.68	292.5762	4615.934	Superstack 1 for SO2 emission
2.	SS006	34.45	574.1542	2.01	516.8056	10.71	31.25	288.638	4613.299	Superstack 2 for SO2 emission

2.2.5 Location of Stacks, Super-stacks, and Monitoring Stations

The stacks, superstack and the monitoring stations are plotted on a Cartesian Grid represented by figure 2.3, 2.4 and 2.5 for years 1990, 1991 and 1992 respectively.

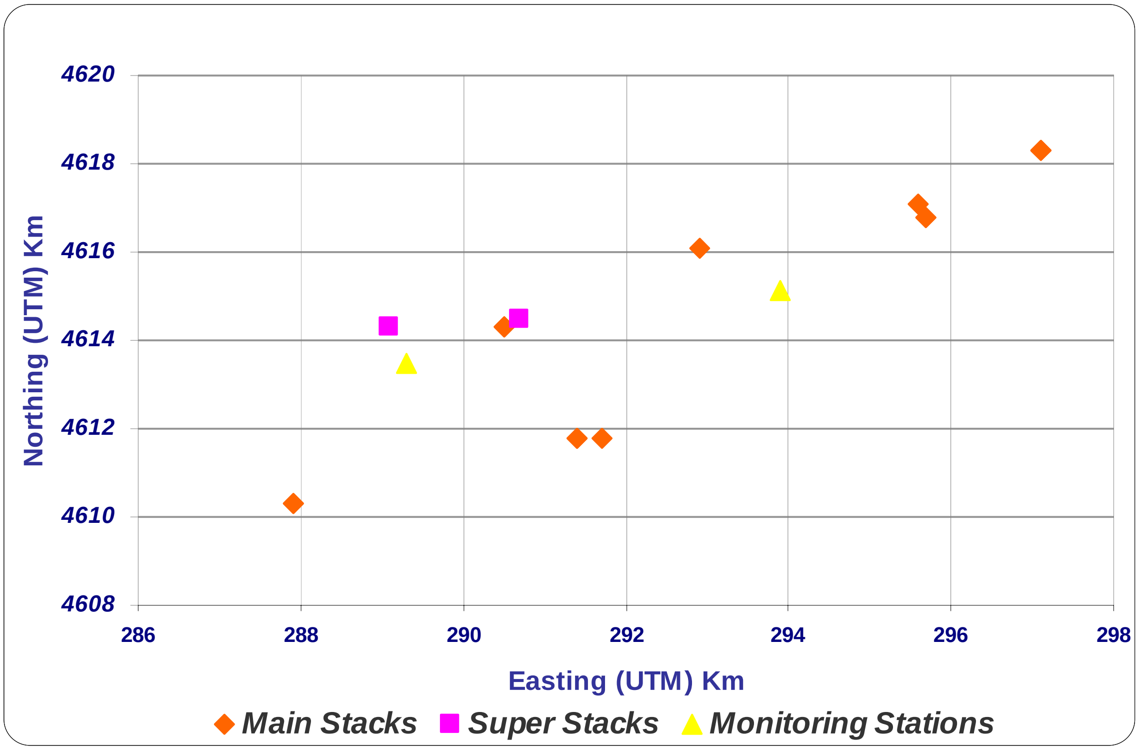

Figure 2.3: Monitor and Source Location for 1990

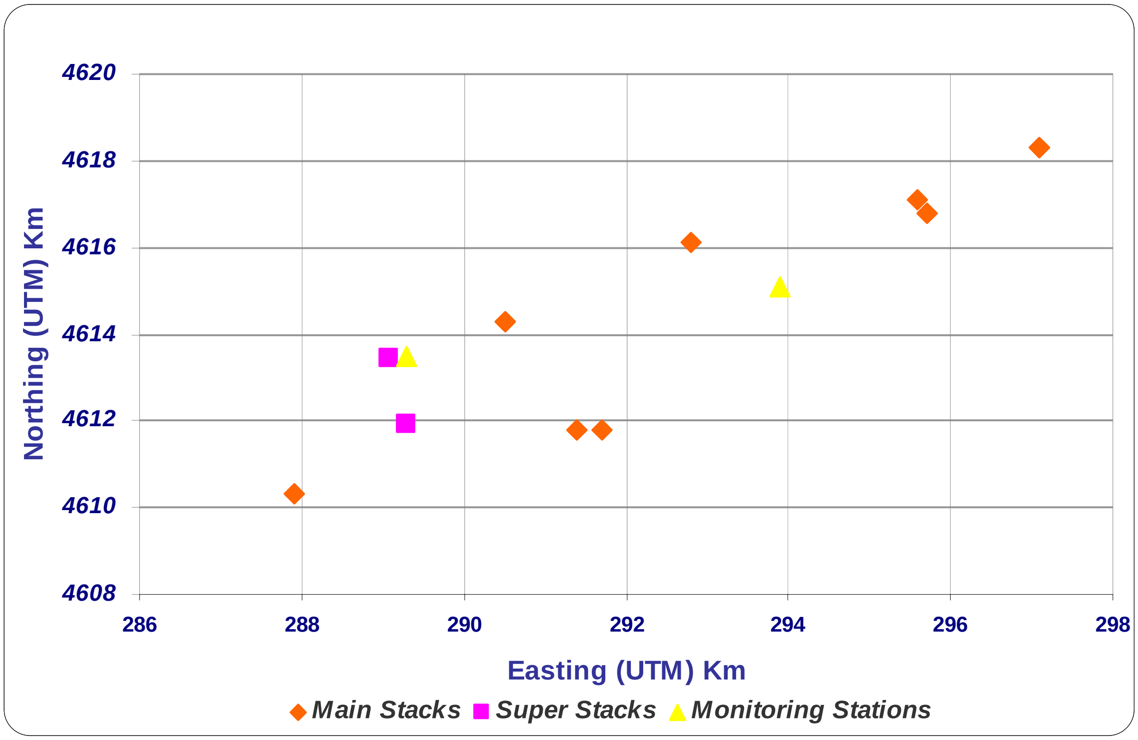

Figure 2.4: Monitor and Source Location for 1991

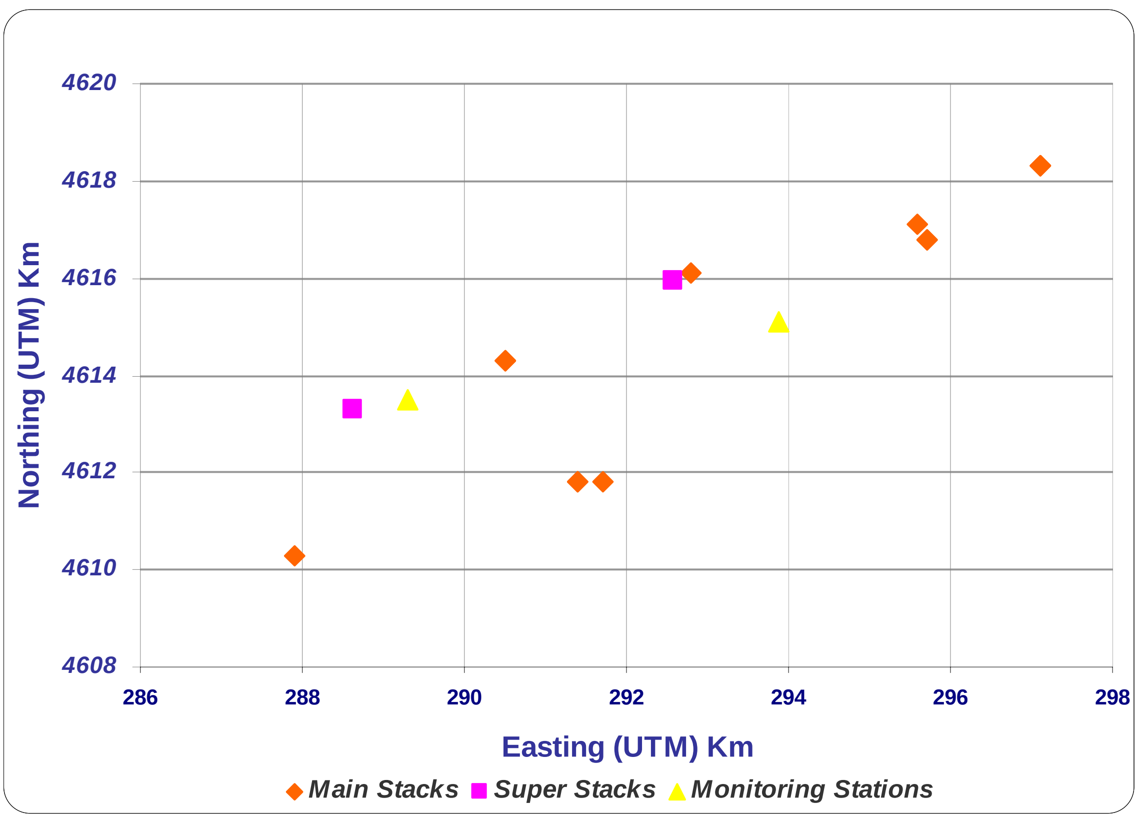

Figure 2.5: Monitor and Source Location for 1992

Chapter 3

MODEL EVALUATION

The study was conducted to evaluate the performance of the AERMOD in an urban area for predicting long-term concentrations. Four other EPA models (CALPUFF, ISCST2, ISCLT2, and SCREEN2) were included in this study. The ambient air mercury concentrations at eight air monitoring stations were used for comparisons. Results for ISCST2, ISCLT2 and SCREEN2 were taken from Patel and Kumar (1998). Comparison of models was done for both quarterly and annual averaging time period option for year 1990 to 1992 in Wayne County, Michigan. The performance of AERMOD, CALPUFF, ISCST2, ISCLT2, and SCREEN2 was evaluated general application as well as for regulatory application.

This thesis examined the performance of models for two different applications. The models were first examined in their ability to predict concentration at any receptor for a given averaging time. This was achieved by qualitative analysis and by the use of seven statistical parameters and the confidence limits on the statistical parameters. The next evaluation was for the use of models for regulatory work. Maximum concentrations are generally used to determine the worst case in regulatory work. This was achieved by calculating RHC for highest concentrations for each model. The conclusions were drawn using RHC values and Q-Q plots.

After the evaluation of all five selected models mentioned above, best models were used to standardize the minimum required meteorological run length time for the long (annual & quarterly) and short (1-hr, 3-hr, 8-hr & 24-hr)averaging time. For AERMOD, It was assumed that urban surface roughness length for whole grid was same as the monitoring station.

3.1 EVALUATION OF EPA'S MODELS FOR GENERAL APPLICATIONS

3.1.1 Graphical Evaluation

3.1.1.1 Quarterly Predicted vs. Observed Concentrations Results

Figure 3.1 through 3.3 represent the observed vs. predicted quarterly concentrations of mercury in Southeast Michigan, with the x-axis representing the corresponding ambient air monitoring stations and the y-axis representing mercury concentration in $\mu g/m^3$. Figure 3.1 shows the relative predictions of all five EPA's models for all three years respectively. Figure 3.2 depicts relative predictions of ISCLT2, ISCLT2, and SCREEN2, whereas Figure 3.3 depicts the relative predictions of AERMOD and CALPUFF. The plots show that SCREEN2 consistently over-predicted the concentrations. ISCST2 predictions were slightly under-predicted as the observed concentrations and ISCLT2 predictions were significantly under-predicted as the observed concentrations. AERMOD and CALPUFF predictions were found better than the ISCST2, ISCSLT2, and SCRREN2.

3.1.1.2 Annual Predicted vs. Observed Concentrations Results

Figure 3.4 through 3.6 represent the observed vs. predicted annual concentrations of mercury in Southeast Michigan, with the x-axis representing the corresponding ambient air monitoring stations and the y-axis representing mercury concentration in µg/m3. Figure 3.4 shows the relative predictions of all five EPA's models for all three years respectively. Figure 3.5 depicts relative predictions of ISCLT2, ISCLT2, and SCREEN2, whereas Figure 3.6 depicts the relative predictions of AERMOD and CALPUFF. The quantitative nature of predictions was almost similar to the quarterly concentration predictions with SCREEN2 consistently over-predicted the concentrations. ISCST2 predictions were slightly under-predicted as the observed concentrations and ISCLT2 predictions were under-predicted as the observed concentrations. AERMOD and CALPUFF predictions were again found better among the all other models.

Detailed results described with Q-Q plots in section 3.3 of this chapter also confirm the above observation.

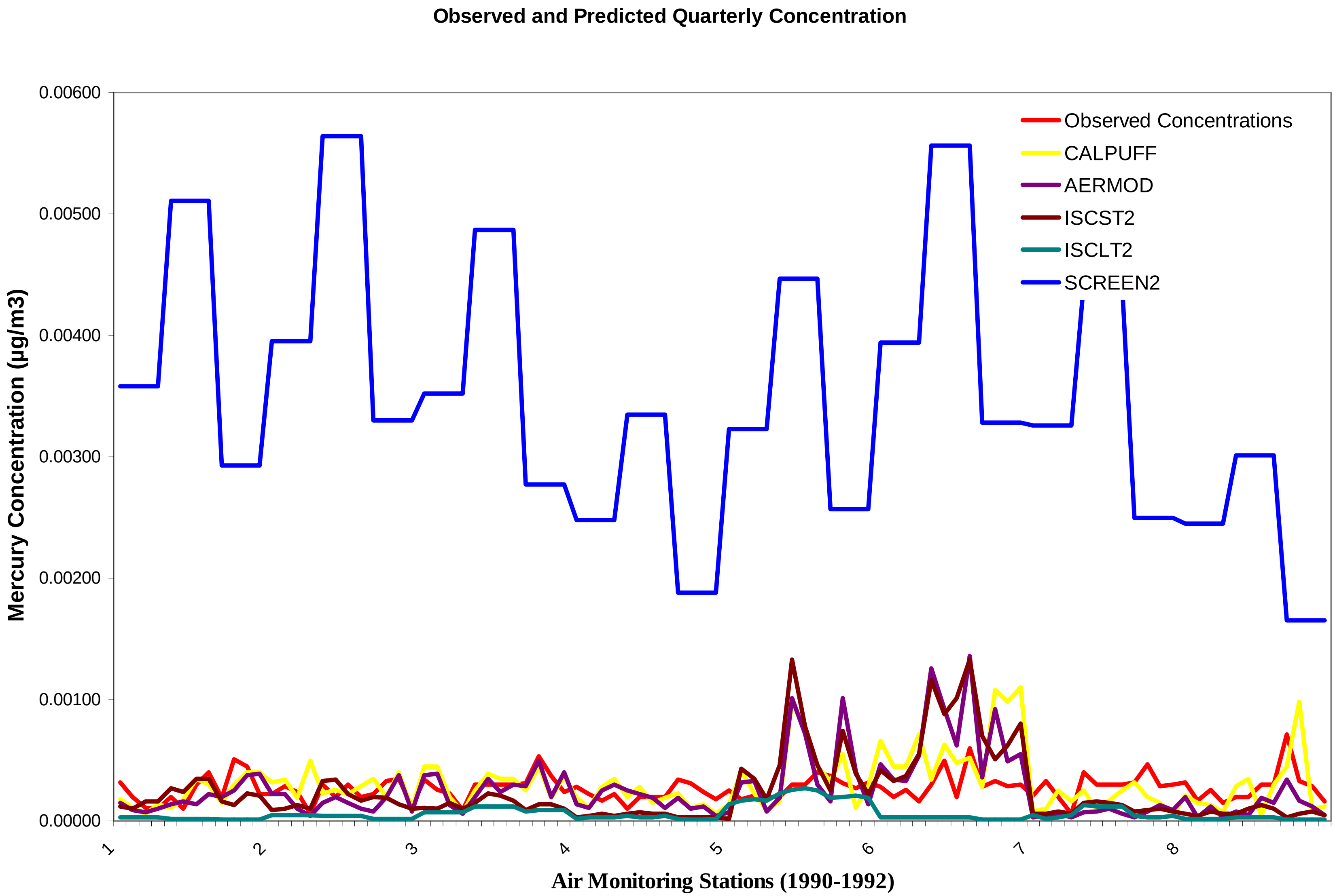

Figure 3.1: Comparison of Quarterly Observed vs. EPA' Model Predicted Mercury concentrations Quarterly Concentration for 1990 to 1992 in Southeast Michigan

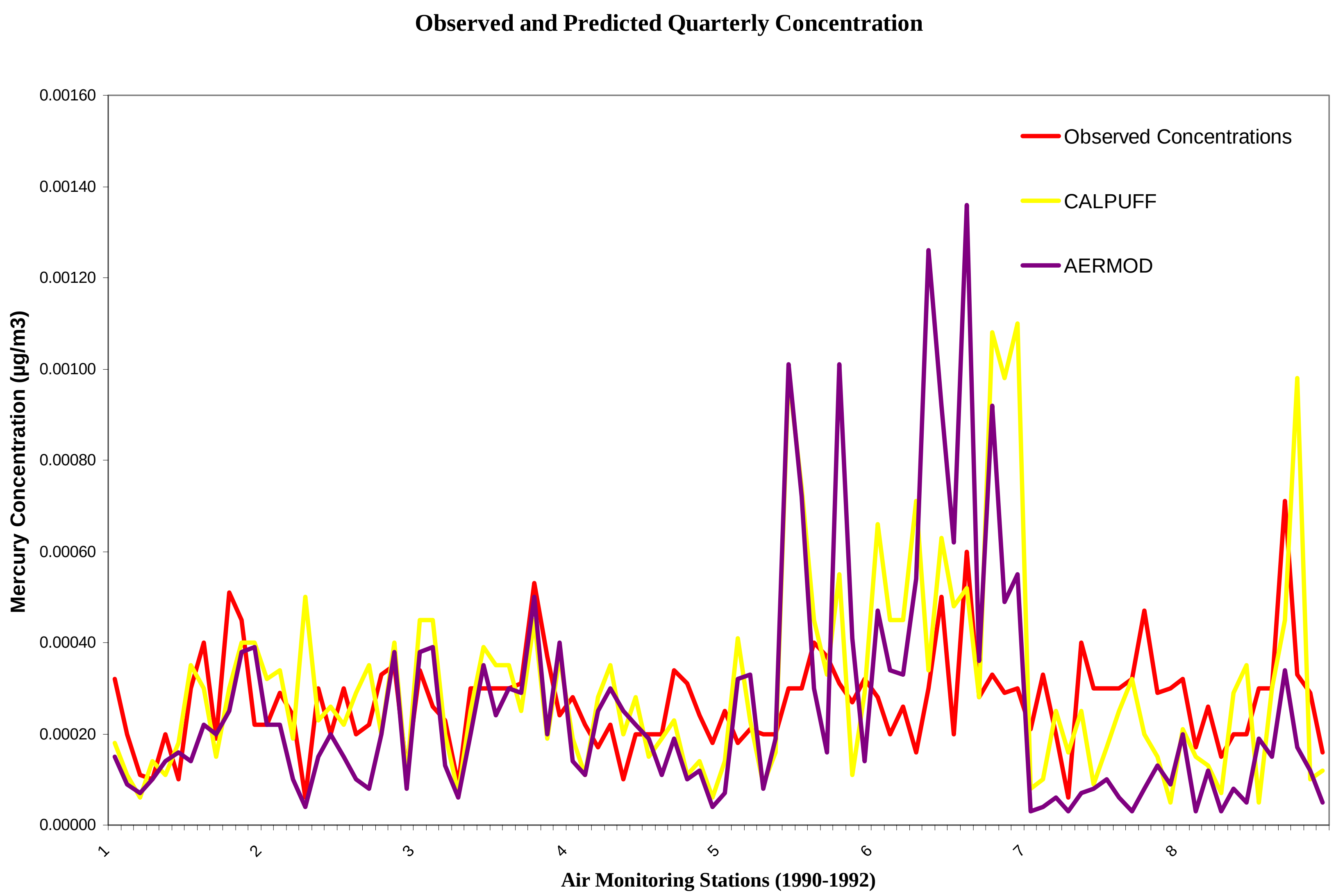

Figure 3.2: Comparison of Quarterly Observed vs. AERMOD & CALPUFF Mercury Concentrations (µg/m^3) for 1990 to 1992 in Southeast Michigan

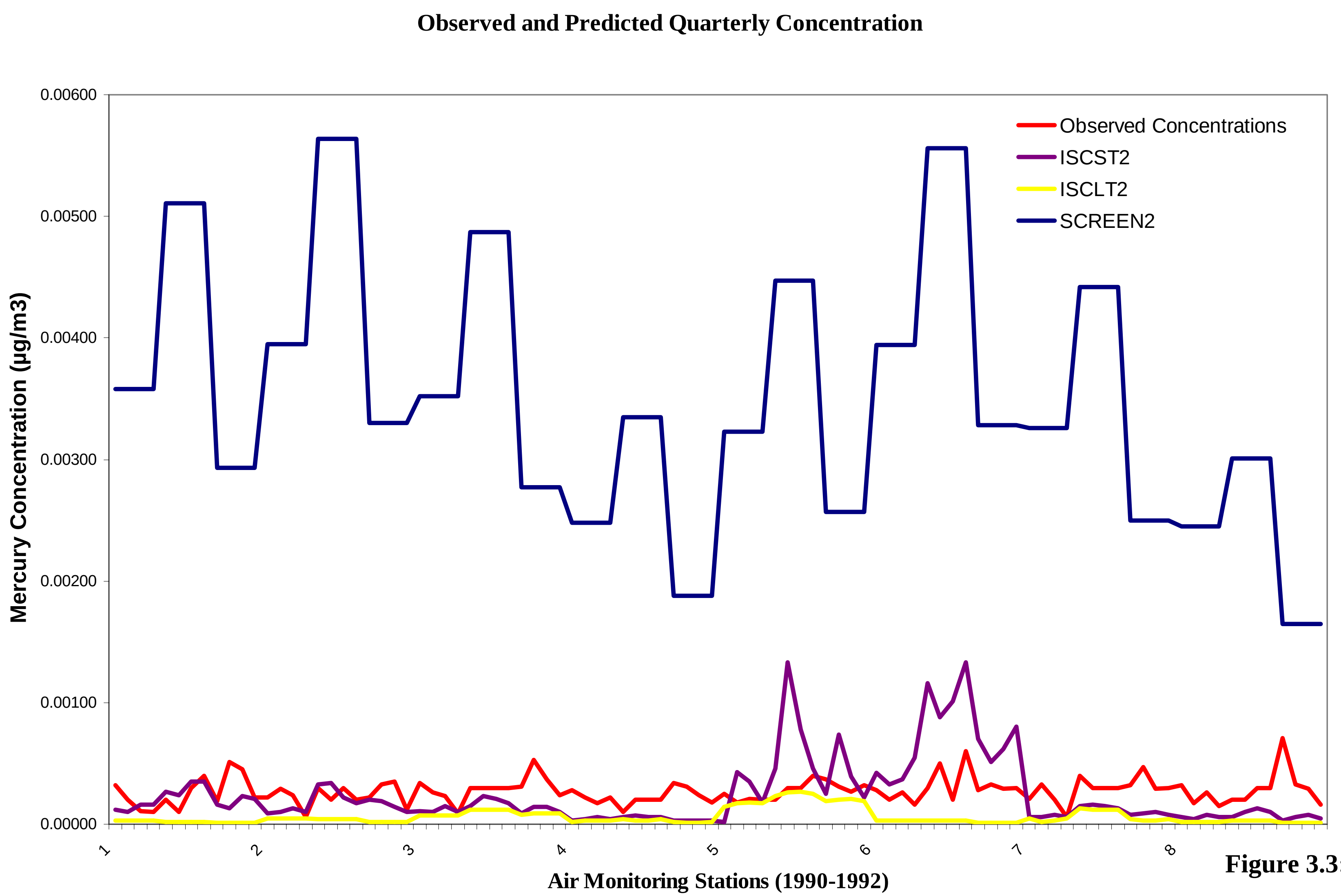

Figure 3.3: Comparison of Quarterly Observed vs. ISCST2, ISCLT2, & SCREEN2 Mercury Concentrations (µg/m^3) for 1990 to 1992 in Southeast Michigan

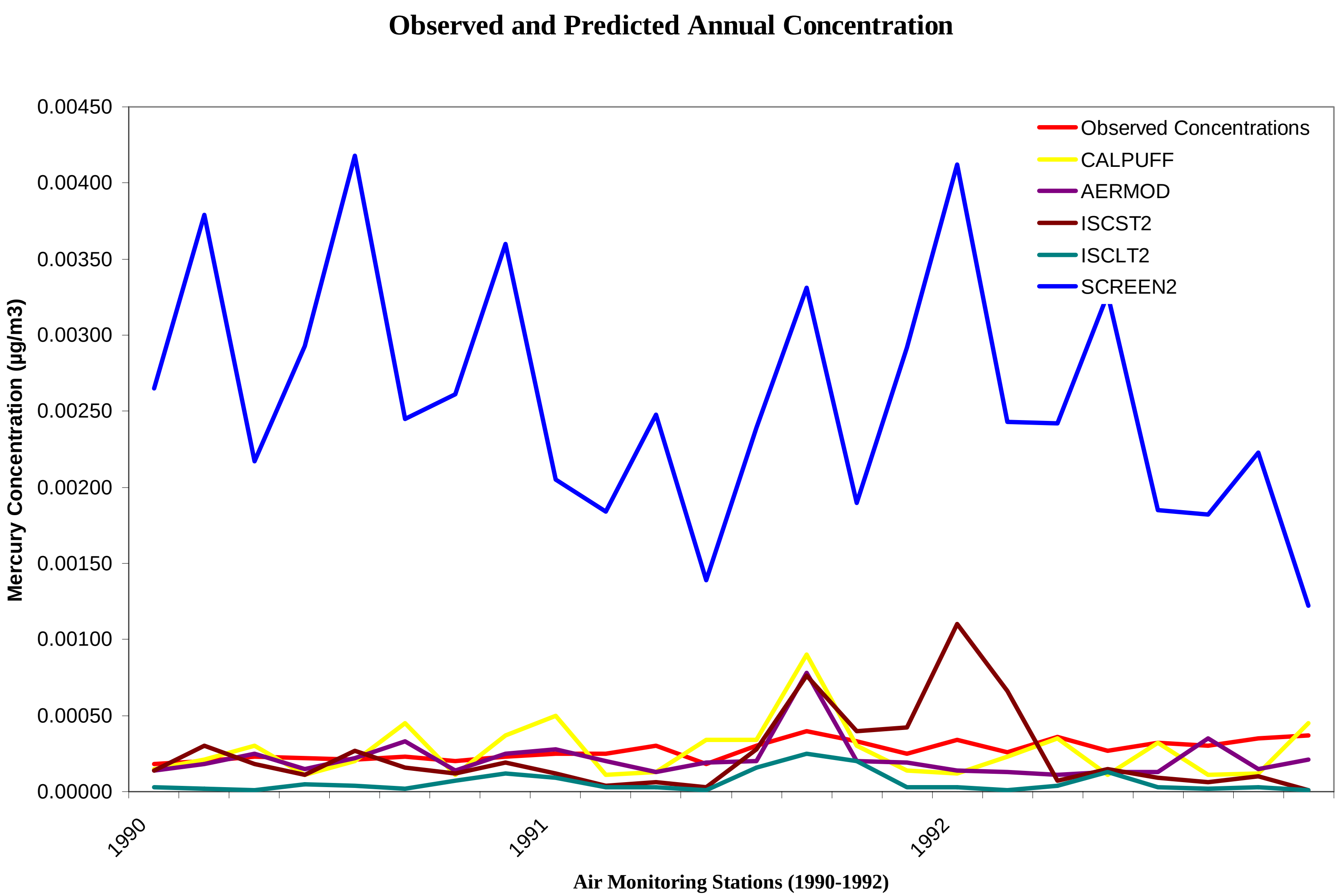

Figure 3.4: Comparison of Annual Observed vs. EPA' Model Predicted Mercury Concentrations (µg/m^3) for 1990 to 1992 in Southeast Michigan

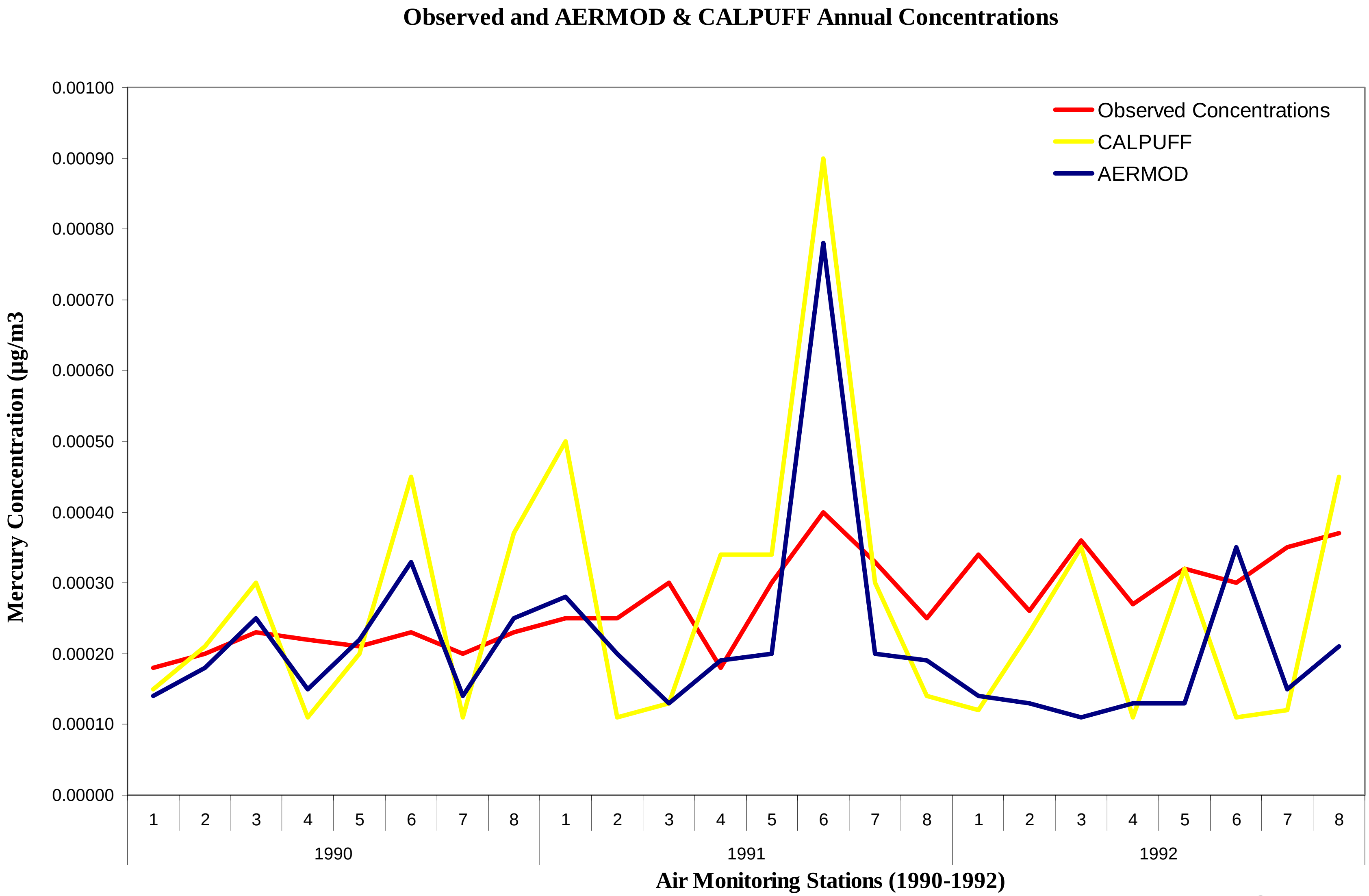

Figure 3.5: Comparison of Annual Observed vs. AERMOD & CALPUFF Mercury Concentrations (µg/m^3) for 1990 to 1992 in Southeast Michigan

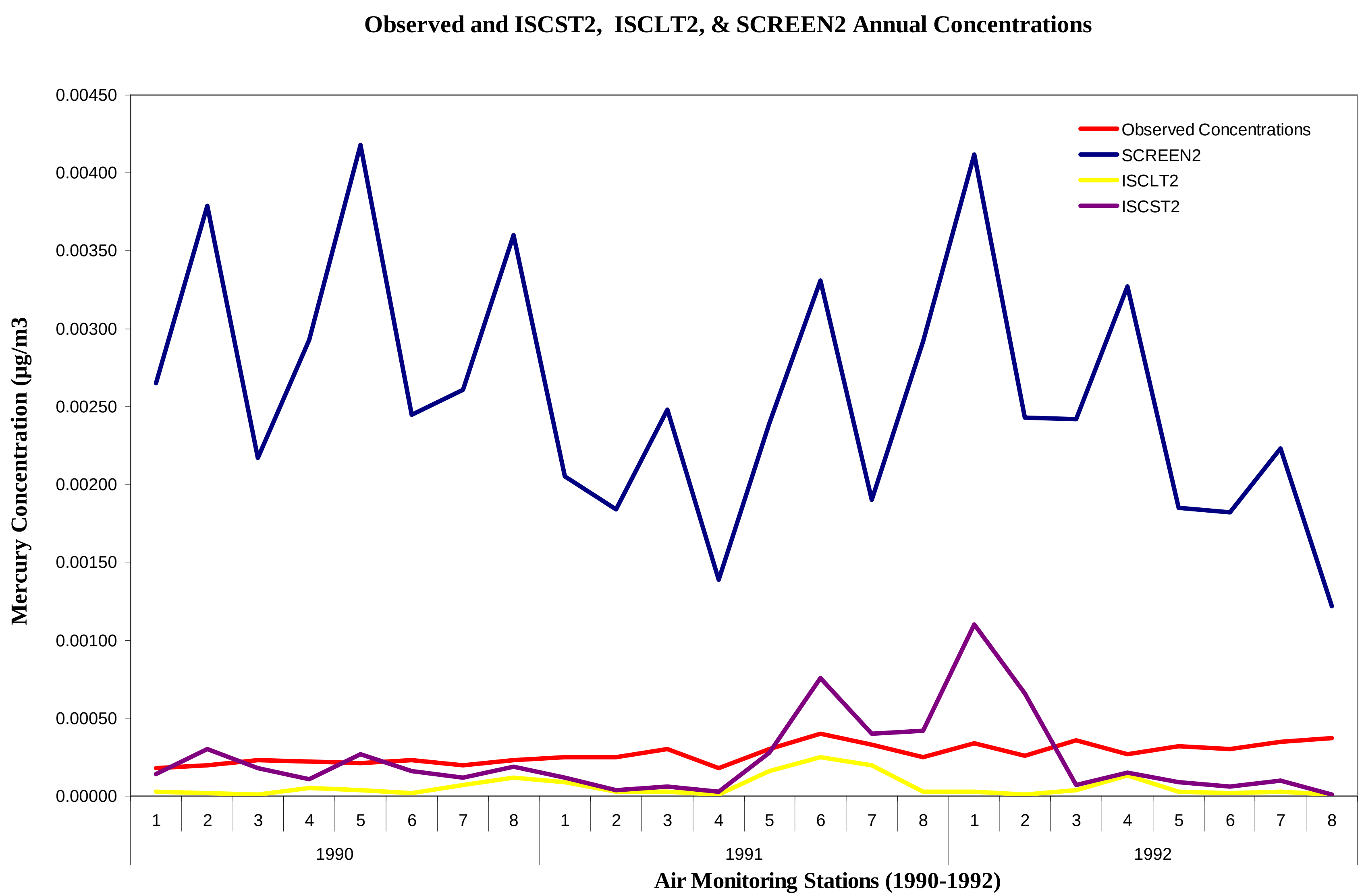

Figure 3.6: Comparison of Annual Observed vs. ISCST2, ISCLT2, & SCREEN2 Mercury Concentrations (µg/m^3) for 1990 to 1992 in Southeast Michigan

3.1.2 Statistical Parameters Evaluation

Quantitative model evaluation was performed by using seven statistical parameters such as fractional bias (FB), fractional variance (FS), normalized mean square error (NMSE), coefficient of correlation (r), and factor of two (Fa2), geometric mean variance (VG), and geometric mean bias (MG) (Kumar et al., 2006). Model performance measures are calculated using four observed concentration (Co) and predicted concentration (Cp) comparison:

- Straight Co and Cp, with no normalization;
- Considering Co/Co and Cp/Co, normalized by Co
- Considering Co/Co and Co/Cp, normalized by Cp
- Considering ln (Co) and ln (Cp).

The first option will result in an emphasis on the highest observed and/or predicted concentrations. The second option will result in an emphasis on the high outliers of Cp/Co. The third option will result in an emphasis on the high outliers of Co/Cp. The last option will result in a balanced emphasis over the entire range of observed and predicted values.

The quality of an ideal and perfect model is to have the fractional bias and the normalized mean square error equal to zero. The ideal value for geometric mean bias and geometric mean variance is one. No model is ideal or perfect. To determine if a model is good or acceptable, certain criteria are to be met. According to Chang and Hanna (2003), a model is acceptable if FB magnitude id ranging from -0.7 to +0.7, NMSE is less than about 0.4 and fraction of predictions within a factor of 2 (Fa2) is more than about 0.5. These criteria have to be relaxed if the points are paired in time and space.

To determine the reliability of the model, the criteria used are as set in a study by Kumar et al., (1993) and Ahuja and Kumar (1996). The performance of a model can be deemed acceptable if:

$$NMSE < 0.5$$

$$-0.5 < FB < +0.5$$

$$Fa2 > 0.8$$

$$0.75 < MG < +1.25$$

$$1.00 < VG < +1.25$$

The statistical significance of performance indicators was further tested by using a Bootstrap resampling method to estimate whether the calculated performance of FB, NMSE, VG, MG, Cor (r), and Fa2 are significantly different from zero for AERMOD, CALPUFF, and ISCST2 and whether the differences in their measure between pairs of models are significantly different from zero (to generate 95% confidence limits).

Evaluation was done for both annual and quarterly time period option. Table 3.1 shows the results for quarterly concentrations, and Table 3.2 shows the results for annual concentrations. The results for statistical parameters indicate an acceptable performance for AERMOD and CALPUFF models for some the above mentioned criteria. The quarterly results for NMSE did not give a satisfactory performance, however annual NMSE results indicated a satisfactory for both the models; FB results found good for both models; results for MG showed that CALPUFF was slightly better than AERMOD; however none of model met the Fa2 and VG criteria. Bootstrap resampling for 99.5 percentile value were supported for above mentioned results. Detailed results are further discussed in section 3.3.

The question to be answered is: ‘the AERMOD and CALPUFF models significant improvement over the competing models?’ The following conclusions were made using 95% confidence limits on NMSE, FB, correlation coefficient, log(VG), and log(MG) using bootstrap resampling method. The summaries of the confidence limit (to generate 95% confidence limits) are tabulated in Table 3.3 and Table 3.4. Results show that NMSE is significantly different from zero for AERMOD and CALPUFF, whereas correlation of r and FB is not significantly different from zero for AERMOD and CALPUFF.

Table 3.1: Performance Measures obtain by Bootstrap Resampling Method for Quarterly Averaging period

Model	NMSE	Cor (r)	Fa2	FB	FS
(1) By Straight Co and Cp i.e. with no Normalization					
AERMOD	0.82	0.386	0.583	0.045	-0.826
CALPUFF	0.60	0.281	0.740	-0.127	-0.707
ISCST2	1.15	0.230	0.417	0.117	-0.876
ISCLT2	3.56	0.064	0.156	1.265	0.515
SCREEN2	12.13	-0.003	0.000	-1.711	-1.630
(2) By Considering Co/Co and Cp/Co i.e. Normalization by Co					
AERMOD	0.71	--	0.583	0.038	--
CALPUFF	1.01	--	0.740	-0.225	--
ISCST2	1.00	--	0.417	0.061	--
ISCLT2	2.46	--	0.156	1.191	--
SCREEN2	20.32	--	0.000	-1.759	--
(3) By Considering Co/Co and Co/Cp i.e. Normalization by Cp					
AERMOD	2.05	--	0.583	0.653	--
CALPUFF	0.81	--	0.740	0.257	--
ISCST2	4.86	--	0.417	0.915	--
ISCLT2	21.42	--	0.156	1.652	--
SCREEN2	9.65	--	0.000	-1.681	--
(4) By Considering ln(Co) and ln(Cp)					
Model	VG		Fa2	MG	FS
AERMOD	2.18	--	0.510	1.430	--
CALPUFF	1.61	--	0.708	1.027	--
ISCST2	3.40	--	0.375	1.680	--
ISCLT2	87.58	--	0.156	6.398	--
SCREEN2	1102.92	--	0.000	0.075	--

Table 3.2: Performance Measures obtain by Bootstrap Resampling Method for Annual Averaging period

Model	NMSE	Cor (r)	Fa2	FB	FS
(1) By Straight Co and Cp i.e. with no Normalization					
AERMOD	0.33	0.31	0.75	0.23	-0.73
CALPUFF	0.38	0.38	0.71	0.01	-0.97
ISCST2	0.94	0.29	0.54	0.12	-1.22
ISCLT2	3.00	0.36	0.17	1.27	-0.02
SCREEN2	8.50	-0.16	0.00	-1.62	-1.71
(2) By Considering Co/Co and Cp/Co i.e. Normalization by Co					
AERMOD	0.22	--	0.75	0.21	--
CALPUFF	0.32	--	0.71	0.00	--
ISCST2	0.73	--	0.54	0.13	--
ISCLT2	3.00	--	0.17	1.29	--
SCREEN2	9.91	--	0.00	-1.64	--
(3) By Considering Co/Co and Co/Cp i.e. Normalization by Cp					
AERMOD	0.48	--	0.75	0.41	--
CALPUFF	0.57	--	0.71	0.34	--
ISCST2	15.84	--	0.54	1.15	--
ISCLT2	15.45	--	0.17	1.64	--
SCREEN2	6.65	--	0.00	-1.58	--
(4) By Considering ln(Co) and ln(Cp)					
Model	**VG**		**Fa2**	**MG**	**FS**
AERMOD	1.35	--	0.71	1.37	--
CALPUFF	1.45	--	0.67	1.19	--
ISCST2	4.44	--	0.50	1.80	--
ISCLT2	94.71	--	0.17	6.89	--
SCREEN2	171.83	--	0.00	0.11	--

Table 3.3: Performance obtained by Bootstrap Resampling Method for Quarterly Averaging Time

Each Model							Among Models						
Model	NMSE		FB		Cor (r)		Model	D(NMSE)		D(FB)		D[Corr. (r)]	
	Yes	No	Yes	No	Yes	No		Yes	No	Yes	No	Yes	No
(1) By Straight Co and Cp i.e. with no Normalization							**(1) By Straight Co and Cp i.e. with no Normalization**						
CALPUFF	X			X	X		CALPUFF-AERMOD		X	X			X
AERMOD	X			X	X		AERMOD-ISCST2	X			X	X	
ISCST2	X			X		X	CALPUFF- ISCST2	X		X			X
(2) By Considering Co/Co and Cp/Co i.e. Normalization by Co							**(2) By Considering Co/Co and Cp/Co i.e. Normalization by Co**						
CALPUFF	X		X		–	–	CALPUFF-AERMOD		X	X		–	–
AERMOD	X			X	–	–	AERMOD-ISCST2	X			X	–	–
ISCST2	X			X	–	–	CALPUFF- ISCST2		X	X		–	–
(3) By Considering Co/Co and Co/Cp i.e. Normalization by Cp							**(3) By Considering Co/Co and Co/Cp i.e. Normalization by Cp**						
CALPUFF	X		X		–	–	CALPUFF-AERMOD	X		X		–	–
AERMOD	X		X		–	–	AERMOD-ISCST2		X		X	–	–
ISCST2	X		X		–	–	CALPUFF- ISCST2	X		X		–	–
(4) By Considering ln(Co) and ln(Cp)							**(4) By Considering ln(Co) and ln(Cp)**						
Model	Log (VG)		Log (MG)		Cor (r)		**Model**	D[Log (VG)]		D[Log (MG)]		D[Corr. (r)]	
	Yes	No	Yes	No	Yes	No		Yes	No	Yes	No	Yes	No
CALPUFF	X			X	–	–	CALPUFF-AERMOD	X		X		–	–
AERMOD	X		X		–	–	AERMOD-ISCST2		X		X	–	–
ISCST2	X		X		–	–	CALPUFF- ISCST2	X		X		–	–

Note: Yes- Indicates significantly different from zero. No- Indicates not significantly different from zero.

Table 3.4: Performance obtained by Bootstrap Resampling Method for Annual Averaging Time

Each Model							Among Models						
Model	NMSE		FB		Cor (r)		Model	D(NMSE)		D(FB)		D[Corr. (r)]	
	Yes	No	Yes	No	Yes	No		Yes	No	Yes	No	Yes	No
(1) By Straight Co and Cp i.e. with no Normalization							**(1) By Straight Co and Cp i.e. with no Normalization**						
CALPUFF	X			X		X	CALPUFF-AERMOD		X	X			X
AERMOD	X			X		X	AERMOD-ISCST2	X			X		X
ISCST2	X			X		X	CALPUFF- ISCST2	X			X		X
(2) By Considering Co/Co and Cp/Co i.e. Normalization by Co							**(2) By Considering Co/Co and Cp/Co i.e. Normalization by Co**						
CALPUFF	X			X	–	–	CALPUFF-AERMOD		X	X		–	–
AERMOD	X		X		–	–	AERMOD-ISCST2	X			X	–	–
ISCST2	X			X	–	–	CALPUFF- ISCST2	X			X	–	–
(3) By Considering Co/Co and Co/Cp i.e. Normalization by Cp							**(3) By Considering Co/Co and Co/Cp i.e. Normalization by Cp**						
CALPUFF	X		X		–	–	CALPUFF-AERMOD		X		X	–	–
AERMOD	X		X		–	–	AERMOD-ISCST2		X	X		–	–
ISCST2		X	X		–	–	CALPUFF- ISCST2		X	X		–	–
(4) By Considering ln(Co) and ln(Cp)							**(4) By Considering ln(Co) and ln(Cp)**						
Model	Log (VG)		Log (MG)		Cor (r)		**Model**	D[Log (VG)]		D[Log (MG)]		D[Corr. (r)]	
	Yes	No	Yes	No	Yes	No		Yes	No	Yes	No	Yes	No
CALPUFF	X			X	–	–	CALPUFF-AERMOD		X		X	–	–
AERMOD	X		X		–	–	AERMOD-ISCST2	X			X	–	–
ISCST2	X		X		–	–	CALPUFF- ISCST2		X		X	–	–

Note: Yes- Indicates significantly different from zero. No- Indicates not significantly different from zero.

3.2 EVALUATION OF EPA'S MODELS FOR REGULATORY APPLICATIONS

3.2.1 Robust Highest Concentration (RHC) Evaluation

First regulatory analysis was assessed by RHC (Cimorelli et al., 2005 and Cox & Tikvart, 1990). The RHC represents a smoothed estimate of the highest concentrations based on an exponential fit to the upper end of the concentration distribution:

$$\mathbf{RHC = X\{n\} + (X-X\{n\}) \ln[(3n-1)/2]}$$

Where,

n = number of values used to characterize the upper end of the concentration distribution,

X = average of the (n-1) largest values, and

X{n} = n^{th} largest value;

For most evaluation comparisons, a value of n is suggested to be 26 (Cox and Tikvart, 1990). RHC is a preferred statistic because it yields a representative high-end estimate while mitigating the undue influence of individual unusual events. In summary, for regulatory applications, a good model would produce a concentration distribution parallel to the slope of the measured distribution and produce high-end concentrations (RHCs) that are similar to that of the observations.

Table 3.5 summarizes the ratio of modeled to observed RHC values for AERMOD, CALPUFF, ISCST2, ISCLT2, and SCREEN2. For quarterly averaging time, number of observation (n) were divided into three categories (26, 50, and 96).

On the RHC values, overall the performance for AERMOD and CALPUFF were better than among all the models. AERMOD and CALPUFF both performed well in all studies with RHC ratios of 0.96-2.15 and 1.35-2.01 respectively. SCREEN2 was consistently high and ISCLT2 was consistently low, in their estimates. However, ISCST2 performances were close to AERMOD and CALPUFF.

Table 3.5: Ratio of modeled to observed robust highest concentration for mercury concentration for Wayne County, Michigan

Time Period	No. of observations	Ratio of modeled to observed robust highest concentrations				
		AERMOD	CALPUFF	ISCST2	ISCLT2	SCREEN2
Quarterly	26	2.04	1.93	2.47	0.60	12.12
	50	2.15	2.01	2.25	0.57	13.23
Annual	24	0.96	1.35	1.67	0.38	12.05

3.2.2 Quantile-Quantile (Q-Q) Plot Evaluation

A Q-Q plot is a plot of quantiles of first data set against the quantiles of the second data set. Concentration distribution can be readily assessed with Q-Q plots (Chamber et al., 1983) that are created by ranking the predicted and observed concentrations and then pairing by rank. Specifically, a good model will have a slope in the plot similar to that of the 1:1 line.

Figure 3.7 depicts the Q-Q plot of model-predicted vs observed for quarterly averaging and figure 3.8 depicts Q-Q plot of model-predicted vs observed for annual averaging time for mercury concentration in Wayne County, Michigan. All Q-Q plots reflect a dropoff in modeled distribution for low concentration. For both time periods, figures show that SCREEN2 consistently over-predicted the concentrations. ISCST2 predictions were slightly under-predicted as the observed concentrations, and ISCLT2 predictions were significantly under-predicted as the observed concentrations. Again

AERMOD and CALPUFF predictions found better than ISCST2, ISCLT2, and SCREEN2.

Graphical representation and Q-Q plots both indicate that AERMOD and CALPUFF performed better than the other EPA's models. Q-Q plots are simple ranked pairings of predicted and observed concentrations, such that any given quantile of the predicted concentration is plotted against the same quantile of the observed concentration. A solid line has been added to the Q-Q plots to indicate an unbiased prediction and two dotted lines have been added to indicate a factor of two under- and over-prediction. Q-Q plots show that model' quarterly concentration distribution was in an agreement with the observed only for lower end concentration maxima. Both of the models, AERMOD and CALPUFF, tend to under-estimate for lower group of concentration, and over-predict for higher group of concentration. The concentration results parallel the 1-1 line below 0.00025 $\mu g/m^3$, until the observed concentration exceed the 0.30000 $\mu g/m^3$. For annual averaged, concentration distribution was a close agreement with the observed, except for few top values, which was over-predicted by both models. Also it appears that AERMOD model has a tendency to under-predict the concentration for annual averaging time. RHC values support the Q-Q plot results. The quarterly RHC results indicate an over-prediction for both model AERMOD (2.04-2.15) and CALPUFF (1.93-2.01), whereas annual RHC results a slightly under-prediction for AERMOD (0.96) and a slightly over-prediction for CALPUFF (1.35).

Results were discussed thoroughly in section 3.3. A sample program for Q-Q plot is attached in Appendix A.

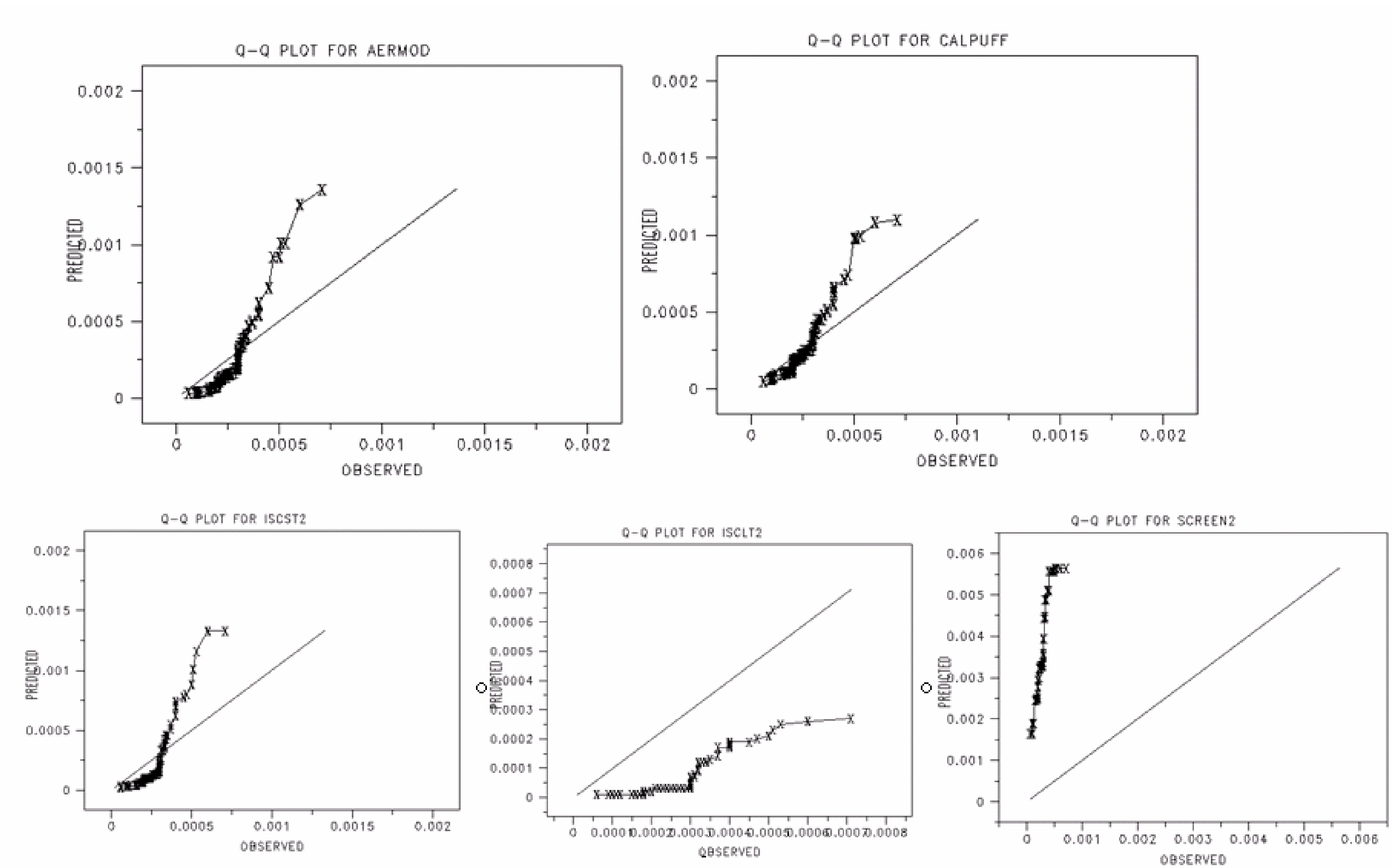

Figure 3.7: Q-Q Plots of Model-Predicted vs Observed Quarterly Averaging Mercury Concentration (µg/m^3) for Wayne County, Michigan

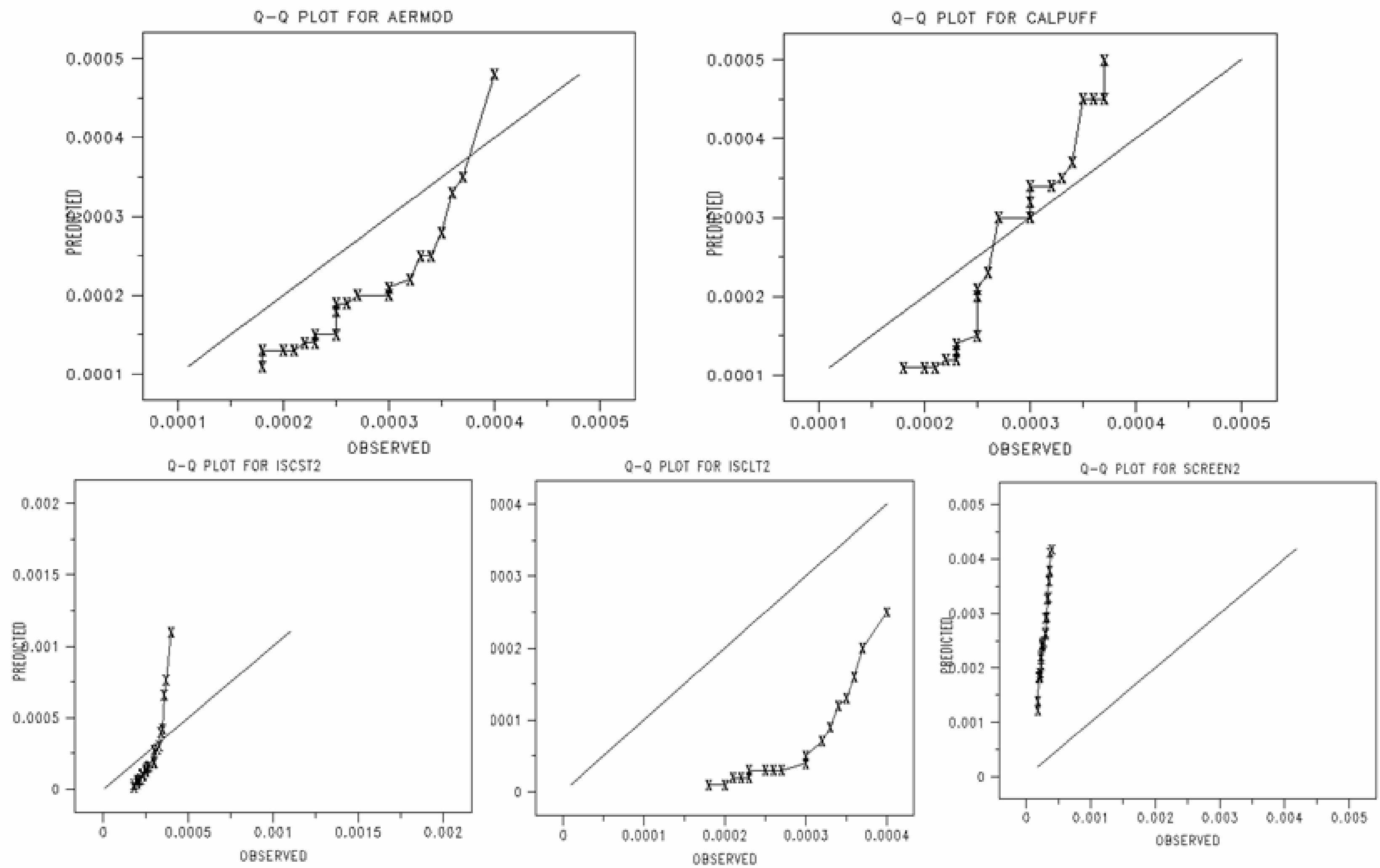

Figure 3.8: Q-Q Plots of Model-Predicted vs Observed Annual Averaging Mercury Concentration (µg/m^3) for Wayne County, Michigan

3.3 EVALUATION RESULTS FOR EPA'S MODELS

3.3.1 Evaluation Results for General Application

- The Results shown figures 3.1 to 3.6 indicate that SCREEN2 consistently over-predicted concentrations and ISCLT2 consistently under-predicted concentrations for both averaging time periods. Overall, performance for AERMOD and CALPUFF were found to be better among all models.
- NMSE: The AERMOD and CALPUFF both showed a significant improvement over all the others models for annual and quarterly averaging period (Table 3.1 and Table 3.2).
- FB: The AERMOD and CALPUFF again showed an acceptable performance and approach to an ideal value (Table 3.1 and Table 3.2).
- MG: The refined model, CALPUFF, showed the overall best performance among all regulatory models; however, performance of AERMOD was satisfactory (Table 3.1 and Table 3.2).
- VG & Fa2: None of the models met the desired criteria; however, AERMOD and CALPUFF showed better performance as compared to all other models (Table 3.1 and Table 3.2).
- All four observed concentration (Co) and predicted concentration (Cp) comparisons give different values for all statistical parameters. However, overall conclusions on model predictions are the same (Table 3.1 and Table 3.2).
- The confidence interval on normalizes mean square error (NMSE), fractional bias (FB), Correlation coefficient (r), geometric mean variance (VG), and geometric

mean bias (MG) implies that the results for CALPUFF and AERMOD are not significantly different from zero for FB and correlation of r (Table 3.3 and Table 3.4).

- The inter-comparison between the models shows that AERMOD and CALPUFF results were not significantly different from each other (Table 3.3 and Table 3.4).

3.4.2 Evaluation Results for Regulatory Application

- For quarterly averaging time, SCREEN2 over-estimated the concentration with a high value of RHC ratios. ISCSLT2 estimated low RHC ratios, which shows concentration was under-estimated by ISCLT2. However, ISCST2 (1.02 and 2.47), AERMOD (2.04 and 2.15), and CALPUFF (1.930 and 2.01) displayed a considerable over-prediction.
- For annual averaging time, SCREEN2 was consistently high in estimates of RHC ratio 12.05. ISCLT2 estimation was again very low, with RHC ratio 0.38. AERMOD performed well with RHC ratio of 0.96. This is a satisfying result (i.e., AERMOD is very capable of estimating the important regulatory concentration). CALPUFF also gives a satisfactory performance with RHC ratio 1.35.
- For quarterly annual averaging time, Q-Q plots show slope of each model concentration distribution from a lower concentration to higher concentration. The concentration distribution slope for SCREEN2 is very high because of its tendency to estimate the worst case scenario. Concentration distribution slope for ISCLT2 is very low, because it is under-estimating the concentration. The slope of ISCST2 concentration distribution shows a high slope. For AERMOD and CALPUFF, results were parallel to 1-1 line up to certain extent; however, for

higher end of concentration maxima, both models over-estimated the observed concentration. This means that the AERMOD and CALPUFF predictions were able to reproduce the distribution similar to observed distribution for low concentration values.

- For annual averaging time, nature of Q-Q plots for SCREEN2 and ISCLT2 were almost similar to quarterly averaging time period with concentration distribution slope for SCREEN2 slope is very high and ISCLT2 is very low. However, concentration distribution slope for ISCST2 is very high as compared to quarterly averaging time period. AERMOD and CALPUFF show a satisfactory performance with combination of under-prediction and over-prediction over the 1-1 line. This shows that the AERMOD and CALPUFF prediction were able to reproduce the distribution similar to observed distribution except for the top value.

On the basis of general and regulatory application evaluations, AERMOD and CALPUFF models were found to be the best among the five EPA's regulatory models; therefore AERMOD and CALPUFF are used for calculating the minimum required meteorological-run-length time for different averaging time intervals.

The following are the possible reasons for not having an ideal performance:

- 7 to 8 % mercury emissions were not considered in modeling.
- Building downwash was not considered.
- Variation in mercury from quarter to quarter is assumed constant.

- All mercury was assumed to be in gaseous form for modeling.
- There may be an error in the reported values of emissions.

Year 1990 emission data was used to check the impact of error in emission inventories. Base (original) emission data varied in four sub-categories (75%, 50%, 125% and 150%) of emissions for additional modeling. The predicted concentrations were obtained for each case. Figure 4.8 compares the Cp/Co with five subcategories of emission inventories and visualizes the model performance of all five categories of emission inventories with four statistical parameters (NMSE, FS, Fa2 and FS). Figure 4.8 depicts, if emission rates are being under-predicted, model performance suffers.

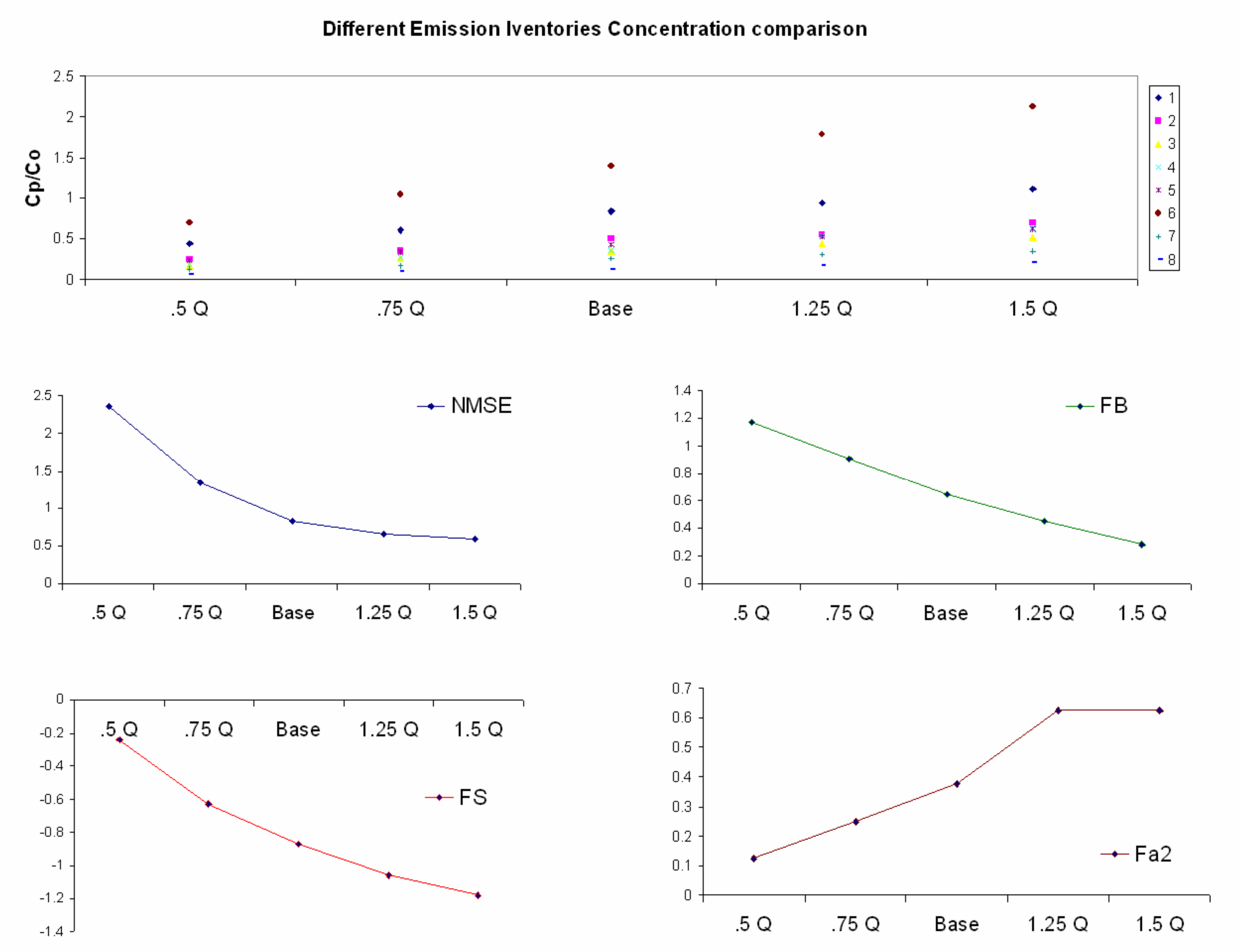

Figure 3.11: Model Performance for five Sub-Categories of Emission Inventories

Chapter 4

METEOROLOGICAL RUN LENGTH ANALYSIS

After in-depth analysis among five selected models mentioned earlier, CALPUFF and AERMOD were proved better than the other model used in the study. Hence only AERMOD & CALPUFF were used to examine the minimum required meteorological-run-length time for long-term (quarterly and annual) periods and short-term (1-hr, 3-hr, 8-hr, and 24-hr) periods. The selected models (AERMOD & CALPUFF) were run using the two pollutants emission inventory data for the selected base years (1990-1992) to predict the ground level-concentration. Using the base year emission inventory and the respective years' meteorological data, predicted concentrations were obtained for 29 consecutive years (1961-1989). This procedure accounted for the meteorological trends during each year of the study period. The impacts of the variation in concentration of pollutants were evaluated by examining the under-predicted periods for each year time interval. The results were used to obtain the required run-length of meteorological data for different averaging time.

4.1 PROCEDURE FOR OBTAINING THE METEOROLIGAL-RUN-LENGTH TIME

First each model (AERMOD and CALPUFF) was run for each of the three years (1990-1992) using the respective year emission inventory and meteorological data. These predicted results will be referred to as "*Base Year Predicted Concentration*" in upcoming chapters. For example, if AERMOD was run for predicting the year 1990 concentration using year 1990 emission inventories and meteorological data, then these results are mentioned as "*1990 year Predicted Concentration*". Annual average predicted base concentration for all three base years (1990-1992) predicted by AERMOD are shown in Table 4.1.

Table 4.1 Annual Average Predicted Base Mercury Concentrations (μg/m^3) for base year 1990, 1991, and 1992 for Wayne County, Michigan

Annual Averaged Predicted Base Concentration (μg/m^3) Results			
Monitoring Stations	**YEAR**		
	1990	**1991**	**1992**
1	0.00014	0.00028	0.00014
2	0.00009	0.00020	0.00013
3	0.00008	0.00007	0.00004
4	0.00009	0.00019	0.00013
5	0.00009	0.00020	0.00013
6	0.00033	0.00078	0.00035
7	0.00006	0.00009	0.00006
8	0.00004	0.00004	0.00002

Predicted concentration results were again obtained for all monitoring stations for 29 consecutive years (1961-1989) keeping the same base year emission inventories and by just changing the meteorological data for each multiple year through running respective model. These concentration results are referred to as "*Year Based Multiple Year Concentration*" in the upcoming chapters. For example, after getting the base predicted concentration for year 1990 from AERMOD, only the AERMET was run by changing the 29 consecutive years meteorological data, keeping all other pathways same in the AERMOD, and therefore these concentration results are referred to as "*1990 Based Multiple Year Concentration*". Annual average multiple year concentrations for all three base years (1990-1992) predicted by AERMOD model are shown in Table 4.2.

The multiple years predicted concentrations from the models were then grouped according to the variable meteorological length of the 5 year, 10 year, 15 year, 20 year, and 25 years time interval. The maximum concentration corresponding to each of these cluster periods was obtained. For instance, for running 5-year time interval, maximum values were obtained for each class (1961-1965, 1962-1966…, 1985-1989) for all monitoring stations from the multiple year concentrations, and then these maximum values were compared with the base year predicted concentration. If maximum concentration was less than the base predicted concentration, then it was referred as an under-predicted period. Finally, the numbers of under-predicted periods were counted for each meteorological length time interval.

Maximum values for annual average predicted concentration over the 5-year interval using AERMOD model is shown in Table 4.3. As mentioned above, these maximum multiple year concentration were then compared with base predicted value to obtain the number of under-predicted periods. The under-predicted periods are shown in the yellow shaded area in the table. Finally, numbers of under-predicted periods were counted to analyze the required length of meteorological run length time. Table 4.4, 4.5, 4.6, 4.7 are shown for 10-year, 15-year, 20-year, and 25-year intervals, respectively.

Most of the time, AERMOD and CALPUFF models under-predicted as compared to the observed concentration that is why multiple year maximum concentrations were compared with base predicted concentrations instead of with observed concentrations. Quantitative value of the under-predicted period represents how many times that particular year-interval failed to predict the worst case scenario from the base predicted concentration. A high numeric value for the under-predicted period demonstrates that selected year-interval is not sufficient for that particular averaging time period, and recommends for a higher year-interval period.

The same procedure was again followed for obtaining the numbers of under-predicted periods for quarterly, 1-hr, 3-hr, 8-hr and 24-hr averaging time periods. Results were obtained for both pollutants (mercury and sulfur dioxide) using AERMOD and CALPUFF. Results for mercury predicted by AERMOD and CALPUFF model were discussed in section 4.4. All other results are mentioned in appendix C.

Table 4.2: Annual Average Predicted Multiple Year Mercury Concentrations (μg/m^3) Results by AERMOD for Wayne County, MI

Annually Averaged Predicted Multiple Year Concentration (μg/m^3) Results (Table Values * 10^{-3})																								
Year	**Monitoring Station**																							
	1			**2**			**3**			**4**			**5**			**6**			**7**			**8**		
	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992
1961	0.11	0.22	0.13	0.10	0.20	0.12	0.06	0.09	0.05	0.07	0.14	0.08	0.12	0.25	0.15	0.30	0.70	0.42	0.06	0.08	0.05	0.03	0.04	0.02
1962	0.11	0.23	0.14	0.12	0.25	0.15	0.06	0.09	0.05	0.08	0.15	0.09	0.14	0.30	0.18	0.28	0.65	0.39	0.06	0.10	0.06	0.03	0.04	0.02
1963	0.14	0.29	0.17	0.09	0.17	0.10	0.07	0.08	0.05	0.07	0.14	0.08	0.10	0.19	0.11	0.34	0.79	0.48	0.06	0.09	0.05	0.03	0.04	0.02
1964	0.15	0.32	0.19	0.09	0.17	0.10	0.06	0.07	0.05	0.08	0.15	0.09	0.10	0.21	0.12	0.34	0.81	0.49	0.04	0.07	0.04	0.04	0.05	0.03
1965	0.13	0.28	0.17	0.10	0.21	0.13	0.06	0.08	0.05	0.08	0.15	0.09	0.12	0.26	0.16	0.32	0.74	0.45	0.04	0.07	0.04	0.04	0.04	0.02
1966	0.13	0.28	0.17	0.09	0.17	0.10	0.05	0.07	0.04	0.07	0.14	0.08	0.11	0.22	0.13	0.29	0.68	0.41	0.05	0.07	0.04	0.04	0.04	0.02
1967	0.13	0.28	0.17	0.09	0.17	0.10	0.06	0.08	0.05	0.08	0.17	0.10	0.11	0.23	0.14	0.34	0.81	0.49	0.04	0.06	0.04	0.04	0.05	0.02
1968	0.12	0.26	0.15	0.08	0.16	0.10	0.07	0.08	0.05	0.07	0.14	0.08	0.10	0.21	0.12	0.32	0.75	0.45	0.04	0.06	0.03	0.03	0.04	0.02
1969	0.12	0.26	0.15	0.11	0.22	0.13	0.06	0.09	0.05	0.09	0.18	0.11	0.14	0.29	0.17	0.28	0.64	0.39	0.05	0.08	0.04	0.04	0.04	0.02
1970	0.14	0.31	0.18	0.11	0.22	0.13	0.06	0.08	0.05	0.08	0.15	0.09	0.13	0.28	0.17	0.30	0.70	0.43	0.05	0.08	0.05	0.04	0.04	0.02
1971	0.12	0.26	0.16	0.09	0.17	0.10	0.05	0.07	0.04	0.08	0.15	0.09	0.11	0.22	0.13	0.28	0.65	0.40	0.04	0.07	0.04	0.03	0.04	0.02
1972	0.12	0.27	0.16	0.08	0.17	0.10	0.06	0.07	0.04	0.10	0.21	0.13	0.10	0.20	0.12	0.30	0.70	0.42	0.05	0.07	0.04	0.04	0.05	0.03
1973	0.15	0.32	0.19	0.09	0.19	0.11	0.05	0.07	0.04	0.09	0.19	0.11	0.11	0.23	0.14	0.33	0.77	0.46	0.05	0.08	0.05	0.04	0.05	0.03
1974	0.17	0.38	0.23	0.09	0.18	0.11	0.06	0.07	0.04	0.10	0.20	0.12	0.10	0.21	0.12	0.34	0.79	0.48	0.05	0.08	0.05	0.05	0.06	0.03
1975	0.13	0.28	0.17	0.09	0.19	0.11	0.06	0.08	0.05	0.09	0.17	0.10	0.11	0.23	0.14	0.29	0.68	0.41	0.05	0.08	0.04	0.04	0.05	0.03
1976	0.14	0.30	0.18	0.07	0.12	0.07	0.05	0.06	0.03	0.11	0.23	0.14	0.07	0.13	0.08	0.31	0.73	0.44	0.04	0.06	0.04	0.04	0.05	0.03
1977	0.13	0.28	0.17	0.09	0.20	0.12	0.06	0.07	0.04	0.08	0.15	0.09	0.10	0.22	0.13	0.31	0.73	0.45	0.05	0.07	0.04	0.04	0.04	0.02
1978	0.14	0.30	0.18	0.09	0.17	0.10	0.06	0.07	0.04	0.09	0.19	0.11	0.10	0.20	0.12	0.30	0.69	0.42	0.05	0.08	0.05	0.04	0.05	0.02
1979	0.14	0.31	0.19	0.09	0.19	0.11	0.07	0.08	0.05	0.08	0.17	0.10	0.10	0.21	0.12	0.28	0.66	0.40	0.05	0.07	0.04	0.04	0.04	0.02
1980	0.15	0.33	0.20	0.09	0.17	0.10	0.06	0.07	0.05	0.11	0.22	0.13	0.10	0.19	0.12	0.26	0.58	0.35	0.05	0.07	0.04	0.05	0.06	0.03
1981	0.14	0.30	0.18	0.10	0.21	0.13	0.06	0.07	0.04	0.10	0.20	0.12	0.11	0.23	0.14	0.28	0.64	0.39	0.06	0.09	0.05	0.05	0.06	0.03
1982	0.15	0.32	0.19	0.10	0.20	0.12	0.07	0.08	0.05	0.08	0.16	0.09	0.11	0.23	0.14	0.29	0.67	0.41	0.05	0.08	0.05	0.04	0.05	0.03
1983	0.12	0.26	0.16	0.11	0.23	0.14	0.06	0.07	0.04	0.09	0.19	0.11	0.12	0.27	0.16	0.30	0.70	0.43	0.05	0.08	0.05	0.04	0.05	0.03
1984	0.13	0.28	0.17	0.09	0.18	0.11	0.07	0.08	0.05	0.08	0.16	0.10	0.11	0.22	0.13	0.30	0.71	0.43	0.05	0.09	0.05	0.04	0.04	0.02
1985	0.14	0.29	0.17	0.11	0.21	0.13	0.06	0.07	0.04	0.07	0.13	0.07	0.11	0.23	0.14	0.35	0.81	0.49	0.07	0.12	0.07	0.04	0.04	0.02
1986	0.13	0.30	0.18	0.11	0.23	0.14	0.06	0.07	0.04	0.08	0.17	0.10	0.12	0.25	0.15	0.29	0.69	0.42	0.05	0.08	0.05	0.04	0.05	0.03
1987	0.13	0.29	0.17	0.12	0.25	0.15	0.06	0.08	0.05	0.09	0.19	0.11	0.13	0.27	0.16	0.29	0.68	0.41	0.05	0.09	0.05	0.04	0.05	0.02
1988	0.14	0.30	0.18	0.08	0.15	0.09	0.06	0.06	0.04	0.08	0.16	0.10	0.08	0.16	0.09	0.32	0.74	0.45	0.05	0.08	0.04	0.04	0.04	0.02
1989	0.13	0.28	0.17	0.10	0.21	0.13	0.07	0.08	0.05	0.09	0.18	0.11	0.10	0.20	0.12	0.28	0.66	0.40	0.06	0.10	0.06	0.04	0.05	0.02

Table 4.3: Maximum Concentration Values for Annual Average Predicted Mercury Concentrations (μg/m^3) for 5-year interval time by AERMOD for Wayne County, Michigan

Maximum Values for Annual Averaged Predicted Concentration (μg/m^3) Results (Table Values * 10-3) for 5-year interval time																								
Time Period	Monitoring Station																							
	1			2			3			4			5			6			7			8		
	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992
1961-1965	0.15	0.32	0.19	0.12	0.25	0.15	0.07	0.09	0.05	0.08	0.15	0.09	0.14	0.30	0.18	0.34	0.81	0.49	0.06	0.10	0.06	0.04	0.05	0.03
1962-1966	0.15	0.32	0.19	0.12	0.25	0.15	0.07	0.09	0.05	0.08	0.15	0.09	0.14	0.30	0.18	0.34	0.81	0.49	0.06	0.10	0.06	0.04	0.05	0.03
1963-1967	0.15	0.32	0.19	0.10	0.21	0.13	0.07	0.08	0.05	0.08	0.17	0.10	0.12	0.26	0.16	0.34	0.81	0.49	0.06	0.09	0.05	0.04	0.05	0.03
1964-1968	0.15	0.32	0.19	0.10	0.21	0.13	0.07	0.08	0.05	0.08	0.17	0.10	0.12	0.26	0.16	0.34	0.81	0.49	0.05	0.07	0.04	0.04	0.05	0.03
1965-1969	0.13	0.28	0.17	0.11	0.22	0.13	0.07	0.09	0.05	0.09	0.18	0.11	0.14	0.29	0.17	0.34	0.81	0.49	0.05	0.08	0.04	0.04	0.05	0.02
1966-1970	0.14	0.31	0.18	0.11	0.22	0.13	0.07	0.09	0.05	0.09	0.18	0.11	0.14	0.29	0.17	0.34	0.81	0.49	0.05	0.08	0.05	0.04	0.05	0.02
1967-1971	0.14	0.31	0.18	0.11	0.22	0.13	0.07	0.09	0.05	0.09	0.18	0.11	0.14	0.29	0.17	0.34	0.81	0.49	0.05	0.08	0.05	0.04	0.05	0.02
1968-1972	0.14	0.31	0.18	0.11	0.22	0.13	0.07	0.09	0.05	0.10	0.21	0.13	0.14	0.29	0.17	0.32	0.75	0.45	0.05	0.08	0.05	0.04	0.05	0.03
1969-1973	0.15	0.32	0.19	0.11	0.22	0.13	0.06	0.09	0.05	0.10	0.21	0.13	0.14	0.29	0.17	0.33	0.77	0.46	0.05	0.08	0.05	0.04	0.05	0.03
1970-1974	0.17	0.38	0.23	0.11	0.22	0.13	0.06	0.08	0.05	0.10	0.21	0.13	0.13	0.28	0.17	0.34	0.79	0.48	0.05	0.08	0.05	0.05	0.06	0.03
1971-1975	0.17	0.38	0.23	0.09	0.19	0.11	0.06	0.08	0.05	0.10	0.21	0.13	0.11	0.23	0.14	0.34	0.79	0.48	0.05	0.08	0.05	0.05	0.06	0.03
1972-1976	0.17	0.38	0.23	0.09	0.19	0.11	0.06	0.08	0.05	0.11	0.23	0.14	0.11	0.23	0.14	0.34	0.79	0.48	0.05	0.08	0.05	0.05	0.06	0.03
1973-1977	0.17	0.38	0.23	0.09	0.20	0.12	0.06	0.08	0.05	0.11	0.23	0.14	0.11	0.23	0.14	0.34	0.79	0.48	0.05	0.08	0.05	0.05	0.06	0.03
1974-1978	0.17	0.38	0.23	0.09	0.20	0.12	0.06	0.08	0.05	0.11	0.23	0.14	0.11	0.23	0.14	0.34	0.79	0.48	0.05	0.08	0.05	0.05	0.06	0.03
1975-1979	0.14	0.31	0.19	0.09	0.20	0.12	0.07	0.08	0.05	0.11	0.23	0.14	0.11	0.23	0.14	0.31	0.73	0.45	0.05	0.08	0.05	0.04	0.05	0.03
1976-1980	0.15	0.33	0.20	0.09	0.20	0.12	0.07	0.08	0.05	0.11	0.23	0.14	0.10	0.22	0.13	0.31	0.73	0.45	0.05	0.08	0.05	0.05	0.06	0.03
1977-1981	0.15	0.33	0.20	0.10	0.21	0.13	0.07	0.08	0.05	0.11	0.22	0.13	0.11	0.23	0.14	0.31	0.73	0.45	0.06	0.09	0.05	0.05	0.06	0.03
1978-1982	0.15	0.33	0.20	0.10	0.21	0.13	0.07	0.08	0.05	0.11	0.22	0.13	0.11	0.23	0.14	0.30	0.69	0.42	0.06	0.09	0.05	0.05	0.06	0.03
1979-1983	0.15	0.33	0.20	0.11	0.23	0.14	0.07	0.08	0.05	0.11	0.22	0.13	0.12	0.27	0.16	0.30	0.70	0.43	0.06	0.09	0.05	0.05	0.06	0.03
1980-1984	0.15	0.33	0.20	0.11	0.23	0.14	0.07	0.08	0.05	0.11	0.22	0.13	0.12	0.27	0.16	0.30	0.71	0.43	0.06	0.09	0.05	0.05	0.06	0.03
1981-1985	0.15	0.32	0.19	0.11	0.23	0.14	0.07	0.08	0.05	0.10	0.20	0.12	0.12	0.27	0.16	0.35	0.81	0.49	0.07	0.12	0.07	0.05	0.06	0.03
1982-1986	0.15	0.32	0.19	0.11	0.23	0.14	0.07	0.08	0.05	0.09	0.19	0.11	0.12	0.27	0.16	0.35	0.81	0.49	0.07	0.12	0.07	0.04	0.05	0.03
1983-1987	0.14	0.30	0.18	0.12	0.25	0.15	0.07	0.08	0.05	0.09	0.19	0.11	0.13	0.27	0.16	0.35	0.81	0.49	0.07	0.12	0.07	0.04	0.05	0.03
1984-1988	0.14	0.30	0.18	0.12	0.25	0.15	0.07	0.08	0.05	0.09	0.19	0.11	0.13	0.27	0.16	0.35	0.81	0.49	0.07	0.12	0.07	0.04	0.05	0.03
1985-1989	0.14	0.30	0.18	0.12	0.25	0.15	0.07	0.08	0.05	0.09	0.19	0.11	0.13	0.27	0.16	0.35	0.81	0.49	0.07	0.12	0.07	0.04	0.05	0.03
Base Predicted	0.14	0.28	0.14	0.09	0.20	0.13	0.08	0.07	0.04	0.09	0.19	0.13	0.09	0.20	0.13	0.33	0.78	0.35	0.06	0.09	0.06	0.04	0.04	0.02
No. of Under-Predicted Periods	1	0	0	0	2	6	25	0	0	4	7	12	0	0	0	8	8	0	13	13	18	0	0	0
Base Observed	0.18	0.36	0.40	0.20	0.22	0.30	0.23	0.18	0.20	0.22	0.18	0.33	0.21	0.21	0.35	0.23	0.30	0.23	0.23	0.32	0.25	0.30	0.23	0.37

Table 4.4: Maximum Concentration Values for Annual Average Predicted Mercury Concentrations (μg/m^3) for 10-year interval time by AERMOD for Wayne County, Michigan

Maximum Values for Annual Averaged Predicted Concentration (μg/m3) Results (Table Values * 10-3) for 10-year interval time																								
Time Period	Monitoring Station																							
	1			2			3			4			5			6			7			8		
	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992
1961-1970	0.15	0.32	0.19	0.12	0.25	0.15	0.07	0.09	0.05	0.09	0.18	0.11	0.14	0.30	0.18	0.34	0.81	0.49	0.06	0.10	0.06	0.04	0.05	0.03
1962-1971	0.15	0.32	0.19	0.12	0.25	0.15	0.07	0.09	0.05	0.09	0.18	0.11	0.14	0.30	0.18	0.34	0.81	0.49	0.06	0.10	0.06	0.04	0.05	0.03
1963-1972	0.15	0.32	0.19	0.11	0.22	0.13	0.07	0.09	0.05	0.10	0.21	0.13	0.14	0.29	0.17	0.34	0.81	0.49	0.06	0.09	0.05	0.04	0.05	0.03
1964-1973	0.15	0.32	0.19	0.11	0.22	0.13	0.07	0.09	0.05	0.10	0.21	0.13	0.14	0.29	0.17	0.34	0.81	0.49	0.05	0.08	0.05	0.04	0.05	0.03
1965-1974	0.17	0.38	0.23	0.11	0.22	0.13	0.07	0.09	0.05	0.10	0.21	0.13	0.14	0.29	0.17	0.34	0.81	0.49	0.05	0.08	0.05	0.05	0.06	0.03
1966-1975	0.17	0.38	0.23	0.11	0.22	0.13	0.07	0.09	0.05	0.10	0.21	0.13	0.14	0.29	0.17	0.34	0.81	0.49	0.05	0.08	0.05	0.05	0.06	0.03
1967-1976	0.17	0.38	0.23	0.11	0.22	0.13	0.07	0.09	0.05	0.11	0.23	0.14	0.14	0.29	0.17	0.34	0.81	0.49	0.05	0.08	0.05	0.05	0.06	0.03
1968-1977	0.17	0.38	0.23	0.11	0.22	0.13	0.07	0.09	0.05	0.11	0.23	0.14	0.14	0.29	0.17	0.34	0.79	0.48	0.05	0.08	0.05	0.05	0.06	0.03
1969-1978	0.17	0.38	0.23	0.11	0.22	0.13	0.06	0.09	0.05	0.11	0.23	0.14	0.14	0.29	0.17	0.34	0.79	0.48	0.05	0.08	0.05	0.05	0.06	0.03
1970-1979	0.17	0.38	0.23	0.11	0.22	0.13	0.07	0.08	0.05	0.11	0.23	0.14	0.13	0.28	0.17	0.34	0.79	0.48	0.05	0.08	0.05	0.05	0.06	0.03
1971-1980	0.17	0.38	0.23	0.09	0.20	0.12	0.07	0.08	0.05	0.11	0.23	0.14	0.11	0.23	0.14	0.34	0.79	0.48	0.05	0.08	0.05	0.05	0.06	0.03
1972-1981	0.17	0.38	0.23	0.10	0.21	0.13	0.07	0.08	0.05	0.11	0.23	0.14	0.11	0.23	0.14	0.34	0.79	0.48	0.06	0.09	0.05	0.05	0.06	0.03
1973-1982	0.17	0.38	0.23	0.10	0.21	0.13	0.07	0.08	0.05	0.11	0.23	0.14	0.11	0.23	0.14	0.34	0.79	0.48	0.06	0.09	0.05	0.05	0.06	0.03
1974-1983	0.17	0.38	0.23	0.11	0.23	0.14	0.07	0.08	0.05	0.11	0.23	0.14	0.12	0.27	0.16	0.34	0.79	0.48	0.06	0.09	0.05	0.05	0.06	0.03
1975-1984	0.15	0.33	0.20	0.11	0.23	0.14	0.07	0.08	0.05	0.11	0.23	0.14	0.12	0.27	0.16	0.31	0.73	0.45	0.06	0.09	0.05	0.05	0.06	0.03
1976-1985	0.15	0.33	0.20	0.11	0.23	0.14	0.07	0.08	0.05	0.11	0.23	0.14	0.12	0.27	0.16	0.35	0.81	0.49	0.07	0.12	0.07	0.05	0.06	0.03
1977-1986	0.15	0.33	0.20	0.11	0.23	0.14	0.07	0.08	0.05	0.11	0.22	0.13	0.12	0.27	0.16	0.35	0.81	0.49	0.07	0.12	0.07	0.05	0.06	0.03
1978-1987	0.15	0.33	0.20	0.12	0.25	0.15	0.07	0.08	0.05	0.11	0.22	0.13	0.13	0.27	0.16	0.35	0.81	0.49	0.07	0.12	0.07	0.05	0.06	0.03
1979-1988	0.15	0.33	0.20	0.12	0.25	0.15	0.07	0.08	0.05	0.11	0.22	0.13	0.13	0.27	0.16	0.35	0.81	0.49	0.07	0.12	0.07	0.05	0.06	0.03
1980-1989	0.15	0.33	0.20	0.12	0.25	0.15	0.07	0.08	0.05	0.11	0.22	0.13	0.13	0.27	0.16	0.35	0.81	0.49	0.07	0.12	0.07	0.05	0.06	0.03
Base Predicted	0.14	0.28	0.14	0.09	0.20	0.13	0.08	0.07	0.04	0.09	0.19	0.13	0.09	0.20	0.13	0.33	0.78	0.35	0.06	0.09	0.06	0.04	0.04	0.02
No. of Under-Predicted Periods	0	0	0	0	0	1	20	0	0	0	2	2	0	0	0	1	1	0	8	8	13	0	0	0
Base Observed	0.18	0.36	0.40	0.20	0.22	0.30	0.23	0.18	0.20	0.22	0.18	0.33	0.21	0.21	0.35	0.23	0.30	0.23	0.23	0.32	0.25	0.30	0.23	0.37

Table 4.5: Maximum Concentration Values for Annual Average Predicted Mercury Concentrations (μg/m^3) for 15-year interval time by AERMOD for Wayne County, Michigan

Maximum Values for Annual Averaged Predicted Concentration (μg/m3) Results (Table Values * 10-3) for 15-year interval time																								
Time Period	Monitoring Station																							
	1			2			3			4			5			6			7			8		
	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992
1961-1975	0.17	0.38	0.23	0.12	0.25	0.15	0.07	0.09	0.05	0.10	0.21	0.13	0.14	0.30	0.18	0.34	0.81	0.49	0.06	0.10	0.06	0.05	0.06	0.03
1962-1976	0.17	0.38	0.23	0.12	0.25	0.15	0.07	0.09	0.05	0.11	0.23	0.14	0.14	0.30	0.18	0.34	0.81	0.49	0.06	0.10	0.06	0.05	0.06	0.03
1963-1977	0.17	0.38	0.23	0.11	0.22	0.13	0.07	0.09	0.05	0.11	0.23	0.14	0.14	0.29	0.17	0.34	0.81	0.49	0.06	0.09	0.05	0.05	0.06	0.03
1964-1978	0.17	0.38	0.23	0.11	0.22	0.13	0.07	0.09	0.05	0.11	0.23	0.14	0.14	0.29	0.17	0.34	0.81	0.49	0.05	0.08	0.05	0.05	0.06	0.03
1965-1979	0.17	0.38	0.23	0.11	0.22	0.13	0.07	0.09	0.05	0.11	0.23	0.14	0.14	0.29	0.17	0.34	0.81	0.49	0.05	0.08	0.05	0.05	0.06	0.03
1966-1980	0.17	0.38	0.23	0.11	0.22	0.13	0.07	0.09	0.05	0.11	0.23	0.14	0.14	0.29	0.17	0.34	0.81	0.49	0.05	0.08	0.05	0.05	0.06	0.03
1967-1981	0.17	0.38	0.23	0.11	0.22	0.13	0.07	0.09	0.05	0.11	0.23	0.14	0.14	0.29	0.17	0.34	0.81	0.49	0.06	0.09	0.05	0.05	0.06	0.03
1968-1982	0.17	0.38	0.23	0.11	0.22	0.13	0.07	0.09	0.05	0.11	0.23	0.14	0.14	0.29	0.17	0.34	0.79	0.48	0.06	0.09	0.05	0.05	0.06	0.03
1969-1983	0.17	0.38	0.23	0.11	0.23	0.14	0.07	0.09	0.05	0.11	0.23	0.14	0.14	0.29	0.17	0.34	0.79	0.48	0.06	0.09	0.05	0.05	0.06	0.03
1970-1984	0.17	0.38	0.23	0.11	0.23	0.14	0.07	0.08	0.05	0.11	0.23	0.14	0.13	0.28	0.17	0.34	0.79	0.48	0.06	0.09	0.05	0.05	0.06	0.03
1971-1985	0.17	0.38	0.23	0.11	0.23	0.14	0.07	0.08	0.05	0.11	0.23	0.14	0.12	0.27	0.16	0.35	0.81	0.49	0.07	0.12	0.07	0.05	0.06	0.03
1972-1986	0.17	0.38	0.23	0.11	0.23	0.14	0.07	0.08	0.05	0.11	0.23	0.14	0.12	0.27	0.16	0.35	0.81	0.49	0.07	0.12	0.07	0.05	0.06	0.03
1973-1987	0.17	0.38	0.23	0.12	0.25	0.15	0.07	0.08	0.05	0.11	0.23	0.14	0.13	0.27	0.16	0.35	0.81	0.49	0.07	0.12	0.07	0.05	0.06	0.03
1974-1988	0.17	0.38	0.23	0.12	0.25	0.15	0.07	0.08	0.05	0.11	0.23	0.14	0.13	0.27	0.16	0.35	0.81	0.49	0.07	0.12	0.07	0.05	0.06	0.03
1975-1989	0.15	0.33	0.20	0.12	0.25	0.15	0.07	0.08	0.05	0.11	0.23	0.14	0.13	0.27	0.16	0.35	0.81	0.49	0.07	0.12	0.07	0.05	0.06	0.03
Base Predicted	0.14	0.28	0.14	0.09	0.20	0.13	0.08	0.07	0.04	0.09	0.19	0.13	0.09	0.20	0.13	0.33	0.78	0.35	0.06	0.09	0.06	0.04	0.04	0.02
No. of Under-Predicted Periods	0	0	0	0	0	0	15	0	0	0	0	0	0	0	0	0	0	0	3	3	8	0	0	0
Base Observed	0.18	0.36	0.40	0.20	0.22	0.30	0.23	0.18	0.20	0.22	0.18	0.33	0.21	0.21	0.35	0.23	0.30	0.23	0.23	0.32	0.25	0.30	0.23	0.37

Table 4.6: Maximum Concentration Values for Annual Average Predicted Mercury Concentrations (μg/m^3) for 20-year interval time by AERMOD for Wayne County, Michigan

Maximum Values for Annual Averaged Predicted Concentration (μg/m3) Results (Table Values * 10-3) for 20-year interval time																								
Time Period	Monitoring Station																							
	1			2			3			4			5			6			7			8		
	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992
1961-1980	0.17	0.38	0.23	0.12	0.25	0.15	0.07	0.09	0.05	0.11	0.23	0.14	0.14	0.30	0.18	0.34	0.81	0.49	0.06	0.10	0.06	0.05	0.06	0.03
1962-1981	0.17	0.38	0.23	0.12	0.25	0.15	0.07	0.09	0.05	0.11	0.23	0.14	0.14	0.30	0.18	0.34	0.81	0.49	0.06	0.10	0.06	0.05	0.06	0.03
1963-1982	0.17	0.38	0.23	0.11	0.22	0.13	0.07	0.09	0.05	0.11	0.23	0.14	0.14	0.29	0.17	0.34	0.81	0.49	0.06	0.09	0.05	0.05	0.06	0.03
1964-1983	0.17	0.38	0.23	0.11	0.23	0.14	0.07	0.09	0.05	0.11	0.23	0.14	0.14	0.29	0.17	0.34	0.81	0.49	0.06	0.09	0.05	0.05	0.06	0.03
1965-1984	0.17	0.38	0.23	0.11	0.23	0.14	0.07	0.09	0.05	0.11	0.23	0.14	0.14	0.29	0.17	0.34	0.81	0.49	0.06	0.09	0.05	0.05	0.06	0.03
1966-1985	0.17	0.38	0.23	0.11	0.23	0.14	0.07	0.09	0.05	0.11	0.23	0.14	0.14	0.29	0.17	0.35	0.81	0.49	0.07	0.12	0.07	0.05	0.06	0.03
1967-1986	0.17	0.38	0.23	0.11	0.23	0.14	0.07	0.09	0.05	0.11	0.23	0.14	0.14	0.29	0.17	0.35	0.81	0.49	0.07	0.12	0.07	0.05	0.06	0.03
1968-1987	0.17	0.38	0.23	0.12	0.25	0.15	0.07	0.09	0.05	0.11	0.23	0.14	0.14	0.29	0.17	0.35	0.81	0.49	0.07	0.12	0.07	0.05	0.06	0.03
1969-1988	0.17	0.38	0.23	0.12	0.25	0.15	0.07	0.09	0.05	0.11	0.23	0.14	0.14	0.29	0.17	0.35	0.81	0.49	0.07	0.12	0.07	0.05	0.06	0.03
1970-1989	0.17	0.38	0.23	0.12	0.25	0.15	0.07	0.08	0.05	0.11	0.23	0.14	0.13	0.28	0.17	0.35	0.81	0.49	0.07	0.12	0.07	0.05	0.06	0.03
Base Predicted	0.14	0.28	0.14	0.09	0.20	0.13	0.08	0.07	0.04	0.09	0.19	0.13	0.09	0.20	0.13	0.33	0.78	0.35	0.06	0.09	0.06	0.04	0.04	0.02
No. of Under-Predicted Periods	0	0	0	0	0	0	10	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0

Table 4.7: Maximum Concentration Values for Annual Average Predicted Mercury Concentrations (μg/m^3) for 25-year interval time by AERMOD for Wayne County, Michigan

Maximum Values for Annual Averaged Predicted Concentration (μg/m3) Results (Table Values * 10-3) for 25-year interval time																								
Time Period	Monitoring Station																							
	1			2			3			4			5			6			7			8		
	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992
1961-1985	0.17	0.38	0.23	0.12	0.25	0.15	0.07	0.09	0.05	0.11	0.23	0.14	0.14	0.30	0.18	0.35	0.81	0.49	0.07	0.12	0.07	0.05	0.06	0.03
1962-1986	0.17	0.38	0.23	0.12	0.25	0.15	0.07	0.09	0.05	0.11	0.23	0.14	0.14	0.30	0.18	0.35	0.81	0.49	0.07	0.12	0.07	0.05	0.06	0.03
1963-1987	0.17	0.38	0.23	0.12	0.25	0.15	0.07	0.09	0.05	0.11	0.23	0.14	0.14	0.29	0.17	0.35	0.81	0.49	0.07	0.12	0.07	0.05	0.06	0.03
1964-1988	0.17	0.38	0.23	0.12	0.25	0.15	0.07	0.09	0.05	0.11	0.23	0.14	0.14	0.29	0.17	0.35	0.81	0.49	0.07	0.12	0.07	0.05	0.06	0.03
1965-1989	0.17	0.38	0.23	0.12	0.25	0.15	0.07	0.09	0.05	0.11	0.23	0.14	0.14	0.29	0.17	0.35	0.81	0.49	0.07	0.12	0.07	0.05	0.06	0.03
Base Predicted	0.14	0.28	0.14	0.09	0.20	0.13	0.08	0.07	0.04	0.09	0.19	0.13	0.09	0.20	0.13	0.33	0.78	0.35	0.06	0.09	0.06	0.04	0.04	0.02
No. of Under-Predicted Periods	0	0	0	0	0	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

4.2 DATA FLOW IN AERMOD RUNS

4.2.1 AERMET

AERMET is the meteorological preprocessor for AERMOD. First, the AERMET preprocessor was run for a base year to produce the meteorological fields necessary for that year to run the AERMOD. To get the multiple year concentrations only, upper air and hourly surface data was continuously changed (from 1961-1989) in AERMET. Hourly surface data (Samson surface met data format) and upper air data (TD 6201 format) both were taken for Flint Bishop Airport (station#14826) wererom WEBMET database (www.webmet.com).

The land use parameters were calculated by analyzing the three kilometer area around the meteorological site using 12 pie-shaped sectors. Surface parameters, namely Albedo, Bowen Ratio, and Surface Roughness for each sector were specified by the sectors that were no smaller than a 30-degree arc. GIS application ARC Map was used for the analysis (Master Thesis, Kanwar 2005). Land use parameters analysis results for all twelve sectors for both Wayne County and Lucas County are given in appendix B.1 and B.2.

The value of anemometer height was taken as 21 ft (6.4 meters). The AERMET model was run on a short regional domain extending westward to 83.75 degree longitude and Northward to 42.96 degree latitude. Data generated by the AERMET preprocessor (includes julian day of the year, the average wind flow factor, wind speed at reference height, height of mixing layer obtained from the upper air data, and hourly observations of surface level parameters such as wind speed temperature and cloud cover from the surface data) were used by AERMET to generate two meteorological files, which used in AERMOD meteorological pathway.

4.2.2 AERMAP

To facilitate the generation of hill height scales and elevation for AERMOD, a terrain preprocessor AERMAP, has been developed. After the AERMET data was complied, the AERMAP was run. AERMAP was run using four separate 1 degree DEM Toledo East, Toledo West, Detroit East, Detroit West to cover the both study area, (www.webgis.com).The details of DEM files are given in Table 4.8. The AERMAP was run using NAD27 datum (North American Datum of 1927). These four DEM files were used same for all AERMOD runs.

Table 4.8: List of USGS DEM 1-degree files used for AERMAP run

NAME	HALF	MIN LONG	MAX LONG	MIN LAT	MAX LAT
DETROIT	W	-84°00'00"	-83°00'00"	42°00'00"	43°00'00"
DETROIT	E	-83°00'00"	-82°00'00"	42°00'00"	43°00'00"
TOLEDO	W	-84°00'00"	-83°00'00"	41°00'00"	42°00'00"
TOLEDO	E	-83°00'00"	-82°00'00"	41°00'00"	42°00'00"

4.2.3 AERMOD

a. Control Pathway: Since the AERMOD model is especially designed to support the EPA's regulatory programs, the default regulatory modeling option is taken into consideration. These options include the use of stack-tip downwash, and a routine for processing averages when calm winds or missing meteorological data occur. Model was run for short-term averaging time period option (1-hr, 3-hr, 8-hr, & 24-hr) and long-term averaging time period option (quarterly & annual). Dispersion coefficient was taken for urban area and, as an input, urban population of Flint area 124943 persons and urban population for Lucas 430459 were taken. For the value of urban surface roughness length, 0.694 meter for Flint and 0.722 meter for Lucas were considered. Elevated terrain height option was used for this study. It was assumed that urban surface roughness length for whole grid was same as the monitoring station.

b. Source Pathway: AERMOD was run using base emission inventories for base year predicted concentration as well as multiple year predicted concentration. Source emission rates were treated as constant throughout the modeling period for both pollutants (mercury and sulfur dioxide), i.e. there were no change in emission factor and wind speed for seasonal, monthly, hourly emission variation.

***c. Receptor Pathway*:** Discrete Cartesian grid receptor monitoring networks option were utilized for both areas. Wayne County was using 8 monitors to predict concentration over a large area and Lucas County was using 2 monitoring stations to predict the concentrations.

d. Meteorology Pathway: The two types of meteorological files, which were generated from the AERMET were utilized for AERMOD run. Wind speed was taken from model default values. Base elevation above MSL was taken 769 ft for Flint Bishop Airport meteorological data. For multiple year concentration, AERMOD was run one by one using 29 years meteorological data generated by AERMET for both pollutants.

e. Output Pathway: The short term averaging results were obtained for the highest second highest 1 hour, 3 hr, 8 hr, and 24 hour & for long term average, results were obtained for quarterly and annual time period options.

4.3 DATA FLOW IN CALPUFF RUNS

The first model was run for three base years (1990-1992) for predicting the base year concentrations. To evaluate the potential for multiple year variation in this study a twenty nine years data set of meteorology has been compiled and runs performed for an array of source locations oriented around all the receptors. The meteorological fields have been produced using the measured National Weather Service (NWS) data sets as inputs, as opposed to the alternative approach, using the prognostic model input from the MM5 model. This is because for this study at least twenty nine years of meteorology are needed and this contiguous time frame is not available for prognostic data sets, such as the MM5 model output. The source locations are oriented with respect to the common receptor location at all directions of the compass and over a range of distances. At each source location CALPUFF runs have occurred for each of the twenty nine years of meteorology including three base years.

4.3.1 CALMET

In this study, the CALMET Model was run on a large regional domain extending westward to 84 degrees longitude and southward to 37 degrees latitude and north and eastward to encompass the entire state of Michigan for both mercury and sulfur dioxide. In the vertical, 8 levels were specified to discern meteorological differences in surface level, transition level, and free atmospheric conditions. This domain is represented in a Lambert - Conformal projection because of its large size. The domain was established at the 40 kilometer resolution to allow reasonable computational times when running the CALMET and CALPUFF model for long time periods. For the CALMET runs the geographical processing to produce terrain heights and land use represented in the model was done using the programs available as recommended by EPA. For the CALMET runs terrain effects have been calculated from an initial guess windfield to produce a first guess windfield, the values of which then were interpolated with surface observations. National Weather Service (NWS), data was used as recommended in the IWAQM guidance which consists of upper air radiosonde data, surface observations, and precipitation measurements (EPA Publication, 1998). For the CALMET domain, meteorological data consists of 48 surface stations, 11 radiosonde stations, and 474 precipitation sites. This data has been processed for the year's 1960 to1989. For the precipitation data, preprocessing was necessary to recode the flag indicating data validity before the data could be read by CALMET. For the meteorological data, data format conversion and data filling was necessary. The data filling and correcting for the radiosonde data was necessary for all missing soundings as well as soundings which, for various reasons, were insufficient to run CALMET.

4.3.2 CALPUFF Runs

CALPUFF was first run using three base years (1990-1991) emission inventories to produce base year predicted concentration. Later on CALPUFF was used to compute the multiple year concentration. For computing the multiple year concentration, CALMET data was compiled for the twenty nine years period (1960 through 1989). CALPUFF runs and the associated CALPOST runs occurred over the 29 years of meteorology for the respective source locations described above. For these runs all input parameters in data files utilized were constant except the year of meteorology. All default CALPUFF settings were chosen so that the model performed in an acceptable manner for multiple year period of time. Similar procedure (like AERMOD) has been adopted for CALPUFF results.

4.4 REQUIRED METEOROLICAL LENGTH RESULTS

This study represents a present situation in the air quality models, which are generally applied for regulatory work. Field data available for mercury from eight ambient air monitoring stations in Wayne County, Michigan, for the year 1990 to 1992, and for sulfur dioxide from two monitoring stations in Lucas County, Ohio, were used for this purpose. Analysis was done using AERMOD and CALPUFF air regulatory models. This analysis could be used to analyze the design value of required meteorological time periods for different averaging time period options rather than using the current EPA requirement of 5-year meteorological data.

4.4.1 Long-Term Averaging Time Period Option

Design length value of meteorological data was obtained for annual as well as quarterly time period options. Results for the quantitative nature of under-predicted periods are shown for mercury pollutants for both AERMOD and CALPUFF model. The perceptible natures of sulfur dioxide long term averaging results are almost similar with mercury results and followed in appendix C.1 and C.2.

Results show that from a regulatory conservatory point, five year of meteorological data for annual time period are sufficient, and 10 year of meteorological data is needed for Quarterly time periods, to produce the stable values. Therefore analysis on annual averaging time supports for current EPA's regulation. However, for results closer to the observed value, at least 15 years of meteorological data will provide reliable and stable values of long-term concentrations. However, 20 years of meteorological data will give the best result for long-term concentrations (Kumar et al., 2006).

4.4.1.1 Quarterly (2^{nd}) Averaging Time Period Option

The quantitative natures of under-predicted periods for quarterly averaging time are shown in Table 4.9 and Table 4.10.

AERMOD Results: Table 4.9 depicts that numbers for under-predicted periods were very noticeable for the 5-year interval (up to 16). However, the numbers were markedly reduced for 10-year interval except for monitoring station 2, 3 and 5, which can be attributed to the larger distance of the monitoring station from the sources.

CALPUFF Results: The quantitative nature of CALPUFF results almost similar to the AERMOD results. Table 4.10 shows that the under-predicted periods were very apparent for 5-year interval (up to 22). It reduced drastically for the 10-year interval, except monitoring stations 2, 3 and 6.

4.4.1.2 Annual Averaging Time Period Option

The quantitative natures of under-predicted period for quarterly averaging time are shown in Table 4.11 and Table 4.12.

AERMOD Results: Table 4.11 summarizes that numbers for under-predicted periods were almost insignificant for 5-year except the monitoring 3 and 7. Hence 5-year interval is the best choice for annual averaging time period.

CALPUFF Results: The quantitative nature of CALPUFF results was very similar to the AERMOD results. Table 4.12 shows under-predicted periods were almost approaching zero for the 5-year interval.

Under-predicted period results for sulfur dioxide for annual averaged are shown in appendix C.2.

Table 4.9: Number of Under-Predicted Periods for Quarterly Averaged for Mercury for all year interval time predicted by AERMOD for Wayne County, Michigan

Numbers of Under-Predicted Periods for Quarterly (2nd) Averaged for all year interval time Predicted by AERMOD																								
Year Time Period	Monitoring Station																							
	1			2			3			4			5			6			7			8		
	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992
5-Year	9	9	9	11	16	16	8	10	16	4	4	12	11	11	15	15	14	14	13	13	13	0	0	8
10-Year	0	0	0	6	10	11	0	5	11	0	0	2	6	6	10	5	2	2	0	6	6	0	0	0
15-Year	0	0	0	0	6	6	0	0	6	0	0	0	0	1	5	0	0	0	0	1	1	0	0	0
20-Year	0	0	0	0	1	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
25-Year	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 4.10: Number of Under-Predicted Periods for Quarterly Averaged for Mercury for all year interval time predicted by CALPUFF for Wayne County, Michigan

Numbers of Under-Predicted Periods for Annual Averaged for all year interval time																								
Year Time Period	Monitoring Station																							
	1			2			3			4			5			6			7			8		
	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992
5-Year	5	16	4	13	16	13	20	22	6	15	14	9	13	16	13	17	7	17	15	15	21	14	13	6
10-Year	0	6	0	8	11	8	10	7	0	4	3	0	0	10	8	12	0	12	5	5	16	4	4	0
15-Year	0	1	0	3	6	3	1	12	0	0	0	0	0	6	3	7	0	7	0	0	11	0	0	0
20-Year	0	0	0	0	1	0	0	7	0	0	0	0	0	1	0	2	0	2	0	0	6	0	0	0
25-Year	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0

Table 4.11: Number of Under-Predicted Periods for Annual Averaged for Mercury for all year interval time predicted by AERMOD for Wayne County, Michigan

Numbers of Under-Predicted Periods for Annual Averaged for all year interval time Predicted by AERMOD																								
Year Time Period	Monitoring Station																							
	1			2			3			4			5			6			7			8		
	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992
5-Year	1	0	0	0	2	6	25	0	0	4	7	12	0	0	0	8	8	0	13	13	18	0	0	0
10-Year	0	0	0	0	0	0	15	0	0	0	0	0	0	0	0	0	0	0	3	3	8	0	0	0
15-Year	0	0	0	0	0	0	15	0	0	0	0	0	0	0	0	0	0	0	3	3	8	0	0	0
20-Year	0	0	0	0	0	0	10	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0
25-Year	0	0	0	0	0	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 4.12: Number of Under-Predicted Periods for Annual Averaged for Mercury for all year interval time predicted by CALPUFF for Wayne County, Michigan

Numbers of Under-Predicted Periods for Annual Averaged for all year interval time																								
Year Time Period	Monitoring Station																							
	1			2			3			4			5			6			7			8		
	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992
5-Year	5	6	4	8	11	0	2	2	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10-Year	0	6	0	3	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
15-Year	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
20-Year	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
25-Year	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

4.4.2 Short-Term Averaging Time Period Option

Design length value of meteorological data was obtained for 1-hr, 3-hr, 8-hr, and 24-hr averaging time period options. The under-predicted period results predicted by AERMOD and CALPUFF model results were shown for mercury pollutants. The results for sulfur dioxide show the almost the same quantifiable nature as mercury results (appendix C.3, C.4, C.5, and C.6).

Results show that for conservative point of view, 20 years of meteorological data for 1-hr, 15-years for 3-hr and 8-hr and, 10 years for 24-hr is sufficient. However, for results closer to the observed value, 25 years of meteorological data are not sufficient to predict reliable and stable values for 1-hr averaging time period. However, a minimum of 25 years of meteorological data are suggested for other short-term time periods (Kumar et al. 2006).

4.4.2.1 1-hr Averaging Time Period Option

The quantitative natures of under-predicted periods for 1-hr averaging time are shown in Table 4.13 and Table 4.14.

AERMOD Results: Table 4.13 depicts that numbers for under-predicted periods were very prominent for the 5-year (up to 22) and the 10-year intervals (up to 15), however the numbers were markedly reduced for 15-year except for the monitoring station 2, 6 and 7. Number of under-predicted periods was approaching to low values in the case of 20-year time intervals except monitoring station 2. For 25-year time intervals variation is almost zero except the monitoring station 2.

CALPUFF Results: The quantitative nature of CALPUFF results was almost identical to the AERMOD results. Table 4.10 shows that the under-predicted periods were very apparent for 5-year, 10- year and 15-year. The numbers were reduced for 20-year interval.

Quantitative natures for all other under-predicted periods for sulfur oxide follow the almost same nature and are mentioned in appendix C.3.

Table 4.13: Number of Under-Predicted Periods for 1-hr Averaging time Mercury for all year interval time predicted by AERMOD for Wayne County, Michigan

Numbers of Under-Predicted Periods for Annual Averaged for all year interval time Predicted by AERMOD																								
Year Time Period	Monitoring Station																							
	1			2			3			4			5			6			7			8		
	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992
5-Year	14	12	15	22	20	20	20	18	18	17	17	17	14	14	17	16	16	16	15	15	15	16	12	12
10-Year	12	5	12	17	15	15	13	13	13	7	7	7	10	10	13	12	12	12	11	11	11	13	5	2
15-Year	7	0	7	12	10	10	8	8	8	1	1	1	5	5	8	7	7	7	6	6	6	8	0	0
20-Year	2	0	2	7	5	5	3	3	3	0	0	0	0	0	3	2	2	2	1	1	1	3	0	0
25-Year	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 4.14: Number of Under-Predicted Periods for 1-hr Averaging time for Mercury for all year interval time predicted by CALPUFF for Wayne County, Michigan

Numbers of Under-Predicted Periods for Annual Averaged for all year interval time																								
Year Time Period	Monitoring Station																							
	1			2			3			4			5			6			7			8		
	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992
5-Year	18	15	14	11	16	16	13	13	18	13	10	13	15	17	12	15	18	12	22	2	25	15	15	21
10-Year	10	9	10	6	10	11	3	3	8	8	5	8	10	9	7	10	13	2	17	0	20	5	5	16
15-Year	5	6	5	0	6	6	3	3	8	3	0	3	5	4	2	5	7	0	12	0	15	0	0	11
20-Year	3	1	0	0	1	1	0	0	3	0	0	0	0	0	0	0	3	0	7	0	10	0	0	6
25-Year	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	5	0	0	1

4.4.2.2 3-hr Averaging Time Period Option

The quantitative natures of under-predicted periods for 3-hr averaging time are shown in Table 4.15 and Table 4.16.

AERMOD Results: Table 4.15 depicts that numbers for under-predicted periods were very salient for 5-year, and 10-year interval, however the numbers were drastically reduced for 15-year except for monitoring station 3, 7 and 8. Number of under-predicted periods was approaching to low values in the case of 20-year time intervals except monitoring station 2.

CALPUFF Results: The quantitative nature of CALPUFF results was almost coincided to the AERMOD results. Table 4.16 shows that the under-predicted periods were very apparent for 5-year, and 10- year. It reduced for 15-year interval.

Results for 3-hr averaging time for sulfur dioxide predicted by AERMOD and CALPUFF are shown in appendix C.4.

Table 4.15: Number of Under-Predicted Periods for 3-hr Averaging time Mercury for all year interval time predicted by AERMOD for Wayne County, Michigan

Numbers of Under-Predicted Periods for Annual Averaged for all year interval time Predicted by AERMOD																								
Year Time Period	Monitoring Station																							
	1			2			3			4			5			6			7			8		
	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992
5-Year	16	15	12	22	8	17	22	15	15	13	15	15	17	17	17	10	12	10	16	21	11	14	9	7
10-Year	6	9	6	17	0	7	17	10	10	4	6	6	12	12	12	2	4	2	11	16	3	6	1	0
15-Year	1	4	1	12	0	0	12	5	5	0	1	1	7	7	7	0	0	0	6	11	0	1	0	0
20-Year	0	0	0	7	0	0	7	0	0	0	0	0	2	2	2	0	0	0	1	6	0	0	0	0
25-Year	0	0	0	2	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0

Table 4.16: Number of Under-Predicted Periods for 3-hr Averaging time for Mercury for all year interval time predicted by CALPUFF for Wayne County, Michigan

Numbers of Under-Predicted Periods for Annual Averaged for all year interval time																								
Year Time Period	Monitoring Station																							
	1			2			3			4			5			6			7			8		
	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992
5-Year	14	11	14	16	17	0	25	0	25	10	4	10	11	1	0	10	17	17	17	8	20	4	0	25
10-Year	9	6	9	11	11	0	20	0	20	0	0	0	6	0	0	5	11	10	12	0	15	0	0	20
15-Year	4	0	4	6	6	0	15	0	15	0	0	0	0	0	0	0	2	1	7	0	10	0	0	15
20-Year	0	0	0	1	1	0	10	0	10	0	0	0	0	0	0	0	0	0	2	0	5	0	0	10
25-Year	0	0	0	0	0	0	5	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5

4.4.2.3 8-hr Averaging Time Period Option

The quantitative natures of under-predicted period for 8-hr averaging time were shown in Table 4.17 and Table 4.18. Quantitative nature of 8-hr averaged time is very similar to 3-hr averaged time period option.

AERMOD Results: Table 4.17 depicts that numbers for under-predicted periods were very remarkable for 5-year, and 10-year interval, however the numbers were significantly reduced for 15-year except few outlier monitoring stations. Number of under-predicted periods was approaching to a low values in the case of 20-year time intervals.

CALPUFF Results: The quantitative nature of CALPUFF results was almost analogous to the AERMOD results. Table 4.18 shows that the under-predicted periods were very apparent for 5-year, and 10- year. It reduced for 15-year interval.

Results for 8-hr averaging time for sulfur dioxide predicted by AERMOD and CALPUFF are shown in appendix C.5.

Table 4.17: Number of Under-Predicted Periods for 8-hr Averaging time Mercury for all year interval time predicted by AERMOD for Wayne County, Michigan

Numbers of Under-Predicted Periods for Annual Averaged for all year interval time Predicted by AERMOD																								
Year Time Period	Monitoring Station																							
	1			2			3			4			5			6			7			8		
	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992
5-Year	20	16	16	18	22	2	25	3	4	1	16	11	4	0	1	2	3	2	12	17	22	11	0	21
10-Year	10	5	5	12	17	0	20	0	0	0	6	1	0	0	0	0	0	0	5	5	17	2	0	16
15-Year	1	1	1	8	12	0	15	0	0	0	0	0	0	0	0	0	0	0	0	0	12	0	0	11
20-Year	0	0	0	3	7	0	10	0	0	0	0	0	0	0	0	0	0	0	0	0	7	0	0	6
25-Year	0	0	0	0	2	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	1

Table 4.18: Number of Under-Predicted Periods for 8-hr Averaging time for Mercury for all year interval time predicted by CALPUFF for Wayne County, Michigan

Numbers of Under-Predicted Periods for Annual Averaged for all year interval time																								
Year Time Period	Monitoring Station																							
	1			2			3			4			5			6			7			8		
	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992
5-Year	5	16	4	13	16	13	20	22	6	15	14	9	13	16	13	17	7	17	15	15	21	14	13	6
10-Year	0	6	0	8	11	8	10	7	0	4	3	0	0	10	8	12	0	12	5	5	16	4	4	0
15-Year	0	1	0	3	6	3	1	12	0	0	0	0	0	6	3	7	0	7	0	0	11	0	0	0
20-Year	0	0	0	0	1	0	0	7	0	0	0	0	0	1	0	2	0	2	0	0	6	0	0	0
25-Year	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0

4.4.2.4 24-hr Averaging Time Period Option

The quantitative natures of under-predicted period for 24-hr averaging time were shown in Table 4.19 and Table 4.20. The quantitative behavior of 24-hr averaging time result was coinciding with the quarterly averaging time period result.

AERMOD Results: Table 4.19 depicts that numbers for under-predicted periods were prominent for 5-year. The number were significantly reduced for 10-year except few outlier monitoring stations.

CALPUFF Results: The quantitative nature of CALPUFF results was almost matched to the AERMOD results. Table 4.18 shows that the under-predicted periods were very apparent for 5-year. It was reduced for 10-year interval.

Results for 24-hr averaging time for sulfur dioxide predicted by AERMOD and CALPUFF are shown in appendix C.6.

Table 4.19: Number of Under-Predicted Periods for 24-hr Averaging time Mercury for all year interval time predicted by AERMOD for Wayne County, Michigan

Numbers of Under-Predicted Periods for Annual Averaged for all year interval time Predicted by AERMOD																								
Year Time Period	Monitoring Station																							
	1			2			3			4			5			6			7			8		
	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992
5-Year	1	2	0	12	2	2	25	22	5	14	14	14	1	1	1	10	13	2	23	15	18	12	0	5
10-Year	0	0	0	2	0	0	20	17	0	4	4	4	0	0	0	0	1	0	18	10	13	2	0	0
15-Year	0	0	0	0	0	0	15	12	0	0	0	0	0	0	0	0	0	0	13	5	7	0	0	0
20-Year	0	0	0	0	0	0	10	7	0	0	0	0	0	0	0	0	0	0	8	0	3	0	0	0
25-Year	0	0	0	0	0	0	5	2	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0

Table 4.20: Number of Under-Predicted Periods for 24-hr Averaging time for Mercury for all year interval time predicted by CALPUFF for Wayne County, Michigan

Numbers of Under-Predicted Periods for Annual Averaged for all year interval time																								
Year Time Period	Monitoring Station																							
	1			2			3			4			5			6			7			8		
	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992	1990	1991	1992
5-Year	7	6	7	15	11	10	12	0	5	15	14	9	13	16	13	7	7	17	15	15	21	4	6	6
10-Year	0	0	0	8	0	5	2	0	0	4	3	0	0	10	8	2	0	12	5	5	16	0	0	0
15-Year	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
20-Year	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
25-Year	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0

Chapter 5

POPULATION SENSITIVITY ANALYSIS FOR AERMOD

Two realistic scenarios were constructed to study the effect of urban population on computing the ground level concentration results in AERMOD. The value for the first case was based on the total population of the grid. The value for the second case was taken as fraction percentage of urban area of total population for the grid. The objective of this study was to find the suitable input value of population that predicts results closest to the observed concentration.

5.1 PROCEDURE FOR POPULATION SENSIVITY IN AERMOD

AERMOD model was first run with whole population and a value of 0.756 for urban surface roughness length in control pathway. Calculation for different types of land use percentage and urban surface roughness length was done for whole grid using GIS application and are shown in appendix D. AERMOD model was again run by changing the urban population in the control pathway, keeping all other parameters same. For this purpose urban population was taken as the fraction of urban area, (i.e., input for population parameter is percentage of urban area multiply by total population taken previously in the AERMOD run). Comparison is performed visually and analytically. For both cases model has been evaluated by again seven statistical parameters using four different comparisons.

In the first run urban population and urban surface length were taken 124943 person (http://www.city-data.com/city/Flint-Michigan.html) and 0.756 meter respectively. From the GIS application percentage of urban area was found 62.4%, therefore, for the second run population input was multiply by 0.624 with the original population of that area. For population sensitivity analysis, AERMOD was run using the urban population as 77964 (i.e., percent of urban area multiplied by the total population). All others parameters were taken the same as previous AERMOD runs. This new AERMOD results are referred as *AERMOD_POP* results in the upcoming chapters.

The sensitivity assessment of AERMOD for urban population option was evaluated qualitatively as well as quantitatively. Qualitative analysis was done by using graphical representation of predicted concentration with observed concentration, whereas quantitative evaluation was done by evaluating statistical parameters respectively using four different methods of Co and Cp comparison. Analysis was conducted for mercury using three years (1990-1992) emission inventories for eight monitoring stations.

Figure 5.1 and Table 5.1 show the quarterly averaged concentration comparison of AERMOD population sensitivity. Figure 5.2 and Table 5.2 show the annual averaged concentration comparison of AERMOD population sensitivity.

The statistical significance performance indicators was further tested by using a Bootstrap resampling method to estimate whether the calculated performance of FB, NMSE, VG, MG, Cor (r), and Fa2 are significantly different from zero for AERMOD and AERMOD_POP, and whether the differences in their measure between pairs of models are significantly different from zero (to generate 95% confidence limits). The summaries of the confidence limits are tabulated in Table 5.3 and Table 5.4. Results show the variation in the input of population has very little impact on computing the ground level concentrations for both time periods.

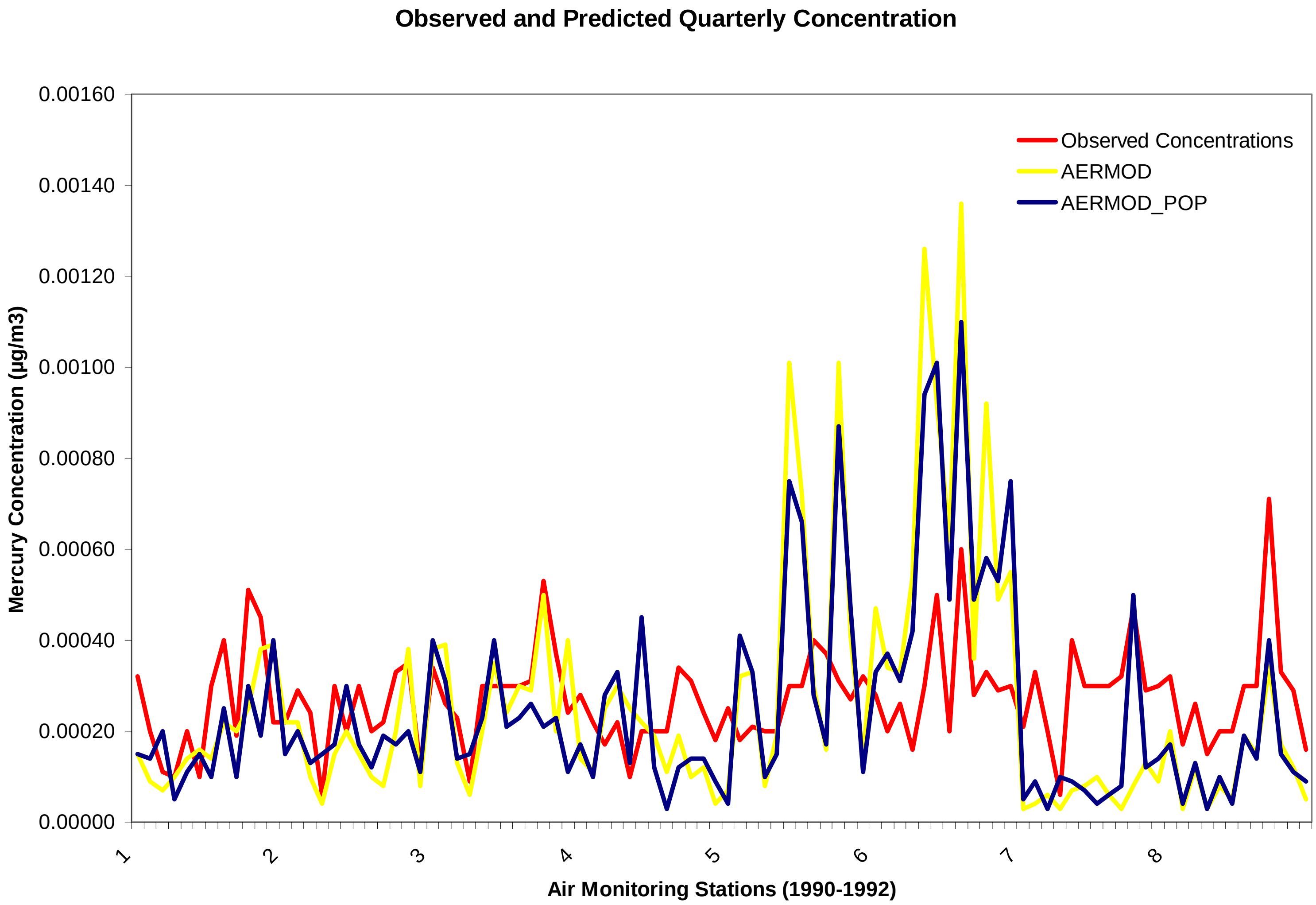

Figure 5.1: Comparison of Quarterly Averaged Concentrations for AERMOD Population Sensitivity Analysis for 1990 to 1992 in Southeast Michigan

Table 5.1: Population Sensitivity Measures obtain by Bootstrap Resampling Method for Quarterly Averaging period for AERMOD

Model	Mean	SIGMA	BIAS	NMSE	Cor (r)	Fa2	FB	FS
(1) By Straight Co and Cp i.e. with no Normalization								
AERMOD	0.00	0.00	0.00	0.82	0.386	0.583	0.045	-0.826
AERMOD_POP	0.00	0.00	0.00	0.62	0.389	0.594	0.090	-0.682
(2) By Considering Co/Co and Cp/Co i.e. Normalization by Co								
AERMOD	0.96	0.82	0.04	0.71	--	0.583	0.038	--
AERMOD_POP	0.96	0.73	0.04	0.56	--	0.594	0.043	--
(3) By Considering Co/Co and Co/Cp i.e. Normalization by Cp								
AERMOD	1.97	1.76	0.97	2.05	--	0.583	0.653	--
AERMOD_POP	1.87	1.52	0.87	1.65	--	0.594	0.608	--
(4) By Considering ln(Co) and ln(Cp)								
Model	**Mean**	**SIGMA**	**BIAS**	**VG**		**Fa2**	**MG**	**FS**
AERMOD	-8.65	0.90	0.36	2.18	--	0.510	1.430	--
AERMOD_POP	-8.63	0.81	0.33	2.05	--	0.563	1.395	--

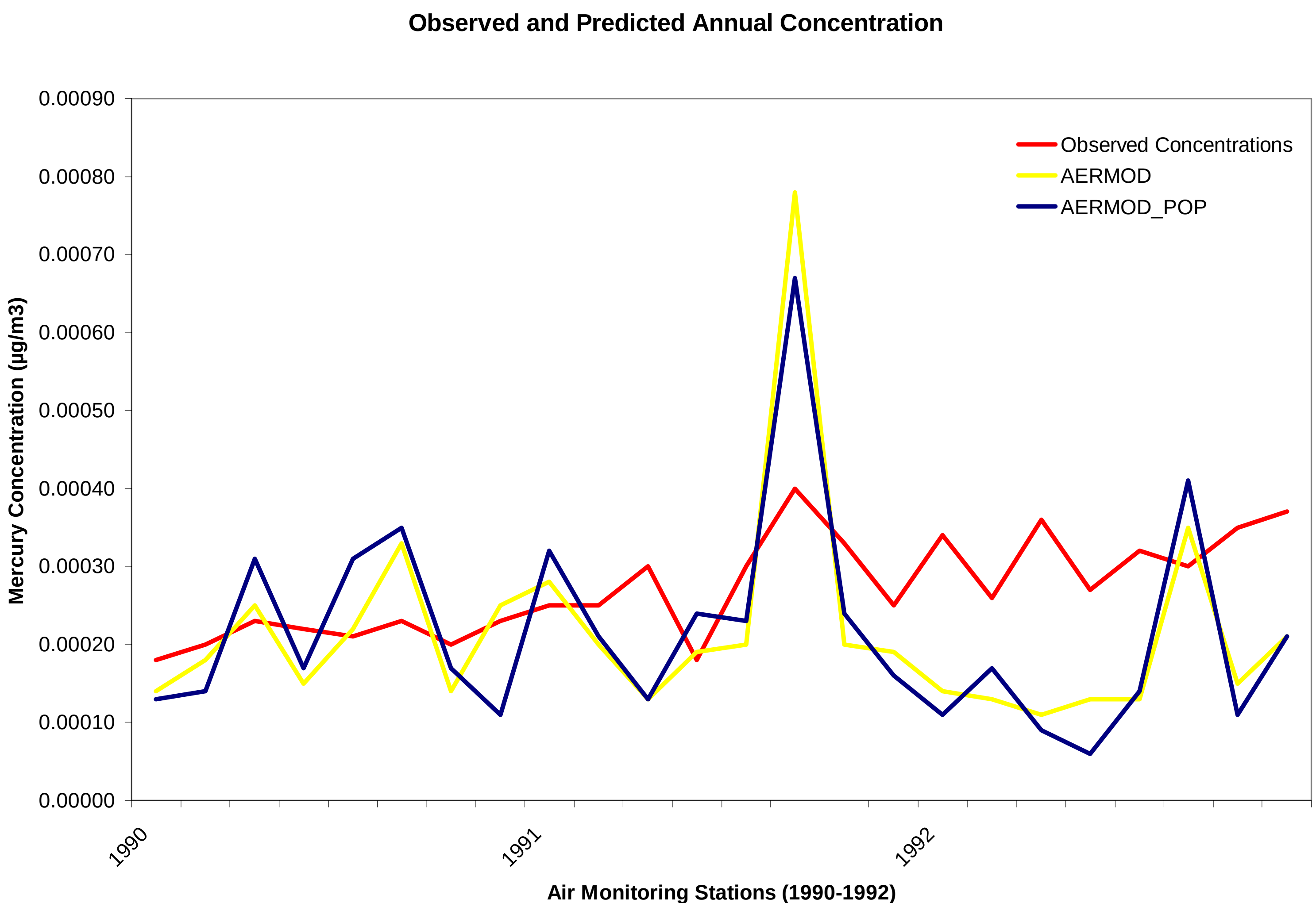

Figure 5.2: Comparison of Annual Averaged Concentrations for AERMOD Population Sensitivity Analysis for 1990 to 1992 in Southeast Michigan

Table 5.2: Population Sensitivity Measures obtain by Bootstrap Resampling Method for Annual Averaging period for AERMOD

Model	Mean	SIGMA	BIAS	NMSE	Cor (r)	Fa2	FB	FS
(1) By Straight Co and Cp i.e. with no Normalization								
AERMOD	0.00	0.00	0.00	0.33	0.309	0.750	0.231	-0.725
AERMOD_POP	0.00	0.00	0.00	0.35	0.196	0.708	0.229	-0.699
(2) By Considering Co/Co and Cp/Co i.e. Normalization by Co								
AERMOD	0.81	0.38	0.19	0.22	--	0.750	0.213	--
AERMOD_POP	0.82	0.43	0.18	0.27	--	0.708	0.197	--
(3) By Considering Co/Co and Co/Cp i.e. Normalization by Cp								
AERMOD	1.51	0.67	0.51	0.48	--	0.750	0.409	--
AERMOD_POP	1.68	1.05	0.68	0.93	--	0.708	0.509	--
(4) By Considering ln(Co) and ln(Cp)								
Model	**Mean**	**SIGMA**	**BIAS**	**VG**		**Fa2**	**MG**	**FS**
AERMOD	-8.55	0.42	0.32	1.35	--	0.708	1.372	--
AERMOD_POP	-8.59	0.53	0.35	1.57	--	0.708	1.419	--

Table 5.3: Performance obtained by Bootstrap Resampling Method for Quarterly Averaging Time

Each Model							Among Models						
Model	NMSE		FB		Cor (r)		Model	D(NMSE)		D(FB)		D[Corr. (r)]	
	Yes	No	Yes	No	Yes	No		Yes	No	Yes	No	Yes	No
(1) By Straight Co and Cp i.e. with no Normalization							**(1) By Straight Co and Cp i.e. with no Normalization**						
AERMOD	X			X	X		AERMOD-AERMOD_POP	X			X		X
AERMOD_POP	X			X	X		CALPUFF-AERMOD_POP		X	X			X
(2) By Considering Co/Co and Cp/Co i.e. Normalization by Co							**(2) By Considering Co/Co and Cp/Co i.e. Normalization by Co**						
AERMOD	X			X	–	–	AERMOD-AERMOD_POP	X			X	–	–
AERMOD_POP	X			X	–	–	CALPUFF-AERMOD_POP		X	X		–	–
(3) By Considering Co/Co and Co/Cp i.e. Normalization by Cp							**(3) By Considering Co/Co and Co/Cp i.e. Normalization by Cp**						
AERMOD	X		X		–	–	AERMOD-AERMOD_POP		X		X	–	–
AERMOD_POP	X		X		–	–	CALPUFF-AERMOD_POP	X		X		–	–
(4) By Considering ln(Co) and ln(Cp)							**(4) By Considering ln(Co) and ln(Cp)**						
Model	Log (VG)		Log (MG)		Cor (r)		**Model**	D[Log (VG)]		D[Log (MG)]		D[Corr. (r)]	
	Yes	No	Yes	No	Yes	No		Yes	No	Yes	No	Yes	No
AERMOD	X		X		–	–	AERMOD-AERMOD_POP		X		X	–	–
AERMOD_POP	X		X		–	–	CALPUFF-AERMOD_POP	X		X		–	–

Note: Yes- Indicates significantly different from zero. No- Indicates not significantly different from zero.

Table 5.4: Performance obtained by Bootstrap Resampling Method for Annual Averaging Time

Each Model							Among Models						
Model	NMSE		FB		Cor (r)		Model	D(NMSE)		D(FB)		D[Corr. (r)]	
	Yes	No	Yes	No	Yes	No		Yes	No	Yes	No	Yes	No
(1) By Straight Co and Cp i.e. with no Normalization							**(1) By Straight Co and Cp i.e. with no Normalization**						
AERMOD	X			X	X		AERMOD-AERMOD_POP	X			X		X
AERMOD_POP	X			X	X		CALPUFF-AERMOD_POP		X	X			X
(2) By Considering Co/Co and Cp/Co i.e. Normalization by Co							**(2) By Considering Co/Co and Cp/Co i.e. Normalization by Co**						
AERMOD	X			X	–	–	AERMOD-AERMOD_POP	X			X	–	–
AERMOD_POP	X			X	–	–	CALPUFF-AERMOD_POP		X	X		–	–
(3) By Considering Co/Co and Co/Cp i.e. Normalization by Cp							**(3) By Considering Co/Co and Co/Cp i.e. Normalization by Cp**						
AERMOD	X		X		–	–	AERMOD-AERMOD_POP		X		X	–	–
AERMOD_POP	X		X		–	–	CALPUFF-AERMOD_POP	X		X		–	–
(4) By Considering ln(Co) and ln(Cp)							**(4) By Considering ln(Co) and ln(Cp)**						
Model	Log (VG)		Log (MG)		Cor (r)		**Model**	D[Log (VG)]		D[Log (MG)]		D[Corr. (r)]	
	Yes	No	Yes	No	Yes	No		Yes	No	Yes	No	Yes	No
AERMOD	X		X		–	–	AERMOD-AERMOD_POP		X		X	–	–
AERMOD_POP	X		X		–	–	CALPUFF-AERMOD_POP	X		X		–	–

Note: Yes- Indicates significantly different from zero. No- Indicates not significantly different from zero.

5.2 POPULATION SENSIVITY RESULTS FOR AERMOD

Graphical evaluation between AERMOD and AERMOD_POP shows that there is not much difference between the both cases. The variation in the input of population has very little impact on the 99.5 percentile value for both time periods and proves that results were almost the same for both scenarios. In both cases, the model was significantly different from zero, and shows a good performance for NMSE and correlation of r. Therefore this study supports that urban algorithms in AERMOD are not sensitive to variation in population. However up to certain extent, the population sensitivity analysis for:

- Annual averaged time period supports for current practice i.e. by taking the whole population for the area.
- Quarterly averaged time period supports for input valued population based on the fraction of urban area multiplied by the whole population.

Chapter 6

CONCLUSION

This chapter summarizes the results of the model performance in two different ways. The first way is to look at the model performance from a regulatory point of view i.e., the prediction of highest concentration, and the second approach is to examine the performance of the model in predicting the concentration for a given sampling time at a receptor. The concept of RHC was used as a proxy for highest concentration because of the uncertainty in predicting the true highest concentration. This chapter also summaries the conclusions for required length of meteorology for different averaging time periods.

The key conclusions from this study are:

- For the general application, AERMOD and CALPUFF were found acceptable among all other models. Performance of AERMOD and CALPUFF were not significantly different from the zero for FB and correlation for r, and also AERMOD and CALPUFF results were not significantly different from each other.
- For regulatory application, AERMOD and CALPUFF were found acceptable for computing RHC for annual averaging period. However, for quarterly averaging time both the models produce conservative estimates of RHC.

- The variation in the input of population has very little impact on computing concentration for both time periods; therefore this study supports that ground level concentration for urban algorithms in AERMOD are not highly sensitive to variation in population.
- For predicting conservation estimates of concentration, 5-year of meteorological run length time is sufficient for annual and 10-year of meteorological data is sufficient for quarterly time periods.
- 20 years of meteorological data are sufficient to predict reliable and stable values for conservative scenario for 1-hr averaging time.
- At least 15-year of meteorological time interval required for conservative scenario for 3-hr and 8-hr averaging time.
- 10-years time interval of meteorological data required for conservative scenario for 24-hr averaging time.

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Appendix A

A.1 Program for obtaining a Q-Q plot in DATA PLOT for annual averaging time period

```
ECHO ON
DEVICE 1 X11
DEVICE 2 POSTSCRIPT
. STEP 0--READ IN THE DATA
READ X Y
0.00018     0.00015
0.00020     0.00021
0.00023     0.00030
0.00022     0.00011
0.00021     0.00020
0.00023     0.00045
0.00020     0.00011
0.00023     0.00037
0.00025     0.00050
0.00025     0.00011
0.00030     0.00013
0.00018     0.00034
0.00030     0.00034
0.00040     0.00090
0.00033     0.00030
0.00025     0.00014
0.00034     0.00012
0.00026     0.00023
0.00036     0.00035
0.00027     0.00011
0.00032     0.00032
0.00030     0.00011
0.00035     0.00012
0.00037     0.00045
END OF DATA
. STEP 1--COMPUTE THE MEAN
.LET M = MEAN Y
. STEP 2 -PLOT THE DATA
TITLE CALIBRATION ANALYSIS
Y1LABEL RESPONSE
XLABEL FORCE
CHARACTERS X BLANK
QUANTILE QUANTILE PLOT Y X
. STEP 3--FIT THE DATA
.FIT Y X
. STEP 4--GENERATE A SUPERIMPOSED PLOT AFTER THE
.CHARACTERS X BLANK
.PLOT Y PRED VERSUS X
```

Appendix B

B.1: Land use parameters for Wayne County, Michigan

Land Use Parameters for Wayne County												
POLYGON	SURFACE ROUGHNESS (m)				ALBEDO				BOWEN RATIO			
	SPRING	SUMMER	AUTUMN	WINTER	SPRING	SUMMER	AUTUMN	WINTER	SPRING	SUMMER	AUTUMN	WINTER
1	0.74	0.79	0.72	0.68	0.14	0.16	0.17	0.4	0.81	1.48	1.61	1.49
2	0.55	0.62	0.52	0.47	0.14	0.16	0.17	0.43	0.65	1.12	1.29	1.46
3	0.59	0.65	0.56	0.51	0.14	0.15	0.16	0.4	0.67	1.15	1.31	1.51
4	0.21	0.3	0.19	0.14	0.14	0.17	0.17	0.5	0.39	0.66	0.84	1.47
5	0.34	0.44	0.32	0.28	0.14	0.17	0.17	0.5	0.52	0.9	1.09	1.48
6	0.71	0.74	0.7	0.67	0.14	0.15	0.17	0.37	0.77	1.45	1.53	1.48
7	0.61	0.63	0.6	0.58	0.13	0.15	0.17	0.35	0.68	1.28	1.35	1.48
8	0.35	0.45	0.32	0.26	0.14	0.16	0.17	0.48	0.51	0.82	1.04	1.5
9	0.41	0.55	0.35	0.24	0.14	0.16	0.16	0.51	0.52	0.67	1.00	1.5
10	0.37	0.51	0.32	0.22	0.14	0.16	0.16	0.5	0.5	0.65	0.96	1.45
11	0.64	0.77	0.57	0.45	0.14	0.15	0.16	0.46	0.7	0.96	1.31	1.57
12	0.8	0.86	0.76	0.7	0.14	0.15	0.17	0.4	0.85	1.47	1.66	1.54

B.2: Land use parameters for Lucas County, Michigan

Land Use Parameters for Lucas County												
POLYGON	SURFACE ROUGHNESS (m)				ALBEDO				BOWEN RATIO			
	SPRING	SUMMER	AUTUMN	WINTER	SPRING	SUMMER	AUTUMN	WINTER	SPRING	SUMMER	AUTUMN	WINTER
1	0.77	0.82	0.75	0.71	0.15	0.16	0.18	0.42	0.84	1.54	1.68	1.55
2	0.57	0.64	0.54	0.49	0.15	0.16	0.17	0.45	0.67	1.17	1.34	1.52
3	0.62	0.68	0.59	0.53	0.14	0.16	0.17	0.41	0.7	1.19	1.36	1.57
4	0.21	0.31	0.2	0.15	0.15	0.18	0.18	0.52	0.41	0.69	0.88	1.53
5	0.36	0.46	0.34	0.29	0.15	0.18	0.18	0.53	0.54	0.94	1.13	1.54
6	0.74	0.77	0.72	0.7	0.14	0.16	0.18	0.38	0.8	1.51	1.59	1.54
7	0.64	0.66	0.62	0.6	0.14	0.15	0.17	0.36	0.71	1.33	1.41	1.54
8	0.36	0.47	0.33	0.27	0.15	0.17	0.18	0.5	0.53	0.86	1.09	1.56
9	0.42	0.58	0.36	0.25	0.14	0.17	0.17	0.54	0.54	0.7	1.04	1.56
10	0.38	0.53	0.33	0.23	0.15	0.16	0.16	0.52	0.52	0.68	1.00	1.51
11	0.66	0.8	0.59	0.47	0.14	0.16	0.16	0.48	0.73	1.00	1.36	1.63
12	0.83	0.89	0.79	0.73	0.14	0.16	0.17	0.42	0.88	1.53	1.72	1.6

Appendix C

C.1 Numbers of under-Predicted Periods for Quarterly Averaged Time Period option for Sulfur Dioxide in Lucas County, Ohio

Predicted By AERMOD

Numbers of Under-Predicted Periods for Quarterly Averaged for all year interval time						
Year Time Period	Monitoring Station					
	1			2		
	1990	1991	1992	1990	1991	1992
5-Year	5	16	4	4	4	12
10-Year	0	6	0	0	0	2
15-Year	0	1	0	0	0	0
20-Year	0	0	0	0	0	0
25-Year	0	0	0	0	0	0

Predicted By CALPUFF

Numbers of Under-Predicted Periods for Quarterly Averaged for all year interval time						
Year Time Period	Monitoring Station					
	1			2		
	1990	1991	1992	1990	1991	1992
5-Year	7	17	15	10	4	10
10-Year	0	12	5	2	0	3
15-Year	0	7	0	0	0	0
20-Year	0	2	0	0	0	0
25-Year	0	0	0	0	0	0

C.2 Numbers of under-Predicted Periods for Annual Averaged Time Period option for Sulfur Dioxide in Lucas County, Ohio

Predicted By AERMOD

Numbers of Under-Predicted Periods for Quarterly Averaged for all year interval time						
Year Time Period	Monitoring Station					
	1			2		
	1990	1991	1992	1990	1991	1992
5-Year	2	4	4	4	4	8
10-Year	0	0	0	0	0	2
15-Year	0	0	0	0	0	0
20-Year	0	0	0	0	0	0
25-Year	0	0	0	0	0	0

Predicted By CALPUFF

Numbers of Under-Predicted Periods for Quarterly Averaged for all year interval time						
Year Time Period	Monitoring Station					
	1			2		
	1990	1991	1992	1990	1991	1992
5-Year	0	2	6	0	0	4
10-Year	0	0	0	0	0	0
15-Year	0	0	0	0	0	0
20-Year	0	0	0	0	0	0
25-Year	0	0	0	0	0	0

C.3 Numbers of under-Predicted Periods for 1-hr Averaging Time Period option for Sulfur Dioxide in Lucas County, Ohio

Predicted By AERMOD

Numbers of Under-Predicted Periods for Quarterly Averaged for all year interval time						
Year Time Period	Monitoring Station					
	1			2		
	1990	1991	1992	1990	1991	1992
5-Year	17	17	17	14	14	17
10-Year	7	7	7	10	10	13
15-Year	1	1	1	5	5	8
20-Year	0	0	0	0	0	3
25-Year	0	0	0	0	0	0

Predicted By CALPUFF

Numbers of Under-Predicted Periods for Quarterly Averaged for all year interval time						
Year Time Period	Monitoring Station					
	1			2		
	1990	1991	1992	1990	1991	1992
5-Year	15	15	15	16	12	12
10-Year	11	11	11	13	5	2
15-Year	6	6	6	8	0	0
20-Year	1	1	1	3	0	0
25-Year	0	0	0	0	0	0

C.4 Numbers of under-Predicted Periods for 3-hr Averaging Time Period option for Sulfur Dioxide in Lucas County, Ohio

Predicted By AERMOD

Numbers of Under-Predicted Periods for Quarterly Averaged for all year interval time						
Year Time Period	Monitoring Station					
	1			2		
	1990	1991	1992	1990	1991	1992
5-Year	15	13	15	15	17	17
10-Year	10	4	6	6	12	12
15-Year	5	0	1	1	7	7
20-Year	0	0	0	0	2	2
25-Year	0	0	0	0	0	0

Predicted By CALPUFF

Numbers of Under-Predicted Periods for Quarterly Averaged for all year interval time						
Year Time Period	Monitoring Station					
	1			2		
	1990	1991	1992	1990	1991	1992
5-Year	0	2	6	0	0	4
10-Year	0	0	0	0	0	0
15-Year	0	0	0	0	0	0
20-Year	0	0	0	0	0	0
25-Year	0	0	0	0	0	0

C.5 Numbers of under-Predicted Periods for 8-hr Averaging Time Period option for Sulfur Dioxide in Lucas County, Ohio

Predicted By AERMOD

Numbers of Under-Predicted Periods for Quarterly Averaged for all year interval time						
Year Time Period	Monitoring Station					
	1			2		
	1990	1991	1992	1990	1991	1992
5-Year	16	18	22	17	22	11
10-Year	5	12	17	5	17	2
15-Year	1	8	12	0	12	0
20-Year	0	3	7	0	7	0
25-Year	0	0	2	0	2	0

Predicted By CALPUFF

Numbers of Under-Predicted Periods for Quarterly Averaged for all year interval time						
Year Time Period	Monitoring Station					
	1			2		
	1990	1991	1992	1990	1991	1992
5-Year	18	18	17	17	17	14
10-Year	13	13	7	7	7	10
15-Year	8	8	1	1	1	5
20-Year	3	3	0	0	0	0
25-Year	0	0	0	0	0	0

C.6 Numbers of under-Predicted Periods for 24-hr Averaging Time Period option for Sulfur Dioxide in Lucas County, Ohio

Predicted By AERMOD

Numbers of Under-Predicted Periods for Quarterly Averaged for all year interval time						
Year Time Period	Monitoring Station					
	1			2		
	1990	1991	1992	1990	1991	1992
5-Year	15	15	14	14	14	14
10-Year	10	5	2	4	4	4
15-Year	5	0	0	0	0	0
20-Year	0	0	0	0	0	0
25-Year	0	0	0	0	0	0

Predicted By CALPUFF

Numbers of Under-Predicted Periods for Quarterly Averaged for all year interval time						
Year Time Period	Monitoring Station					
	1			2		
	1990	1991	1992	1990	1991	1992
5-Year	15	14	9	15	18	12
10-Year	4	3	0	10	13	2
15-Year	0	0	0	5	7	0
20-Year	0	0	0	0	3	0
25-Year	0	0	0	0	0	0

Appendix D

D.1 Calculation for Land use type and Urban surface Length in Wayne County

LAND USE TYPE	Percentage
Urban	62.40
Agriculture	15.24
Grassland	1.50
Forest	12.58
Water	4.65
Swamp	3.39
Desert	0.22
Total	100.00

SURFACE ROUGHNESS				
LAND USE	**SPRING**	**SUMMER**	**AUTUMN**	**WINTER**
URBAN	1.00	1.00	1.00	1.00
	0.62	0.62	0.62	0.62
AGRICULTURE	0.03	0.20	0.05	0.01
	0.06	0.06	0.06	0.06
GRASSLAND	0.05	0.10	0.01	0.00
	0.13	0.13	0.13	0.13
FOREST	1.00	1.30	0.80	0.50
	0.13	0.13	0.13	0.13
WATER	0.00	0.00	0.00	0.00
	0.05	0.05	0.05	0.05
SWAMP	0.20	0.20	0.20	0.05
	0.03	0.03	0.03	0.03
DESERT	0.30	0.30	0.30	0.15
	0.02	0.02	0.02	0.02

	SPRING	SUMMER	AUTUMN	WINTER
TOTAL	0.77	0.82	0.74	0.69

Average 0.76