University of Alberta

MODELLING OF URBAN AIR POLLUTION IN THE EDMONTON STRATHCONA INDUSTRIAL AREA USING ARTIFICIAL NEURAL NETWORKS

by

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Abstract

Exposure to air pollution has become an exceedingly inescapable part of urban living. An important facet of the control and abatement of urban air pollution (UAP) is the use of modelling. Current modelling techniques generally use mathematics to describe transport and dispersion mechanisms of pollutants, and predict their levels at given locations away from a source. However, due to mathematical constraints, these models have limited success in dealing with complex airsheds containing many point and non-point sources of UAP.

Artificial Neural Network (ANN) modelling is a technique that effectively models non-linear type processes, such as those governing complex urban air pollution situations. The objective of this study was to investigate the use of ANN to model UAP, namely oxides of nitrogen, in the Strathcona Industrial Area, east of the City of Edmonton. This study found that ANN is a promising and effective technique for modelling hourly oxide of nitrogen fluctuations in an urban environment.

To all my friends who listened to me complain, hopefully it will stop now. To my mom Naz, dad Ali, and sister Farrah, thanks for all the support and understanding. To Karim, Almina, Suru, and Keith, thank you for all the advise and motivation. And to Safeena, thanks for the listening and the caring.

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1.0 Introduction

1.1 Thesis Organisation

This document reports on the feasibility of using of Artificial Neural Networks to model urban air pollution in the form of hourly oxides of nitrogen in the Strathcona Industrial Area of the City of Edmonton. It is split into 5 major sections. In the first section a brief introduction of this topic is given. The second section contains a detailed literature review analysing facets of urban air pollution (UAP) and Artificial Neural Network (ANN) modelling. It also contains information from literature pertaining more specifically to aspects of the problem at hand. The third section looks at the detailed modelling process of this study, outlining the methods used in the different stages of modelling. The fourth section of this document discusses a sensitivity analysis of the developed model. The fifth section provides general conclusions as well as recommendations for future research in the area.

1.2 Project Background and Summary

The modelling of UAP is an important facet of air pollution control and abatement. Models provide a means of predicting and forecasting measures of urban air quality. Current techniques used for modelling UAP use dispersion characteristics of pollutants to predict pollutant levels at locations away from defined sources. They work well in relatively simple situations with few sources in consideration. However it is very difficult for these models to handle the mathematics in an airshed with many point and non-point sources of UAP.

This study investigates and presents the results of applying ANN modelling to an airshed in the City of Edmonton, Alberta. The airshed comprises of an area containing industries such as oil refineries and power plants, and a residential zone. The Strathcona Industrial Association (SIA), consisting of ten industry members, has monitored air quality in and around the airshed since 1979. Currently, seven continuous air monitoring stations and twenty-one static air monitoring stations are operated by the SIA, and they measure many common air quality indicators, including NO_x (oxides of nitrogen). Hourly NO_x was chosen to be the output parameter for this study because data are readily available and it has diverse sources, principally from the transportation and industrial sectors. Of particular interest to this study was attempting to determine the influence of traffic volumes in the airshed on observed hourly NO_x levels.

The reproduction of NO_x concentrations by the model requires a variety of input data to be evaluated over the same time period. This includes local meteorological data (wind speed, wind direction, atmospheric stability, temperature), industrial emission data, and local traffic flow data in the airshed. Meteorological data sets were available from Environment Canada monitoring stations, industrial emission data were available from SIA members, and traffic flow data were available from the City of Edmonton Transportation Department and the County of Strathcona Engineering and Environmental Planning Department.

ANN modelling is a technique that offers advantages in modelling non-linear type processes such as those that govern complex urban air pollution situations. ANN modelling uses historical data and then extrapolates and "learns" the patterns that occur between given inputs and outputs of the model. The method is a "black-box" method, where equations describing the complex situations are not known or required. Therefore, ANN may be suitable for air pollution modelling of situations where the governing equations are too complex to solve or expensive to derive.

1.3 Research Objectives

The main objective of this study was to assess the feasibility of using ANN to model UAP in the Strathcona Industrial Area. As part of this objective, another objective of this study was to apply ANN modelling to reproduce ambient hourly NO_x concentrations measured at a selected monitoring station in the Strathcona Industrial area. The ANN model developed provided a mapping between model input parameters (the parameters that affect the hourly NO_x concentration at a monitoring station) and the hourly NO_x concentration reported at the monitoring station. The study modelled hourly NO_x concentrations so that distinct variations of levels during a day could be seen. The last objective of this study was to use the results of the ANN model to provide a means of evaluating the effect of proposed control measures on urban air quality in the monitored area. Specifically, a sensitivity analysis was done to evaluate how sensitive hourly NO_x readings in the area were to motor vehicle traffic counts on roadways directly adjacent to the air monitor.

2.0 Literature Review

2.1 Organisation of Literature Review

This literature review comprises of three main areas: ANN modelling, UAP, and an investigation of information more specific to the study at hand. As an aside, it is noted that there were very few references that encompassed both ANN modelling and UAP at the same time, as the application of ANN modelling to UAP is a relatively new undertaking.

The literature review of ANN modelling had to be general as well as specific to environmental engineering applications. Topics such as a history of ANN, general artificial intelligence modelling, types of learning and training in ANN models, and designing with various model architectures were all examined. Successful applications of ANN modelling were also investigated.

In exploring UAP for the purposes of this literature review, it was important to search out general information as well as information specific to the Edmonton region. Topics such as a history of UAP, measures of UAP, natural and anthropogenic sources of UAP, and current modelling techniques were all investigated.

Finally, the literature review contains information specific and pertinent to this study. Topics such as the selection of an appropriate output parameter, selection of model input parameters, and climatological and meteorological data for the City of Edmonton were all investigated.

2.2 *Artificial Neural Network Modelling*

2.2.1 General Overview

Artificial Neural Network (ANN) modelling is a technique that falls in the subset of Artificial Intelligence (AI) modelling. AI modelling has come to the forefront as a viable modelling technique in many areas. AI systems have three general subsets, and those are knowledge based (expert) systems, fuzzy-logic systems, and the aforementioned ANN systems.

The knowledge based or expert systems use an external human judgement skill pool to determine a set of rules. These rules are then followed to solve the situations that are demonstrated in the data set. Typically then, the set of rules is quite site specific making transference to another problem or site quite difficult. The fuzzy-logic technique encodes an ambiguity into the decision making process and composes inferences from the data set based on the fuzzy logic procedure. In other words, a fact need not be true or false, but it can be mostly true or mostly false.

ANN models show strength in solving non-linear processes efficiently, accurately, and rapidly (Rege and Tock, 1996). Resurgence in the application of ANN modelling techniques is currently in progress, in various fields of civil engineering and many other areas (Garrett, 1992). The ANN technique is unique in that is simulates the learning process that takes place inside the human brain in an effort to learn patterns directly from the data set. The key facet of ANN models that makes them desirable is their ability to learn patterns from a data set and apply these patterns to accurately forecast future events. An ANN model comprises of interconnected neuron-type processing units. These neurons, known as perceptrons, function on recognition of patterns in a data set through use of computations such as threshold logic and summation (Zhang, 1996). Once interconnected with each other, the result is a highly powerful processor with the ability to self-organise and to learn from an extensive data set.

ANN models work differently than traditional urban air models, which are based on mathematics or statistical methods. ANN models are essentially nonparametric regression models, or "black box" models. ANN models are not programmed, nor do they have set functions that attempt to approximate real-life situations. They learn directly from historical data, analysing the relationships between the inputs and the outputs of the situation at hand. They require significant knowledge on the factors that impact the process being modelled. Once the model has learned from the historical data, it can then be applied to forecast future events.

ANN models offer advantages over other current modelling techniques due to their rapid information processing, and their ability to construct a map between the input factors and the output factors initially fed into the network. This mapping not only provides a means for forecasting, it also gives a general idea of how important each of the inputs is to the model.

It is important to recognise that ANN models work best in certain situations, but may not be applicable in others. Successful applications of ANN modelling tend to fall in the following areas:

1) The algorithm to solve the problem is unknown, complex, or expensive to discover.
2) The heuristics or rules that are required to solve the problem are unknown or difficult to express.
3) There is a good base of data (in terms of quality and quantity) available for the given problem.

Some areas where ANN may not be applicable are:

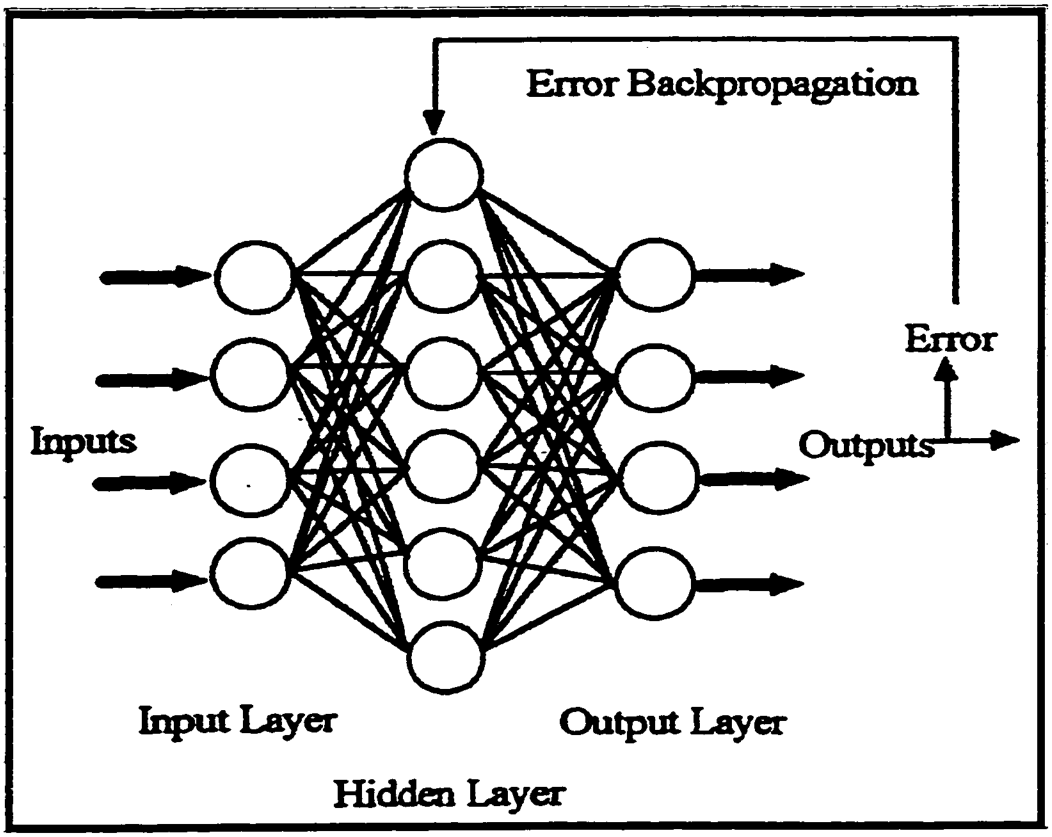
1) Linear problems for which it would be much faster and easier to solve the problem using linear problem solving techniques.
2) Problems where it is unknown as to what inputs may be affecting the output.
3) Those problems which need precise mathematical computation. It is important to remember that ANN modelling can be seen as a black-box type approach. No information about the mathematics behind the effect of the inputs on the outputs is known.

ANN applications are abundant in the realm of the stock market and are just now gaining acceptance into engineering, and in particular, environmental engineering. There are many examples of ANN applications in environmental engineering. Rege and Tock (1996) applied ANN modelling to estimate emission rates of H_2S and NH_3 from point sources. Boznar et al. (1993) used ANN modelling for short term predictions of ambient SO_2 concentration in highly polluted industrial areas in Slovenia. Zhang (1996) applied ANN modelling to the field of water treatment.

2.2.2 ANN Model Components

ANN models essentially consist of perceptrons and the interconnections between them. The weights of the interconnections between the neurons or perceptrons modify inputs into each of them (Daniell, 1991). A simple neural network is conceptually composed of perceptrons organised into an input layer, hidden layer(s), and an output layer. A simple neural network is shown in Figure 1:

Figure 1. Schematic of a Simple Artificial Neural Network (modified from Zhang, 1996)



The input layer is where the data are brought into the model. The data are transformed into an input pattern that can then be used by the hidden layer(s). The hidden layer(s) are where the majority of processing is done. The hidden layer(s) then transfer a new pattern to the output layer, which in turn creates an output pattern.

2.2.3 Learning and Training an ANN Model

There are two distinct learning techniques that can be used by ANN models. One is known as supervised learning, and the other is known as unsupervised learning. In supervised learning, input and actual output data are available for learning. This means that there is a set of input data and a set of actual output data, and the model can adjust itself and predict the output values based on the input values. The output pattern from the model can be used to readjust the input pattern to help the model improve its predictive ability. The model therefore learns from itself and readjusts itself so as to get closer to the actual output values. In unsupervised learning, there are no available actual output values, so the model must make guesses and categories based on the inputs (Zhang, 1996). In other words, outputs are generated by the network during the course of training (Daniell, 1991). This type of learning has limited applications in most engineering problems. As data are available for the output parameter, NO_x, supervised learning was used for this study.

In supervised learning, the training of the model occurs in phases. Initially, a detailed set of data consisting of input and output values is fed into the network. These data are split into three sets, the training set, the testing set, and the production set. The model uses the training set in the actual training of the model. It then uses the test set to check the model and make corrections. The production set is kept separate from the learning process and is used after the model is developed to assess model performance on entirely new data that the model has never seen before. The ANN model uses an attribute based object recognition technique (Zhang, 1996). Various levels of the different inputs to the model result in perceptrons being either stimulated or not stimulated by each learning event. When stimulated, the pattern is recognised and stored for future reference.

Supervised learning consists of the General Backpropagation (GB) technique and its variations. GB neural network models are known to be very effective at capturing the non-linear relationships that exist between variables in complex systems (Cote et. al., 1994). During the learning stage, the model outputs are compared to the actual outputs. The network learns from itself, readjusts internal weighting factors, and attempts to predict again. This "backpropagation" minimises the mean square error between the generated output in the output layer and the desired or ideal output, from the data set (Boznar et. al., 1993). This technique makes adjustments to the hidden layers in a backward propagation to allow the ANN model to learn how to predict the output more effectively.

This technique continues until the number of learning stages (epochs) reaches a specified value, or the error of the model output compared to the actual output reaches a desired minimum value. Variations of the GB technique are the recurrent network and jump connection network. In these cases, there are some interconnections between the input and output layer perceptrons that bypass the hidden layer(s), and there are some backward connections that feed the data backward through the network. In these cases, the network may take longer to converge, but might model time-series data more accurately (Zhang, 1996).

2.2.4 Topology

The input layer, output layer, and hidden layer design is referred to as the topology design of the ANN model. Topology determines the number of hidden layers, the number of neurons in the hidden layers, the number of neurons in the input and output layers, the type of learning, and the type of functions that determine the weighting of the data in the network. Selection of the best topology for the system being modelled is an important component of the modelling process. Many factors make up the topology of the model. Therefore a systematic approach must be used to determine the characteristics of the ANN model that are important for a given modelling situation. In this study, factorial design concepts were used to assess model topology and its effect on model performance in Stage 1 of the modelling process. More detail can be found in Zhang and Stanley (1997).

2.2.5 Successful Applications of ANN Models for UAP

As mentioned previously, environmental engineering applications of ANN modelling techniques are growing. In the realm of urban air pollution modelling, there are a few successful applications worth mentioning. Rege and Tock (1996) applied ANN modelling to develop a simple neural network to estimate emission rates of hydrogen sulphide (H_2S) and ammonia (NH_3) from single point sources. They used a supervised, simple backpropagation type model. The inputs used in the model were downwind distance, crosswind distance, wind speed, downwind concentration, atmospheric stability, ambient temperature, and relative humidity. They found that for the test set of data, the predictions of most emission rates were found to be within 10% of measured values, with worst case predictions within 20% of measured values.

ANN modelling was also applied to develop a model to predict ambient sulphur dioxide concentrations (SO_2) in highly polluted industrial areas with complex terrain in Slovenia (Boznar et. al., 1993). Traditional Gaussian type dispersion modelling was attempted but was found ineffective due to the complexity of the problem, specifically in the interaction of the pollutants and the terrain. The results obtained showed promise for the use of ANN modelling to predict short-term concentrations of any urban air pollutant. On the basis of these two papers and the literature review, the prospects of applying ANN modelling to predict NO_x concentrations were positive.

2.3 Urban Air Pollution

2.3.1 Definition and History of Urban Air Pollution

Urban air pollution can be defined as the infusion of pollutants into the air, from natural and anthropogenic sources within an urban area. This infusion can adversely affect human health, affect animal and plant health, damage materials and structures, and cause an aesthetic nuisance in and around urban centres. Urban air pollution is a problem that has increased in the last century. From a global perspective, it is also a problem that will continue to grow in the future due to the detrimental environmental effects of the rapid onset of urbanisation and industrialisation. The United Nations Environment Programme and World Health Organisation estimate that by the year 2000, 47% of the global population will be living in urban areas (UNEP & WHO, 1992). This creates the potential for a significant increase in the levels of air pollution in the urban environment from industry, transportation, power generation, and other sources. This rapid influx of people into urban areas also causes a significant rise in the number of people that will be exposed to urban air pollution (UNEP & WHO, 1992).

The study of urban air pollution as an environmental engineering issue is relatively new. Urban air pollution issues have their roots in England, the first area to undergo an industrial revolution that drastically affected air quality in an urban environment. The combustion of coal resulted in highly increased emissions of particulate matter and sulphur dioxide (SO_2). The effects of these emissions on human health were quite pronounced in many cases. For example, an urban air quality episode during the industrial revolution in England in 1880 resulted in a 27 percent increase in mortality during a two-week period. Another urban air quality episode resulted in 1300 excess deaths in a four-day period of heavy fog (Henry and Heinke, 1989). In addition to the health effects of some of these incidents, there have been other associated effects, which include significant damage to forest and crops, detrimental effects on animals, and damage to materials. It is estimated that these effects have cost in the billions of dollars (Halvorsen and Ruby, 1982).

This has led the way to the development of standards for air quality. These standards attempt to control ambient air quality through setting limits for emissions of certain air pollutants. Early emphasis in these standards was almost solely based on controlling sulphur dioxide, nitrogen oxide, and particle counts in the air to a level that was safe for humans (Henry and Heinke, 1989). The British Clean Air act was passed in 1956, the U.S. Clean Air act was passed in 1963, and the Canadian Clean Air act was passed in 1971. Amendments to these acts have followed, as more is understood about the complexity of urban air pollution problems. It is important to note that the science of setting urban air pollution standards is still relatively new. Many of the instruments used to measure urban air pollution indicators have been developed in the last two decades. Therefore, as more is understood about the nature of UAP, many of the standards are continually changing.

2.3.2 Urban Air Pollution Modelling

2.3.2.1 General Overview

Pollutants that are emitted into the air undergo the processes of transport, dispersion, transformation, and wet and dry deposition (Lyons and Scott, 1990). The need to understand these physical and chemical processes and how they affect the ambient concentration of urban air pollutants has led to the development of urban air pollution models.

Urban air pollution models can provide the user with a scientific means of relating source emissions to changes in the overall urban air quality. These models can be either empirical or deterministic. In an empirical model, measurements of gases and particles are done at the source and at the air monitor to estimate the contribution of the source to the readings at the monitor (Patrick, 1994). ANN models are purely empirical models, where the relationship between the inputs and the output are found by the model. Deterministic models, which are the more commonly used in terms of air pollution modelling, use mathematical processes to mimic the physical and chemical processes that affect urban air pollutant levels.

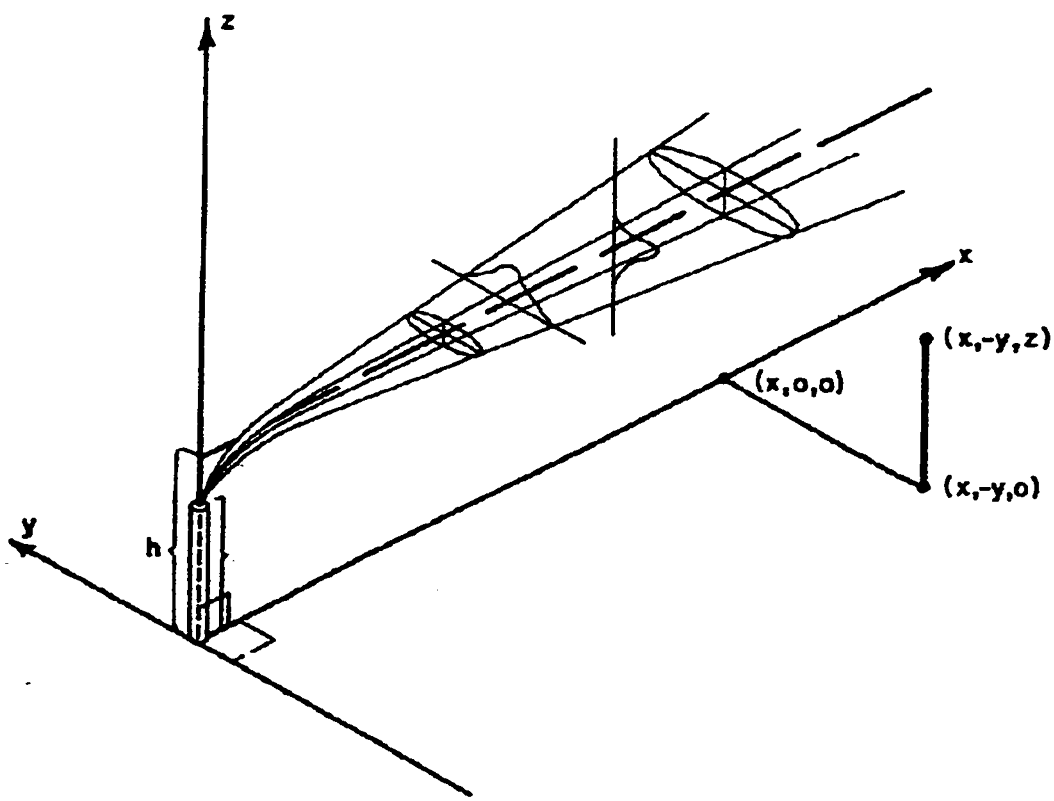
Deterministic urban air pollution models generally begin by analysing the physical processes of transport and dispersion in the atmospheric boundary layer. Then, an understanding of the chemical processes and the removal processes that affect air pollutants are incorporated. This leads to an air pollution model that accounts for many of the processes that affect urban air pollutant levels, even if only in a broad sense.

The complexity of the deterministic air pollution model depends on the number of processes that are simulated and the sophistication of the numerical methods employed (Lape, 1994). Specifically, air pollution models have been developed and applied in many variations of time frames and distances (Lape, 1994). The air pollution monitor location, or the location at which the predictions of air quality are to be made, can vary from a few metres to hundreds of kilometres from air pollution sources, depending on the model type. In other words, certain models can be applied at very short distances or at far distances from the emission sources being considered. They can be also be applied through time frames ranging from hours to years (Lape, 1994).

2.3.2.2 Gaussian Plume Dispersion

When a pollutant is released into the air, it generally has defined boundaries inside which it is contained. This is known as the plume of the emission if the release is continuous, and a puff if the release is instantaneous (Lape, 1994). The key to traditional urban air models is in the modelling of the dispersion and movement of pollutants from their source within the plume or puff. There are various ways that this can be approximated, and the most popular method is through Gaussian Plume Dispersion. This approximation assumes that the concentration of an urban air pollutant once it leaves a source spreads out in the shape of a normal distribution or bell curve. According to Lyons and Scott (1990), the Gaussian function provides a general description of average dispersion, because of the random nature of this phenomenon, by analogy with the central limit theorem of statistics. Figure 2 shows the Gaussian distributions in the horizontal and vertical directions.

Figure 2. Coordinate System showing Gaussian Distributions in the Horizontal and Vertical Directions (modified from Lyons and Scott, 1990)



The general equation of Gaussian dispersion is shown below (Lyons and Scott, 1990):

$$\bar{\chi} = \frac{Q}{(2\pi\sigma_y\sigma_z\bar{u})}\exp(-\frac{y^2}{2\sigma_y{}^2})(\exp(-\frac{(z-h)^2}{2\sigma_z{}^2}) + \exp(-\frac{(z+h)^2}{2\sigma_z{}^2}))$$

$\bar{\chi}$ =	concentration in grams/cubic metre [M/L^3]
y,z =	Cartesian coordinates
Q =	source strength in grams [M/T]
$\bar{u}$ =	mean wind speed [L/T]
σ^2_n =	variance of distribution of dispersing cloud in n direction [L^2]
h =	elevation of the source above the ground plane [L]

The strength of Gaussian dispersion is in its ability to give a general idea of the concentration of urban air pollutants at various distances away from the source. The weakness comes from the implicit assumptions made when using Gaussian dispersion. These are identified in Lyons and Scott, 1990:

1) A plume-diffusion formula assumes that the release and sampling times are long compared with travel time from source to receptor. If the release or sampling time is short compared to the travel time then we are considering an instantaneous puff and cannot neglect diffusion in the direction of travel. This represents one of the differences between continuous plume diffusion and puff diffusion.
2) The material diffused is a stable gas or aerosol (less that 20μm diameter), which remains suspended in the air over long periods of time.
3) The equation of continuity holds. That is, none of the material emitted is removed from the plume and there is complete reflection at the ground.
4) Except where specifically mentioned, the plume constituents are assumed to have

a Gaussian distribution in both the crosswind and vertical directions.

5) The Gaussian approach assumes steady-state conditions during the time interval for which the model is used, usually one hour. Of course, during rapidly changing meteorological conditions, such as the passage of a front or the arrival of a sea breeze, this assumption does not hold.

6) A constant wind speed, $\bar{u}$, is assumed. However, we have seen that wind speed increases with height near the surface. Hence for a moderate to strong vertical wind shear this assumption may introduce a considerable error. Furthermore, when the wind speed is variable, so no mean direction can be specified, and when the wind speed approaches zero, so the denominator in the Gaussian Plume equation approaches zero, the model cannot be applied.

7) The surface-wind direction in the xy plane is assumed constant. This is a reasonable assumption for a uniform mesoscale area under steady conditions. However, hills and valleys have a profound influence on the surface-wind direction and tend to channel flow.

8) The wind-shear effect on horizontal diffusion is not considered. This is a good approximation over short distances, but it becomes significant at distances greater than 10km.

9) The dispersion parameters σ_y and σ_z are assumed to be independent of z and functions of x (and hence $\bar{u}$) alone. However, eddy diffusivity increases with height near the surface. When $\bar{u}$, σ_y, or σ_z are considered independent of height, boundary-layer flow in the first several hundred metres may not be simulated. In addition σ_y and σ_z are functions of surface roughness, so that for varying terrain (for example when the plume crosses a lakeshore) they are not constant.

10) The averaging time of all quantities ($\bar{u}$, σ_y, σ_z, $\bar{\chi}$) is the same.

Other dispersion prediction techniques have also been used. The most sophisticated techniques use numerical techniques such as finite difference analysis. This analysis requires extensive data and computer resources, as well as technical expertise (Lape, 1994).

Gaussian plume dispersion and other dispersion prediction techniques are what can be referred to as a predictive approach. This approach uses mathematics in an effort to simulate the dispersion and transport of urban air pollutants. As mentioned before, the ANN modelling approach is an empirical approach, where simulation of the process is not used. What is used is an understanding of the relationship between the factors that affect urban air pollutants and the pollutants themselves.

2.3.2.3 Types of Traditional Models

Many of the dispersion models that have been developed can be classified as screening or refined models based on their level of refinement. Refined models can be classified as climatological, time-series, mesoscale, or traffic (Davies, 1984).

1) Screening Models

These models address point sources of pollutants or point sources in combination with area sources and line sources. They are quick and fairly inexpensive models to use, and have the ability to generally distinguish between problem areas and non-problem areas. These models are designed to assist in the initial design of air quality management systems. They tend to overestimate the actual concentrations due to the assumptions made. Some examples of Alberta Environmental Protection (AEP) screening models used during the 1980's are the STACKS model, the FLARES model, and the PLUMES model. They were all steady state Gaussian type dispersion models (Davies, 1984). The USEPA currently uses a model known as SCREEN3. SCREEN3 allows the user to select one of a number of pre-set scenarios that fit the situation to be evaluated. The SCREEN3 model allows the user to input the wind speed and stability, and can treat building downwash, buoyancy induced dispersion, fumigation, and plume impact on elevated terrain. It determines maximum concentrations of urban air pollutants under worst-case scenario meteorological conditions (Lape, 1994). The "worst-case" scenario is one that may not even occur for the situation being modelled. However, by evaluating this "worst-case," the model provides a quick method of identifying if the situation could be a problem. The United States Environmental Protection Agency (USEPA) approaches modelling using a tiered approach, which allows the user to begin with a simple analysis and move into more complex analyses where needed.

2) Climatological Models

As with the screening models, the climatological models address point sources, area sources, and/or line sources. These models use general meteorological data to try to determine the short-term and/or long-term urban air quality impact of various pollutant discharges. The generalised meteorological information includes things such as general wind direction, general wind speed, and general stability of the overlying air mass. Some examples of AEP climatological screening models used are the SULDEP model and the SULDEP2 model, which both use a rectangular plume model to determine the distribution of sulphur deposition from a conventional stack. Note that some of the simplifying assumptions made in these models are that there is flat terrain and that there is no chemical transformation of the pollutants that takes place (Davies, 1984). The USEPA uses the RAM model to determine both short and long term concentrations, for single or multiple point, line or area sources. The RAM model applies the user-specified locations for sources and monitors and calculates concentrations based on the distance between them. The CDM 2.0 model is exclusively used by the USEPA to calculate long term concentrations for multiple sources in an urban environment. The Industrial Source Complex (ISC3) models are the most commonly used refined USEPA models for simple and/or complex terrain applications. The ISC3 models evaluate dry deposition, building downwash conditions, stack tip downwash, and chemical transformation (using exponential decay). These models are also the preferred models to evaluate complicated sources in which refined models are not adequate to use (Lape, 1994).

3) Time Series Models

These models can only address point sources, or point sources in combination with area and line sources. Time series models attempt to simulate the urban air quality changes that occur on an hourly basis. They use previous data in the form of hourly data from a representative year. The hourly predictions obtained can be multiplied to represent time periods that are multiples of an hour, for example daily and weekly values. In the 1980's, AEP used a time series model that had 3 model components. These were GLCGEN, FRQDTN, and TIMSER. GLCGEN was a steady state Gaussian model that predicted the hourly concentrations based on single or multiple point sources. FRQDTN used the ground level concentration file produced by GLCGEN and generated average ground level concentrations for selected averaging times. The TIMSER model used the hourly concentration data files and put them into a time series file which could then be used by FRQDTN (Davies, 1984). The USEPA uses the previously mentioned SCREEN3 model to evaluate and predict the maximum 1-hour concentration of an air pollutant at the source of the air pollutant or a user defined location. AEP now uses the ISC models as time series models.

4) Mesoscale Models

Mesoscale models are specifically designed to look at impacts of urban air pollution from effluent sources over a large area. This differs from the first three types of models discussed as they focus on smaller areas. Screening, climatological, and time series models are generally applied at distances up to 10 km away (some models have been applied at distances up to 100 km) (Davies, 1984). Mesoscale models are generally designed for prediction of medium and long-range pollution transport/removal processes at distances of up to 1,000 km away. Mesoscale models should not be applied for this type of prediction close to the sources, because many simplifying assumptions are made that give poor results near the source and better results in the 100 km to 1,000 km ranges. There are other applications of mesoscale models at close proximity to sources. Table 1 shows the applications of meteorological mesoscale type models.

Table 1. Applications of Meteorological Mesoscale Models (adapted from Jandali and Hrebenyk, 1985)

Scales (km)	Application
2.5 to 25	power plant siting highway siting industrial plant siting windmill siting urban heat island lake breeze mountain valley breeze
25 to 250	sea breeze short-range weather prediction medium-range pollution transport/removal
250 to 2500	subsynoptic weather prediction long-range pollution transport/removal
All scales	mesoscale climatology severe weather trajectory calculations dynamics/energetics of mesoscale systems

Some examples of the United States Environmental Protection Agency (USEPA) mesoscale models used are the MESOPLUME, MESOPUFF, MESOPAC, and MESOFILE models (Lape, 1994).

5) **Traffic Models**

Traffic models are designed to simulate urban air quality changes due to non-point pollutant sources, specifically those derived from urban automobile traffic. These sources are considered line sources for single highways, and area sources for urban areas. AEP currently recommends use of the MOBILE-SC model, while some examples of USEPA traffic models are the APRAC, HIWAY, and ROADWAY models (Davies, 1984).

2.3.2.4 Previous Urban Air Pollution Modelling in Edmonton

Modelling urban air pollution in the City of Edmonton has essentially been restricted to the application of dispersion modelling techniques (Jandali and Hrebenyk, 1985). Western Research and Development Ltd. applied a simple advective, non-diffusive air column trajectory method to try to predict concentration of nitrogen oxides, carbon monoxide, and excess water vapour as a function of the meteorological variables (Western Research, 1976). Some of the assumptions made by this model were species conservation (i.e. chemical stability), constant spatial and temporal horizontal wind velocity, and uniform pollutant distribution in the mixing layer. The model concluded with some general observations, such as that the highest concentrations of the three parameters occurred downwind of the city (coincidentally the location of the Strathcona Industrial Area). The R^2 value, a measure of the fit of the model to the data, was 0.36, indicating a fairly poor fit (a value of 1.0 indicates an exact fit, and a value of 0 indicates an extremely poor fit). More information on R^2 is contained in Section 3.5: Discussion of Error Analysis.

Another study was conducted by Western Research that made some additions to the previous model. The atmospheric assimilative capacity, based on the stability of the overlying air mass, was considered (thermal inversions). The model also accounted for chemically reactive pollutants. One conclusion of this model was that the worst urban air quality conditions in the area were attributed to the presence of a stable air mass. This coupled with temperature inversions tends to trap the pollutants close to the surface where they remain until the air mass dissipates. Another relevant conclusion of this model was that the contributions of industrial source emissions of the Strathcona Industrial Area were relatively small under most conditions.

The final study that will be noted is the one by Hage and Hopps (1981). This study used a numerical modelling approach for predicting surface concentrations of carbon monoxide from lower level area sources in the city. The model was applied during stable atmospheric conditions, the scenarios most likely to produce extreme pollution events. This study had an R^2 value of 0.62 for predicting CO concentrations.

2.3.3 Urban Air Pollutants

Indicators of urban air pollution have evolved as the standards of urban air pollution control have progressed. In the past, urban air pollution indicators were largely based on the human senses. For example, an indicator of urban air pollution could be the colour of the sky or the smell of the air. Presently, urban air pollution standards have taken advantage of developments in measurement instrumentation, and measure levels of the actual urban air pollutants.

Essentially, urban air pollutants can be identified as primary air pollutants, secondary air pollutants, or air toxics. A primary urban air pollutant is defined as one that is produced directly in the form it remains. An example of a primary urban air pollutant is sulphur dioxide (SO_2). A secondary urban air pollutant is defined as one that is produced through a reaction of primary air pollutants and other factors. An example of a secondary urban air pollutant is ground level ozone (O_3), which is formed by the photochemical reaction of nitrogen oxides, volatile organic compounds (VOC's), and sunlight. An air toxic is defined through the use of four major criteria (Patrick, 1994). These criteria are as follows:

1) It is measurable in the air
2) It is for the most part produced by the activities of man
3) It is not a primary or secondary air quality pollutant as defined by the USEPA
4) It causes serious adverse human health effects

2.4 Research Focus

2.4.1 Strathcona Climatological and Geographical Information

The region or airshed modelled in this study is located at the east-end of the City of Edmonton. Edmonton is the fifth largest city in Canada, with a population of 635,000, and total population of 890,000 if surrounding communities are included. Edmonton is geographically situated at 53°34' N latitude and 113°35' W longitude. The metropolitan area of the City is approximately 400km^2. Elevations in the city and surrounding areas vary from 633m above sea level to 709m above sea level (Klemm and Gray, 1982).

The climate in the city can be described as sub-arctic continental. The humidity of the region is of a dry to sub-humid nature. The mean annual precipitation is 40 to 46cm. Mean summer temperatures average 13°C, while average winter temperatures fall down to -10°C. Winds are westerly 70% of the time, and the average wind velocity is 16km/h (Klemm and Gray, 1982).

Temperature inversions are important meteorological phenomena that occur frequently in this region. The mixing layer (layer the pollutants are contained in) is greatly reduced in this situation, and tends to trap the pollutants close to the ground surface. Inversions can be expected to occur almost every night of the year in this region, as well as during the day in cold winter periods.

The airshed modelled is comprised of industries such as oil refineries, chemical plants, fibreglass plants, and power plants. It also contains a residential zone, which is located east of the industrial area. The Strathcona Industrial Association (SIA), consisting of ten industry members, has monitored air quality in and around the airshed since 1979. Two continuous monitoring stations operated by the SIA are located in the airshed along with a station monitored by the Alberta Environmental Protection Agency (AEP). These monitors were used as sources of data for the ANN model.

2.4.2 Choosing an Output Parameter for the ANN Model

Literature has identified many urban air pollutants. As a whole, there is some consensus on what are considered major urban air pollutants. Those that have been consistently identified are as follows. The designation of these pollutants as primary or secondary is also noted below:

Sulphur Dioxide (SO_2)	Primary
Carbon Monoxide (CO)	Primary
Ground Level Ozone (O_3)	Secondary
Volatile Organic Compounds (VOC) / Total Hydrocarbons (THC)	Primary
Airborne Particulate Matter (PM)	Primary
Oxides of Nitrogen (NO and NO_2)	Primary and Secondary

The modelling of urban air pollution using Artificial Neural Networks requires the definition of an output parameter, or a parameter that will be modelled.

One criterion for choosing this output parameter is that it must have readily available and complete data sets. This is because the quality of an ANN model is entirely dependent on the quality and quantity of data available. The data had to be available in the hourly form, as the goal of this study was to model urban air pollution hourly so that the distinct variations of levels during a day could be seen. Another criterion is that the output parameter must adequately represent sources from various sectors of urban air pollution, such as transportation related, or industrial related. This is so the resulting model can be used to extrapolate information about a large range of air pollution sources. For these reasons, no air toxics could be used as the output parameter. An in-depth analysis of each of the 7 major pollutants was conducted, so that an output parameter could be chosen.

2.4.2.1 Sulphur Dioxide (SO_2)

Description:

SO_2 is the most common of the sulphur oxides found in the lower atmosphere. The sulphur oxides are compounds of the sulphur molecule and the oxygen molecule. SO_2 is a colourless gas that can be detected by taste and even smell in fairly small concentrations of 1,000 $\mu g/m^3$. If the concentrations surpass 10,000 $\mu g/m^3$, the result is a pungent smell (World Bank, 1996). SO_2 is a major precursor to acid rain. About 30% of the total concentration in the atmosphere is converted to a sulphate acid aerosol which can be carried for many miles and deposited by wet or dry deposition. The mechanism for this transformation in the atmosphere is that SO_2 is converted to SO_3, which is then rapidly converted to sulphuric acid (H_2SO_4) (World Bank, 1996).

Guidelines:

Alberta Environmental Protection has adopted the most stringent objectives of Environment Canada in setting guidelines for SO_2 emissions. Alberta Environmental Protection currently uses a volume/volume relationship to express concentration guidelines of air pollutants (i.e. ppm or ppb). To convert to appropriate SI units (μg/L) at 0°C and 1 atm pressure, the following conversion was done for all of the air pollutants discussed (Zumdahl, 1989):

$$y(ppm) = x(\mu g / m^3) \bullet \frac{22.4 L / mol}{MW_p} \bullet \frac{1}{1000}$$

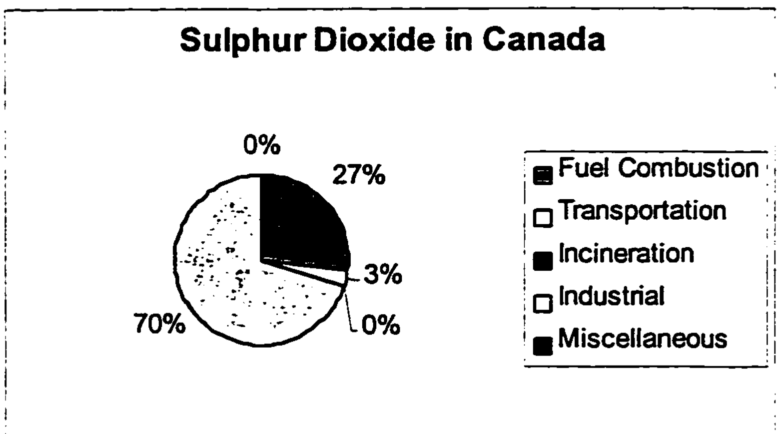
y =	concentration of air pollutant in parts per million by volume (ppm)
x =	concentration of air pollutant in SI units of micrograms/litre ($\mu g/m^3$)
22.4 L/mol =	ideal gas constant at 0°C and 1 atm pressure
MW_p =	molar weight of the pollutant (grams/mole)

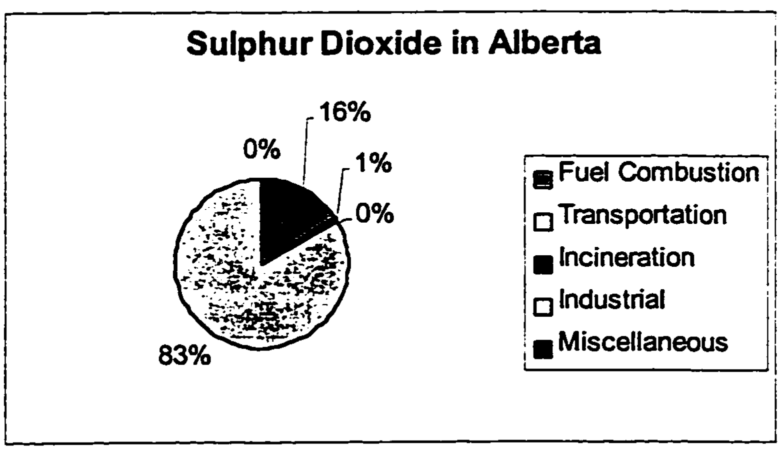
The 1-hour average concentration guideline is 490 $\mu g/m^3$ (0.17 ppm). The 24-hour average concentration guideline is 170 $\mu g/m^3$ (0.06 ppm). The annual average concentration guideline is 29 $\mu g/m^3$ (0.01 ppm) (Myrick and Byrne, 1996).

Sources:

Many sources of SO_2 have been described in literature. UNEP & WHO (1992) identified combustion in stationary sources, industrial as well as domestic wood and coal use, as being major sources of SO_2. Henry and Heinke (1989) acknowledged that sulphur dioxides are emitted primarily from the combustion of fuel oil and coal at stationary sources, and also noted that small amounts of SO_2 and SO_3 are emitted from the combustion of gasoline and diesel fuels. Kosteltz and Deslauriers (1990) reported that of total SO_2 emissions in Canada, about 70% were associated with industrial and manufacturing processes. In general, most references indicate that SO_2 is primarily an industrial effluent, and that it is associated with the combustion at stationary sources of coals, woods, and fuel oils. In addition to the anthropogenic sources of SO_2, some natural sources of SO_2 are volcanoes and forest fires. Figure 3 shows the distribution of anthropogenic SO_2 emissions based on source category in Canada and in Alberta.

Figure 3. Canadian and Alberta Emissions by Source Category for SO_2 in 1985 (adapted from Kosteltz and Deslauriers, 1990)





Health Effects:

Exposure to elevated SO_2 levels in the urban air regime can adversely affect human health directly and indirectly. An example of a direct pathway that can affect human health is exposure through direct inhalation (UNEP & WHO, 1992). An example of an indirect pathway is exposure through drinking water contamination and food contamination (UNEP & WHO, 1992). Most adverse health effects from SO_2 exposure occur in brief, high exposure situations. Exposure has been associated with decreased lung function, irritation of the eyes, nose, and throat, and increased irritation in asthmatics, children, and the elderly. Acid aerosols of SO_2 have been known to affect respiratory and sensory functions. Table 2 shows some of the health effects associated with certain concentrations of SO_2.

Table 2. Summary of reported effects of inhalation of SO_2 (adapted from Jandali and Hrebenyk, 1985)

Concentration ($\mu g/m^3$ **at 1atm, 0°C**)	**Effect or Comments**
100	WHO-estimated threshold for respiratory effects from long-term exposure (increased respiratory symptoms in adults and children above this level)
230	WHO-estimated threshold for worsening the condition of patients with existing respiratory disease from short-term exposure (e.g., increased asthma attack rate, increased illness score among bronchitics)
510	WHO-estimated threshold for excess mortality among the elderly or chronically sick from short-term exposure
1000	Mortality rate three times normal in epidemiological study, London, England
860 – 2,800	Detectable by taste
2,100 – 2,800	Lowest level causing detectable decrease in FEV, FVC, and MMFR in human lab studies (2-h exposure)
23,000 – 34,000	Immediate irritation to throat
57,000 – 140,000	Immediate irritation to eyes, nose, and throat, inducing sneezing, rhinorrhea, and cough

Ecological and Other Effects:

SO_2 is believed to cause adverse impacts to forest area, crops, and other vegetation. The WHO (1996) reported that high ambient concentrations of SO_2 could cause a loss in productivity and foliage in many types of vegetation. The acidic aerosols are even more harmful through wet and dry deposition. Sulphuric acid can damage not only vegetation, but also freshwater lake and stream systems. In terms of materials, SO_2 and the sulphate aerosols may damage stone and iron structures, which can affect many buildings and even historical monuments. Marble, limestone, paper, and leather, are other materials that may be affected by SO_2 and its other forms.

Suitability as an Output Parameter:

SO_2 data was readily available for use, and it was in the hourly form, which was needed for this study. However, the problem with using SO_2 as the output parameter is that it does not have a range of sources that adequately represent the broad sources of urban air pollution. Essentially, SO_2 represents the industrial side of urban air pollution well, but not the transportation side. If an ANN model were run using hourly SO_2 as the output parameter, the resulting model would only address the contribution of industrial sources of urban air pollution. Therefore SO_2 was not chosen as the output parameter.

2.4.2.2 Carbon Monoxide (CO)

Description:

Carbon monoxide (CO) is a colourless and odourless gas indicative of urban air pollution. It is emitted in greater quantities than any other urban air pollutant

(Alberta Environment, 1983). It is predominantly formed from the incomplete combustion of fossil fuels.

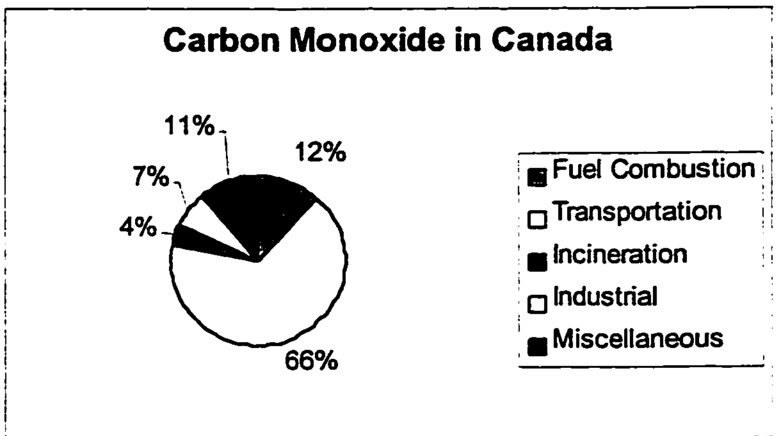
Guidelines:

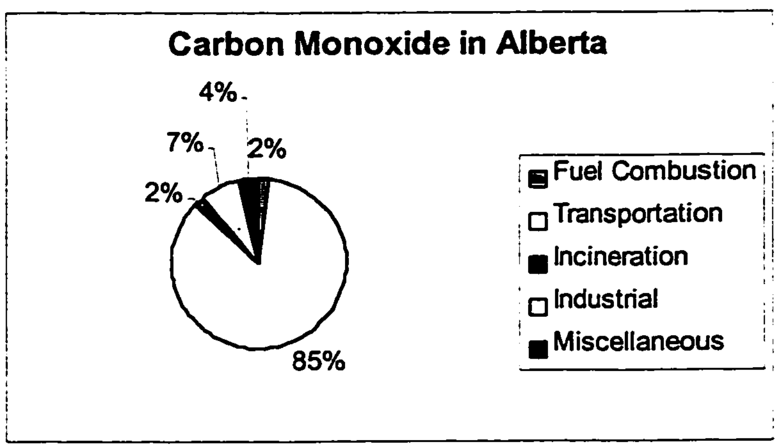
Alberta Environmental Protection has adopted the most stringent objectives of Environment Canada in setting guidelines for CO emissions. The maximum permissible concentrations are as follows. The 1-hour average concentration guideline is 16,000 $\mu g/m^3$ (13.0 ppm). The 8-hour average concentration guideline is 6,000 $\mu g/m^3$ (5.0 ppm) (Myrick and Byrne, 1996).

Sources:

The majority of carbon monoxide found in the air is from anthropogenic sources. Only trace quantities are due to natural sources (Furmanczyk, 1994). Alberta Environment (1983) indicated that of the anthropogenic sources in the Edmonton area, 96.4% came from vehicular emissions, 1.0% came from fireplaces, 1.0% came from major industrial sources, and 0.8% came from natural gas combustion and others. A common issue mentioned in many references was the discrepancy between carbon monoxide readings from sensors at elevated levels as compared to those from street levels. At elevated levels, the CO readings may appear to be within guideline values, but at the street level close to the source, CO readings can be extremely high (Jandali and Hrebenyk, 1985). Figure 4 shows the anthropogenic source category emissions for carbon monoxide in Alberta and in Canada in 1985.

Figure 4. Canadian and Alberta Emissions by Source Category for Carbon Monoxide in 1985 (adapted from Kosteltz and Deslauriers, 1990)





Health Effects:

Carbon monoxide is a highly toxic gas that can be harmful in small amounts over a certain period of time. It has a high affinity for the hemoglobin in blood, and is able to displace oxygen from the blood. The results can be cardiovascular problems and neurobehavioral effects. With high enough concentrations over a given period of time, carbon monoxide can lead to death. CO has also been known to cause headaches and dizziness (UNEP & WHO, 1992).

Suitability as an Output Parameter:

CO data was readily available for use, and it was also available in the hourly form. However, the problem with using CO as the output parameter is that it does not have a broad range of sources that adequately represent the sources of urban air pollution. CO represents the transportation side of urban air pollution but not the industrial side. This is opposite to the situation with sulphur dioxide. Essentially, a model developed using CO as an output parameter would only provide information and make observations based predominantly on the transportation side of urban air pollution. Therefore CO was not chosen as the output parameter.

2.4.2.3 Ground Level Ozone (O_3)

Description:

Ozone (O_3) is a colourless reactive gas and oxidant, and at ground levels is a major contributor to atmospheric smog. Ozone does have a characteristic sharp odour when it is highly concentrated, such as during lightning storms (Myrick and Byrne, 1996). It is formed through the photochemical reaction of oxides of nitrogen, volatile organic compounds (VOC), and sunlight.

Guidelines:

The guidelines for ozone are as follows. The 1-hour average concentration guideline is 180 $\mu g/m^3$ (0.082 ppm). The 24-hour average concentration guideline is 50 $\mu g/m^3$ (0.025 ppm) (Myrick and Byrne, 1996).

Sources:

Ground level ozone can be formed thousands of kilometres away from the source of its precursors. It is different than the other major urban air pollutants because it is not directly emitted, but rather formed from other urban air pollutants. The following simplified sequence outlines the formation of ozone from its precursors (Henry and Heinke, 1989):

$2NO + O_2 \rightarrow 2NO_2$

NO_2 + short wave radiation $\rightarrow NO + O$

$O + O_2$ + VOC catalyst $\rightarrow O_3$ + VOC catalyst

Both natural and anthropogenic sources can act as precursors to ozone formation. In terms of the anthropogenic sources, automobile emissions have been widely identified as the largest precursor source. Other anthropogenic sources of precursors include emissions from chemical and petroleum industries, and organic solvents from sources such as drycleaners (World Bank, 1996). It is interesting to note that Edmonton is reported to have naturally high background ozone levels (Alberta Environment, 1983).

Health Effects:

Ambient ozone has a marked effect on the pulmonary function of human beings. Short-term concentration spikes can cause eye and respiratory irritation, coughing, eye and chest discomfort, thoracic pain, and headaches (World Bank, 1996). As well, besides short term impacts, the potential for irreversible damage over the longer term is a concern with ozone.

Ecological and Other Effects:

Agriculture and crops can be affected by elevated ozone exposures. These exposures can cause damage to leaves and other vegetation, and this damage is manifested visibly in defoliation and plant discolouring (World Bank, 1996). Ozone may also decrease plant resistance to bacteria, viruses, and insects. This can result in reduced plant growth and inhibited yield.

Suitability as an Output Parameter:

O_3 data was readily available in the hourly form. However, the value of hourly ozone depends on the concentration of other urban air pollutants hours before, and this creates a difficulty in modelling on an hourly basis. Ozone concentrations in an area may be due to precursors from entirely different areas that are transported into the area of interest. Therefore it is difficult to use this as the output parameter, as it is not entirely known where the precursors that affect ozone originate. Therefore, ozone was not chosen as the output parameter.

2.4.2.4 Volatile Organic Compounds (VOC) / Total Hydrocarbons (THC)

Description:

VOC's are chemicals that contain hydrogen, carbon, and possibly other elements, that evaporate easily. There are many hundreds of these compounds in the atmosphere (Alberta Environment, 1993). THC's refers to a broad range of chemicals that contain carbon and hydrogen atoms (Myrick and Byrne, 1996). Methane is by far the largest (by mass) form of THC. VOC's can be seen as the volatile component of the THC measure. Therefore the two measures are closely related. VOC's contribute to the formation of ground level ozone in urban areas, as they react with nitrogen oxides and sunlight to form ozone.

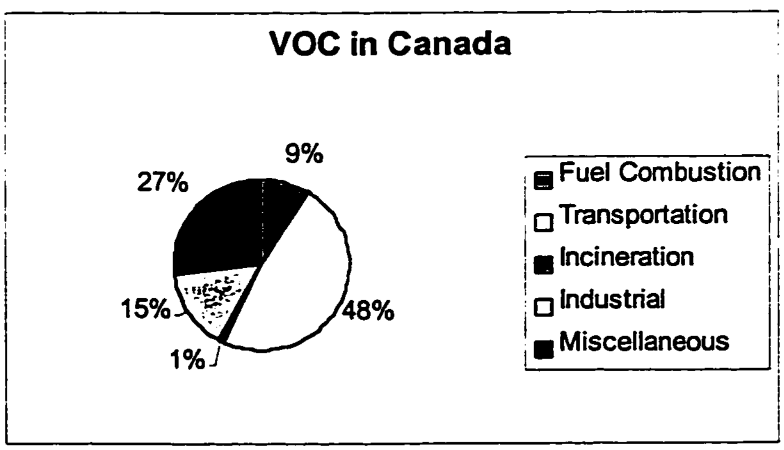
Guidelines:

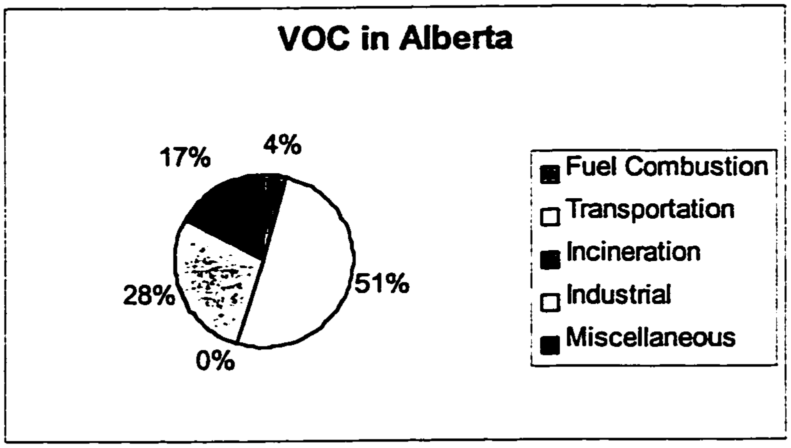
Alberta Environmental Protection currently does not have any guidelines for ambient VOC concentrations or THC concentrations.

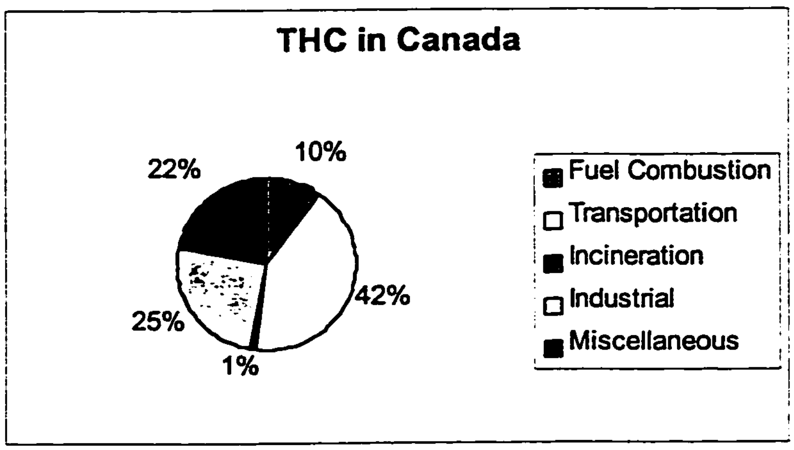
Sources:

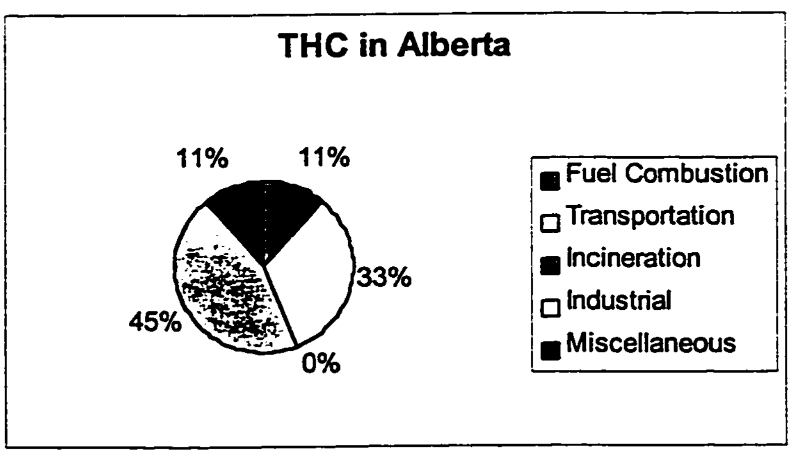
Natural sources of VOC's and THC's include fossil fuel deposits (including oil sands), volcanoes, vegetation, and bacteria. The anthropogenic sources are transportation, solvent use, industrial processes, and gasoline evaporation. In terms of the relative VOC and THC amounts produced by different sources, a breakdown for Canada and Alberta in 1985 is shown in Figure 5.

Figure 5. Canadian and Alberta Emissions by Source Category for VOC's and THC's in 1985 (adapted from Kosteltz and Deslauriers, 1990)




VOC in Alberta
17%
4%
28%
51%
0%
Fuel Combustion
Transportation
Incineration
Industrial
Miscellaneous


THC in Canada
22%
10%
42%
25%
1%
Fuel Combustion
Transportation
Incineration
Industrial
Miscellaneous


THC in Alberta
11%
11%
33%
45%
0%
Fuel Combustion
Transportation
Incineration
Industrial
Miscellaneous

Health Effects:

First and foremost, VOC's act as a precursor to ozone formation, and this is the primary means by which VOC's and therefore THC's present a human health risk. In addition, long-term exposure to certain VOC's is believed to be a threat to human health. According to the Alberta Environment (1993), benzene has been implicated as a cancer-causing agent, and hexane has been implicated in the formation of nervous system disorders.

Suitability as an Output Parameter:

Data sets for VOC are not readily available in the hourly form. Data sets for the closely related measure of THC were available in the hourly form. VOC's and THC's are indicative of petroleum industries and the transportation sector. In other words, using THC's and VOC's as the output parameter would give a complete representation of all the sources that contribute to urban air pollution. However, because of the fact that there is currently no VOC or THC guideline set by Alberta Environmental Protection, the analysis of the results would have less of a significance than with an urban air pollutant with a guideline. Therefore the VOC measure was not chosen as the output parameter.

2.4.2.5 Airborne Particulate Matter

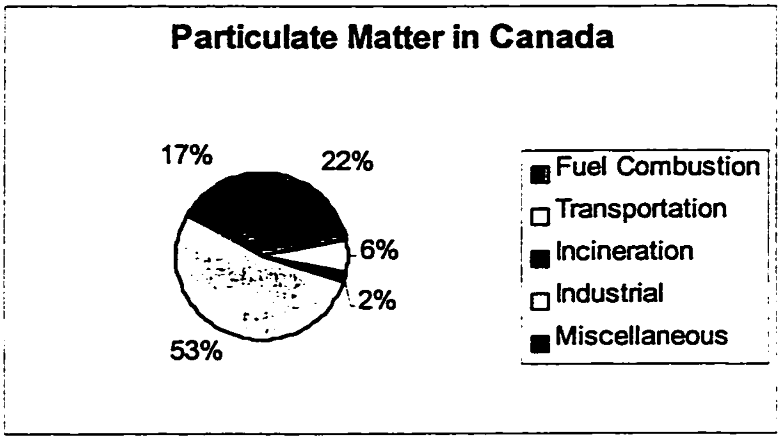
Description:

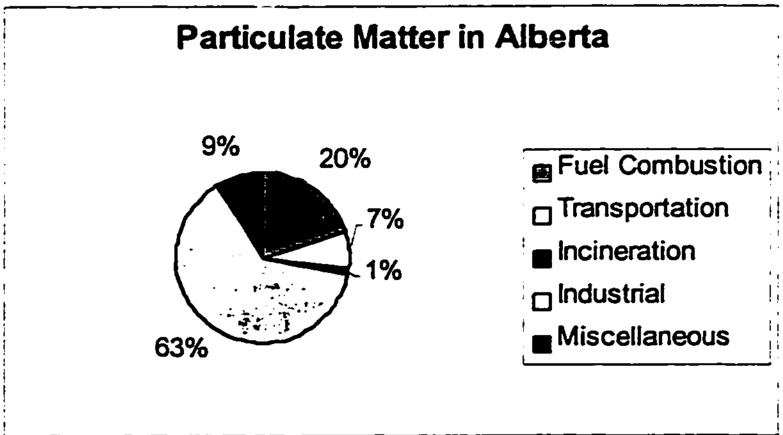
Airborne particles are defined as those particles which are small and light enough to remain suspended in the atmosphere. They include dust, dirt, soot, and liquid droplets emitted into the air (World Bank, 1996). Particles greater than 2.5 μm ($PM_{2.5}$) in aerodynamic diameter are considered to be coarse particulate and those smaller than 2.5 μm are considered fine particulate. The coarse particulate is composed of approximately 90% crustal material, and the fine particulate is composed of 60% to 90% soot and combustion by-products (Furmanczyk, 1994). Historically and presently, airborne particulate is the most identifiable form of urban air pollution. The particulate matter manifests itself by interfering with visibility, soiling material, and acting as a respiratory irritant (Alberta Environment, 1983). Particles that are airborne tend to interact with the gaseous or solid compounds in the air, thus forming organic and inorganic chemical compounds. Many of the fine particles combine with sulphates. Products of incomplete combustion may make up the carbonaceous portion of the particles (World Bank, 1996). Many of the coarse particles tend to be comprised of silicon, aluminium, calcium, and iron, reflecting elemental components of the Earth's crust.

Sources:

Natural sources for airborne particulate matter include evaporated water spray, wind-borne pollen, dust, forest fires, soil cultivation, and volcanic eruptions. In most cases, particulate matter that is natural in origin tends to be coarse. The anthropogenic sources of airborne particulate matter mainly stem from combustion processes. These may include space heating, agricultural burning, engine combustion for transportation, thermal power generation facilities, cement manufacturing facilities, and metallurgical processes. One point of interest is that in Edmonton, the use of particulate matter levels as an index for urban air pollution may not be effective simply due to the large amount of airborne particulate matter that is derived from the soil and the geography (Jandali and Hrebenyk, 1985). Figure 6 outlines the source breakdown of anthropogenic sources of airborne particulate matter:

Figure 6. Canadian and Alberta Emissions by Source Category for Airborne Particulate Matter 1985 (adapted from Kosteltz and Deslauriers, 1990)

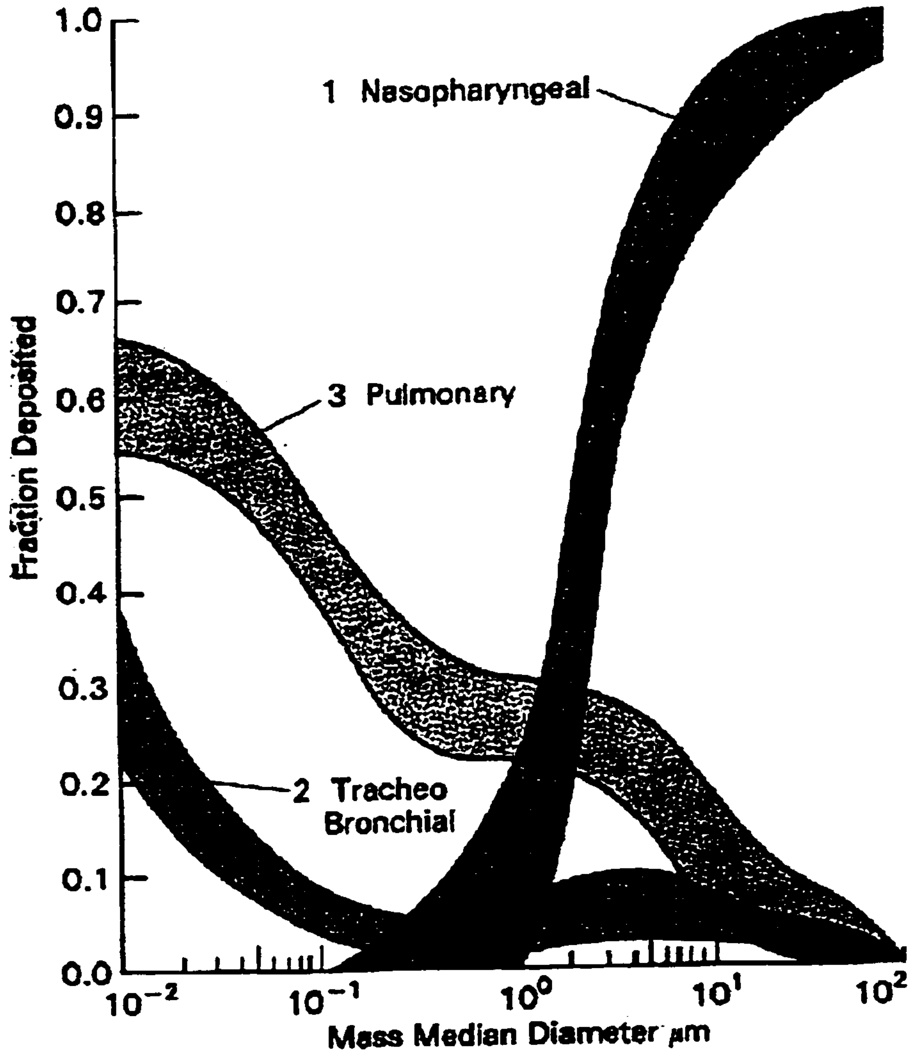




Health Effects:

Airborne particles primarily enter humans through the respiratory system. According to the particle size, shape, density, and the breathing pattern of the individual, deposition may occur at various points throughout the respiratory system (World Bank, 1996). It has been found that although most particles smaller than 10 μm (PM_{10}) can enter the respiratory system, only those particles in the fine range will be retained. Figure 7 illustrates the deposition characteristics of particles based on their size.

Figure 7. Aerodynamic deposition of particles by size in the respiratory tract (modified from Henry and Heinke, 1989)



PIC's, or products of incomplete combustion, can form a large portion of fine airborne particulate matter. They can contribute significantly to the health effects associated with exposure to smaller particles. Mortality rates have been found to significantly increase in areas with high concentrations of airborne particulate matter. Heart disease and lung disease have also been documented as being caused by higher particulate levels. It has been said also that it is possible that there may be no safe threshold below which particulate matter does not damage human health (World Bank, 1996).

Ecological and Other Effects:

In terms of vegetation, plants exposed to wet and dry deposition of particulate matter may be injured, especially in the cases where other pollutants have attached to the particulate matter. Gas exchange can be disturbed, thus stunting growth in vegetation. Heavy metals and other toxic substances can infiltrate the soil, which may also lead to reduced plant growth and yield. Other effects may be reduced visibility and soiling and erosion of buildings and materials.

Suitability as an Output Parameter:

The measure of PM_{10}, or particulate matter that is smaller than 10 μm in diameter, is readily available in the hourly form. However, as mentioned previously, high background levels of particulate matter may interfere with the use of this measure as an indicator of urban air pollution. As well, similar to the situation with VOC's, there are no guidelines set by Alberta Environmental Protection on airborne particulate matter. This means that the analysis of the results would have less of a significance than with using an urban air pollutant with a guideline. Therefore, airborne particulate matter was not chosen as the output parameter for the ANN model.

2.4.2.6 Oxides of Nitrogen (NO_x)

Description:

Oxides of Nitrogen (NO_x) are formed by natural and human activities. The natural activities that form NO_x include bacterial action in the soil, lightning, and volcanic eruptions. The human activities that lead to NO_x formation occur during combustion processes when oxygen (O_2) and nitrogen (N_2) combine at temperatures generally greater than 1000°C (Elsom, 1992). In ambient air, the two most important forms of NO_x for pollution studies are nitric oxide (NO) and nitrogen dioxide (NO_2). This is because the other forms of NO_x such as nitric acid (HNO_3), nitrous oxide (N_2O), dinitrogen trioxide (N_2O_3), dinitrogen tetroxide (N_2O_4) and dinitrogen pentoxide (N_2O_5) are not known to have any biological significance (Elsom, 1992). Nitric oxide (NO) is colourless and odourless. It is the most predominant nitrogen oxide emitted at the source of the emission. It is however, readily converted into the nitrogen dioxide (NO_2) form.

$N_2 + O_2 + \text{heat} \rightarrow NO_x$

$2NO + O_2 \rightarrow 2NO_2$

NO_2 has an orange brown colour and a very pungent odour, and many have thought that it contributes to the familiar discoloration of the sky associated with urban air pollution. NO_2 is a more toxic form than NO (Alberta Environment, 1983). A portion of the nitrogen dioxide in the atmosphere is converted to nitric acid (HNO_3) which, like the sulphate aerosols, contributes to acid rain through deposition in the wet and dry forms. Oxides of Nitrogen are also precursors to ozone (O_3) formation.

Guidelines:

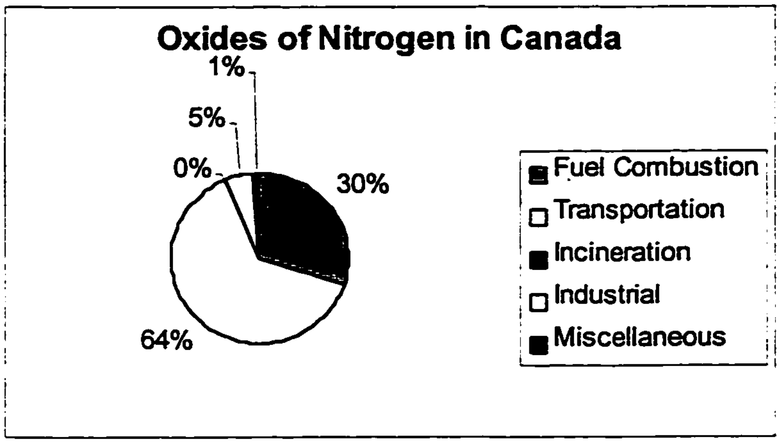
Alberta Environmental Protection has guidelines for NO_x emissions based on prevention of human health effects. Therefore the guidelines are placed on the NO_2 form of NO_x. The 1-hour average concentration guideline is 430 $\mu g/m^3$ (0.21 ppm). The 24-hour average concentration guideline is 230 $\mu g/m^3$ (0.11 ppm). The annual average concentration guideline is 60 $\mu g/m^3$ (0.03 ppm) (Myrick and Byrne, 1996).

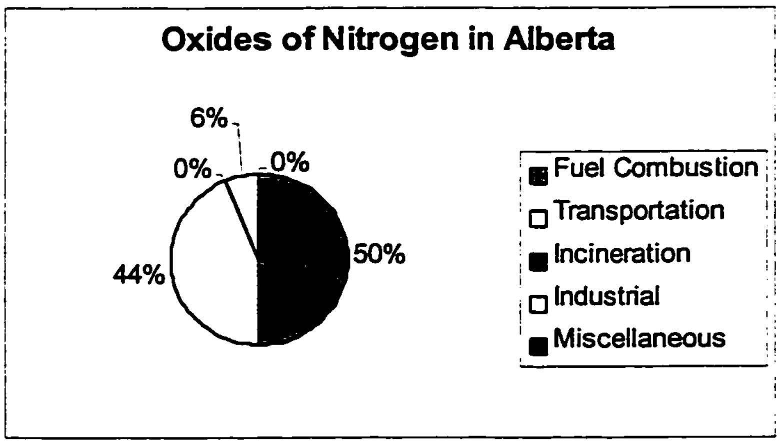
Sources:

According to Godish (1991), anthropogenic or man made sources make up about 10% of total NO_x emissions. The other 90% of NO_x emissions is accounted for by natural sources, such as anaerobic biological processes, lightning, and volcanoes. In an urban environment however, most of the NO_x concentration can be attributed to anthropogenic sources. Many sources pinpoint the combustion of fossil fuels as the leading man-made source of NO_x compounds (Myrick and Byrne, 1996). UNEP & WHO (1992) identified the automobile as the major source of NO_x emissions in an urban environment.

Other sources of nitrogen oxides are industrial boilers, incineration, space heating, electricity generation, and mining explosives (World Bank, 1996). In Edmonton in 1995, Alberta Environmental Protection estimated that 43% of nitrogen emissions were from transportation, 37% from industrial sources, and 20% from power plants and other sources in the Edmonton area (Myrick and Byrne, 1996). Figure 8 shows the distribution of anthropogenic nitrogen oxide emissions based on source category in Canada and in Alberta (note that fuel combustion includes stationary fuel sources including those from industry).

Figure 8. Canadian and Alberta Emissions by Source Category for Oxides of Nitrogen in 1985 (adapted from Kosteltz and Deslauriers, 1990)





Objectives for NO_x concentrations for Canada are set out in the National Ambient Air Quality Objectives. These objectives outline what are considered as desirable, acceptable, tolerable, and intolerable levels of NO_x in terms of annual means, daily (24hr) means, and hourly means. Table 3 shows the percentage of stations across Canada falling within the various ranges for NO_2 levels. Note that all values of concentration in $\mu g/m^3$ are for 0°C and 1atm pressure.

Table 3. Nitrogen Dioxide – Percentage of Stations with Reading in Various Ranges with Respect to the National Ambient Air Quality Objectives (1984 to 1990) (adapted from Furmanczyk, 1994)

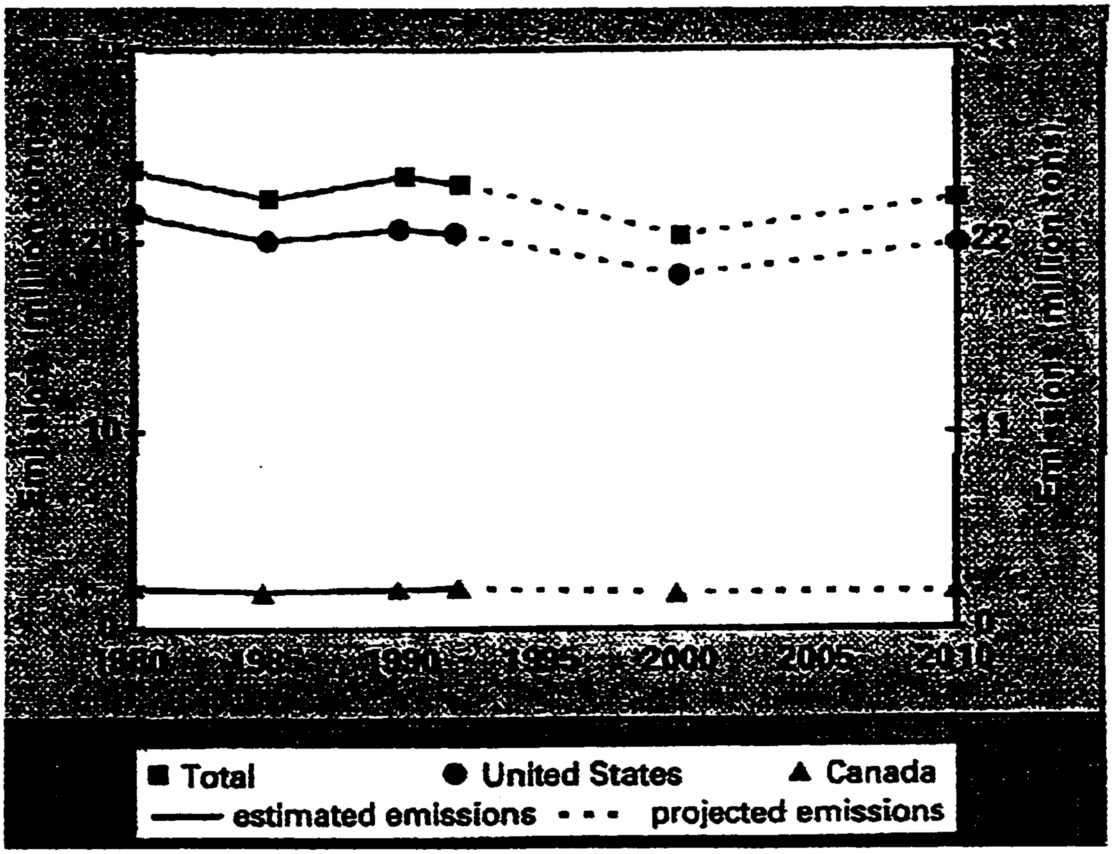
Range (μg/m^3)	1984	1985	1986	1987	1988	1989	1990
A) Annual Means							
0 to 68*	87	90	89	87	86	88	91
68 to 110**	13	10	11	13	14	12	9
>110	-	-	-	-	-	-	-
No. of Stations	39	41	36	32	44	42	34
B) 24-hour Maximum							
0 to 220**	96	96	100	100	100	88	100
220 to 330***	4	4	-	-	-	10	-
>330	-	-	-	-	-	2	-
No. of Stations	51	51	50	49	51	52	45
C) 1-hour Maximum							
0 to 440*	98	100	100	100	100	100	100
440 to 1090**	2	-	-	-	-	-	-
>1090	-	-	-	-	-	-	-
No. of Stations	51	51	50	49	51	52	45

* desirable level
** acceptable level
*** tolerable level

In recent years, many changes have occurred in technology to decrease the release of NO_x compounds to the urban air environment. However, the general increase in automobile numbers and industry in urban centres has continued to contribute to the rise in NO_x levels. The 1994 Progress Report on the Canada-United States Air Quality Agreement reports that NO_x emissions are actually expected to decline slightly by the year 2000, and then begin to rise in both of the countries (Air Quality Committee, 1994). NO_x emissions in Canada are expected to reach 2.2

million tonnes per annum by the year 2010. Figure 9 shows NO_x emission trends from 1980 until predicted values in 2010 for both the United States and Canada:

Figure 9. NO_x Emission Estimates (modified from Air Quality Committee, 1994)



Health Effects:

The health effects associated with exposure to NO_x in the urban air environment are mainly associated with pulmonary function. NO_2 is the form of NO_x that is predominantly associated with health effects. As one of the components of smog, the NO_2 component of NO_x can cause an irritation of lungs and an increased susceptibility to respiratory infections (Alberta Environment, 1993). Asthmatics, the very young, and the elderly are the most sensitive in terms of pulmonary effects to NO_2. According to World Bank (1996), levels above 3,760 $\mu g/m^3$ cause normal subjects to show significant changes in pulmonary function. Table 4 lists some of the health effects of NO_2 at various concentrations. Note that all values of concentration in $\mu g/m^3$ are for 0°C and 1atm pressure.

Table 4. Summary of reported effects of inhalation of NO_2 (adapted from Jandali and Hrebenyk, 1985)

Concentration ($\mu g/m^3$ at 1atm, 0°C)	**Effect or Comments**
100 to 155	No effect on prevalence of chronic respiratory symptoms
155 to 310	Increased respiratory disease in children
225-860	Odour threshold
1,025	WHO-estimated threshold for respiratory effects of short-term exposure
1,440 to 10,300	Increased airways resistance in laboratory studies after 10 min to 2 hour exposure
20,500 to 41,000	No discomfort
205,000 to 308,000	Delayed pulmonary edema after 30 min to 60 min exposure
410,000 to 1,400,000	Fatal pulmonary edema after less than one minute exposure
More than 3,500,000	Lethal in minutes

Ecological and Other Effects:

Oxides of nitrogen are major precursors to acid rain and deposition, as well as to ozone production, both of which can injure plants and materials. Agriculture, in terms of growth, is not adversely affected as the nitrogen contained in the nitrogen oxides is well below levels applied in the form of fertilisers. NO_2 also can cause discoloration and harm to fabrics. It is a serious enough problem that industry has devoted research and resources to developing textiles and dyes that are more resistant to NO_2 exposure.

Suitability as an Output Parameter:

Data sets for NO_x were readily available in the hourly form, which is a requirement of an output parameter for this study. Also, NO_x is representative of a broad range of urban air pollution sources, ranging from the transportation sector, to the industrial sector, to power generation. A model that used NO_x as the output parameter would therefore be able to show the effect of these sectors on urban air pollution as a whole. There also are guidelines set by Alberta Environmental Protection on NO_x. Analysis from a model developed using NO_x as the output parameter would have more of an impact than with an urban air pollutant without a guideline. The effect of reducing NO_x levels could be seen relative to the NO_x guideline. Therefore NO_x was chosen as the output parameter. Specifically, the hourly NO_x was chosen as the output parameter, as it allows for the prediction of variations during a typical day, related to the cyclic bi-modal variation in motor vehicle traffic along roadways.

2.4.3 Parameters Affecting NO_x

The selection of NO_x as the output parameter for this study was one of the first steps in the development of an ANN model for a specific situation. The next step was the identification of the factors that affect the output in general and in specific in the area of concern. This is because ANN relates the model output to the model inputs and identifying the patterns that exist between them. The parameter of hourly NO_x was used as the measurable output of the model, therefore the factors that affect hourly NO_x concentrations in ambient air were identified as the model inputs. Literature identifies many of these input parameters, or parameters that affect hourly NO_x levels. These parameters generally fall into three general classes: industry and power related, traffic related, and meteorologically related. The industry, power, and traffic related parameters represent where the NO_x is produced, and the meteorologically related parameters represent how the NO_x disperses and travels to the monitor where it is measured.

The ANN model is only as effective as the data incorporated into it. It is crucial that an understanding of the problem is well incorporated into the model through the input parameters chosen. One could choose an input parameter to be the NO_x concentration the day before, but that does not give a true representation of what actually physically affects NO_x concentrations. Parameters such as traffic counts or ambient air temperature have an actual effect on the NO_x concentrations in a physical sense, and these are the types of parameters that helped to create a flexible model with broad applications.

2.4.3.1 Industry Related Parameters

The industry and power related inputs represented the effect that industry and power generation has on the hourly NO_x levels. The availability of data from these sources was limited. Data were collected in the form of stack tests from major industries and power generating facilities that emit NO_x within the study airshed. However, it was not possible to get an hourly emission breakdown, as stack tests are typically done twice a year. The data from these stack tests were collected and average hourly values were extrapolated from them. These average values were not a true representation of the actual hourly NO_x emissions. This is because some variation in hourly emission rates would be expected relative to rates measured during stack tests. However, industries and power generating facilities in the area all stated that production was quite steady with major fluctuations only due to plant shutdowns (for which data was not available). Hourly fluctuations could then be considered small for normal operating conditions for the industries in question. These fluctuations appear even smaller when compared to the fluctuations of other input parameters used. Therefore it was judged that the average hourly values extrapolated from the stack tests were a satisfactory estimate of actual hourly values for normal operating conditions, and would be sufficient for the use in this study.

2.4.3.2 Transportation Related Parameters

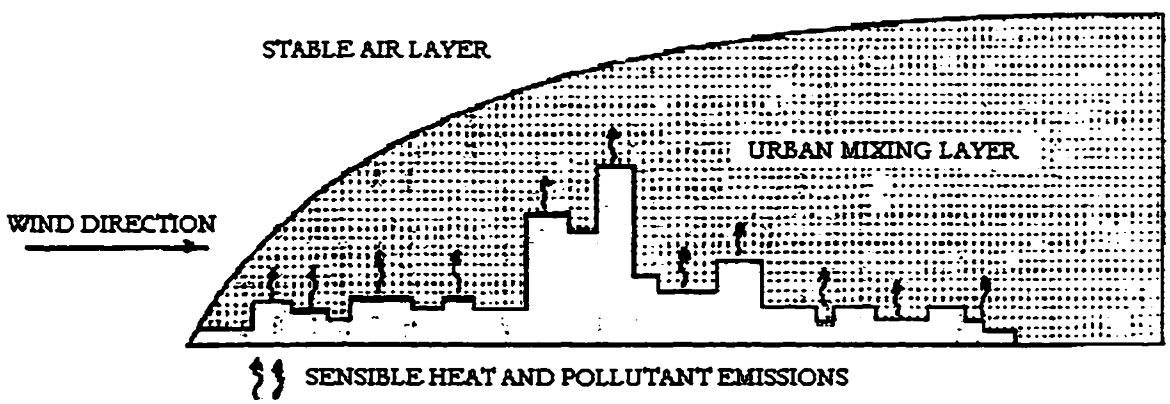
The traffic related inputs represented the effect that traffic and transportation has on hourly NO_x levels. Hourly traffic counts for the City of Edmonton and the adjacent County of Strathcona were available from the City of Edmonton Transportation Department and the Strathcona County Engineering and Environmental Planning Department. The traffic counts record the number of vehicles that pass a point on a given roadway, travelling in a given direction. The counts typically are done for a three to seven day period every few years, and usually incorporate a weekday and a weekend. Traffic counts were the best way to represent the amount of traffic in the study area. The dilemma came in addressing which traffic counts should be used. Traffic counts for the study area were available, as were traffic counts from outside the study area, which also could affect NO_x through transport processes. An ANN model takes the inputs into the model and scales them to a value between 0 and 1. Therefore, the difference of using 20 road counts or 2 road counts is negligible as long as the relative increases and decreases in hourly traffic flow are the same among the roads. It was decided that the nearfield traffic counts would be used. These are counts from roads that are surrounding and within a 5km radius of the air monitoring station where the output parameter was measured.

2.4.3.3 Meteorological Related Parameters

The meteorologically related inputs represented the effect that meteorology has on transport and transformation of NO_x. Literature has identified many meteorological parameters that may affect air pollution in general. The key was to identify the parameters with the greatest effect and use those in the model.

One aspect of meteorology that has been frequently cited in literature as significant in its effect on NO_x is the temperature profile and mixing height or the atmospheric boundary layer of the atmosphere. It is defined as the space between the Earth's surface and the lowest level in the atmosphere at which the ground surface no longer influences the meteorological variables through the turbulent transfer of mass (Lyons and Scott, 1990). It can also be defined as the mixing layer because it is the layer where urban air pollutants mix and dilute (Lape, 1994). Figure 10 shows the idea of a conceptual mixing or atmospheric boundary layer.

Figure 10. Schematic of a Mixing Layer (adapted from Western Research and Development Ltd., 1976)



Both the horizontal and vertical variation of the urban temperature field have an effect on the levels of urban air pollution, specifically NO_x concentrations (Jandali and Hrebenyk, 1985). The ambient temperature profile in the atmosphere defines the height of the mixing layer. Based on the conditions of this mixing layer, the dispersion and transport characteristics of the urban air pollutants contained within it will be different. Therefore, model inputs were needed that described the mixing layer, the stability of the air, and the atmospheric temperature. The first input chosen for use in the ANN model was ambient air temperature. These data were available in the hourly form from Environment Canada at the Edmonton City Centre Airport.

A closely related meteorological aspect to temperature profile that needed to be addressed in the ANN model is the stability of the air. This is defined as the tendency of the air to resist vertical movement or suppress existing turbulence. The stability of the atmosphere is one of the most important meteorological characteristics in terms of air pollution, as it directly affects the dispersion characteristics of pollutants in the atmosphere (Wark and Warner, 1981). Atmospheric stability can be described through the use of the dry adiabatic lapse rate. This is the rate of temperature decrease in the atmosphere with elevation wherein there is no heat added or removed from a parcel of air (Lyons and Scott, 1990). If the dry adiabatic lapse rate is compared to the actual lapse rate in the atmosphere at a given time, it can be used to indicate the stability of the atmosphere. If the actual lapse rate is greater than the dry rate, the atmosphere is unstable, which enhances the dispersion of air pollutants. On the other hand, a strongly stable atmosphere would have an adiabatic lapse rate inverse to the dry adiabatic lapse rate, which causes pollutants to remain trapped in close to the ground. In other words, when temperature increases with altitude, the lapse rate is negative, and the atmospheric condition is termed an inversion.

Inversions are quite common in the Edmonton area, more common in the autumn and winter (Klemm and Gray, 1982). They produce stagnant atmospheric conditions that have the potential to create elevated urban air pollution episodes. The mixing layer is greatly reduced in these situations, and tends to trap the pollutants close to the ground surface. Inversions can be expected to occur almost every night of the year, as well as during the day in cold winter periods. There are two main forms of inversions. Subsidence inversions are where an air mass acts as a cap to the air below it and as it sinks, the air below is trapped. In cases where this condition prevails for days, it is possible for a pollution episode to occur. These types of inversions generally occur in the wintertime, and occur above the mixing layer. Another type of inversion that can occur is a radiation inversion. This is where surface layers of the atmosphere are warmed through various means by the Earth's surface. The lower atmosphere then may cool during a clear night, and the lower layer of the Earth's atmosphere may be cooler than the upper layers. These types of inversions mostly occur during cloudless and windless nights, and tend to occur directly in the mixing layer (Wark and Warner, 1981).

In defining input parameters that described the stability of the atmosphere, issues of availability and suitability needed to be addressed. Alberta Environmental Protection did not have representative data on atmospheric temperature profiles at the location of the monitor in the Strathcona Industrial Area. Data were not consistent with the period of record for which data on other modelled variables were available. Alberta Environmental Protection measures horizontal wind direction fluctuations and computes the standard deviation of these fluctuations to define local stability conditions. It is important to note that because of the anisotropy of boundary layer turbulence, horizontal wind fluctuations may not always be a suitable representation of the vertical wind fluctuations for certain situations. However, data on horizontal wind direction fluctuations were available, and in most situations give an idea of the stability of the air based on its gustiness (Angle and Sakiyama, 1991). Table 5 shows turbulence classifications based on horizontal wind fluctuations.

Table 5. Turbulence classifications based on wind fluctuations (adapted from Angle and Sakiyama, 1991)

Stability Description	Standard Deviation of the Horizontal Wind Direction Fluctuations (in degrees)	Standard Deviation of the Vertical Wind Direction Fluctuations (in degrees)
Very unstable	Greater than 22.5	Greater than 11.5
Moderately unstable	17.5 to 22.5	10.0 to 11.5
Slightly unstable	12.5 to 17.5	7.8 to 10.0
Neutral	7.5 to 12.5	5.0 to 7.8
Slightly stable	3.8 to 7.5	2.4 to 5.0
Moderately stable	2.1 to 3.8	1.2 to 2.4
Very stable	< 2.1	< 1.2

Notes:

(1) These criteria are appropriate for steady-state conditions, a measurement height of 10m, level terrain, and an aerodynamic surface roughness length of 15cm. Care should be taken that the wind sensor is responsive enough for use in measuring wind direction fluctuations.

(2) A surface roughness factor of $(z_0/15\text{cm})^{0.2}$ where z_0 is the average surface roughness measured in centimetres within a radius of 1-3 km of the source, may be applied to the tabulated values.

(3) For nighttime hours with horizontal wind fluctuations indicated to be unstable, the following corrections should be applied:

If the indicated Stability Category is:	And the Wind Speed at 10 m is: (m/s)	Then the Corrected Stability Category is:
Extremely unstable	< 2.4	Very stable
	2.4 to 2.9	Moderately stable
	2.9 to 3.6	Slightly stable
	> or equal to 3.6	Neutral
Moderately unstable	< 2.4	Moderately stable
	2.4 to 3.0	Slightly stable
	> or equal to 3.0	Neutral
Slightly stable	< 2.4	Slightly stable
	> or equal to 2.4	Neutral

Therefore, the input parameter of standard deviation of horizontal wind direction was chosen. Measurements of the horizontal wind direction are taken every 5 minutes, and the standard deviation of these measurements inside of an hour is the value recorded every hour at the Alberta Environmental Protection monitoring station.

The next aspect of meteorology that needed to be incorporated in some form as an input parameter was the dispersion and transport of the pollutants from their respective sources to the air pollution monitor in the Strathcona Industrial Area. The input parameters of hourly horizontal wind speed and hourly horizontal wind direction were chosen as they describe the travel of pollutants to the monitoring station. At the same time, these two input parameters also give an idea of the stability of air.

3.0 ANN Modelling of NO_x in the Strathcona Industrial Area

3.1 *Organisation of Section*

This section discusses the application of ANN Modelling to model hourly NO_x concentrations in the Strathcona Industrial Area. The modelling protocol used to develop the ANN model is outlined. The results of the various stages of model development are also presented. The neural network development software package used for this entire modelling study was Neuroshell ® 2 developed by the Ward Systems Group ®.

3.2 *Modelling Protocol*

ANN modelling is a very subjective process. There are a number of possible ways to design a model, so it is of utmost importance that a protocol be developed to provide a direction. Without a protocol, ANN modelling becomes more of a random trial and error process that may not identify the best solutions for the modelling situation. The modelling protocol allows the user to develop a model that works with the available data and the modelling situation. The process used in this study is as follows:

1) Literature Review of Problem
2) Collection of Data
3) Source Data Analysis
4) Stage 1 Modelling: Identification of General Model Architecture Type
5) Stage 2 Modelling: ANN Feasibility Through ANN Pilot Model

6) Stage 3 Modelling: Full-Scale ANN Model

The literature review was the first step of this modelling protocol. This identified the input and output parameters for the model. In other words, this step identified what was to be modelled (output), and what affected that parameter (inputs). The second step of the modelling protocol was the collection of data. Both these steps for the modelling of hourly NO_x in the Strathcona Industrial Area were already outlined in the Literature Review (Section 2.0), particularly in the Research Focus (Section 2.4).

3.3 Source Data Analysis

Source data analysis investigates the situation to be modelled along with the data available, and allows the user to determine the feasibility of ANN modelling for the situation. Source data analysis also allows the user to get a general sense as to the type of backpropagation model that would best be able to model the situation. The source data analysis answers the following questions:

1) Is ANN modelling applicable in this situation?
2) Is the domain study an open system or a closed system?
3) What are the cause-effect relationships in the study domain?
4) What is the behaviour or characteristics of the output?
5) Is there any unusable data?
6) Are all the input data used justifiable?

The feasibility of modelling of hourly NO_x in the Strathcona Industrial Area and the factors used in modelling it are discussed below:

1) Is ANN modelling applicable in this situation?

ANN modelling may be applicable in cases where there are no other cheaper and more efficient modelling techniques available. This means that the study domain is quite complex with various cause/effect relationships that may not all be understood, or that the governing mathematical equations are too complex or expensive to discover. In this situation, the mini-airshed in question has many inputs that act differently and that are interrelated. It would be difficult to apply other modelling techniques, such as Gaussian plume dispersion models, to this situation as the airshed is complex and there are many input factors to consider. The non-linearity of the modelling situation also lends itself well to the application of ANN modelling.

2) Is the domain study an open system or a closed system?

An open system is one where the relationships between the model inputs and the model outputs are not fully understood. A closed system is one where more is known about these relationships, and the domain is restricted to an area that is understood well. The domain in question is an open system. In other words, there are many input factors that are known to affect the NO_x levels in the airshed, but the relationships between the inputs and outputs are not fully understood.

3) What are the cause-effect relationships in the study domain?

This relates to knowing what inputs affect the output. As stated previously, this is more of an open system, so the exact relationships between the inputs and the outputs are not known. As outlined in the research focus (Section 2.4), the input parameters of importance are split into three major classes: industry related, transport related, and meteorologically related. All of these input parameters are known to affect the hourly NO_x levels at the monitor. The input parameters chosen are listed as follows:

INPUT PARAMETER	UNITS	SOURCE
Atmospheric Temperature	degrees C*	Environment Canada
Wind Speed	km/h*	AEP and SIA
Wind Direction Sector	no units	AEP and SIA
Wind Direction Degree	degrees*	AEP and SIA
Atmospheric Stability (standard deviation of horizontal wind direction)	degrees (hourly average)	AEP
Industry Emission Data	kg/s	SIA
Traffic Data	traffic counts	City of Edmonton and County of Strathcona

* data sampled and archived at the beginning of every hour

It is known that an increase of atmospheric stability results in the potential of an increase in hourly NO_x levels. An increase in traffic volume also results in the potential increase in hourly NO_x levels. An increase in industry emissions may result in an increase in the background NO_x concentrations seen by the model. Certain wind directions may cause the hourly NO_x readings at the monitors to be higher based on the source of the NO_x. A higher wind speed generally results in potentially lower NO_x, as mixing in the atmosphere is promoted and pollutant dispersion is enhanced. And generally speaking, a lower temperature can promote a higher level of NO_x because winter conditions result in predominantly more stable air in the Edmonton area.

4) What is the behaviour or characteristics of the output?

The output seems to sway between lower values with slight variation to higher values associated with events, which can last for days on end and have sharp variations. The lower values are likely situations in which the stability of the atmosphere is low, and the higher values are likely from inversions.

5) Is there any unusable data?

There are some cases where there are data gaps in the records. For example, there may be a few days where the temperature readings go off-line, so that even though all of the other input data are available, the entire set of data for those time periods cannot be used. Generally speaking, there seem to be very few of these data gaps over the entire record. All of the input and output data for situations where there was a data gap for a given hour were taken out of the set so that the model had complete data sets to work with.

6) Are all the input data used justifiable?

All the input data used is justifiable. The standard deviation of horizontal wind direction and the wind speed and direction indicate the mixing characteristics of the atmosphere. The temperature data gives an indication of the weather patterns present and the stability of the atmosphere. The actual horizontal wind direction also indicates the significance of different inputs that are in different directions from the monitor. The traffic and industry emissions indicate the source of NO_x in the system.

3.4 Detailed Overview of General Backpropagation Networks

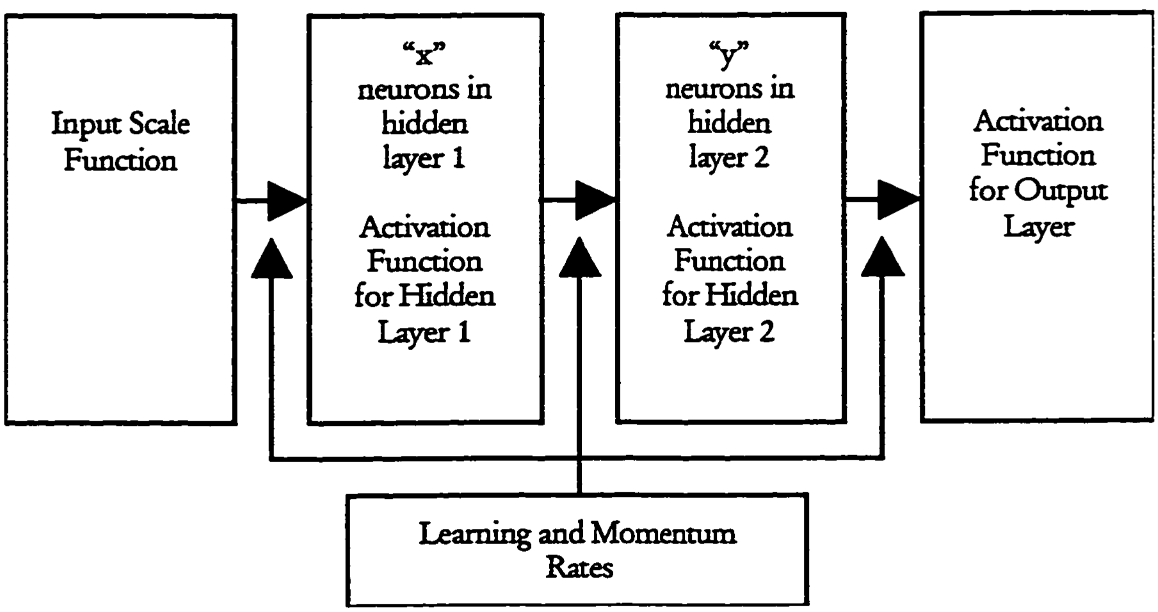
There are different general architecture types of ANN models that can be used to model a given situation. The general model architecture type investigated in this study was the backpropagation architecture, due to its' strength in modelling non-linear situations. Backpropagation networks are able to generalise well for a wide variety of problem types. They are classified as supervised networks, which means that there are both inputs and an output that are used to train the model. Within the realm of backpropagation architecture, there are many sub-types that are classified based on the connections between the layers of the network. The backpropagation network sub-types investigated in detail in this study were as follows:

1. Standard 4-layer Backpropagation Network
2. Standard 3-layer Backpropagation Network
3. 4 layer Jump-Connection Network

3.4.1 Variable Parameters in Backpropagation Networks

Backpropagation training requires many parameters to be set or defined for model training to take place. Some of these parameters are schematically shown in Figure 11.

Figure 11. Detailed Schematic of a Backpropagation Network



The parameters that need to be set or defined for model training are as follows:

1) Number of neurons in the hidden layer(s)
2) Input Scale Function
3) Hidden Layer and Output Layer Activation Functions
4) Learning and Momentum Rates in Layer Links
5) Pattern Selection and Weight Updates
6) Stop Training Criteria

1) Number of neurons in the hidden layer(s)

The number of neurons in the input layer is equal to the number of inputs used for the modelling, and the number of neurons in the output layer is equal to the number of outputs used. Therefore the only numbers that vary are the numbers of neurons in the hidden layer(s). General heuristic rules exist that can help provide a direction for selecting the number of neurons, but generally speaking, this is a trial and error process. Some of the heuristics suggest using the same number of hidden layer neurons as there are in the input and output layers. Other heuristics attempt to use a formula to set the number of hidden layer neurons based on the number of neurons in the input layer. For networks with 2 or more hidden layers, some heuristics suggest that each subsequent layer should be 75% or the previous hidden layer. However, the specific set-up for a particular problem will vary, and the best way to find the optimum is through experimenting with the problem.

2) Input Scale Function

The input scale function of the input layer serves to adjust the scale of all the inputs so that they can be fed into the hidden layers where the processing takes place. There are two main types of scaling functions: those that scale the inputs from –1 to 1 and those that scale the inputs from 0 to 1. Because the input data used for this study can have negative values (temperature), the scaling functions should scale the inputs from –1 to 1. Therefore, the choices of scale functions are the linear function and the tanh function. The linear function may be further subdivided into two functions. The linear[-1,1] denotes that the network will cut off numbers below and above the ranges it encounters later in new data. The linear <-1,1> denotes that new data falling outside the range will be accepted into the model.

3) Hidden Layer and Output Layer Activation Functions

The hidden layer and output layer activation functions represent how the data will be propagated within the network. Essentially, the hidden layers produce an output that is based on the sum of the weighted values from the preceding connection. The activation function is then applied, re-scaling the sums into an output that is then fed into the next layer. The different functions are as follows (Ward Systems Group Inc., 1996):

a) logistic
b) linear
c) tanh
d) tanh15
e) sine
f) symmetric logistic
g) Gaussian
h) Gaussian complement

4) Learning and Momentum Rates in Layer Links

Each connection between layers in a model has its own learning rate and momentum rate. Learning rate refers to the rate that the network learns and retains patterns from the data. A slower learning rate is generally needed for more complex and noisy inputs, and a quicker learning rate can be used for simpler problems.

Momentum rate is analogous to momentum in physics. A high momentum rate will give the network a higher inertia or tendency to proceed in a straight direction. A low momentum rate results in a slower modelling process, but a reduced probability of being stuck in a local minimum as a solution.

5) Pattern Selection and Weight Updates

The pattern selection refers to the method by which data are input into the model. A rotational input refers to a method whereby every n^{th} input pattern is used on a rotational basis. An input pattern is defined as data from all of the inputs for a single output data point. A random input refers to a method whereby random patterns are chosen to input into the network. Certain pattern selections fit with certain methods for weight updates. The weight update types analysed in this study were the momentum method and the Turboprop method. The momentum method is suggested for use with a random pattern selection. The momentum method makes use of the learning and momentum rates input into the network. The Turboprop method is only used with rotational weight updates. This method uses different weights rather than a single learning and momentum rate. The results are generally poorer with the Turboprop method, but generally faster. The Turboprop method also gives the user a general idea of how the model type being used is working at modelling the situation.

6) Stop Training Criteria

The criteria with which the training of the model is ended are referred to as the stop training criteria. The model training process can be terminated based on the error in the training set or the error in the testing set. This study uses the testing set error as the criteria for ending training, as it is a more accurate representation of actual model performance, rather than an assessment of training set fit. The actual testing set error value that terminates training can be specified. The number of intervals since the minimum testing error can also be specified.

3.5 *Discussion of Error Analysis*

Reporting results from the different stages of modelling required a consistent means of error measurement that would allow comparison between models and evaluation of model effectiveness. The quality of the models throughout the optimisation process was measured through an analysis of the errors. The errors had to be analysed within the model and then across the model. The main statistical values used for measuring the error across the model were the R^2 error and the root mean square error (RMS).

The R^2 error is a statistical indicator that is usually applied in multiple regression analysis (Ward Systems Group Inc., 1996). A perfect model fit would result in an R^2 of 1. An R^2 of 0 indicates that the model predicts no better than using the mean of all the outputs as the model output. The R^2 value can be seen as a method of comparing the model output values to an arbitrary benchmark, the average of the output values. The formula used by the ANN modelling software Neuroshell® 2 is shown as follows (Ward Systems Group Inc., 1996):

$$R^2 = 1 - \frac{SSE}{SS_{YY}}$$

where $SSE = \Sigma(y - \hat{y})^2$

$SS_{YY} = \Sigma(y - \bar{y})^2$

y = actual value of output

$\hat{y}$ = predicted value of y

$\bar{y}$ = mean of all the y values

The root mean square error (RMS) is a statistical measure of the differences between the actual output values and the model output values. It is defined as the mean of the squares of all of the residuals between actual outputs and the model outputs. The formula can be shown as follows:

$$RMS = \frac{\sum_{n}^{1}(actual - predicted)^2}{n}$$

where n = total number of output values

actual = the actual output values

predicted = the model predicted output values

The use of these measures of error across the model enables a model that has relatively well distributed prediction errors to be chosen, as large areas are strongly penalised (Zhang, 1996). To measure the error within the model, two types of residual plots were done. These were the residual error versus time, and the residual error versus NO_x concentration. In Stage 1 of the modelling, the R^2 error was used as the means of error analysis because only a preliminary indication of future model direction was needed. In later stages, a more detailed error analysis was conducted to give a complete indication of model performance.

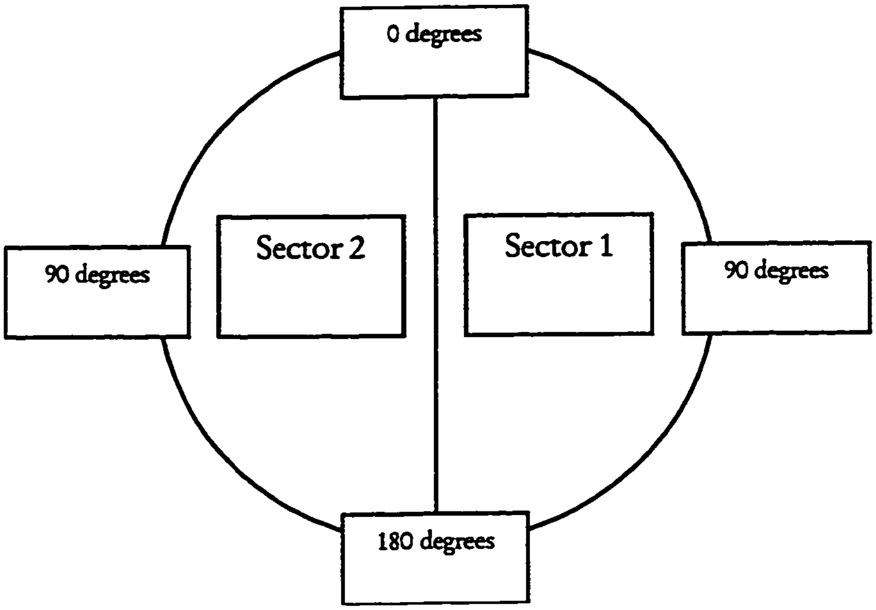
3.6 Input Data for the ANN Model

The inputs into the model were temperature, wind speed, wind direction, standard deviation of horizontal wind direction, and traffic counts of motor vehicles in nearfield roadways. These were in fact the inputs for all of the models throughout this study, as they were identified as the most important inputs from the literature review.

The NO_x data were obtained from the Alberta Environmental Protection (AEP) monitor located in the Strathcona Industrial Area. The NO_x data are in parts per million (ppm) as NO_2, and are measured to the nearest thousandth of a ppm. The temperature data were obtained from the Environment Canada City Centre Airport monitor, located approximately 10 km from the Strathcona Industrial Area. The temperature data are in degrees Celsius, and are measured to the nearest $1/10^{th}$ of a degree. The wind speed data were obtained from the AEP monitor in the Strathcona Industrial Area, and are measured to the nearest $1/10^{th}$ of a kilometre per hour.

The wind direction data were obtained from the AEP monitor as well and were recorded hourly to the nearest degree from north (bearing). There was an additional issue with wind direction. An ANN model looks at the data from a purely numerical point of view. A reading of 359 degrees from North is numerically very different from a reading of 1 degree from North. However, in reality the two values point to almost exactly the same direction. This discrepancy needed to be incorporated into the model. Boznar et. al. (1993) identified the same problem in the modelling of ambient SO_2 in Slovenia. It was decided that two inputs would be created from the wind direction input. The two inputs would be a sector and a degree reading. This is schematically shown in Figure 12.

Figure 12. Schematic Representation of Wind Direction Input



Therefore an angle of 45 degrees would become sector 1, 45 degrees. An angle of 185 degrees would become sector 2, 5 degrees. In this way, the discrepancy is remedied, and the model should find it easier to decipher and use the wind direction data.

Traffic data were obtained from the City of Edmonton Transportation Department and the Strathcona County Engineering and Environmental Planning Department. The traffic counts were recorded in terms of vehicles per hour. As described in the research focus section of the literature review (Section 2.4), it was decided that traffic counts from nearfield sources to the monitor would be used. Counts from roads directly adjacent to the monitor were used. These were as follows:

1) Station 8545E (City of Edmonton) at 17 Street North of Baseline Road
2) Station 13S (County of Strathcona) at Baseline Road East of Broadmoor Boulevard
3) Station 8S (County of Strathcona) at 17 Street South of 90 Avenue
4) Station 512E (City of Edmonton) at Baseline Road East of 34 Street

Refer to the map in Appendix A to observe the location of the traffic counts in relation to the AEP monitor location. This map also shows the location of the Strathcona Industrial Area in relation to the City of Edmonton.

3.7 Stage 1 Modelling

3.7.1 Overview

There were two main purposes of Stage 1 of the modelling process. This stage allowed the identification of the general architecture type that fit the modelling situation the best. It also allowed for a preliminary indication of the feasibility of the use of ANN modelling in this situation.

The source data analysis prepared the data for use in an ANN model. The next step was to create an input file with the data in the form that was to be used for this stage of the modelling process. To assess the feasibility of applying ANN to this situation, it was decided that a trial data set be made consisting of data from two specific hours every day from a given year be used. In other words, instead of using all 24 hours in a day to conduct the modelling, only 2 hours were used, with the time frame of the data set being the year 1995. The two hours used corresponded to the general high and low NO_x hours during a day and these were assumed to correspond with the high and low traffic the data from 4am and from 5pm. Appendix B contains a sample of the actual data set used for Stage 1 modelling.

One point of interest for all the models in Stage 1 and the other stages of the modelling process is mentioned. The industry emission input, as previously discussed in the research focus (Section 2.4), was in the form of a continuous, static input (averaged from stack tests). The ANN models developed reduce the industry emissions to zero when the input function is applied because there is no change in the emission. In other words, the model extrapolates that the change in NO_x from one hour to the next cannot be attributed to a change in industry emissions because industry emissions are static. The model uses other inputs to account for the variance in NO_x. The sensitivity analysis at the end of Stage 3 allows the background levels of NO_x due to industry to be extrapolated. Therefore the models did not use industry emissions to predict hourly NO_x concentrations, but this does not mean that industries do not affect the levels of NO_x.

In Stage 1 of the ANN modelling process, three types of backpropagation networks were investigated in detail. These were the standard 4-layer, standard 3-layer, and 4-layer jump connection networks. Parameters within these models were varied. These parameters were discussed in Section 3.4.1: Variable Parameters in Backpropagation Models. Varying these parameters gave an idea as to what factors were important to backpropagation networks in general and specific to the types of backpropagation models investigated. This also gave a means of comparison between the three backpropagation model types investigated. A factorial design approach was used to facilitate Stage 1 of the modelling process. This allowed an investigated into the factors as well as the interaction between the factors. A fractional factorial design of 2^{4-1} was used throughout Stage 1. For more information on Factorial Design Analysis, refer to Box et. al. (1978).

Detailed results of the factorial design analysis and the results from all of the tested ANN models are shown in Appendix B.

3.7.2 Results

3.7.2.1 Standard 4-layer Backpropagation Network

The standard 4-layer backpropagation network consists of an input layer, 2 hidden layers, and an output layer (Refer to Section 2.2.4: Topology for more information on layers). Various factors within the network were varied. These factors were:

1) The use or omission of the standard deviation of horizontal wind direction as an input
2) The use or omission of atmospheric temperature as an input
3) The number of hidden layer neurons in the two hidden layers
4) The ratio of the neurons between these layers
5) The activation functions in the two hidden layers and the output layer
6) The input scale function
7) The percentage of source data split into the training, test, and production sets
8) The momentum and learning rates of the links in the network

Stage 1 of the modelling process for standard 4-layer backpropagation networks indicated that the preliminary best-fit model, with an $\mathbf{R^2}$ **of 0.42**, had the following major properties:

1) linear [-1,1] input scale function
2) Gaussian – Logistic – Gaussian activation functions in the 2 hidden layers and the output layer respectively
3) 50% of source data for training set, 30% for testing, and 20% for production
4) 60 neurons in the first hidden layer and 12 neurons in the second hidden layer
5) momentum rate = 0.2, learning rate = 0.2

Although the R^2 demonstrated a fairly average fit, this stage of the modelling process provided a direction for 4-layer Backpropagation models to be used in the next step of modelling. It was noted that many of the R^2 values for the 4-layer backpropagation networks were above 0.3. This indicated that the 4-layer backpropagation models were fairly consistent and stable.

3.7.2.2 Standard 3-layer Backpropagation Network

The standard 3-layer backpropagation network consists of an input layer, a hidden layer, and an output layer. Various factors within the network were varied. These factors were:

1) The use or omission of the standard deviation of horizontal wind direction as an input
2) The use or omission of atmospheric temperature as an input
3) The number of hidden layer neurons in the hidden layer
4) Turboprop or momentum learning
5) The activation functions in the hidden layer and the output layer
6) The input scale function
7) The percentage of source data split into the training, test, and production sets

Stage 1 of the modelling process for standard 3-layer backpropagation networks indicated that the preliminary best-fit model, with an **R^2 of 0.31**, had the following major properties:

1) linear <-1,1> input scale function
2) Logistic – Logistic activation functions in the hidden layer and the output layer respectively

3) 50% of source data for training set, 30% for testing, and 20% for production
4) 15 neurons in the hidden layer
5) momentum learning

Although the R^2 demonstrated a poor fit, this stage of the modelling process provided a direction for 3-layer Backpropagation models to be used in the next step of modelling. It also provided a means of comparison between the use of this type of backpropagation model and the use of the other types investigated.

3.7.2.3 4-layer Jump Connection Network

The 4-layer Jump connection network consists of an input layer, 2 hidden layers, and an output layer. It is different from a standard 4-layer backpropagation network in that there are additional connections between layers. These connections are from the input layer to the second hidden layer and the output layer, as well as from the first hidden layer to the output layer (Refer to Section 2.2.4: Topology for more information on layers). Various factors within the network were varied. These factors were:

1) The use or omission of the standard deviation of horizontal wind direction as an input
2) The number of hidden layer neurons in the two hidden layers
3) The activation functions in the output layer
4) The input scale function

Stage 1 of the modelling process for 4-layer jump connection networks indicated that the preliminary best-fit model, with an **R^2 of 0.45**, had the following major properties:

1) linear [-1,1] input scale function
2) Logistic – Logistic – Logistic activation functions in the 2 hidden layers and the output layer respectively
3) 70% of source data for training set, 20% for testing, and 10% for production
4) 40 neurons in the first hidden layer and 60 neurons in the second hidden layer

The R^2 value indicated a fairly good fit. However, it was noted that a slight variance from this exact architecture would cause the R^2 value to drop substantially. This indicated a very unstable network type. Results are detailed in Appendix B.

Based on the results of Stage 1 of the modelling process, it was decided that the 4-layer backpropagation network was the best type of network to model this particular situation. This was because of the stability of the 4-layer backpropagation models and their stability in modelling the problem at hand. However, after Stage 1, it was still not known if ANN was feasible to use in modelling hourly NO_x in the Strathcona Industrial Area. This was because the results in terms of R^2 were quite average. A typical R^2 value should be 0.60 or higher to indicate a good model fit. Therefore Stage 2 of the modelling process needed to address raising the R^2.

3.8 Stage 2 Modelling

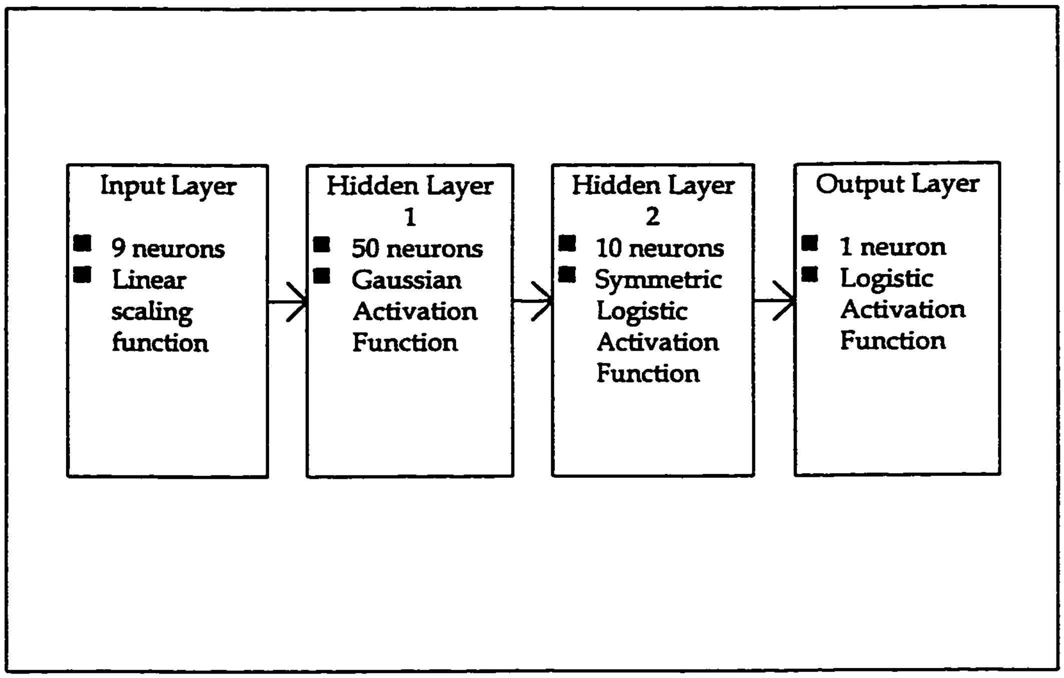
3.8.1 Overview

This stage allowed a further investigation into the feasibility of ANN modelling for this situation. In other words, it expanded on the results from Stage 1 of the modelling process to further investigate not only if ANN was viable, but how well it modelled. It also looked at a data optimisation process for distributing data within the training, test, and production sets in an effort to aid model training. This data optimisation process involved splitting up the data into the three sets, so that each set had a similar breakdown of data based on the number and properties of the input data. This was done in an effort to aid model training and increase model performance. This stage also made an attempt to model urban air pollution in a real time format. This meant using a continuous set of data with all hours of the day used, rather than only a few points per day.

The first model developed in Stage 2 of the modelling process looked at a pilot data set with two data points per day over a given year. In this case, the hours of 7am and 7pm were used, and the year used was 1995. This is because further analysis of the input data showed that maximum and minimum values of NO_x occur closer to 7am and 7pm then 4am and 5pm (used in Stage 1). Based on the previous modelling stage, a 4-layer standard backpropagation network was chosen for modelling. As in the last modelling stage, there were many settings that had to be optimised. These were the scaling function, the activation functions, the number of neurons in the two hidden layers, and the breakdown of the data set into the training, testing and production sets.

The first model developed in Stage 2 of the modelling process was developed using not only the R^2 as a measure of model fit, but also the RMS error and residual plots. Further discussion on error analysis is contained in Section 3.5: Discussion of Error Analysis. It was decided that factorial design analysis would not be used in this stage of the modelling process. This is because the major properties of the model had already been determined in Stage 1, and only a fine-tuning of the model was needed. The best-fit model (based on the error analysis) specifics for this first model developed in Stage 2 are shown in Figure 13:

Figure 13. Architecture of Neural Network, Stage 2 Modelling, Model 1

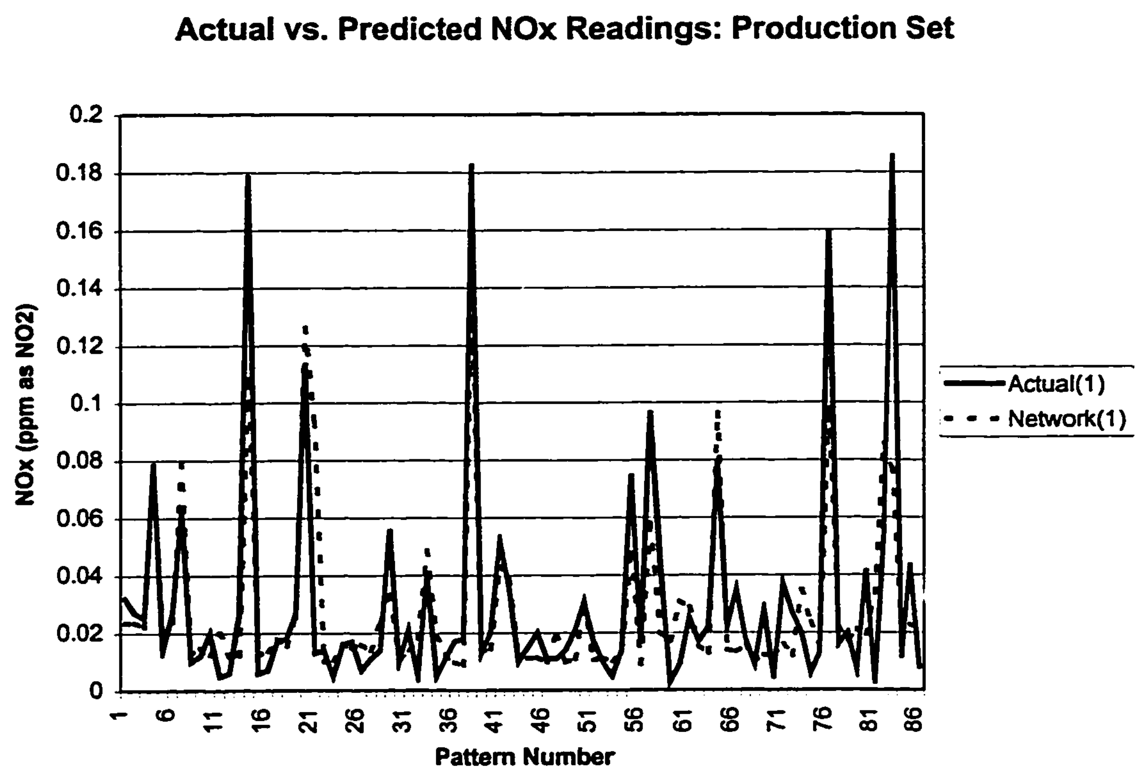


3.8.2 Results

The results of this model showed that ANN was feasible and provided a fairly good fit between the actual output data and the model predicted data. The error analysis of the model was done on the production set of data. The production set of data is that data which the model has not seen during the model training. Detailed analysis of this first model developed in Stage 2 of the modelling process is shown in Appendix C.

The use of R^2 as a measure of model fit should be done cautiously. A model may have a high R^2 but not be able to model the peak values of the output set effectively. It is important to have a model with not only a high R^2, but also one that follows the general trends of the actual output data well. Therefore, the analysis of the model that was developed had to show this. Figure 14 shows a graph of the actual output data plotted with the model output data.

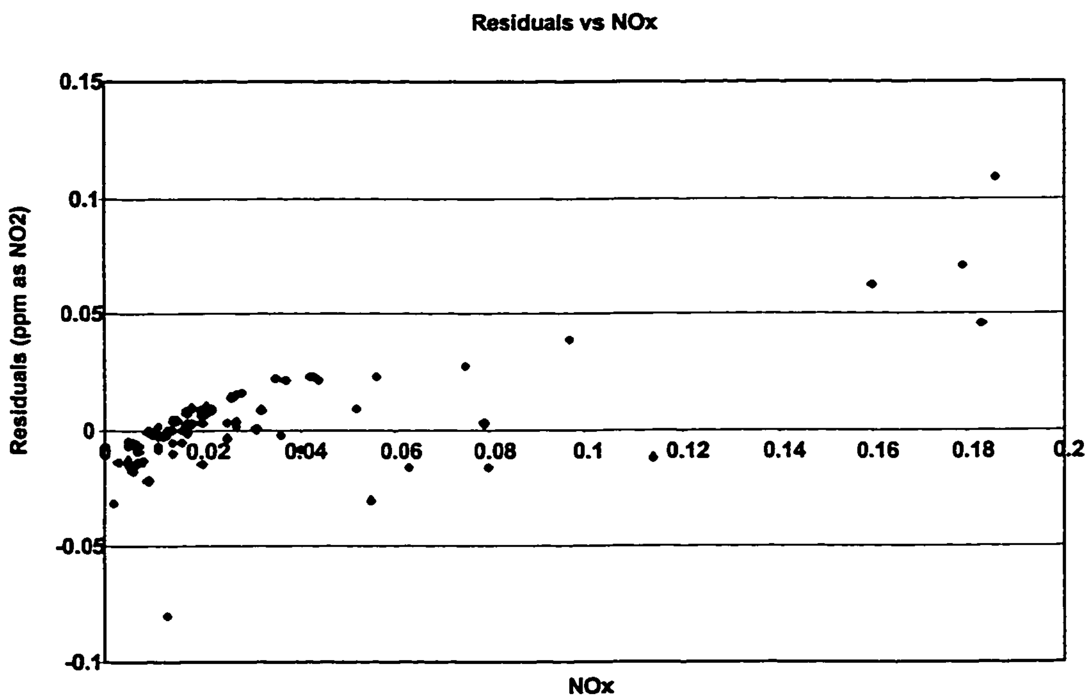
Figure 14. Actual Output Compared with Predicted Model Output, Stage 2 Modelling, Model 1



By looking at Figure 14, it can be seen that the model generally followed the trends of the actual data quite well. The model identified the times when actual NO_x was fairly low and also when it was fairly high. This indicated that the model was able to extrapolate from the inputs those values that caused high and low values of hourly NO_x to occur. The model had a slight bit of difficulty assessing the exact value of the extreme peak events, and seemed to slightly underestimate in those cases.

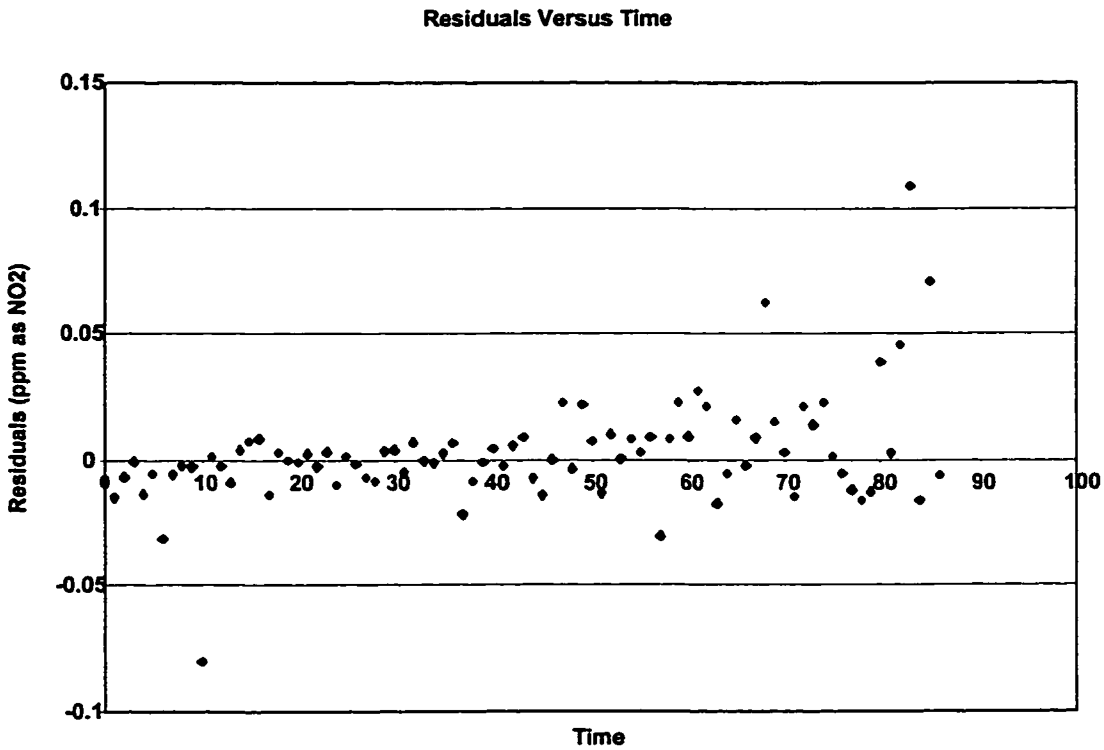
The next step in the analysis of this model was to look at the residuals versus NO_x and time to get an idea of the model fit within the model. Figure 15 shows a graph of the residuals (actual-predicted output) versus the actual NO_x.

Figure 15. Residuals vs. Actual NO_x, Stage 2 Modelling, Model 1



This residuals plot shows that most of the data fall within a residual of 0.05 and –0.05. It also shows a fan shape where the higher the NO_x concentration, the higher the residual. Again, this could be attributed to the model having a slight bit of difficulty in predicting the magnitude of the extreme NO_x concentration events. The next residual plot, Figure 16, shows the residuals plotted versus time.

Figure 16. Residuals vs. Time, Stage 2 Modelling, Model 1



This residuals plot shows that most of the data are in a tight band around the x-axis, indicating that there is no time dependency in the residuals. In terms of the error across the model, the values for R^2 and the RMS Error are as follows:

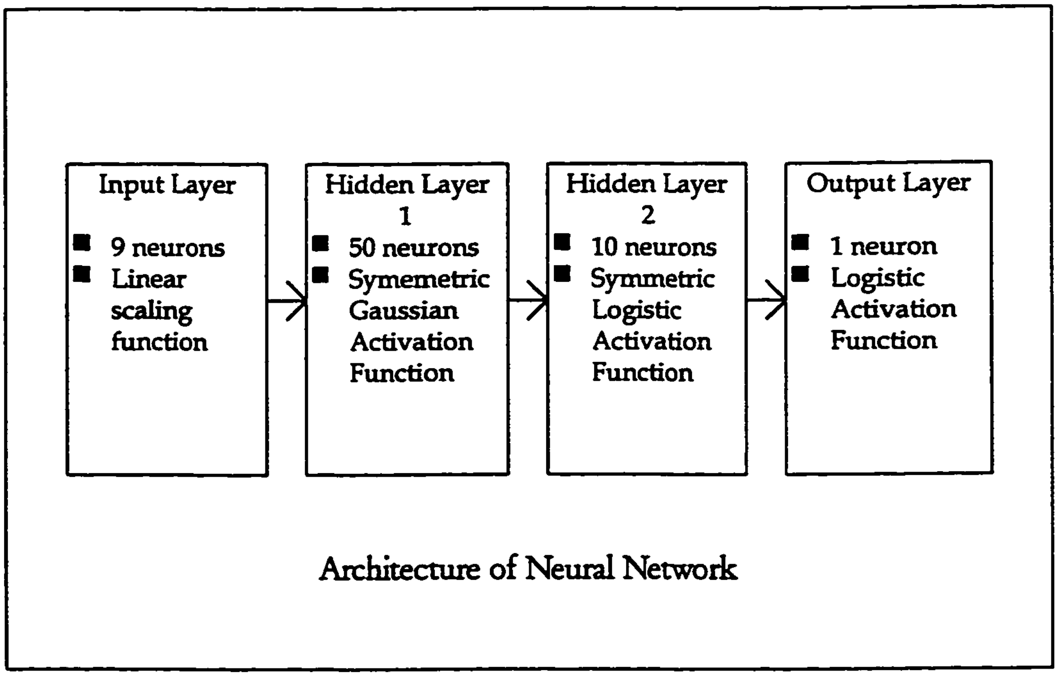
R Square:	0.67
Root Mean Square Error:	4.8E-4 ppm as NO_2

This first model developed in Stage 2 of the modelling process was deemed successful in determining the feasibility of ANN modelling to this situation, and improving the fit of the model output to the actual output data.

The next step in Stage 2 modelling was to attempt to model hourly NO_x in a real time situation. The models created to this point were based on only 2 hours of data a day for a given time period. Therefore, attempting to create a model that used all 24 hours of data in a given day and modelled them sequentially was the next step. By doing this, a better understanding of real time model performance would be gained, which was the final goal of the modelling process.

This model was developed using trial set of data, consisting of hourly input and output data from the month of March in 1995. The reason for choosing March was because through an analysis of the data, it was found that March contained within it the most variations and fluctuations of the data than any other month. As with previous models, the model type chosen was a four-layer backpropagation net. The model was developed through a fine-tuning process of the architecture used in the previous model developed in Stage 2 modelling. The architecture of the best-fit model developed on the data from March 1995 is shown in Figure 17.

Figure 17. Architecture of Neural Network, Stage 2 Modelling, Model 2



As with the previous models, the R^2 error and the root mean square error (RMS) were the main statistical values used for measuring the error across the model. As well, residual error plots of error versus time and error versus NOx concentration were done to measure error within the model. Figure 18 shows a plot of the actual output plotted with the model output.

Figure 18. Actual Output Compared with Predicted Model Output, Stage 2 Modelling, Model 2

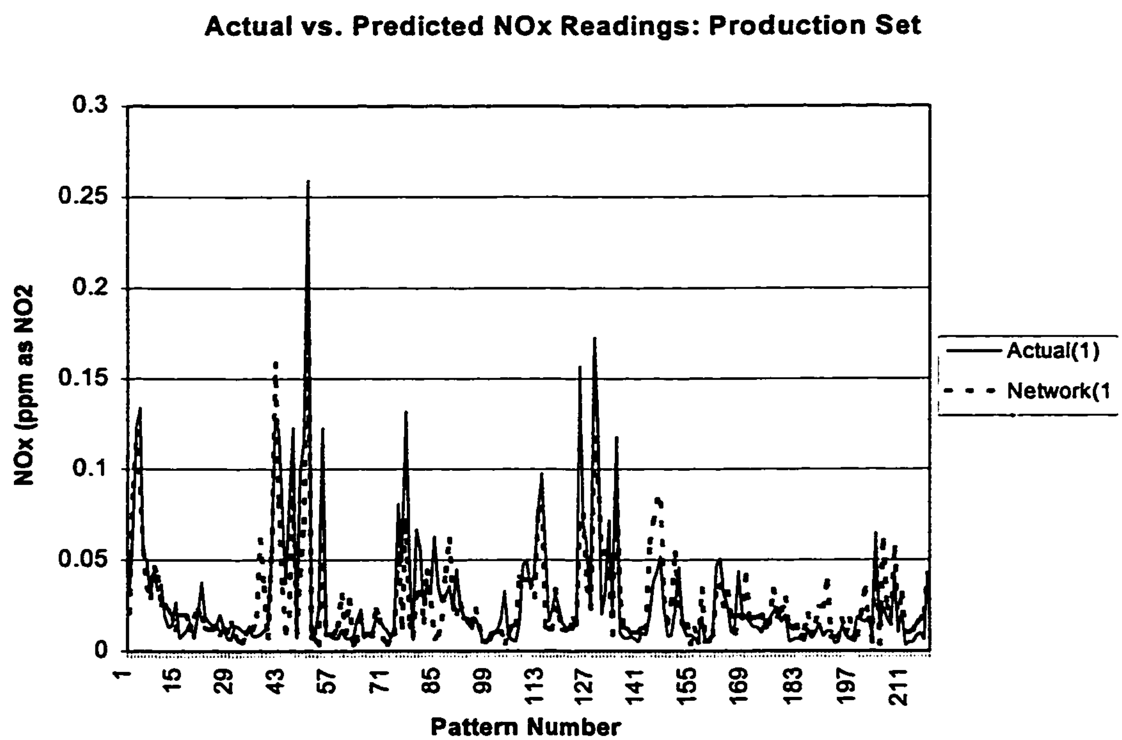
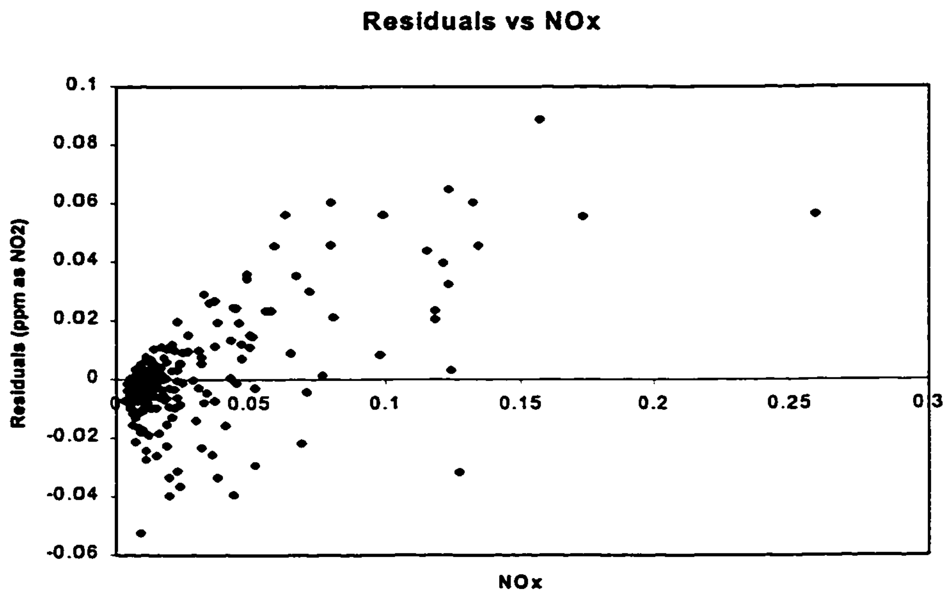


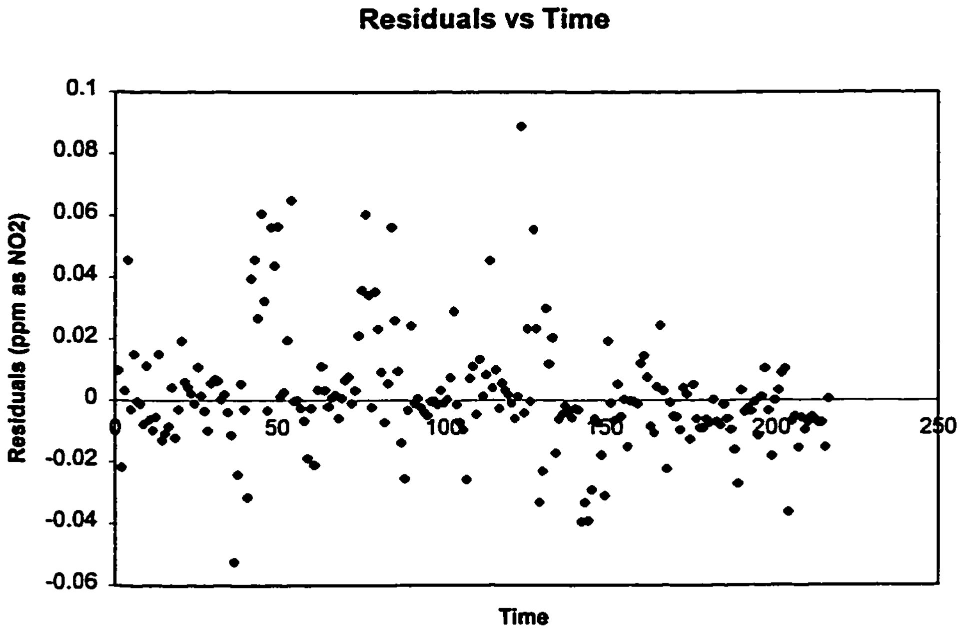
Figure 18 shows that the model output fit the actual output very well. In many cases, the model was able to predict the occurrence and magnitude of the extreme events, which is an improvement over the previous model developed in Stage 2 modelling. The model was successful in predicting the occurrence of either extreme events or low events. Figure 19 shows a plot of residuals versus the actual NO_x in an effort to learn more about the fit within the model.

Figure 19. Residuals vs. Actual NO_x, Stage 2 Modelling, Model 2



This residuals plot shows that most of the residuals are between 0.05 and – 0.05, which is similar to the model developed at the beginning of Stage 2 modelling. Again, a fan shape is present indicating that the higher NO_x values tend to have higher residuals. This is natural as the model has a harder time in predicting the magnitude of extreme NO_x event than it does for more typical NO_x values. The next plot, Figure 20, shows the residuals plotted versus time.

Figure 20. Residuals vs. Time, Stage 2 Modelling, Model 2



The plot shows that most of the data are in a fairly tight band around the x-axis, which is desirable. It also shows that there is not trend of an increasing residual with time. This indicates no time dependency of the residuals. The values for error across the model (RMS error and R^2) were as follows:

R Square:	0.70
Root Mean Square Error:	3.7E-4 ppm as NO_2

3.9 Stage 3 Modelling

3.9.1 Overview

The main purpose of Stage 3 of the modelling process was to develop a real time working model for the modelling of hourly NO_x in the Strathcona Industrial Area. This model would then be used in a sensitivity analysis to gain insight into the parameters that affect NO_x in the Strathcona Industrial Area.

The set of data used for Stage 3 modelling used the months of January and July for the year 1995. These two months were chosen as they essentially represent the maximum range of the input and output parameters. Appendix D contains a sample of the data used for modelling.

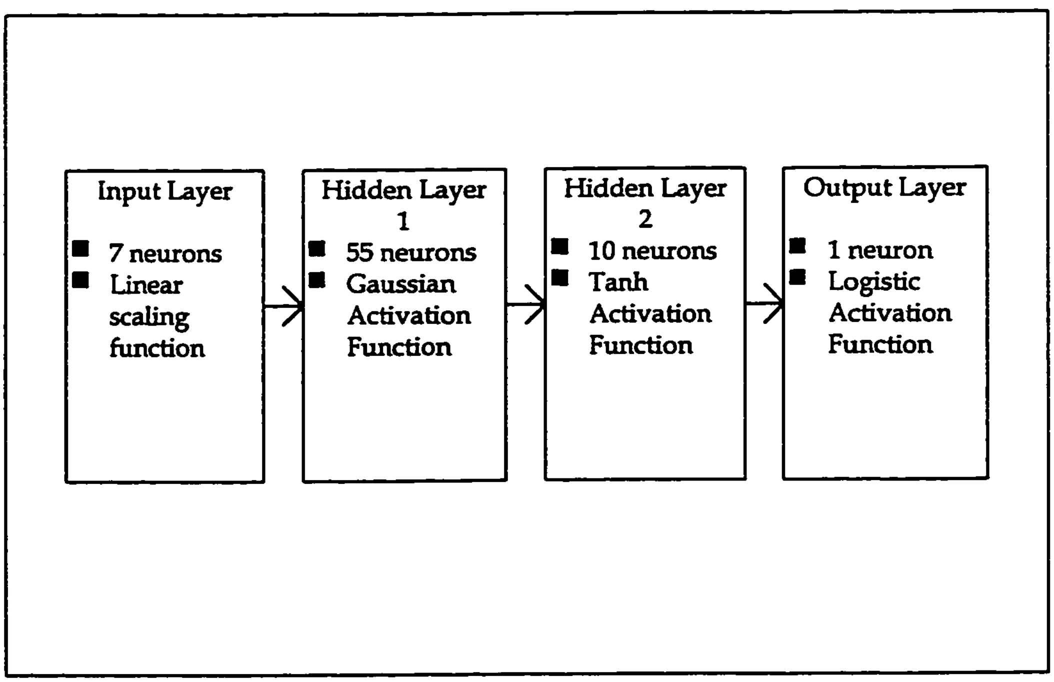
The inputs for this model were essentially the same as the inputs from previous models developed in Stage 1 and 2 of the modelling process, with two exceptions. The first exception was an additional input called the season index. The season index was a numerical value of 1, 2, or 3 that was dependent on the season of the particular data used. A season index value of 1 signified data from the months of November to February inclusive. A season index value of 2 signified data from the months of March to June inclusive, and a value of 3 represented data from the months of July to October inclusive. The reason that this index was added was that it was found to improve results of some of the initial models tested early in Stage 3 modelling. Data from the winter months tended to contain the majority of extreme NO_x events due to atmospheric inversions and stable air tendencies. This index helped the model to distinguish events based on season in addition to the other input factors.

The second exception was that instead of four separate inputs for traffic counts in nearfield streets, a single, summation input was used. In previous models developed in Stage 1 and 2, there were four separate inputs, representing traffic counts in four nearfield quadrants surrounding the air monitoring station. It was found that a better model fit could be achieved in Stage 3 modelling by adding the four nearfield traffic count inputs into a single input.

Stage 3 of the modelling process used previous models developed in Stage 1 and 2 of the modelling process and fine-tuned them in an effort to create a satisfactory working model. The results in Stage 3 modelling were expected to drop slightly from Stage 2 (in terms of R^2 and model fit) due to the fact that there were many extreme events that occurred in January 1995. The same data optimisation process used in Stage 2 modelling was used again in Stage 3. The only difference was that Stage 2 modelling split the data into three approximately equal in number sets (training, test, and production), and Stage 3 modelling had an approximate ratio of 2:1:1 between the three sets respectively. The reason that more data were used in the training set than in Stage 2 was that the data were extremely noisy with sharp fluctuations and many extreme events. By including more data in the training set, the model was to use more data in the learning process and was able to improve model prediction from initial models attempted in Stage 3 modelling.

The specifics of the best-fit model developed in Stage 3 of the modelling process (based on an overall error analysis) are shown in Figure 21.

Figure 21. Architecture of Neural Network, Stage 3 Modelling



3.9.2 Results

The results of this model were obtained from a complete evaluation of the actual output data versus the model output. The error analysis of this model was done on the production set of data. Figure 22 shows a graph of the actual output data plotted with the model output data.

Figure 22. Actual Output Compared with Predicted Model Output, Stage 3 Modelling

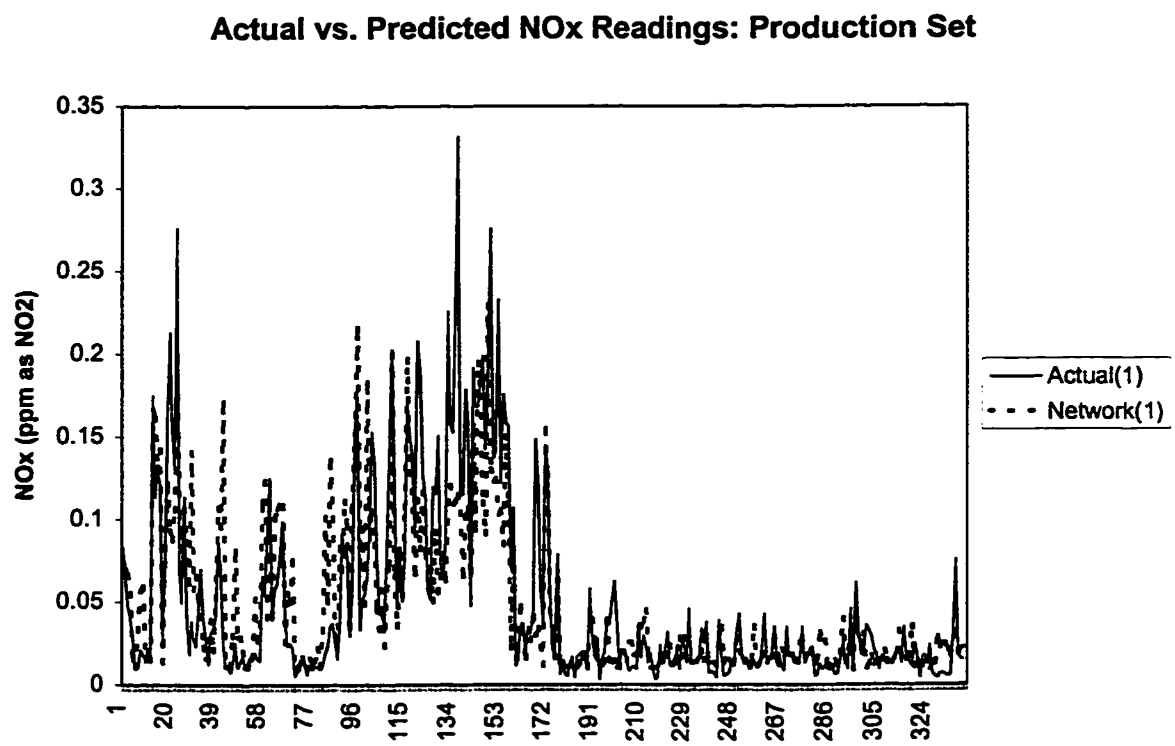
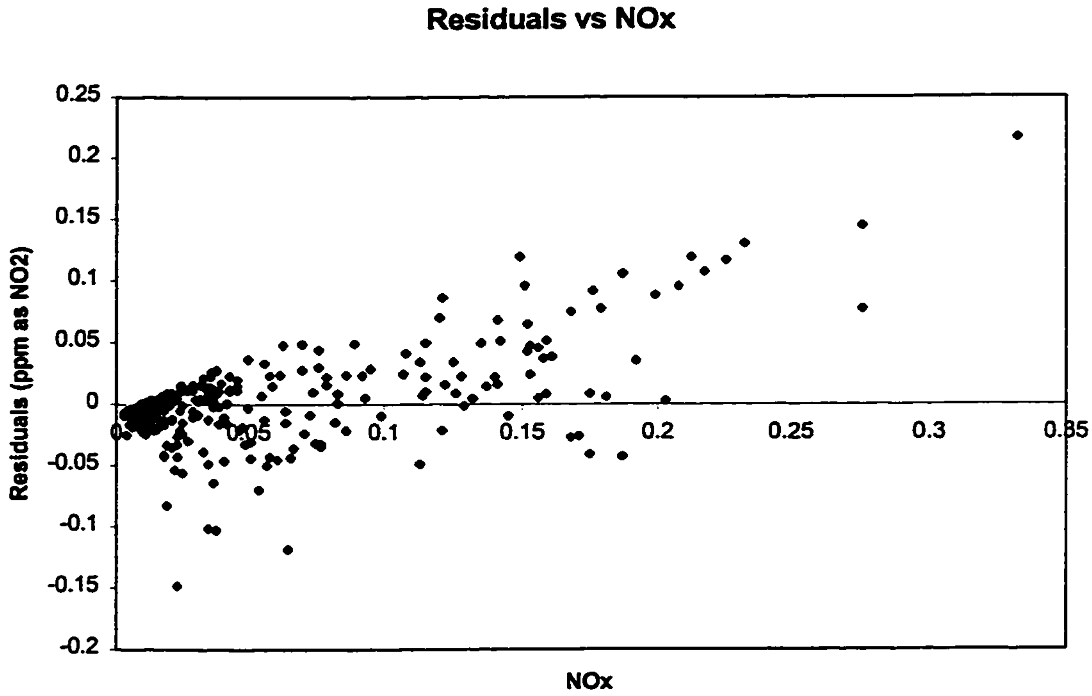


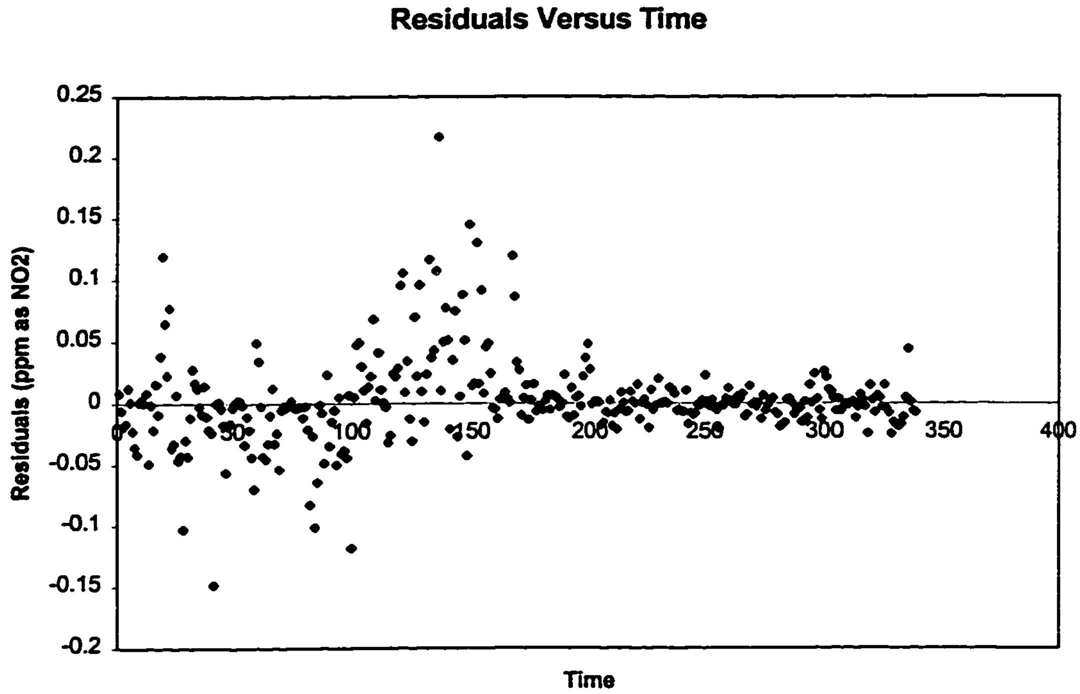
Figure 22 shows that the model once again was able to predict the occurrence of either extreme NO_x events or low NO_x events. The model was fairly successful in predicting the magnitude of extreme NO_x events except between patterns 130 and 140, where the model under predicted the magnitude of two events. Figure 23 shows a residual plot of the residuals versus the actual NO_x.

Figure 23. Residuals vs. Actual NO_x, Stage 3 Modelling



The residuals plot shows the typical fan shape that has been characteristic to many of the models developed in the various stages of the modelling process. This fan shape indicates that at higher values of NO_x, the value of the residuals tends to increase. The model tends to predict the occurrence of extreme NO_x events, but not quite catch the magnitude of some of these events. The next plot, Figure 24, plots the residuals versus time.

Figure 24. Residuals vs. Time, Stage 3 Modelling



The plot shows most of the data within a fairly tight band around the x-axis. It shows that there is no apparent time dependency of the model. The values for error across the model (RMS error and R^2) are as follows:

R Square:	0.63
Root Mean Square Error:	1.8E-3 ppm as NO_2

These values indicated that the model output fit the actual output well, and that a model was successfully developed for use in the sensitivity analysis. There was a slight drop in model performance from the models developed in Stage 2 of the modelling process. The change in these values can mainly be attributed to two things. The RMS error and R^2 value tend to heavily punish those instances where the error is quite large. The model had fairly significant errors in predicting the magnitude of two extreme events, as previously mentioned. The R^2 and RMS values would have been significantly higher were it not for the two events. Another reason for the change was the fact that winter months tend to contain the majority of extreme NO_x events. Half of the data used to develop this model was from the month of January 1995, which is one of the more difficult months for the model to predict in.

4.0 Model Application

4.1 Organisation of Section

This section applies a model developed in Stage 3 of the modelling process to extrapolate information about the nature of urban air pollution in the Strathcona Industrial Area. A sensitivity analysis allowed an analysis on the dependence of hourly NO_x values on traffic counts of nearfield streets. This analysis also allowed for an investigation into the relative input of NO_x from industrial and other sources.

This section begins by applying the ANN model developed in Stage 3 modelling to an arbitrary week of data not seen before by the model. The traffic counts are changed in positive and negative increments to observe the effect on hourly NO_x values. Following that, the model uses a value for the expected increase in traffic by the year 2020 to predict the increase in average hourly NO_x concentrations. Finally, the model is used to predict the relative input of industrial and other emissions to hourly NO_x values.

4.2 Sensitivity Analysis

4.2.1 Description

There were essentially two main phases in the sensitivity analysis. The first phase was to apply the model to a randomly chosen week of data. The model input of nearfield traffic counts was then varied in increments of 5% in the positive and negative direction in an effort to understand the sensitivity of NO_x to these counts. This step included adjustment of the counts to the value corresponding to the expected growth in traffic estimated in the City of Edmonton in the year 2020, and calculating the increase in average hourly NO_x concentration. The second phase of the sensitivity analysis was to back-calculate (based on the sensitivity of the traffic counts to the hourly NO_x) the influence of other factors on hourly NO_x (industry and other).

4.2.2 Sensitivity of Hourly NO_x to Nearfield Street Traffic Counts

The ANN model developed in Stage 3 of the modelling process was applied to an arbitrarily chosen week of data. The week of February 8^{th} to 14^{th} in 1995 was the week of data chosen. This data set contained data on the 7 input parameters used to develop the model from Stage 3 modelling. A dynamic link library (DLL) file was created to link the ANN model developed in Stage 3 modelling to the spreadsheet file containing the week of data. This allowed the model to be used to predict the hourly NO_x based on the data. Appendix E contains a sample of the data set used.

The performance of the model used was evaluated based on a visual observation of the actual hourly NO_x for the week of data used and the model predicted hourly NO_x. This is because the detailed evaluation of the model was already completed in Stage 3 modelling, which found the model to be quite satisfactory for use. Essentially, the visual check of model fit was done to ensure that the model was able to follow the general trends of the data well, and to ensure the proper functioning of the DLL file. Figure 25 shows a graph of the actual NO_x values plotted with the model predicted NO_x values. Note that patterns (x-axis) are in real-time order such that pattern 1 refers to hour 1 on February 8^{th}, 1995.

Figure 25. Actual Output Compared with Predicted Model Output, Sensitivity Analysis

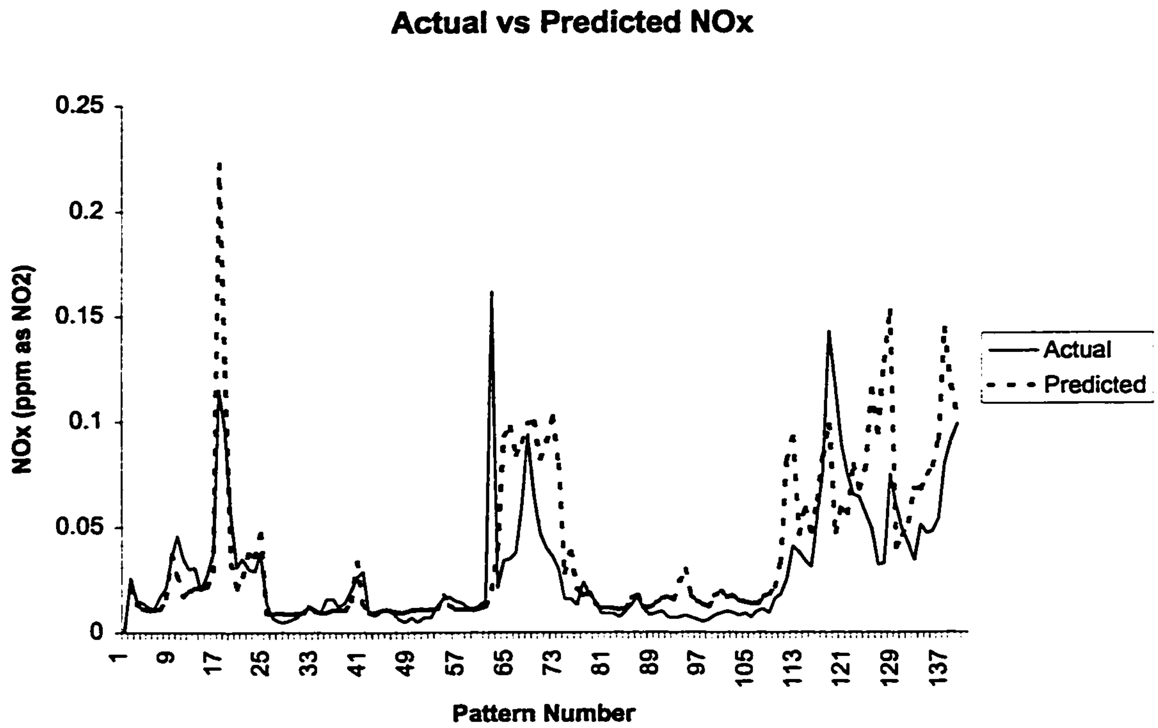


Figure 25 shows that the model fit the data quite well, in that it was able to predict extreme NO_x events and normal events. It was also able to predict the magnitude of extreme NO_x events satisfactorily, with the exception of an over-prediction at pattern 17 and an under-prediction at pattern 63. This step showed that the model was functioning well and could be used for the sensitivity analysis.

The next step was to begin varying the input of traffic counts on nearfield streets and observing the effect on the NO_x concentration for the week of data used. The counts were varied in increments of 5% from –40% to +40% of original counts. Appendix E shows the changed traffic count data. Figure 26 shows a graph of the initial hourly NO_x model output compared with the output in the case where the traffic data is increased by 40%.

Figure 26. Original Model Output Compared to Output for 40% Increased Traffic Counts

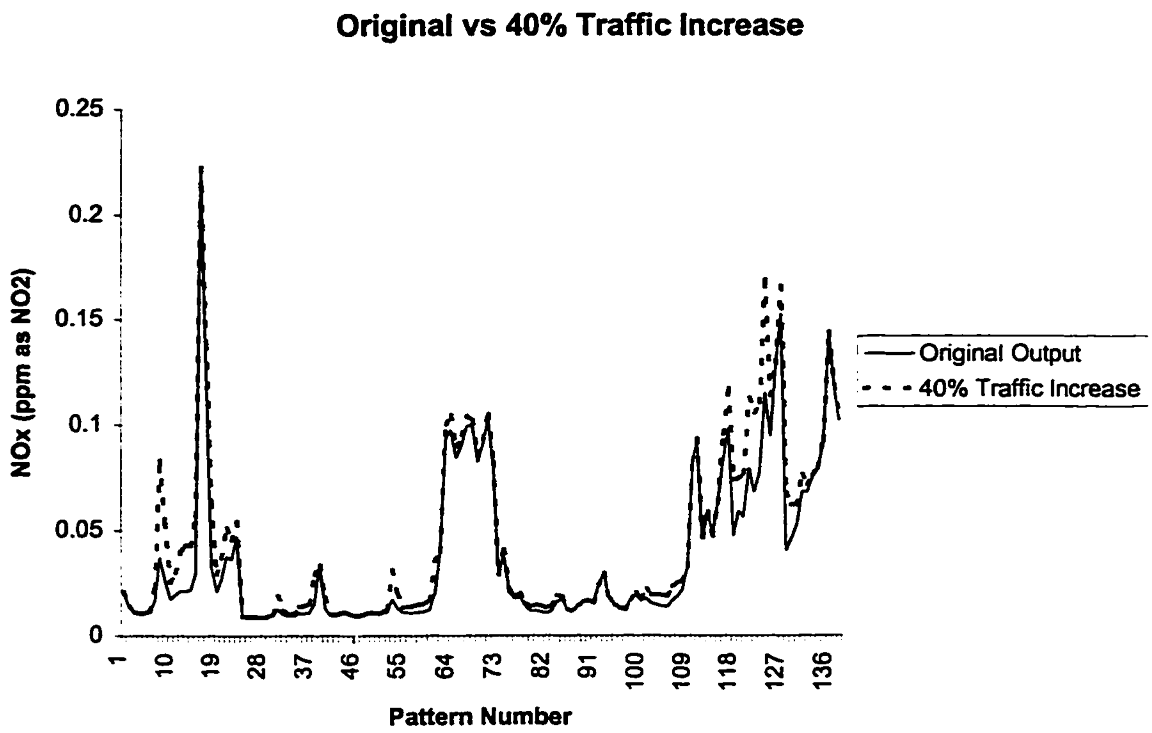


Figure 26 shows that an increase in the traffic counts of nearfield streets caused an increase in the overall hourly NO_x concentrations throughout the test. There were instances where the hourly NO_x values were almost unchanged, and the logical inference was that those particular hourly NO_x values were not strongly influenced by traffic counts on nearfield streets. One thing to note is that Pattern 17 exceeded the range of the model when increased by 40%, and the model responded by keeping the NO_x concentration at the same level as before the traffic increase. There were also instances where the hourly NO_x values were significantly changed by the increase in NO_x. The logical inference in that case was that for those particular hours, the hourly NO_x values read at the monitor were strongly dependent on the traffic counts on nearfield streets. Figure 27 shows the initial output compared to the new output when the traffic data is decreased by 40%.

Figure 27. Original Model Output Compared to Output for 40% Decreased Traffic Counts

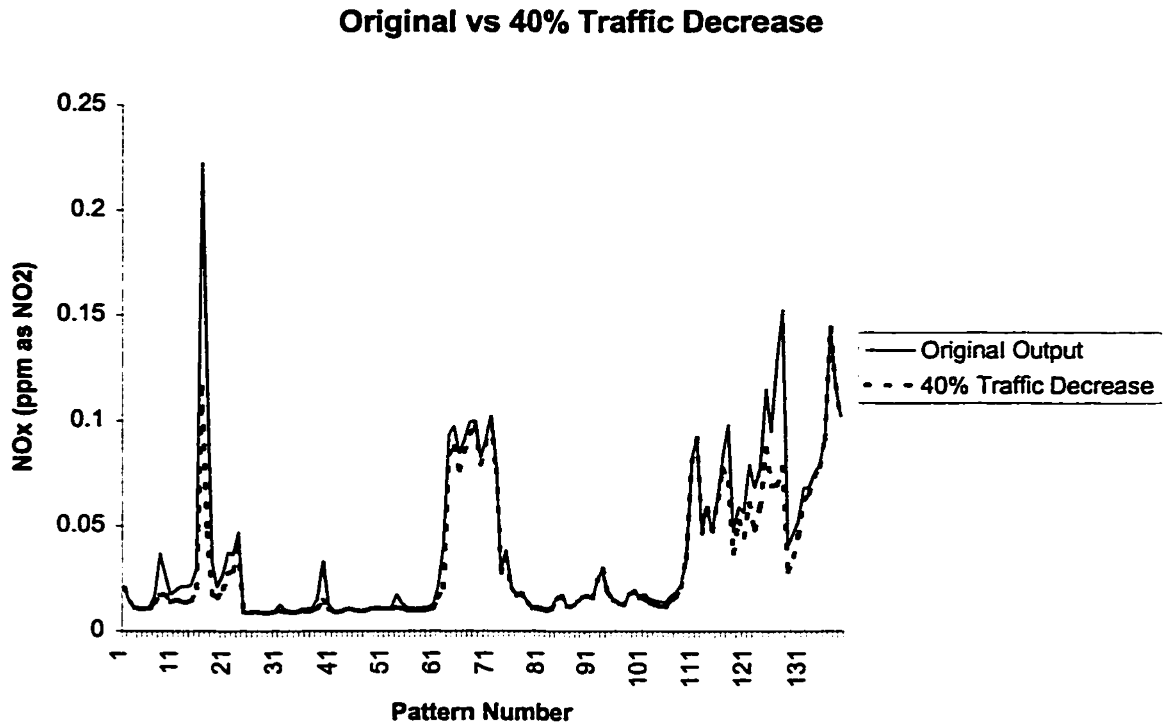
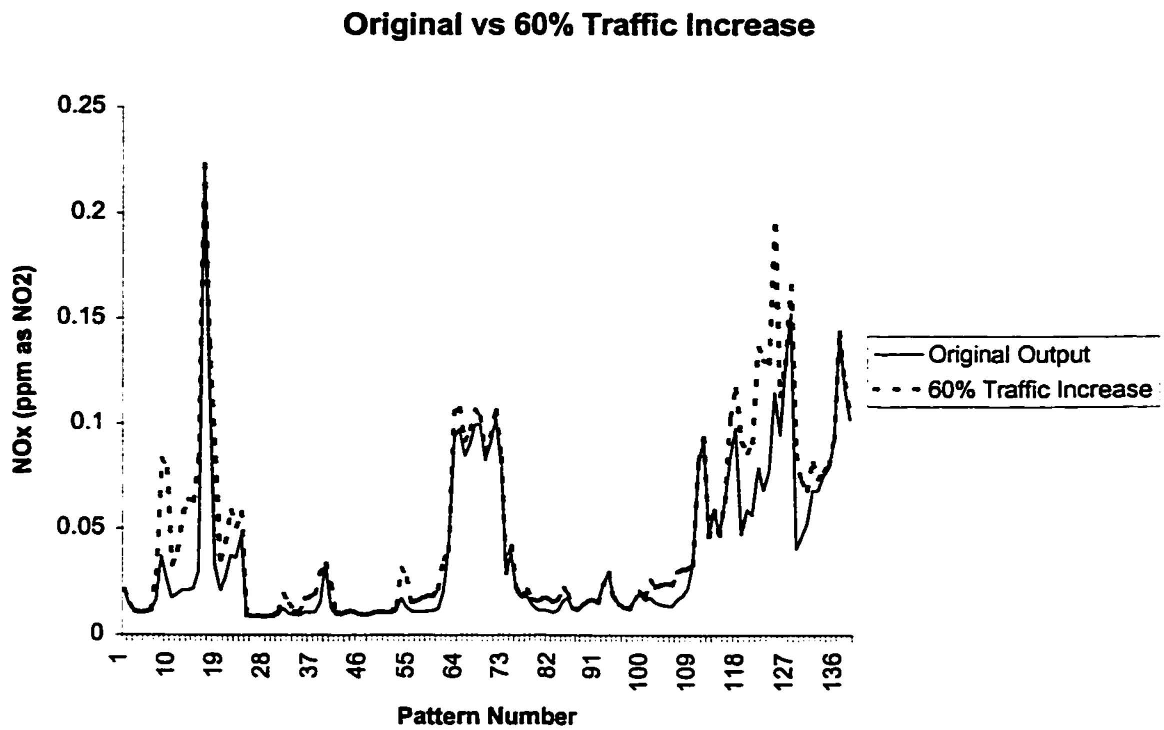


Figure 27 shows that a decrease in the traffic counts of nearfield streets decreased the overall hourly NO_x concentrations during the test week. What was interesting to note was that some peaks were substantially decreased while others remained relatively unchanged, which was analogous to the case with a traffic increase.

The City of Edmonton Transportation Department has an overall general estimate for the increase in vehicular traffic expected between 1997 and the year 2020, and that is a 60% increase. Applying this to the model, it predicted a 26% increase in overall average NO_x concentrations would occur with a 60% increase in traffic (assuming vehicular traffic on nearfield streets follows the same percent increase as the rest of the city). Figure 28 shows graphically the change in NO_x concentrations that would occur.

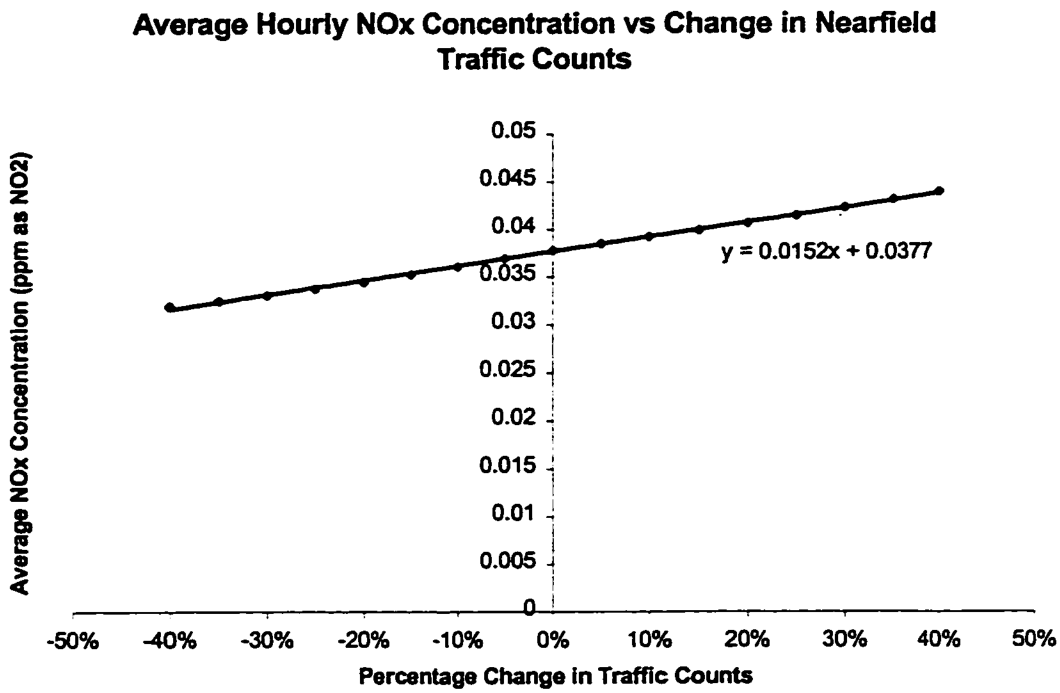
Figure 28. Original Model Output Compared to Output for 60% Increased Traffic Counts (forecast for 2020)



4.2.2 Extrapolating the Influence of Other Sources

The second phase of the sensitivity analysis involved taking the results from the first phase and extrapolating the influence of factors other than nearfield traffic counts on hourly NO_x values. Traffic counts were varied from an increase of 40% to a decrease of 40%. The resulting plot showed the effect of the change in traffic counts on the average hourly NO_x concentration for the week. Figure 29 shows the relationship between average NO_x concentration and change in traffic counts.

Figure 29. Effect of Change in Traffic Counts on Average Hourly NO_x



A linear regression was done on the points to give the linear relationship between average NO_x and traffic count change. From the 40% increase to the 40% decrease (80% decrease total) in traffic counts, the average hourly NO_x decreased by 32% (calculated through use of the linear relationship). A 100% reduction in traffic counts would therefore decrease the average hourly NO_x concentration by 40%. The model therefore concluded that for the test week in February, 1995, 40% of the hourly NO_x concentrations were from the input from vehicle emissions and the other 60% were from other sources. This breakdown is similar to findings reported by Myrick and Byrne (1996) indicating that 43% of NO_x emissions in Edmonton during 1995 were from transportation sources. The other sources could include industrial emissions, power generation, and space heating. Other possible sources of NO_x in an urban environment are outlined in Section 2.4.2.6 – Oxides of Nitrogen.

5.0 Conclusions

5.1 General Conclusions

This study had three main objectives, outlined in Section 1.3 – Research Objectives. The main objective of the study was to assess the feasibility of modelling urban air pollution, specifically hourly NO_x concentrations, in the Strathcona Industrial Area of the City of Edmonton, using ANN modelling. This objective was successfully met through Stages 1 and 2 of the modelling process, Sections 3.7 and 3.8. The measure of success was the error analysis of the models developed in these stages.

Models developed in Stages 1 of the modelling process focussed on three main backpropagation architecture types. The first was a standard 4-layer backpropagation network, and this type achieved an R^2 of 0.42. The next was a standard 3-layer backpropagation network, and this achieved an R^2 of 0.31. The last type was the 4-layer jump connection network, which had an R^2 of 0.45. It was decided at the end of Stage 1 to pursue modelling with a 4-layer backpropagation network, because of the overall stability in the results compared with the 4-layer jump connection network. If any of the inputs were varied slightly, the 4-layer jump connection network would not converge and would give an R^2 of 0. The 4-layer backpropagation network however was more stable and continued to converge with slight variations of the input parameters.

Stage 2 of the modelling process was able to further prove the feasibility of using ANN to model the problem. The first model created in Stage 2 was able to model better than the 4-layer backpropagation network developed in Stage 1. This first model used a data optimisation process that enhanced the learning process of the model, and was able to significantly improve the performance of the model in all aspects. This model had an R^2 of 0.67, a RMS error of 4.8E-4 ppm as NO_2, and residual plots that showed no apparent time dependency trends.

The next objective of this study was to apply ANN modelling to reproduce hourly NO_x concentrations in a real-time format. Essentially this meant using all available data from a given day to model, rather than two points per day, as was used in Stage 1 and the first model of Stage 2. The second model developed in Stage 2 used data from the month of March in 1995 in a real-time format. The model had an R^2 of 0.70, a RMS error of 3.7E-4 ppm as NO_2, and residual plots that again showed no apparent time dependency trends.

Stage 3 of the modelling process (Section 3.9) also sought to model hourly NO_x in a real-time format. This stage used data from the months of January and July 1995 to develop the model. The model developed was expected to drop in performance from the second model of Stage 2 modelling because of the fact that many extreme events (high NO_x concentrations) occur during the winter months, and January 1995 was no exception. The data was markedly noisier with more severe fluctuations than the data set used to model the second model in Stage 2. This model had an R^2 of 0.63 and a RMS error of 1.8E-3 ppm as NO_2, and residual plots that again showed no apparent time dependency trends.

The last objective of this study was to use the results from an ANN model to provide a means of evaluating the effect of proposed control measures on urban air quality (measured in terms of hourly NO_x) specifically in terms of traffic counts on nearfield streets. The model developed in Stage 3 of the modelling process was applied to an arbitrary week of data, and then the effect of varying the traffic counts was found (Section 4.2). A straight-line relationship was developed through use of a linear regression, and it was concluded that a 100% drop in traffic would result in a 40% drop in average hourly NO_x concentrations. This was important, in that it also showed the percentage of hourly NO_x concentrations that could be attributed to inputs other than the transportation sector. It also showed the sensitivity of average hourly NO_x concentrations to the traffic counts.

Another part of the sensitivity analysis involved obtaining an estimate for the average increase in vehicular traffic expected by the year 2020 from the City of Edmonton Transportation Department. Once the estimate was obtained, the effect of this increase on the average hourly NO_x concentration was found. The estimate was an increase in vehicular traffic of 60%. The corresponding modelled increase in average hourly NO_x concentrations was 26%.

Overall, the objectives set out for this study were met. There are, however, some recommendations for future research in the field that are outlined in the next section.

5.2 Recommendations for Future Research

It is important to note that this study was essentially an introduction into the use of ANN modelling to model urban air pollution. The main objective of the study, as mentioned before, was to assess the feasibility of using ANN modelling in the field of urban air pollution modelling. There are many possible avenues for future research in this area, and following are some recommendations.

1) Investigate the use of other output factors and observe whether they can be successfully modelled. This includes O_3, PM, SO_2, VOC/THC, and CO. It is possible that these other outputs may be able to be modelled successfully using either the current set of inputs or a different set. This could generate more information as to the characteristics of urban air pollution in the Strathcona Industrial Area in a more thorough manner.

2) Investigate the use of other input factors on model performance. This can include measures such as relative humidity, atmospheric pressure, hours of bright sunshine, and various other meteorological measures. These other input parameters may provide the model with more information on the creation, dispersion, and transport of urban air pollutants in the Strathcona Industrial Area.
3) The model that was developed was a single model used to predict hourly NO_x for many situations throughout a year. A possible avenue for investigation would be the development of separate ANN models that model for different levels of inputs. For example, a model could be developed for use throughout the winter months, where the characteristics of hourly NO_x concentrations in the Edmonton area are drastically different than in the other times of the year. By developing different models for different times of the year, the model fit may turn out to be much better.
4) Another interesting avenue for research could be the application of this model to other geographical areas. The model could extrapolate characteristics that are common between the other area and the Strathcona Industrial Area. It would shed light onto what characteristics are important to hourly NO_x concentrations specific to the Strathcona Industrial Area and what characteristics are important to concentrations regardless of location.
5) The sensitivity analysis was done specifically on vehicle counts on streets adjacent to the monitor used to measure hourly NO_x concentrations. The analysis of sensitivity could be expanded to other inputs in the model. This may also give more information regarding the effect of all inputs on the hourly NO_x concentrations.
6) This study focussed on the use of general backpropagation type neural networks. Future studies could attempt to use other types of ANN models and see how they function. Examples are GRNN type models and the use of genetic algorithms.

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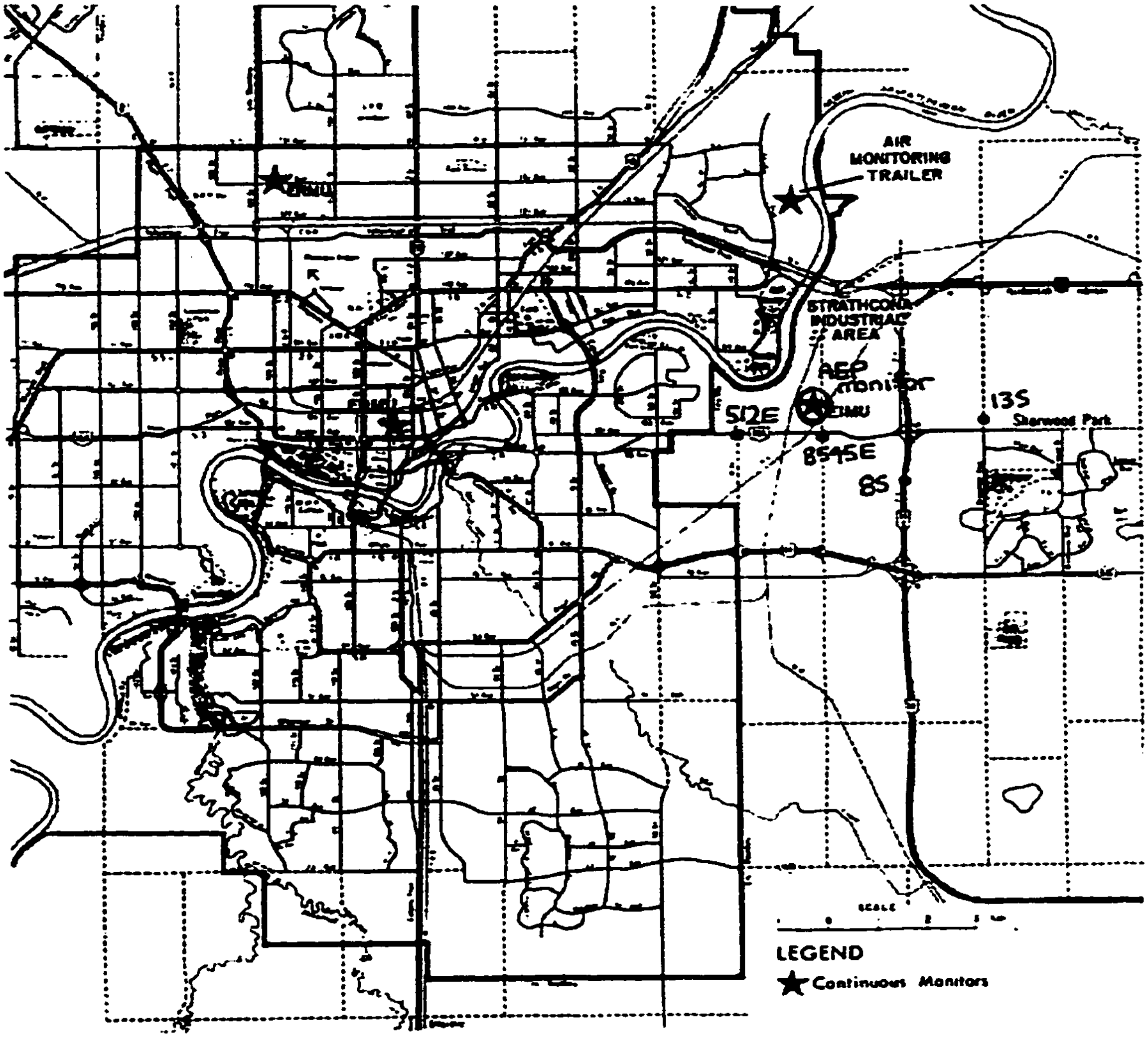
APPENDIX A – The Study Airshed in the Strathcona Industrial Area of the City of Edmonton and the County of Strathcona



Ref: Alberta Environment, 1991

APPENDIX B – Detailed Results and Analysis from Stage 1 of the ANN Modelling Process

Standard 4-layer Backpropagation Network: Results and Analysis

DEV =	standard deviation of horizontal wind direction
HL =	hidden layer
Act. =	activation function
Last Error Trn. =	last average training error
Min. Error Trn. =	minimum average training error
Min. Error Tst. =	minimum average testing error
R2 Production =	R^2 value from applying the model to the production set
x:y ratio =	x:y ratio between neurons in hidden layers 1 and 2
N =	percentage of input data used for test set
M =	percentage of input data used for production set
mom =	momentum rate
l =	learning rate
G-G-G =	Gaussian – Gaussian – Gaussian activation functions in hidden layers 1 and 2 and the output layer
G-L-G =	Gaussian – Logistic – Gaussian activation functions in hidden layers 1 and 2 and the output layer

Architecture Type 1 - Standard 4 layer backpropagation net

	Positive	Negative
A	with DEV	without DEV
B	40 neurons HL1	60 neurons HL1
C	40 neurons HL2	60 neurons HL2
D=ABC	Gaussian Act.	Logistic Act.

Results:

	Last Error Trn.	Min. Error Trn.	Min. Error Tst.	R2 Production
Trial 1	0.0016003	0.0013497		0.2597
Trial 2	0.0193618	0.0193618	0.0280005	0
Trial 3	0.0048306	0.0040126	0.0115825	0.2881
Trial 4	0.0015144	0.0015144	0.0072485	0.1239
Trial 5	0.0017543	0.0016935	0.0074151	0.2564
Trial 6	0.0019683	0.0016515	0.0113582	0
Trial 7	0.0031952	0.0031952	0.0114674	0
Trial 8	0.0011614	0.001137	0.0070806	0.2494

Significant Effects:	**A effect**	The effect of having the DEV data are to actually reduce the R2.
	AB effect	Therefore, it will not be used in further Stage 1 4 hidden layer nets.

Architecture Type 1.1 - Standard 4 layer backpropagation net

	Positive	Negative
A	2:1 ratio	3:1 ratio
B	30 neurons HL1	36 neurons HL1
C	Linear[-1,1]	Linear<-1,1>
D=ABC	Gaussian Act.	Tanh Act.

Results:

	Last Error Trn.	Min. Error Trn.	Min. Error Tst.	R2 Production
Trial 1	0.0208282	0.0208282	0.0532618	0.3353
Trial 2	0.005569	0.0050089	0.012229	0.0432
Trial 3	0.0071127	0.0049247	0.0108558	0.2933
Trial 4	0.0434505	0.0228035	0.0434453	0.1469
Trial 5	0.0189367	0.0189367	0.045788	0.1887
Trial 6	0.005569	0.0050089	0.012229	0.0432
Trial 7	0.0070325	0.0034753	0.0118333	0
Trial 8	0.0434505	0.0228035	0.0434453	0.1469

Significant Effects:	**C effect**	**AB effect**	The linear [-1,1] scale function is preferred
	A effect	**AC effect**	as is the 3:1 neuron ratio.

Architecture Type 1.2 - Standard 4 layer backpropagation net

	Positive	Negative
A	3:1 ratio	4:1 ratio
B	36 neurons HL1	48 neurons HL1
C	N=20,M=10	N=30,M=20
D=ABC	with temp	without temp

Results:

	Last Error Trn.	Min. Error Trn.	Min. Avg. Tst.	R2 Production
Trial 1	0.0049359	0.0049359	0.0128032	0.1023
Trial 2	0.0033392	0.0025959	0.0107425	0.3374
Trial 3	0.003951	0.001678	0.0109563	0.2513
Trial 4	0.0043338	0.0043338	0.0124708	0.1533
Trial 5	0.0074633	0.002944	0.0111988	0
Trial 6	0.0061319	0.0061203	0.0147946	0.1824
Trial 7	0.0055939	0.0055939	0.0149316	0.082
Trial 8	0.0028541	0.0028541	0.0122117	0.043

Significant Effects:	**C effect**	**AB effect**	The strongest effect is the interaction AB. It tends
	A effect		be better at the lower settings of A and B, so a higher Number of neurons, and a 4:1 ratio. However, A is Important at 3:1 as well. N=30 and N=20 also is better.

Architecture Type 1.3 - Standard 4 layer backpropagation net

	Positive	Negative
A	G-G-G	G-L-G
B	mom=0.15, l=0.15	mom=0.2, l=0.2
C	2:1 ratio	5:1 ratio
D=ABC	50 neurons	60 neurons

Results:

	Last Error Trn.	Min. Error Trn.	Min. Error Tst.	R2 Production
Trial 1	0.0036294	0.0019316	0.009943	0.4153
Trial 2	0.0011295	0.0010761	0.0098675	0.3383
Trial 3	0.0158977	0.0126049	0.0154211	0.0334
Trial 4	0.0014809	0.0011603	0.104317	0.2955
Trial 5	0.0204516	0.0065013	0.0109372	0.3281
Trial 6	0.0065709	0.0023669	0.0087533	0.2063
Trial 7	0.0204509	0.0069881	0.0111085	0.3191
Trial 8	0.0028324	0.0016914	0.0102605	0.2922

Significant Effects:	**BC effect**	The interaction between B and C is significant. The other significant
	B effect	effect is the learning and momentum rate, which strongly favour the setting of l=0.2 and mom=0.2 over l=0.15 and mom=0.15.

Standard 3-layer Backpropagation Network: Results and Analysis

DEV =	standard deviation of horizontal wind direction
HL =	hidden layer
Act. =	activation function
Last Error Trn. =	last average training error
Min. Error Trn. =	minimum average training error
Min. Error Tst. =	minimum average testing error
R2 Production =	R^2 value from applying the model to the production set
x:y ratio =	x:y ratio between neurons in hidden layers 1 and 2
N =	percentage of input data used for test set
M =	percentage of input data used for production set
mom =	momentum rate
l =	learning rate
L-G =	Logistic – Gaussian activation functions in the hidden layer and the output layer
L-L =	Logistic – Logistic activation functions in the hidden layer and 2 and the output layer

Architecture Type 2 - Standard 3 layer backpropagation net

	Positive	Negative
A	with DEV	without DEV
B	40 neurons HL1	60 neurons HL1
C	Gaussian Act.	Logistic Act.
D=ABC	Linear [-1,1]	Linear <-1,1>

Results:

	Last Error Trn.	Min. Error Trn.	Min. Error Tst.	R2 Production
Run 1	0.0031318	0.0031318	0.0080706	0.2457
Run 2	0.002015	0.0018796	0.0068654	0.1729
Run 3	0.0028117	0.0024513	0.0076051	0.1942
Run 4	0.0035537	0.0033196	0.007067	0.1921
Run 5	0.016563	0.0108009	0.0231428	0
Run 6	0.0019684	0.0019684	0.010438	0.0419
Run 7	0.0349752	0.0069808	0.0133807	0.1887
Run 8	0.0238983	0.0150034	0.0279355	0

Significant Effects:	**C effect**	The effect of having a Gaussian Activation function is to
	B effect	decrease the R2. The effect of having 40 neurons is to
	BC effect	increase the R2. Therefore the direction for future 3 hidden
		layer tests is towards Logistic Activation functions and less neurons.

Architecture Type 2.1 - Standard 3 layer backpropagation net

	Positive	Negative
A	20 neurons HL	30 neurons HL
B	Logistic HL	tanh HL
C	Logistic output	tanh output
D=ABC	Linear [-1,1]	Linear <-1,1>

Results:

	Last Error Trn.	Min. Error Trn.	Min. Error Tst.	R2 Production
Run 1	0.0251556	0.0203517	0.0450785	0.306
Run 2	0.0234767	0.0234767	0.0489733	0.3056
Run 3	0.0163245	0.0162778	0.0466555	0.2101
Run 4	0.0161196	0.0149541	0.0473099	0.277
Run 5	0.0036295	0.0033505	0.0078942	0.0759
Run 6	0.0043797	0.0043797	0.0077654	0.2821
Run 7	0.0032607	0.0032542	0.007235	0.3074
Run 8	0.0026998	0.0026798	0.0075419	0.2849

Significant Effects:

ABC effect
BC effect

Having a linear <-1,1> is seen to be quite significant in improving the value of R2. The next set of tests will use the linear <-1,1> as well as tanh output, and between 15 and 25 neurons in the hidden layer.

Architecture Type 2.2 - Standard 3 layer backpropagation net

	Positive	Negative
A	15 neurons HL	25 neurons HL
B	N=20,M=10	N=30,M=20
C	with temp	without temp
D=ABC	turboprop	momentum

Results:

	Last Error Trn.	Min. Error Trn.	Min. Error Tst.	R2 Production
Run 1	0.007661	0.0039927	0.0074991	0.139
Run 2	0.0057091	0.0057091	0.0075891	0.1495
Run 3	0.0050825	0.0050825	0.0090064	0.2319
Run 4	0.0073509	0.0035311	0.0089838	0.1019
Run 5	0.0018717	0.0016884	0.0062993	0.2996
Run 6	0.0049929	0.0031284	0.0066385	0.3142
Run 7	0.0056459	0.0029365	0.0079316	0.1557
Run 8	0.0032607	0.0032542	0.007235	0.3074

Significant Effects:		
	C effect	It seems that the largest effect is from the combination of having no
	B effect	temp included as well as having a larger production and test set.
	BC effect	As well, it seems that it is more advantageous to have a larger production and test set as well as including temperature.

Architecture Type 2.3 - Standard 3 layer backpropagation net

	Positive	Negative
A	mom=0.15	mom=0.3
B	l=0.15	l=0.3
C	12 neurons	18 neurons
D=ABC	L-L	L-G

Results:

	Last Error Trn.	Min. Error Trn.	Min. Error Tst.	R2 Production
Run 1	0.0143385	0.0065455	0.0101396	0.2341
Run 2	0.0038546	0.0017137	0.0057759	0.1345
Run 3	0.0049465	0.0028584	0.0062819	0.2403
Run 4	0.0112971	0.0052907	0.0096167	0.1885
Run 5	0.0028449	0.0016912	0.0058981	0.0859
Run 6	0.0261568	0.0057475	0.0102559	0.2174
Run 7	0.010304	0.0052039	0.0094363	0.1534
Run 8	0.0042496	0.0018248	0.0058804	0.1327

Significant Effects:	**AC effect**	The largest effect is the confounded interaction between A and C.
	ABC effect	The next significant effect is the number of neurons, which favours
	C effect	18 over 12. As well, the activation functions (ABC) appear significant towards having L-G instead of L-L.

4-layer Jump Connection Network: Results and Analysis

DEV =	standard deviation of horizontal wind direction
HL =	hidden layer
Act. =	activation function
Last Error Trn. =	last average training error
Min. Error Trn. =	minimum average training error
Min. Error Tst. =	minimum average testing error
R2 Production =	R^2 value from applying the model to the production set
x:y ratio =	x:y ratio between neurons in hidden layers 1 and 2

Architecture Type 3 - 4 Layer Jump Connection Net

	Positive	Negative
A	with DEV	without DEV
B	40 neurons HL1	60 neurons HL1
C	40 neurons HL2	60 neurons HL2
D=ABC	Gaussian Act.	Logistic Act.

Results:

	Last Error Trn.	Min. Error Trn.	Min. Error Tst.	R2 Production
Model 1	0.0012878	0.0012774	0.0081268	0.024
Model 2	0.0131341	0.0122305	0.0248806	0.0165
Model 3	0.0036059	0.0011149	0.0128805	0
Model 4	0.0013245	0.0012197	0.0069536	0.4519
Model 5	0.0018566	0.0018566	0.0072116	0.3223
Model 6	0.0087632	0.0087632	0.028	0
Model 7	0.0075357	0.0075313	0.0153239	0
Model 8	0.0009128	0.0009128	0.0067342	0.2887

Significant Effects:	**AC effect**	It seems that in this case, the 2 factor interactions are significant
	BC effect	There is a confounding pattern, so the AC is confounded with BD
	AB effect	the BC is confounded with the AD, and the AB is confounded with the CD. A full factorial design should be conducted.

Architecture Type 3.1 - 4 Layer Jump Connection Net

	Positive	Negative
A	2:1 ratio	3:1 ratio
B	30 neurons HL1	36 neurons HL1
C	Linear [-1,1]	Linear <-1,1>
D=ABC	Gaussian Act.	Tanh Act.

Results:

	Last Error Trn.	Min. Error Trn.	Min. Error Tst.	R2 Production
Model 1	0.1188676	0.118775	0.2102616	0
Model 2	0.0098821	0.0076381	0.0181293	0.0554
Model 3	0.0064628	0.0051434	0.0199645	0
Model 4	0.160058	0.1580243	0.1864138	0
Model 5	0.1188676	0.118775	0.2102616	0
Model 6	0.0098821	0.0076381	0.0181293	0.0554
Model 7	0.0064628	0.0051434	0.0199645	0
Model 8	0.160058	0.1580243	0.1864138	0

Significant Effects:	**A effect**	This particular set of runs seemed to greatly reduce the values of R2.
	B effect	Therefore, it is prudent that the first set of results be used for the 4
	AB effect	layer backpropagation net, and a different direction be chosen.

Architecture Type 1 - Standard 4 layer backpropagation net

	Positive	Negative
A	with DEV	without DEV
B	40 neurons HL1	60 neurons HL1
C	40 neurons HL2	60 neurons HL2
D=ABC	Gaussian Act.	Logistic Act.

Results:

	Last Avg. Error Trn.	Min. Avg. Error Trn.	Min. Avg. Error Tst.	R2 Production
Trial 1	0.0016003	0.0013497		0.2597
Trial 2	0.0193618	0.0193618	0.0280005	0
Trial 3	0.0048306	0.0040126	0.0115825	0.2881
Trial 4	0.0015144	0.0015144	0.0072485	0.1239
Trial 5	0.0017543	0.0016935	0.0074151	0.2564
Trial 6	0.0019683	0.0016515	0.0113582	0
Trial 7	0.0031952	0.0031952	0.0114674	0
Trial 8	0.0011614	0.001137	0.0070806	0.2494

Architecture Type 2 - Standard 3 layer backpropagation net

	Positive	Negative
A	with DEV	without DEV
B	40 neurons HL1	60 neurons HL1
C	Gaussian Act.	Logistic Act.
D=ABC	Linear [-1,1]	Linear <-1,1>

Results:

	Last Avg. Error Trn.	Min. Avg. Error Trn.	Min. Avg. Error Tst.	R2 Production
Run 1	0.0031318	0.0031318	0.0080706	0.2457
Run 2	0.002015	0.0018796	0.0068654	0.1729
Run 3	0.0028117	0.0024513	0.0076051	0.1942
Run 4	0.0035537	0.0033196	0.007067	0.1921
Run 5	0.016563	0.0108009	0.0231428	0
Run 6	0.0019684	0.0019684	0.010438	0.0419
Run 7	0.0349752	0.0069808	0.0133807	0.1887
Run 8	0.0238983	0.0150034	0.0279355	0

Architecture Type 3 - 4 Layer Jump Connection Net

	Positive	Negative
A	with DEV	without DEV
B	40 neurons HL1	60 neurons HL1
C	40 neurons HL2	60 neurons HL2
D=ABC	Gaussian Act.	Logistic Act.

Results:

	Last Avg. Error Trn.	Min. Avg. Error Trn.	Min. Avg. Error Tst.	R2 Production
Model 1	0.0012878	0.0012774	0.0081268	0.024
Model 2	0.0131341	0.0122305	0.0248806	0.0165
Model 3	0.0036059	0.0011149	0.0128805	0
Model 4	0.0013245	0.0012197	0.0069536	0.4519
Model 5	0.0018566	0.0018566	0.0072116	0.3223
Model 6	0.0087632	0.0087632	0.028	0
Model 7	0.0075357	0.0075313	0.0153239	0
Model 8	0.0009128	0.0009128	0.0067342	0.2887

Architecture Type 1.1 - Standard 4 layer backpropagation net

	Positive	Negative
A	2:1 ratio	3:1 ratio
B	30 neurons HL1	36 neurons HL1
C	Linear[-1,1]	Linear<-1,1>
D=ABC	Gaussian Act.	Tanh Act.

Results:

	Last Avg. Error Trn.	Min. Avg. Error Trn.	Min. Avg. Error Tst.	R2 Production
Trial 1	0.0208282	0.0208282	0.0532618	0.3353
Trial 2	0.005569	0.0050089	0.012229	0.0432
Trial 3	0.0071127	0.0049247	0.0108558	0.2933
Trial 4	0.0434505	0.0228035	0.0434453	0.1469
Trial 5	0.0189367	0.0189367	0.045788	0.1887
Trial 6	0.005569	0.0050089	0.012229	0.0432
Trial 7	0.0070325	0.0034753	0.0118333	0
Trial 8	0.0434505	0.0228035	0.0434453	0.1469

Architecture Type 2.1 - Standard 3 layer backpropagation net

	Positive	Negative
A	20 neurons HL	30 neurons HI
B	Logistic HL	tanh HL
C	Logistic output	tanh output
D=ABC	Linear [-1,1]	Linear <-1,1>

Results:

	Last Avg. Error Trn.	Min. Avg. Error Trn.	Min. Avg. Error Tst.	R2 Production
Run 1	0.0251556	0.0203517	0.0450785	0.306
Run 2	0.0234767	0.0234767	0.0489733	0.3056
Run 3	0.0163245	0.0162778	0.0466555	0.2101
Run 4	0.0161196	0.0149541	0.0473099	0.277
Run 5	0.0036295	0.0033505	0.0078942	0.0759
Run 6	0.0043797	0.0043797	0.0077654	0.2821
Run 7	0.0032607	0.0032542	0.007235	0.3074
Run 8	0.0026998	0.0026798	0.0075419	0.2849

Architecture Type 3.1 - 4 Layer Jump Connection Net

	Positive	Negative
A	2:1 ratio	3:1 ratio
B	30 neurons HL1	36 neurons HL1
C	Linear [-1,1]	Linear <-1,1>
D=ABC	Gaussian Act.	Tanh Act.

Results:

	Last Avg. Error Trn.	Min. Avg. Error Trn.	Min. Avg. Error Tst.	R2 Production
Model 1	0.1188676	0.118775	0.2102616	0
Model 2	0.0098821	0.0076381	0.0181293	0.0554
Model 3	0.0064628	0.0051434	0.0199645	0
Model 4	0.160058	0.1580243	0.1864138	0
Model 5	0.1188676	0.118775	0.2102616	0
Model 6	0.0098821	0.0076381	0.0181293	0.0554
Model 7	0.0064628	0.0051434	0.0199645	0
Model 8	0.160058	0.1580243	0.1864138	0

Architecture Type 1.2 - Standard 4 layer backpropagation net

	Positive	Negative
A	3:1 ratio	4:1 ratio
B	36 neurons HL1	48 neurons HL1
C	N=20,M=10	N=30,M=20
D=ABC	with temp	without temp

Results:

	Last Avg. Error Trn.	Min. Avg. Error Trn.	Min. Avg. Error Tst.	R2 Production
Trial 1	0.0049359	0.0049359	0.0128032	0.1023
Trial 2	0.0033392	0.0025959	0.0107425	0.3374
Trial 3	0.003951	0.001678	0.0109563	0.2513
Trial 4	0.0043338	0.0043338	0.0124708	0.1533
Trial 5	0.0074633	0.002944	0.0111988	0
Trial 6	0.0061319	0.0061203	0.0147946	0.1824
Trial 7	0.0055939	0.0055939	0.0149316	0.082
Trial 8	0.0028541	0.0028541	0.0122117	0.043

Architecture Type 2.2 - Standard 3 layer backpropagation net

	Positive	Negative
A	15 neurons HL	25 neurons HL
B	N=20,M=10	N=30,M=20
C	with temp	without temp
D=ABC	turboprop	momentum

Results:

	Last Avg. Error Trn.	Min. Avg. Error Trn.	Min. Avg. Error Tst.	R2 Production
Run 1	0.007661	0.0039927	0.0074991	0.139
Run 2	0.0057091	0.0057091	0.0075891	0.1495
Run 3	0.0050825	0.0050825	0.0090064	0.2319
Run 4	0.0073509	0.0035311	0.0089838	0.1019
Run 5	0.0018717	0.0016884	0.0062993	0.2996
Run 6	0.0049929	0.0031284	0.0066385	0.3142
Run 7	0.0056459	0.0029365	0.0079316	0.1557
Run 8	0.0032607	0.0032542	0.007235	0.3074

Architecture Type 4 - 3 Layer Jump Connection Net

	Positive	Negative
A	30 neurons	25 neurons
B	N=20,M=10	N=30,M=20
C	with temp	without temp
D=ABC	turboprop	momentum

Results:

	Last Avg. Error Trn.	Min. Avg. Error Trn.	Min. Avg. Error Tst.	R2 Production
Model 1	0.0215683	0.0107682	0.0158367	0
Model 2	0.0266969	0.0115191	0.0135914	0.031

* This type of model ruled out after trial Model 2

Architecture Type 1.3 - Standard 4 layer backpropagation net

	Positive	Negative
A	G-G-G	G-L-G
B	mom=0.15, l=0.15	mom=0.2, l=0.2
C	2:1 ratio	5:1 ratio
D=ABC	50 neurons	60 neurons

Results:

	Last Avg. Error Trn.	Min. Avg. Error Trn.	Min. Avg. Error Tst.	R2 Production
Trial 1	0.0036294	0.0019316	0.009943	0.4153
Trial 2	0.0011295	0.0010761	0.0098675	0.3383
Trial 3	0.0158977	0.0126049	0.0154211	0.0334
Trial 4	0.0014809	0.0011603	0.104317	0.2955
Trial 5	0.0204516	0.0065013	0.0109372	0.3281
Trial 6	0.0065709	0.0023669	0.0087533	0.2063
Trial 7	0.0204509	0.0069881	0.0111085	0.3191
Trial 8	0.0028324	0.0016914	0.0102605	0.2922

Architecture Type 2.3 - Standard 3 layer backpropagation net

	Positive	Negative
A	mom=0.15	mom=0.3
B	l=0.15	l=0.3
C	12 neurons	18 neurons
D=ABC	L-L	L-G

Results:

	Last Avg. Error Trn.	Min. Avg. Error Trn.	Min. Avg. Error Tst.	R2 Production
Run 1	0.0143385	0.0065455	0.0101396	0.2341
Run 2	0.0038546	0.0017137	0.0057759	0.1345
Run 3	0.0049465	0.0028584	0.0062819	0.2403
Run 4	0.0112971	0.0052907	0.0096167	0.1885
Run 5	0.0028449	0.0016912	0.0058981	0.0859
Run 6	0.0261568	0.0057475	0.0102559	0.2174
Run 7	0.010304	0.0052039	0.0094363	0.1534
Run 8	0.0042496	0.0018248	0.0058804	0.1327

APPENDIX C – Detailed Results and Analysis from Stage 2 of the ANN Modelling Process

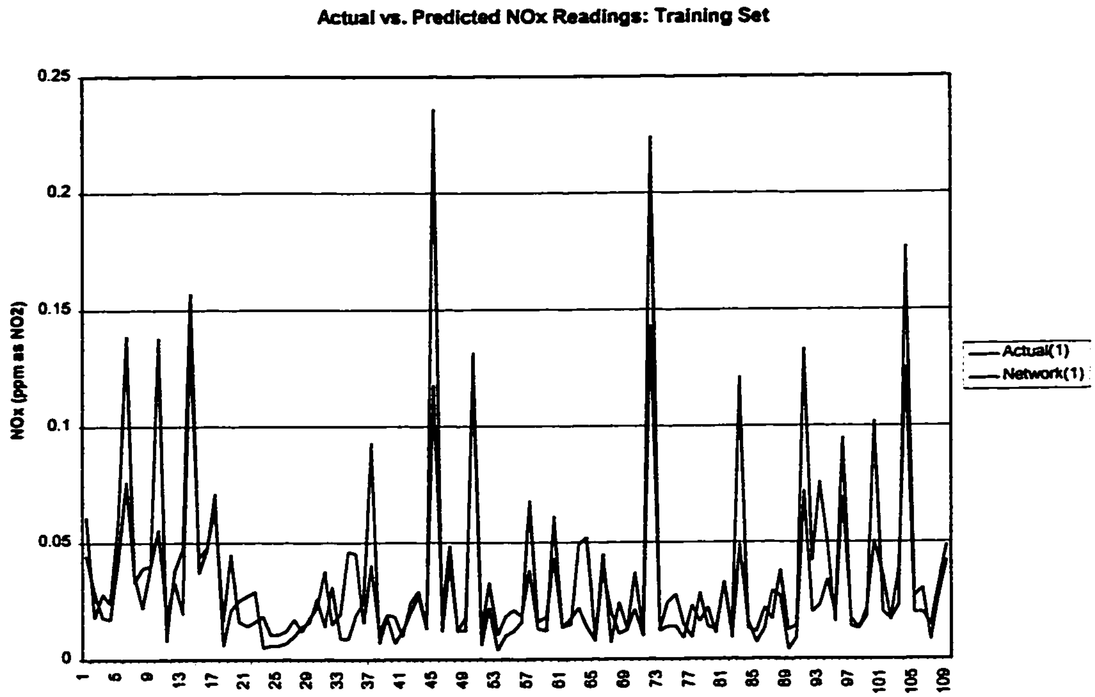
Sample of Data Used For Stage 2 Modelling, Models 1 and 2

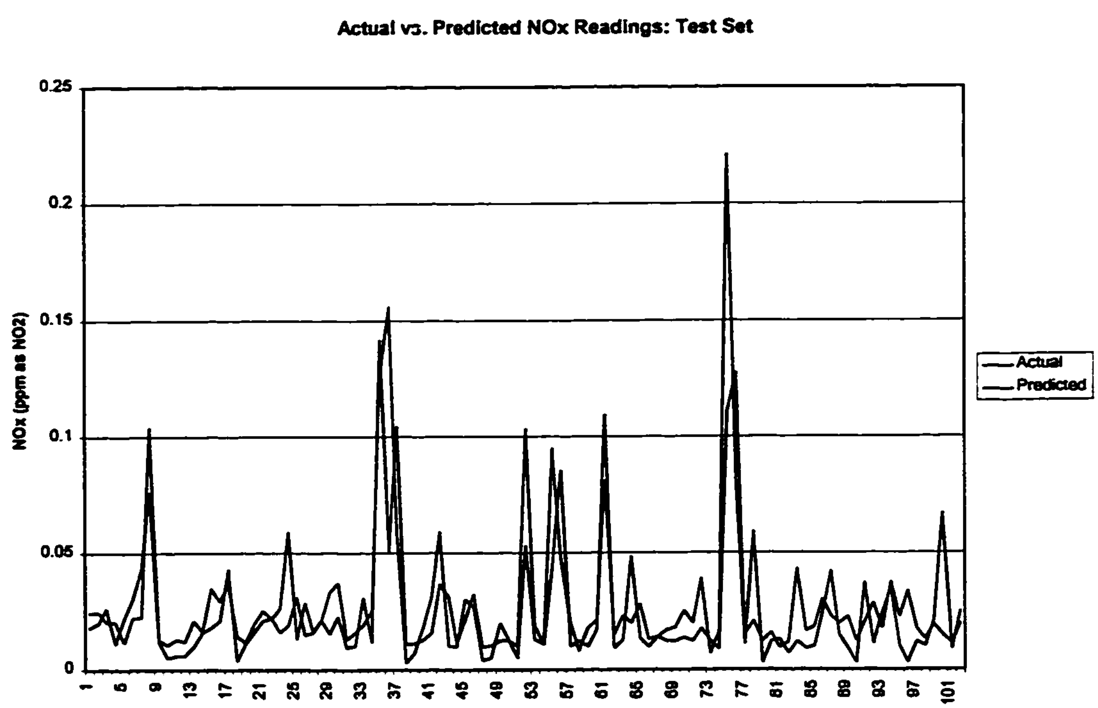
YR	MTH	DAY	HR	DEV	Tmp(Muni)	WDR	WDR Deg	WDR Sec	WSP	NOX	TR Sec 1	TR Sec 2	TR Sec 3	TR Sec 4	Class
95	1	1	17	10	-9.5	262	98	2	15.2	0.016	1832	254	367	2653	T
95	1	2	4	9	-14.3	253	107	2	10.4	0.01	122	8	25	76	P
95	1	3	17	88	-18.8	247	113	2	0.4	0.177	1832	254	367	2653	V
95	1	5	4	14	-15.5	229	131	2	7.1	0.059	122	8	25	76	P
95	1	5	17	24	-12.8	226	134	2	6.3	0.081	1832	254	367	2653	P
95	1	7	4	10	-13.3	219	141	2	18.5	0.014	122	8	25	76	T
95	1	8	4	12	-23.9	309	51	2	2.9	0.093	122	8	25	76	P
95	1	11	4	28	-12.1	319	41	2	2	0.02	122	8	25	76	P
95	1	12	4	20	-12.1	260	100	2	0.8	0.053	122	8	25	76	V
95	1	13	4	71	-8	180	180	2	0.1	0.02	122	8	25	76	T
95	1	18	17	11	-10.2	324	36	2	1.2	0.114	1832	254	367	2653	V
95	1	19	4	45	-10	248	112	2	2.4	0.023	122	8	25	76	T
95	1	24	17	13	-9.3	326	34	2	0.3	0.126	1832	254	367	2653	V
95	1	25	4	41	-16.2	225	135	2	0	0.221	122	8	25	76	T
95	1	26	17	17	-10.2	320	40	2	1.4	0.122	1832	254	367	2653	P
95	1	30	4	7	-5.6	196	164	2	12.5	0.027	122	8	25	76	V
95	1	30	17	13	4.5	205	155	2	5.4	0.058	1832	254	367	2653	V
95	1	31	4	67	3.3	340	20	2	0.7	0.102	122	8	25	76	T
95	2	1	4	68	-0.9	339	21	2	3.4	0.035	122	8	25	76	P
95	2	2	17	8	-5.4	267	93	2	9.4	0.047	1832	254	367	2653	V
95	2	4	4	9	1.1	207	153	2	15.4	0.016	122	8	25	76	P
95	2	4	17	9	3.3	201	159	2	15.4	0.021	1832	254	367	2653	P
95	2	5	4	18	-4.5	185	175	2	8.1	0.052	122	8	25	76	V
95	2	6	17	10	-5.3	305	55	2	3.7	0.179	1832	254	367	2653	T
95	2	8	4	9	1.1	201	159	2	17.6	0.012	122	8	25	76	V
95	2	9	4	10	1.8	229	131	2	32.8	0.005	122	8	25	76	T
95	2	9	17	10	-8.8	242	118	2	14.9	0.026	1832	254	367	2653	T
95	2	10	4	9	-16	238	122	2	19	0.005	122	8	25	76	P
95	2	10	17	10	-14.7	268	92	2	11.9	0.021	1832	254	367	2653	P
95	2	11	4	16	-21.3	246	114	2	4	0.04	122	8	25	76	V
95	2	11	17	9	-18.9	258	102	2	18.3	0.01	1832	254	367	2653	V
95	2	12	4	10	-20.9	223	137	2	17	0.007	122	8	25	76	T
95	2	12	17	12	-17.2	220	140	2	16.2	0.009	1832	254	367	2653	T
95	2	14	17	69	-13.6	191	169	2	1.5	0.055	1832	254	367	2653	V
95	2	15	17	22	-15.8	312	48	2	4.1	0.047	1832	254	367	2653	T
95	2	16	4	16	-17.8	321	39	2	4.4	0.027	122	8	25	76	P
95	2	16	17	36	-19.3	198	162	2	3.4	0.049	1832	254	367	2653	P
95	2	18	4	20	-13.5	270	90	2	2.9	0.043	122	8	25	76	T
95	2	19	17	13	7.4	210	150	2	12.4	0.019	1832	254	367	2653	P
95	2	22	4	9	0.3	204	156	2	21.6	0.006	122	8	25	76	P
95	2	22	17	14	1.1	269	91	2	17.1	0.031	1832	254	367	2653	P
95	2	25	17	15	-5.8	217	143	2	14.4	0.01	1832	254	367	2653	P
95	2	26	4	10	-15.5	224	136	2	17.9	0.006	122	8	25	76	V
95	2	26	17	14	-18.6	270	90	2	14.8	0.007	1832	254	367	2653	V
95	2	27	17	12	-13.1	278	82	2	8.6	0.019	1832	254	367	2653	T
95	3	1	4	5	-19.9	190	170	2	11.9	0.025	122	8	25	76	V
95	3	1	17	9	-2.1	293	67	2	18.1	0.02	1832	254	367	2653	V
95	3	2	4	4	-7.6	204	156	2	14.9	0.028	122	8	25	76	T
95	3	2	17	9	-2.6	350	10	2	14.2	0.027	1832	254	367	2653	T
95	3	5	4	12	-23.6	192	168	2	5.7	0.009	122	8	25	76	T
95	3	5	17	9	-17.7	220	140	2	11	0.021	1832	254	367	2653	T
95	3	6	4	11	-24.6	197	163	2	9.1	0.016	122	8	25	76	P
95	3	6	17	12	-14.6	336	24	2	9.8	0.037	1832	254	367	2653	P
95	3	7	4	3	-22.6	216	144	2	5.7	0.061	122	8	25	76	V
95	3	11	17	33	7.9	220	140	2	8.2	0.033	1832	254	367	2653	T
95	3	12	4	5	-2.2	196	164	2	14	0.026	122	8	25	76	P
95	3	16	4	10	3.1	283	77	2	15	0.026	122	8	25	76	V
95	3	16	17	13	5	360	0	2	12.6	0.016	1832	254	367	2653	V
95	3	17	17	43	7.4	195	165	2	4.4	0.027	1832	254	367	2653	T
95	3	19	4	12	0.6	191	169	2	3.4	0.013	122	8	25	76	V
95	3	19	17	34	11.8	322	38	2	6.9	0.009	1832	254	367	2653	V
95	3	22	4	15	-0.7	281	79	2	13.5	0.021	122	8	25	76	V

Sample of Output from Best-Fit Model, Model 1

Production			Test			Training		
Actual(1)	Network(1)	Act-Net(1)	Actual(1)	Network(1)	Act-Net(1)	Actual(1)	Network(1)	Act-Net(1)
0.032	0.023575	0.008425	0.018	0.0243228	-0.006323	0.061	0.0445127	0.016487
0.027	0.0237046	0.003295	0.02	0.0244973	-0.004497	0.018	0.0283588	-0.010359
0.025	0.022324	0.002676	0.026	0.020485	0.005515	0.028	0.0178303	0.01017
0.079	0.0765366	0.002463	0.011	0.0203528	-0.009353	0.024	0.0173216	0.006678
0.014	0.0198035	-0.0058	0.022	0.0116968	0.010303	0.059	0.0425184	0.016482
0.027	0.0239734	0.003027	0.03	0.0221595	0.007841	0.139	0.0762038	0.062796
0.063	0.0794308	-0.01643	0.043	0.0225458	0.020454	0.033	0.0356646	-0.002665
0.01	0.0123132	-0.00231	0.076	0.1039746	-0.027975	0.039	0.0218665	0.017133
0.012	0.0149376	-0.00294	0.012	0.0127131	-0.000713	0.04	0.039644	0.000356
0.02	0.0125474	0.007453	0.005	0.0105728	-0.005573	0.138	0.055612	0.082388
0.005	0.0201481	-0.01515	0.006	0.0130294	-0.007029	0.008	0.0185743	-0.010574
0.006	0.0120204	-0.00602	0.006	0.0119017	-0.005902	0.038	0.0327313	0.005269
0.026	0.0121975	0.013803	0.01	0.0209371	-0.010937	0.047	0.0195107	0.027489
0.179	0.1082391	0.070761	0.016	0.0164862	-0.000486	0.157	0.1384054	0.018595
0.006	0.0122708	-0.00627	0.018	0.0346166	-0.016617	0.037	0.0433194	-0.006319
0.007	0.01382	-0.00682	0.021	0.0292965	-0.008296	0.047	0.0477289	-0.000729
0.017	0.01832	-0.00132	0.043	0.0365033	0.006497	0.071	0.0642357	0.006764
0.018	0.0156177	0.002382	0.004	0.0144819	-0.010482	0.006	0.0164526	-0.010453
0.027	0.0255302	0.00147	0.011	0.0113804	-0.00038	0.021	0.0449397	-0.02394
0.114	0.1262659	-0.01227	0.016	0.0194705	-0.00347	0.025	0.0161673	0.008833
0.013	0.0932829	-0.08028	0.021	0.02522	-0.00422	0.027	0.014238	0.012762
0.014	0.0100956	0.003904	0.022	0.0216543	0.000346	0.029	0.016217	0.012783
0.005	0.010671	-0.00567	0.016	0.0263853	-0.010385	0.005	0.0184001	-0.0134
0.016	0.0163801	-0.00038	0.019	0.0588368	-0.039837	0.006	0.0105426	-0.004543
0.017	0.0147739	0.002226	0.031	0.0132468	0.017753	0.006	0.0107432	-0.004743
0.007	0.0160956	-0.0091	0.015	0.0285625	-0.013563	0.007	0.0123166	-0.005317
0.011	0.0138533	-0.00285	0.016	0.0163057	-0.000306	0.01	0.017131	-0.007131
0.014	0.0240447	-0.01004	0.021	0.021169	-0.000169	0.014	0.0120687	0.001931
0.056	0.0333007	0.022699	0.033	0.0153161	0.017684	0.016	0.0177707	-0.001771
0.01	0.0109016	-0.0009	0.037	0.0227276	0.014272	0.026	0.021977	0.004023
0.021	0.0141516	0.006848	0.013	0.0094578	0.003542	0.014	0.0378207	-0.023821
0.005	0.0180904	-0.01309	0.016	0.0103314	0.005669	0.031	0.0148992	0.016101
0.04	0.0485896	-0.00859	0.019	0.0308597	-0.01186	0.009	0.0196269	-0.010627
0.005	0.018728	-0.01373	0.025	0.0118528	0.013147	0.009	0.0460946	-0.037095
0.011	0.0127312	-0.00173	0.126	0.1417608	-0.015761	0.019	0.0451707	-0.026171
0.017	0.0097983	0.007202	0.156	0.0503889	0.105611	0.024	0.0155763	0.008424
0.018	0.0088606	0.009139	0.058	0.1045658	-0.046566	0.093	0.0402995	0.052701
0.183	0.1373765	0.045623	0.003	0.0109576	-0.007958	0.007	0.0113444	-0.004344
0.013	0.0136831	-0.00068	0.007	0.0111759	-0.004176	0.018	0.0190736	-0.001074
0.02	0.0144902	0.00551	0.018	0.0128035	0.005197	0.007	0.018142	-0.011142
0.052	0.0429314	0.009069	0.031	0.0156924	0.015308	0.012	0.0098624	0.002138
0.036	0.0386467	-0.00265	0.059	0.0365297	0.02247	0.02	0.0241441	-0.004144
0.01	0.0124339	-0.00243	0.01	0.0310982	-0.021098	0.027	0.0292939	-0.002294
0.015	0.0111256	0.003874	0.01	0.0113498	-0.00135	0.013	0.0145522	-0.001552
0.02	0.0114009	0.008599	0.03	0.0217109	0.008289	0.236	0.1176003	0.1184
0.011	0.0099797	0.00102	0.027	0.0323536	-0.005354	0.012	0.0196763	-0.007676
0.011	0.0195625	-0.00856	0.004	0.009699	-0.005699	0.04	0.0485896	-0.00859
0.014	0.0096813	0.004319	0.005	0.0101007	-0.005101	0.012	0.0123727	-0.000373
0.021	0.0111266	0.009873	0.02	0.0123751	0.007625	0.018	0.0123521	0.005648
0.031	0.0307879	0.000212	0.013	0.0126207	0.000379	0.122	0.1316927	-0.009693
0.017	0.010475	0.006525	0.005	0.0100512	-0.005051	0.006	0.0110078	-0.005008
0.01	0.0112496	-0.00125	0.053	0.1033636	-0.050364	0.022	0.0327515	-0.010751

Training and Test Set Actual NO_x and Predicted NO_x, Model 1





APPENDIX D – Detailed Results and Analysis from Stage 3 of the ANN Modelling Process

<u>**Sample of Data Used For Stage 3 Modelling**</u>

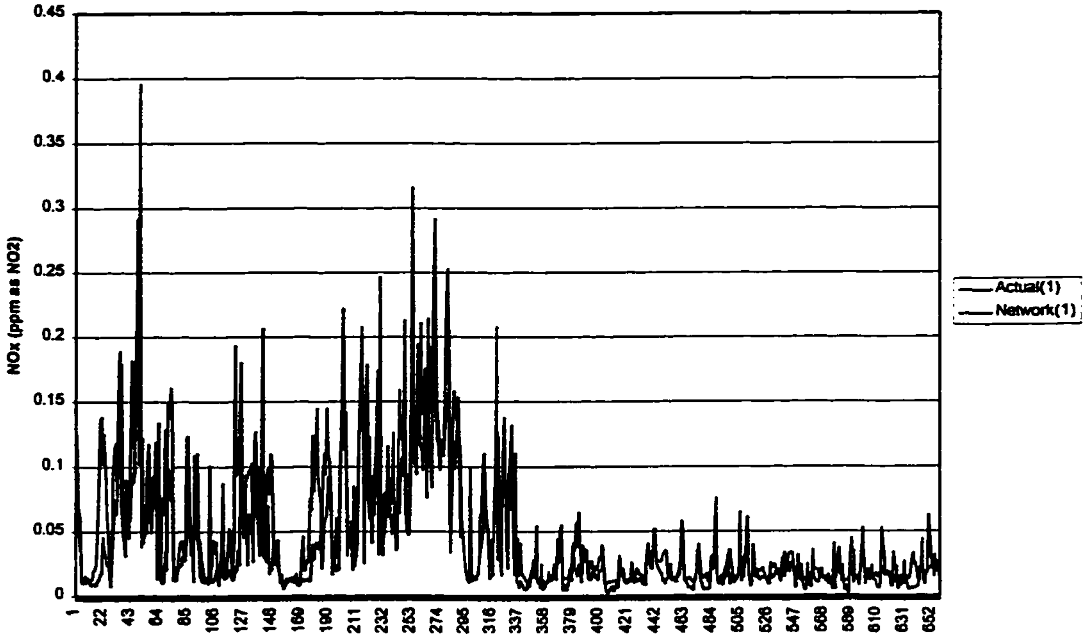
Yr	Mth	Day	Hour	Temp	NOX PPM	WSP KPH	WDR SEC	WDR DEG	DEV DEG	sum transport	Season Index	Class
1995	1	1	1	-12.2	0.127	6.5	1	158	21	718.3010064	1	T
1995	1	1	2	-12.6	0.109	8.9	1	129	6	651.9056661	1	T
1995	1	1	3	-13.9	0.083	9.1	1	128	7	420.1656479	1	V
1995	1	1	4	-14.6	0.064	9.6	1	125	4	269.3354311	1	V
1995	1	1	5	-14.3	0.051	9.9	1	122	3	300.2339375	1	T
1995	1	1	6	-15.4	0.048	10.7	1	127	3	356.8569695	1	V
1995	1	1	7	-16.1	0.039	11.8	1	121	3	887.80509	1	V
1995	1	1	8	-15.5	0.031	12	1	117	6	1195.807192	1	P
1995	1	1	9	-16.2	0.036	13.3	1	128	3	1366.39152	1	T
1995	1	1	10	-15.4	0.037	13.4	1	135	5	1463.989991	1	P
1995	1	1	11	-16.3	0.064	10.8	2	180	18	2323.145147	1	P
1995	1	1	12	-12.5	0.035	8.5	2	150	14	2466.991325	1	P
1995	1	1	13	-11.4	0.029	12.1	2	121	19	2742.060078	1	V
1995	1	1	14	-8.5	0.014	18	2	92	14	2935.911401	1	T
1995	1	1	15	-8.1	0.011	22.6	2	84	8	3004.09567	1	T
1995	1	1	16	-8.6	0.011	19	2	85	10	3058.555494	1	T
1995	1	1	17	-8.2	0.016	15.2	2	98	10	2951.027746	1	T
1995	1	1	18	-9.5	0.011	20.6	2	84	8	2892.431249	1	V
1995	1	1	19	-10.9	0.013	18	2	84	9	2080.746124	1	T
1995	1	1	20	-10.0	0.011	16.5	2	82	8	1573.088522	1	P
1995	1	1	21	-10.6	0.014	12.9	2	93	8	1245.228279	1	T
1995	1	1	22	-11.3	0.012	13.3	2	101	8	1046.317437	1	P
1995	1	1	23	-12.5	0.012	13.8	2	92	8	825.6113452	1	T
1995	1	2	1	-12.0	0.008	13.2	2	96	11	469.3	1	T
1995	1	2	2	-13.0	0.009	12.5	2	93	13	272.6	1	T
1995	1	2	3	-14.0	0.009	10	2	99	13	198.4	1	T
1995	1	2	4	-15.0	0.01	10.4	2	107	9	194.7	1	T
1995	1	2	5	-14.0	0.008	8.9	2	104	12	271.7	1	T
1995	1	2	6	-14.0	0.01	8.1	2	112	12	652.2	1	V
1995	1	2	7	-14.5	0.012	7.3	2	119	16	2197.9	1	T
1995	1	2	8	-14.5	0.013	5.7	2	122	19	4211.7	1	T
1995	1	2	9	-15.1	0.017	2.4	2	104	18	3259.7	1	T
1995	1	2	10	-15.5	0.018	1.4	2	104	41	2477	1	T
1995	1	2	11	-15.1	0.046	4.3	1	151	126	2596.4	1	T
1995	1	2	12	-15.3	0.038	8.6	1	143	12	2953.7	1	T
1995	1	2	13	-15.4	0.032	9.7	1	125	8	3156.2	1	T
1995	1	2	14	-15.4	0.024	10.1	1	113	12	3117	1	T
1995	1	2	15	-15.3	0.021	11.2	1	110	9	3278.8	1	V
1995	1	2	16	-14.9	0.017	9.7	1	97	11	4055.1	1	P
1995	1	2	17	-15.4	0.018	8.6	1	79	12	5573.9	1	V
1995	1	2	18	-16.0	0.025	9.8	1	76	8	5161.6	1	T
1995	1	2	19	-16.6	0.015	15.6	1	79	6	3261.4	1	V
1995	1	2	20	-16.0	0.022	10.2	1	89	11	2144.9	1	V
1995	1	2	21	-15.6	0.015	10.2	1	80	11	1708.1	1	V
1995	1	2	22	-15.7	0.015	9.1	1	86	11	1604	1	P
1995	1	2	23	-16.5	0.02	4.7	1	69	14	1178.5	1	T
1995	1	2	24	-11.8	0.007	14.3	2	94	11	708.0058839	1	T
1995	1	3	1	-18.4	0.026	4.5	1	62	32	469.3	1	T
1995	1	3	2	-17.9	0.051	3.2	1	118	12	272.6	1	T

Sample of Output from Best-Fit Model, Stage 3 Modelling

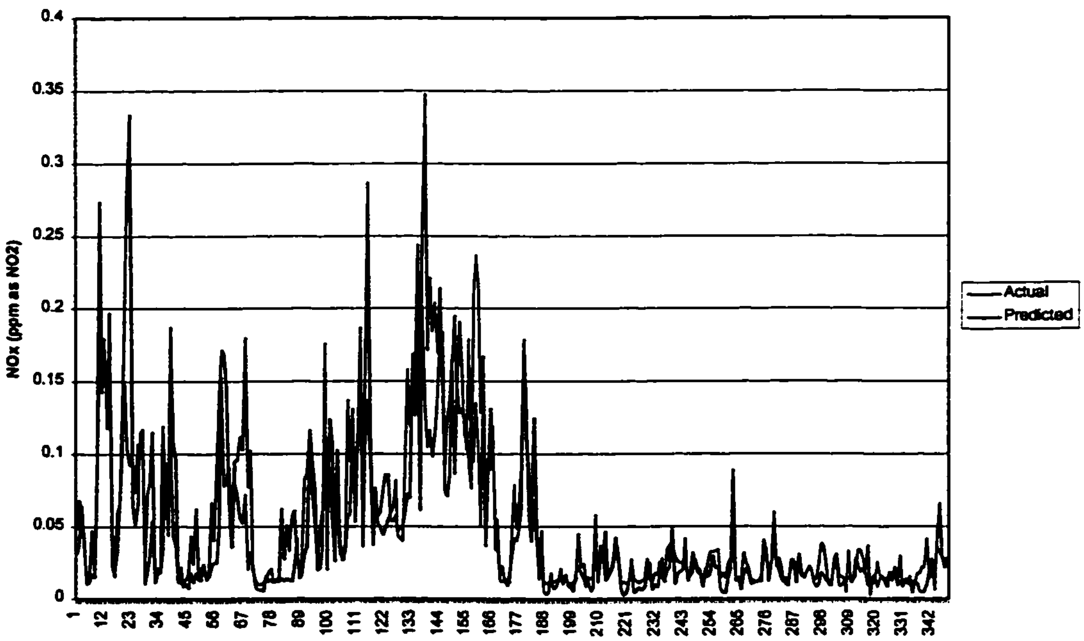
	Production			Test			Training	
Actual(1)	Network(1)	Act-Net(1)	Actual(1)	Network(1)	Act-Net(1)	Actual(1)	Network(1)	Act-Net(1)
0.083	0.0748091	0.008191	0.031	0.0481199	-0.01712	0.127	0.100242	0.026758
0.064	0.0698064	-0.00581	0.037	0.0679598	-0.03096	0.109	0.077536	0.031464
0.048	0.0666322	-0.01863	0.064	0.0615599	0.00244	0.051	0.065064	-0.01406
0.039	0.0555696	-0.01657	0.035	0.0426	-0.0076	0.036	0.060013	-0.02401
0.029	0.0165654	0.012435	0.011	0.0101239	0.000876	0.014	0.010546	0.003454
0.011	0.009967	0.001033	0.012	0.012652	-0.00065	0.011	0.009778	0.001222
0.01	0.0324478	-0.02245	0.017	0.0475583	-0.03056	0.011	0.010394	0.000606
0.021	0.0565174	-0.03552	0.015	0.0185673	-0.00357	0.016	0.012054	0.003946
0.018	0.0594478	-0.04145	0.085	0.0903661	-0.00537	0.013	0.009964	0.003036
0.015	0.0142352	0.000765	0.274	0.1795884	0.094412	0.014	0.012808	0.001192
0.022	0.0189221	0.003078	0.142	0.1483001	-0.0063	0.012	0.012042	-4.2E-05
0.015	0.0145537	0.000446	0.175	0.1795306	-0.00453	0.008	0.012234	-0.00423
0.175	0.1665469	0.008453	0.141	0.1174688	0.023531	0.009	0.013058	-0.00406
0.113	0.1620654	-0.04907	0.177	0.1968236	-0.01982	0.009	0.019516	-0.01052
0.129	0.1302647	-0.00126	0.047	0.0224708	0.024529	0.01	0.020254	-0.01025
0.121	0.1426309	-0.02163	0.02	0.0154689	0.004531	0.008	0.024976	-0.01698
0.029	0.0132903	0.01571	0.032	0.0598384	-0.02784	0.012	0.048558	-0.03656
0.073	0.0818579	-0.00886	0.065	0.0649105	8.95E-05	0.013	0.086245	-0.07325
0.161	0.1224495	0.03855	0.128	0.1023915	0.025609	0.017	0.135609	-0.11861
0.213	0.09369	0.11931	0.201	0.1483758	0.052624	0.018	0.138622	-0.12062
0.152	0.0871854	0.064815	0.282	0.1037561	0.178244	0.046	0.101639	-0.05564
0.128	0.1052626	0.022737	0.334	0.0926259	0.241374	0.038	0.125168	-0.08717
0.276	0.1987621	0.077238	0.065	0.0934148	-0.02841	0.032	0.101259	-0.06926
0.067	0.1031727	-0.03617	0.051	0.0736618	-0.02266	0.024	0.06285	-0.03885
0.049	0.0816083	-0.03261	0.065	0.1071496	-0.04215	0.025	0.050538	-0.02554
0.114	0.1070579	0.006942	0.114	0.097258	0.016742	0.02	0.030574	-0.01057
0.041	0.0872462	-0.04625	0.117	0.1075118	0.009488	0.007	0.011277	-0.00428
0.018	0.0608219	-0.04282	0.01	0.0166866	-0.00669	0.026	0.032795	-0.00679
0.038	0.1409581	-0.10296	0.019	0.0725809	-0.05358	0.051	0.096166	-0.04517
0.027	0.0570262	-0.03003	0.029	0.0798883	-0.05089	0.075	0.113927	-0.03893
0.023	0.0661584	-0.04316	0.054	0.1151927	-0.06119	0.063	0.118824	-0.05582
0.041	0.0524806	-0.01148	0.021	0.0108689	0.010131	0.066	0.081016	-0.01502
0.07	0.0422175	0.027783	0.021	0.0183367	0.002663	0.124	0.178742	-0.05474
0.04	0.0232314	0.016769	0.02	0.0181809	0.001819	0.105	0.189102	-0.0841
0.028	0.0158783	0.012122	0.033	0.1191522	-0.08615	0.179	0.069976	0.109024
0.012	0.0145993	-0.0026	0.094	0.0744228	0.019577	0.105	0.052245	0.052755
0.031	0.039618	-0.00862	0.044	0.0595385	-0.01554	0.041	0.040008	0.000992
0.034	0.0199849	0.014015	0.118	0.1874344	-0.06943	0.031	0.055901	-0.0249
0.041	0.0516157	-0.01062	0.043	0.1064119	-0.06341	0.064	0.090525	-0.02652
0.086	0.1074787	-0.02148	0.037	0.0973256	-0.06033	0.076	0.085608	-0.00961
0.071	0.094847	-0.02385	0.012	0.0115653	0.000435	0.045	0.056823	-0.01182
0.023	0.171292	-0.14829	0.022	0.0112964	0.010704	0.106	0.060566	0.045434
0.011	0.0110108	-1.1E-05	0.008	0.0100532	-0.00205	0.182	0.094795	0.087205
0.011	0.0101896	0.00081	0.01	0.0131924	-0.00319	0.115	0.087706	0.027294
0.007	0.0111551	-0.00416	0.007	0.0164174	-0.00942	0.117	0.095972	0.021028
0.011	0.0285212	-0.01752	0.018	0.0437144	-0.02571	0.171	0.204616	-0.03362
0.025	0.0814948	-0.05649	0.011	0.0239096	-0.01291	0.292	0.20691	0.08509
0.01	0.0284455	-0.01845	0.018	0.0625714	-0.04457	0.221	0.101441	0.119559

Training and Test Set Actual NO_x and Predicted NO_x

Actual vs. Predicted NOx Readings: Training Set



Actual vs. Predicted NOx Readings: Test Set



APPENDIX E – Detailed Results and Analysis from Sensitivity Analysis

Sample of Data Set Used in Model Application for the Sensitivity Analysis

YR	MTH	DAY	HOUR	Temp	WSP	WDR Sec	WDR Deg	DEV	Sum Trans	Season Index	Actual NOx
95	2	8	1	1.5	10.6	2	161	10	469.3	1	0.026
95	2	8	2	1.4	14	2	162	8	272.6	1	0.015
95	2	8	3	1.1	16.5	2	167	11	198.4	1	0.014
95	2	8	4	1.0	17.6	2	159	9	194.7	1	0.012
95	2	8	5	1.1	17.6	2	163	10	271.7	1	0.011
95	2	8	6	0.4	17.1	2	159	9	652.2	1	0.017
95	2	8	7	-0.3	15.3	2	156	9	2197.9	1	0.021
95	2	8	8	-0.8	15.3	2	154	11	4211.7	1	0.036
95	2	8	9	-1.5	14.7	2	158	10	3259.7	1	0.046
95	2	8	10	-1.2	15.5	2	155	11	2477	1	0.035
95	2	8	11	-0.4	14.6	2	157	11	2596.4	1	0.03
95	2	8	12	0.7	16	2	158	10	2953.7	1	0.031
95	2	8	13	2.1	16.6	2	155	10	3156.2	1	0.02
95	2	8	14	3.2	14.2	2	156	12	3117	1	0.027
95	2	8	15	3.6	10.3	2	161	15	3278.8	1	0.038
95	2	8	17	3.3	11.2	1	126	11	5573.9	1	0.115
95	2	8	18	2.6	11.6	1	97	7	5161.6	1	0.097
95	2	8	19	2.4	17.8	1	93	8	3261.4	1	0.055
95	2	8	20	2.0	22.9	1	98	6	2144.9	1	0.031
95	2	8	21	1.1	20.3	1	111	11	1708.1	1	0.035
95	2	8	22	0.9	18.4	1	119	7	1604	1	0.03
95	2	8	23	0.3	17.9	1	124	6	1178.5	1	0.029
95	2	8	24	2.4	19.5	1	151	19	782.4	1	0.038
95	2	9	1	4.2	24.2	2	163	11	469.3	1	0.014
95	2	9	2	5.5	29.7	2	145	10	272.6	1	0.007
95	2	9	3	4.5	36.6	2	127	8	198.4	1	0.005
95	2	9	4	2.4	32.8	2	131	10	194.7	1	0.005
95	2	9	5	1.8	31.1	2	143	9	271.7	1	0.006
95	2	9	6	1.4	32.9	2	137	12	652.2	1	0.007
95	2	9	7	1.9	30	2	126	12	2197.9	1	0.01
95	2	9	8	1.1	34.7	2	96	8	4211.7	1	0.012
95	2	9	9	-2.4	32.8	2	86	10	3259.7	1	0.011
95	2	9	10	-4.3	32.4	2	83	9	2477	1	0.009

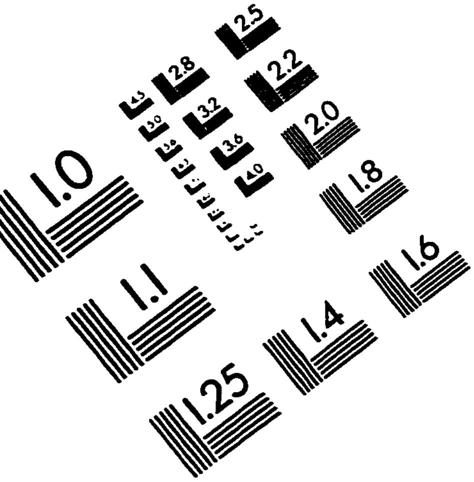
Data for Relationship between Traffic Counts and Average Hourly NO_x

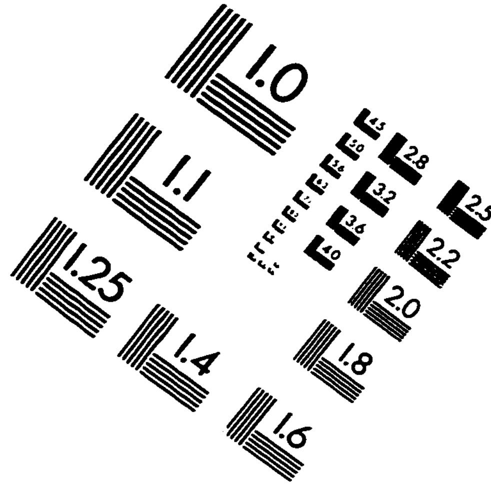
Percent Increase or Decrease	Average Hourly NOx Concentration
40%	0.043933553
35%	0.043115096
30%	0.042269783
25%	0.041421563
20%	0.040629659
15%	0.039891927
10%	0.039206034
5%	0.038501885
0%	0.037780349
-5%	0.036913786
-10%	0.036065663
-15%	0.035245015
-20%	0.03446298
-25%	0.033730919
-30%	0.033060206
-35%	0.032457773
-40%	0.031922972

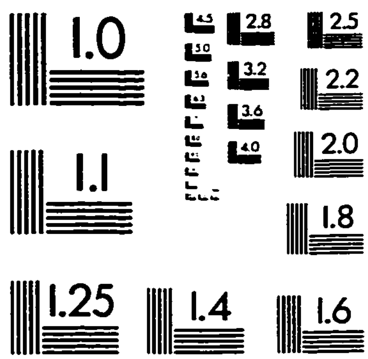
Sample of Model Output for Varying Traffic Counts

15% Traffic	10% Traffic	5% Traffic	-5% Traffic	-10% Traffic	-15% Traffic
0.02076	0.020739	0.020719	0.020681	0.020662	0.020645
0.013925	0.013908	0.013892	0.01386	0.013845	0.013829
0.011251	0.011241	0.011232	0.011219	0.011219	0.011219
0.010527	0.01052	0.010513	0.010506	0.010506	0.010506
0.010633	0.010621	0.010609	0.010587	0.010576	0.010565
0.011429	0.011386	0.011345	0.011267	0.011229	0.011193
0.018674	0.018004	0.017393	0.016331	0.015871	0.015452
0.05397	0.047551	0.041957	0.032993	0.029475	0.026497
0.033896	0.031191	0.028806	0.024871	0.02326	0.02185
0.019676	0.018812	0.018034	0.016704	0.016137	0.015628
0.022358	0.021257	0.020269	0.018591	0.01788	0.017244
0.026306	0.02439	0.022696	0.019886	0.018728	0.017711
0.026841	0.024631	0.022694	0.019527	0.018244	0.017128
0.027388	0.025323	0.023515	0.020552	0.019345	0.018292
0.036813	0.034126	0.031781	0.02796	0.026415	0.025075
0.222579	0.222579	0.222579	0.213118	0.201347	0.187603
0.137953	0.137953	0.133109	0.113015	0.101705	0.090375
0.041948	0.038545	0.03541	0.029915	0.027538	0.025396
0.023638	0.022679	0.021781	0.020158	0.019428	0.018748
0.030362	0.029158	0.028014	0.025899	0.024929	0.024014
0.042322	0.040686	0.039101	0.036093	0.034676	0.03332
0.0396	0.038467	0.037365	0.035261	0.03426	0.033294
0.049729	0.048843	0.047964	0.046231	0.045378	0.044534

IMAGE EVALUATION TEST TARGET (QA-3)

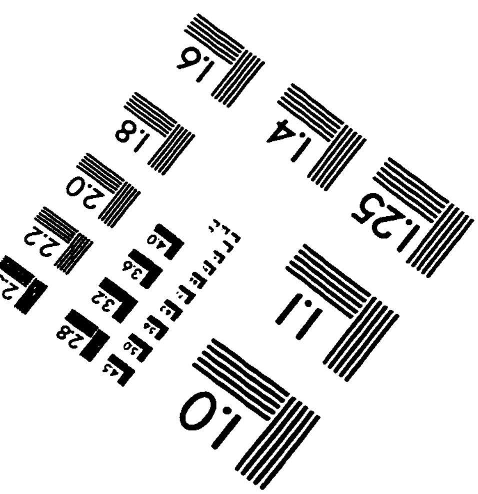






150mm

6"



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