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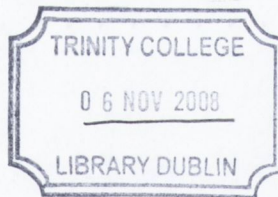
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Modelling the Impact of Traffic Emissions on Local Air Quality

A thesis submitted to the University of Dublin in fulfillment of the requirements for the degree of Doctor of Philosophy in the Faculty of Engineering.

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June 2008.



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DECLARATION

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Abstract:

Air quality modelling can be used to complement monitoring networks and to obtain information at lower cost. A primary advantage of modelling is that it can be used for the prediction of future air quality, which often forms an important part of Environmental Impact Assessment (EIA) studies. The research described in this thesis represents an in - depth atmospheric dispersion modelling study carried out at highway and street canyon locations in the Dublin area for the pollutants CO, NO_x and NO₂.

In this context, appropriate dispersion models GFLSM and CALINE4 for highways and STREET and OSPM models were studied and validated for local conditions.

Three separate cases were studied for the highway modelling problem. The DMRB model, which is a screening model was first applied at the M4 (Leixlip) study site and modelling analysis was carried out using a more up to date version of the DMRB model (version 1.02, 2003) and compared to those modelling results previously presented by Budd (2004). Two Gaussian based dispersion models CALINE4 and GFLSM model were also evaluated at this site, with an emphasis on temporal variation of concentrations over the 12 month study period. The pollutants studied were CO and NO_x. A constant background value was selected while modelling CO concentrations and it was observed that the performances of the GFLSM and CALINE4 models were very similar to each other and that the GFLSM model is a suitable alternative to the CALINE4. Analysis was carried out using both composite and hourly Emission factors, but there was no significant difference in either of the modelling results obtained. A detailed study of background concentration assumptions was carried out for NO_x, wherein the modelled NO_x concentrations obtained using GFLSM and CEF were combined with different background concentrations and compared with monitored data. A new method of classifying the background concentrations as per stability class and diurnal variation was proposed and validated at the end of the study.

The second study was carried out at the M50 motorway. The major objective of this study was to assess the ability of modelling to capture spatial variation in hydrocarbon concentrations at the study site. To this end, receptors were placed at either side of the road at 25m, 120m and 240m and 'background corrected' concentrations were recorded. The hydrocarbons were predicted using the GFLSM model and compared to those previously obtained with CALINE4 by O'Donoghue (2005). It was observed that the model performances decreased with receptor distance from the roadside, though the performances of both models at 240m were very similar. Both models effectively represented spatial variation observed in the monitored data. The third study on highway modelling assessment was carried out at Monasterevin town. The major aim of the study was to predict the change in air quality due to the opening of a new bypass. Monitored data (before and after) showed that a significant change in the air quality occurred due to the opening of the bypass. Modelled data obtained using the GFLSM model also showed the same trend, though the model evaluation parameters indicated poor model performance. The model performed best for the after case scenario.

Street canyon modelling techniques are very different from those used for highway modelling system as it involves a recirculation component that is missing in highway modelling systems. Special models are used for this case. In this study the STREET and OSPM models, both semi-empirical in nature were evaluated and validated at Pearse Street, Dublin for CO and NO_x. The detailed modelling study carried out showed that the OSPM was better at modelling the CO and NO_x concentrations than the STREET model, although the STREET model given its very basic nature was also reasonably accurate. Hourly background concentrations obtained from an urban background source were utilised in the study. A study on the background concentration assumptions for NO_x, similar to that mentioned earlier was followed and similar conclusions were drawn using both models. Model predictions were calculated using CEFs and HEFs and no significant changes in modelling results were observed.

One of the major reasons for monitoring or predicting NO_x concentrations in urban areas is to determine the ambient NO_2 concentrations for comparison with limit values. Standard methods like that of Stedman and Wilson and Laxen methods are readily available. The standard methods were modified as per local conditions and compared with the original methods. A new method i.e., the power method was proposed in this context, and improved model evaluation parameters achieved. Modelled NO_x concentrations obtained using STREET and OSPM with CEFs and HEFs were also assessed for calculating NO_2 concentrations. These modelled NO_2 concentrations were then compared against monitored data and it was observed that the power method offered the best representation of the conversion rate at the Pearse Street study site. This was also observed at the M4 highway study site. One of the significant drawbacks of Gaussian based highway models is their inability to predict concentrations under parallel wind conditions. A new model, viz, a hybrid model is proposed in this context. Two gaussian based models, the GFLSM and the IITLS models are combined together to give a better predicting capabilities under parallel wind conditions. It was observed that the hybrid model performed better than the GFLSM stand alone model for predicting concentrations under parallel wind conditions.

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This chapter sets the background in which this work is relevant (Section 1.1), outlines the objectives proposed (Section 1.2), the research methodology (Section 1.3) and the structure of the thesis.

1.1 Background

Air is one of the most essential components of life. It is humanly impossible to choose the air we breathe. Hence it is of utmost importance that the air we breathe is protected and maintained. The atmosphere of the world's cities has been affected by air pollution, thereby degrading air quality and this is one of the most pressing environmental concerns of our time. The concern of degrading air quality in cities is well documented; however changes have occurred regarding the type and nature of air pollution over the years.

In the past, the major sources of air pollution were from domestic and the industrial sources and the pollutants of concern were smoke, SO₂ and TSP. Over a number of years, legislation and control have led to a marked decrease in the air pollution impacts of industries in many developed countries. However, there has also been a substantial increase in urban air pollution from motor vehicles due to increased demand to meet transportation needs (Nagendra and Khare, 2002). The pollutants of major concern nowadays are NO₂, PM₁₀, PM_{2.5}, CO and VOC (WHO, 1992). Traffic also emits green house gases like CO₂ and CH₄. A report on Ireland's environment (EPA, 2000) mentioned that 'Road traffic has replaced stationery combustion sources as the greatest threat' to air quality in Ireland. The report also concluded that, 'it is clear from the limited monitoring for nitrogen dioxide and fine particulate matter that meeting future EU limits for these pollutants will present a difficult challenge'.

Pollutant emission has a varied effect on the environment including degradation of buildings and health effects. The final impact is also an amalgamation of the effects of several individual

Chapter 1

Introduction

pollutants. An air quality analysis can be carried out in two methods. The more detailed one would involve large scale monitoring approaches at varied sites and for long durations. One of the significant drawbacks of this approach is the cost involved, both initial and recurrent. Another drawback of this method is that it does not aid in future prediction and evaluate abatement strategies. The second option involves the development of an air quality model. Modelling of air quality can be used in tandem with monitoring for the estimation of air quality and can also be used for future forecasts and hence is generally employed for Environmental Impact Assessment (EIA) studies.

Air quality modelling for mobile sources is complex in nature and involves generally a combination of different types of models (FHA, 2000). In a broad sense three different types of model are required for performing a complete air quality analysis. The first involves estimation of traffic activity and fleet composition and is generally computed using a traffic model. Localised traffic monitoring data where the model is to be used is also applicable for this purpose. The second type of analysis involves the estimation of vehicular emission rates in grams per unit time or distance (or both) computed using an emission rate model. The combination of the first two model types leads to a spatial and temporal estimation of emissions leading to the development of an emission inventory. The last step involves the computation of ambient pollutant concentration using a pollutant dispersion model. These may incorporate deposition and photochemistry modules.

The estimation of emission factors is crucial as it links the traffic and pollutant dispersion components and errors involved can have heavy consequences for the final output of the air quality model. The majorities of the traffic models are well developed and can be easily evaluated as they output straightforward parameters like average speed, flow, queues, etc. On

the other hand, the validation of emission rates is expensive and hence a variety of methods have to be employed to validate emission rate models.

Further to the above, certain fundamental but pertinent questions arise regarding the estimation of pollutant concentrations in urban areas. For example, what degree of temporal and spatial accuracy is required? What are the important traffic parameters required? Also as there are many different types of traffic, emission rate and pollutant dispersions models – what type and complexity of model should be employed?

Ireson (1999) has mentioned that a lack of compatibility amongst the three classes of model poses another difficulty for current air quality analysis. The development of these three classes of models has evolved separately over time and output of one model may not be suitable as inputs for the next. Policy makers need a fully integrated system of models to be able to redress local urban air quality problems accurately and efficiently. Only when all three classes of model, i.e; traffic, emissions and dispersion components, are linked together with similar level of precision and accuracy, can successful strategies for abating urban air pollution can be formulated.

The roadway air pollution models generally used in Ireland, the DMRB and CALINE4, both developed outside the country, have already been evaluated for use in local conditions to a certain extent by Budd (2004). One of the important themes of this thesis involves the similar validation of alternative line source models like the General Finite Line Source Model, GFLSM (Luhar and Patil, 1989) and its modification for application in local conditions depending on site characteristics. The GFLSM model which is generally applicable for

highway sources, was investigated for predicting CO, NO_x and hydrocarbons at motorway locations. The GFLSM model predictions were compared with CALINE4 for CO, a suitable alternative for handling background concentrations based on stability class has been proposed, while the modelling of NO_x and the prediction of hydrocarbon concentrations has been carried out under 'background corrected' situations. The model has also been tested for predicting the change of air quality at Monasterevin town, before and after the opening of a bypass to divert regional traffic flow. Urban street canyon modelling was performed using the STREET and OSPM modelling techniques for CO and NO_x. Further to this, a NO₂ modelling approach has also been carried out, making relevant changes to the mathematical methods used for predicting NO₂ concentrations and a new method has been proposed. Finally, a hybrid model was developed for better prediction capabilities under parallel wind conditions.

1.2 Objective of Research

The broad objectives of the research described in this thesis are:

- Present an in-depth review of the current situation in air quality assessment for traffic sources.
- Determine appropriate models to predict dispersion of pollutants from vehicular exhausts giving due respect to the suitability of the model in its particular application.
- Assess the suitability of existing highway and urban street air quality models by performing statistical and graphical analysis of monitored and modelled data.
- Propose modeling techniques which are computationally efficient and analytically solvable as alternatives to cumbersome numerical models. These are to be applicable in urban air quality assessment, traffic management and in EIAs of new road schemes.
- Develop and evaluate improved modelling techniques and compare results with observed air quality.

1.3 Research Methodology.

The main tasks completed to meet these objectives are:

- Review of available models and their suitability for different air quality assessment requirements.
- Investigation of current modelling practice, particularly for urban air quality management and EIA of road schemes.
- Selection of two possible locations, a highway and an urban street canyon junction, for investigation of different dispersion models.
- Modelling of air quality at the M4 motorway using the GFLSM model and comparison of modelling results with monitored data using statistical and graphical analysis. This also included proposing a new method for incorporating emission factors and a novel way of treating background concentrations.
- Intercomparison of temporal variation in modelled data obtained using GFLSM and CALINE4.
- Assessment of the applicability of the GFLSM model at another highway site (M50 motorway) and comparison of the modelled spatial variation of concentrations with monitored data and modelled data using CALINE4.
- Application of the GFLSM to an actual air quality assessment and comparison of its outcome with monitored and CALINE4 modelled data.
- Application of the STREET and OSPM urban street canyon models to the urban street site.
- Comparison of street canyon model output with monitored data and intercomparison of the modelled datasets obtained using STREET and OSPM.
- Assessment of methods for NO₂ modelling at urban street canyon and highway locations, including a new method for determining NO₂ concentrations from NO_x concentrations.

- Development of a new hybrid model for improved prediction capability under parallel wind concentrations.

1.4 Novel aspects of PhD Research

The contributions of this research to the scientific field of air quality include the following:

1. An up-to-date research review on modelling the dispersion of traffic emissions has been completed.
2. In Ireland, generally, numerical models like CALINE4 are used irrespective of site considerations. New mathematical models that have not been previously used have now been evaluated for Irish road considerations with proper respect to site conditions.
3. Prior to this project, the GFLSM model, an analytical model whose formulation is based on similar technique as per CALINE4 (a complex numerical modelling application) had not been used in Ireland. The GFLSM model was applied at *highway locations* to study the accuracy of the modelled spatial and temporal variation of pollutant concentrations, and it was found to be more suitable than CALINE4 when modelling for *highway conditions*.
4. A new concept of using Hourly Emission factor (HEF) in place of the existing Composite Emission Factor (CEF) to increase model performance was investigated and proposed for further use. The concept was applied and investigated at both *highway* and the *urban street canyon* sites.
5. A new method of determining background concentrations based on stability class analysis (stable, unstable and neutral) was proposed and its performance in improving model predictions for ambient NO_x concentrations at both *highway* and *urban street canyon* sites was demonstrated.
6. Two typical street canyon models, STREET and OSPM were evaluated for urban street conditions in Dublin.

7. In an urban scenario, one of the pollutants of most importance is NO_2 and there exists no direct models for its prediction. The concentration of roadside NO_2 is computed from roadside NO_x data. The general expressions which are generally used for NO_2 determination were modified for local conditions and were compared with the original methods. Further to this, modelled NO_x concentrations were also used to determine the NO_2 concentrations and compared with monitored data to test its applicability. Generally, the roadside NO_2 follows a logarithmic pattern for determination from roadside NO_x ; however a new pattern, namely the power method was observed and reported in the thesis.
8. A hybrid model was proposed and tested with success. This included a modification to the GFLSM model by incorporating the parallel concentration term from the IITLSM model.
9. A major contribution is the identification of cases where computationally straightforward models based on analytical solutions can achieve similar accuracy to more complex numerical models. This will promote the development of integrated transport air quality modelling.

1.5 Layout of the thesis

The thesis is divided into eight chapters:

Chapter one introduces the problem considered and presents the objectives of the research. The research methodology carried out and the novel aspects of the research study are also mentioned.

Chapter two reviews the literature related to the various modeling techniques used for air quality assessment. Some pertinent background details on the pollutants modelled in this study are also given.

Chapter three outlines the first part of Highway Modeling study. A Step-by-step approach describing the requirements for modelling, modelling analysis, new proposals (emission factors) and modifications to data sets (background data) is followed and inferences drawn

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from the study are presented. In summary, a detailed temporal variation analysis of the pollutants (CO and NO_x) is highlighted in this chapter. The modeling applications were carried out using CALINE4 and GFLSM, the first of which was generally used for highway modeling and the second one finds its application first time for study in Ireland.

Chapter four deals with the second part of the Highway Modeling study. An interesting application of the above mentioned models was used to determine the spatial variation of VOC's, comprising seven individual hydrocarbons, in the vicinity of the roadway. Results of the application of the GFLSM model at a rural town to predict the change in air quality due to the construction of a new bypass is also presented in this chapter.

Chapter five presents the modeling results at an urban street canyon using STREET and OSPM for CO and NO_x. The new proposals regarding emission factors and modifications of background data proposed in the highway study in chapter three for NO_x are further investigated at the street canyon site.

Chapter six outlines the modeling of the NO₂ concentrations from NO_x concentrations using standard techniques. Modifications to the standard techniques are made which are more suitable for local conditions and a new method for determining NO₂ concentrations from NO_x concentrations as observed in the urban street canyon is proposed and evaluated.

Chapter seven describes the development and validation of a hybrid model based on the GFLSM model for better estimation in parallel wind concentrations.

Chapter eight summaries the work carried out during the course of this project and the main conclusions drawn from the research. The major contributions of this research to 'air quality modelling' are laid down. Furthermore, some recommendations for future work are proposed.

Chapter 2 Background and Literature Review

The increase of man's self sufficiency has led to an increase in his wants and desires. The personal motor vehicle has given the owners a personal mobility and freedom that would have been unheard of hundred years ago. Although a single car consumes little fuel and emits small amount of pollutants, the cumulative effect of all vehicles magnify any effects greatly. This chapter outlines an introduction to the transport sector as a source of air pollution, presents a discussion on selected traffic related air pollutants that are considered in later chapters in this thesis, including a review on their health effects, sources and fate in the atmosphere. This chapter also gives an in-depth review on the various dispersion models in usage, their suitability, drawbacks and a comprehensive statement of their applications. The chapter signs off by presenting a comprehensive report of air pollution study carried out in Ireland.

2.1 Transport sector as a source of air pollution.

2.1.1 Introduction

The transport sector emerged as a significant source of air pollution in urban areas after the solution to the problem of sooty smog generated from coal burning was obtained (Colvile et al, 2001). The transport sector has been primarily accused of being responsible for causing acid rain, ozone depletion and causing climatic changes to a certain extent (Colvile et al, 2001). Road traffic emissions are of much concern for their adverse effects on human health (Colvile et al, 2001). To a certain degree reality has set in amongst people and urban residents are now much more aware of air pollution and its consequences, leading to legislation governing abatement methods like installation of catalytic converters. This step has been probably the best and biggest exercise carried out for abatement of air pollution emissions from tail pipe sources (Colvile et al, 2001). It has been reported that fixing of catalytic converters leads to an increased NO₂ emissions. On a broader scale, urban air quality and global climate change are identified as major issues but regional air quality and acidification are also considered.

Chapter 2 Background and Literature Review

2.1.2 Contribution of transport sector to emission.

On an overall basis, all modes of transport cause air pollution due to the combustion of liquid fossil fuel. Major significant pollutants emitted by transport sector are CO₂, water vapor and hydrocarbons from incomplete combustion of fuel. Incomplete combustion leads to emission of carbon monoxide. An impurity like sulphur gets oxidized to sulphur dioxide and sulphate which assists nucleation of particles in exhaust. Vanadium also contributes further to particulate formation. Organic lead in High Octane Petrol also forms particles in exhaust and at high combustion temperatures atmospheric nitrogen gets oxidized to NO and NO₂ (Colvile et al, 2001).

Air pollution emissions generated during the use of any form of transport are only a part of the total amount of air pollution generated by transport related activities. Life Cycle Assessment (LCA) techniques can be used to determine which state of production, use and disposal of a given transport technology is responsible for the most significant atmospheric emissions. For example, 60-65% of lifecycle greenhouse gases from a petrol engined car are CO₂ exhaust emissions during use with a further 10% being non-CO₂ exhaust emissions during use of the remainder, 10% is associated with the car's manufacture, and a further 10-20% is emitted during extraction, refinery and transport of its fuel (Colvile et al, 2001)

The quantification of emissions from transport can be performed using two types of techniques, namely top down and bottom up approaches (Colvile et al, 2001).

The 'top down approach' involves data that describes total polluting activities throughout the whole geographical area of interest. These are related to the magnitude of the associated air pollution source by means of an emission factor which is obtained in laboratory measurements of representative samples of engines or vehicles which are simulated to emulate real conditions.

Chapter 2 Background and Literature Review

The ‘bottom down approach’ starts with geographically resolved data. For large stationary sources, emission data are determined by measurement of each individual source. The total emission is determined by summation of the individual contributions. Its drawback lies in the fact that it requires large amount of data and involves lots of assumptions and approximations. Colville (2001) summarised the factors that need to be considered when quantifying a given impact of transport emissions. They are as follows:

- emissions during the complete life cycle of vehicle, fuel and associated infrastructure;
- significance of transport emissions compared with other sources of the same pollutants within a given geographical region, as shown by emissions inventory data;
- contribution of sources outside the geographical area covered by the emission inventory;
- source – receptor relationships;
- other pollutants contributing to or exacerbating the impact of interest;
- other impacts of the pollutants of interest.

Vehicular exhaust emissions emit a variety of pollutants. A detailed review of the pollutants modelled in this study along with their health impacts are presented below.

2.2 Description of pollutants and their effects.

2.2.1 Carbon Monoxide

2.2.1.1 Introduction

Carbon monoxide (CO) is a colourless odourless and tasteless gas discovered by Joseph Priestly in 18th century (Brimblecombe, 1986). It is a diatomic molecule having a molecular weight of 28g/mole. It is known that at low ambient levels, CO has no definite impact on property, vegetation and materials (Peavy, 1985). However at higher levels CO can have adverse health effects. The primary health effect on humans is a condition termed as ‘CO poisoning’ and over exposure can cause death by hypoxia. The mechanism involves formation

Chapter 2

Background and Literature Review

of carboxyhemoglobin (COHb) complex in blood, which lowers the ability and alertness to work at concentrations exceeding 5% (Brimblecombe, 1986). The maximum risk involves smokers. An Irish EPA report (2004) mentions that exposure to high doses of CO can lead to blindness, decreased learning ability and difficulty performing complex tasks.

2.2.1.2 Sources of CO

There are a variety of sources that lead to the generation of CO. The major sources can be identified as (a) anthropogenic sources (b) emission from seas and oceans (c) burning of biomass (d) oxidation of non-methane hydrocarbons (e) production by vegetation and (f) oxidation of methane (Meszaros, 1981). Table 2.1 presents a range of estimated emission rates as reported by Jacob (1999).

Sources	Range of estimates (Tg CO/year)
Fossil Fuel combustion/industry	1800-2700
Biomass Burning	300-550
Vegetation	60-160
Oceans	20-200
Oxidation of methane	400-1000
Oxidation of other hydrocarbons	200-600

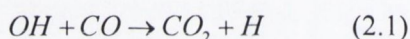
Table 2.1 Sources of CO

The major anthropogenic source of CO nowadays is transport related emissions. Incomplete combustion of fuels in vehicle engines leads to the formation of CO. High levels of CO are generally observed at places of high traffic intensity and congestion (Han, 2005) when vehicle engines operate at lower efficiency. Other sources include domestic heating and industrial non transportable fuel combustion.

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2.2.1.3 Atmospheric chemistry of CO

The removal of CO generally takes place in three major mechanisms, soil uptake which accounts for 250-640 Tg /yr, stratospheric reactions accounting for 100 Tg/year and the hydroxyl radical (OH) which accounts for 1400-2600 Tg/yr (Jacob, 1999). Hence it is quite obvious that the major removal involves tropospheric oxidation by OH. The reactions involved are shown in Equation 2.1 and 2.2. Oxidation causes the formation of carbon dioxide and a free hydrogen atom. The hydrogen atom reacts with oxygen forming an HO₂ radical, which then self reacts to form hydrogen peroxide (H₂O₂), which is highly soluble in water and is removed from the atmosphere by wet deposition (Jacob, 1999). The presence of CO aids in formation of CO₂, a greenhouse gas.



The major factor involved in the process is the availability of the hydroxyl ions to react with CO. The presence of hydroxyl radicals provide the main driving force behind tropospheric chemistry and play a crucial role in the formation of VOC's (Jacob, 1999).

2.2.2 Oxides of Nitrogen

2.2.2.1 Introduction

Traffic generated nitrogen oxides exist mainly in form of nitric oxide (NO) and nitrogen dioxide (NO₂) in the atmosphere. Trace quantities of nitrogen trioxide, nitrous oxide and nitrogen pentoxide also exists depending upon the oxidation state. Together they are classified as nitrogen oxides (NO_x), however in the remainder of this thesis the term NO_x shall indicate NO and NO₂. Nitrogen dioxide is formed in the environment from primary emissions of oxides of nitrogen. Although there are natural sources of NO_x (e.g., forest fires), the

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combustion of (fossil) fuels has been, and remains, the major contributor in European urban areas. Over the past 50 years vehicular traffic has substantially replaced other sources (e.g., domestic heating, local industry) as the major outdoor source of NO_x from fossil fuel combustion, and hence NO_2 . Other, stationary, sources (e.g., power plants or domestic) also contribute to NO_x emissions, and, therefore to outdoor concentrations of NO_2 in certain areas. Traffic related sources emanate from direct exhaust emissions of NO , which then gets converted to NO_2 by a series of chemical and photochemical reactions, as described in the following section. NO_2 is a reddish brown gas and is highly reactive in nature. Of primary importance is its role in photochemical smog formation. Adverse health effects have been documented after short-term exposure to elevated concentrations, as well as long-term exposure to relatively low concentrations of NO_2 . Short term exposure may cause lung function injury, whereas at higher doses it may reduce immunity and cause respiratory infections (Han, 2005). Some studies have documented that subjects living close to busy roads experience more adverse short- term and long-term effects from air pollution than subjects living further away (WHO, 1995). In urban areas, up to 10% of the population may be living at such “hot spots” and the public health burden of such exposures is therefore significant.

In the European Union, vehicular traffic contributes more than half of the emissions of NO_x . This is more than in the United States of America, and the contribution to total NO_x emissions is even higher in some European cities, based on data from the 1990s. In London, for example, road transport contributes 75% of NO_x emissions (WHO 2003, 2004). Due to their characteristics (low emission heights; high emission densities in urbanised areas), traffic emissions are often the dominating source of urban outdoor NO_2 exposure. The EU air quality directive pertaining to NO_2 levels in ambient (CEC, 1999) sets limit values for hourly and

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mean levels to be achieved by 2010. This limit value is considered to be the most difficult limit to meet in urban areas in Ireland and the UK (EPA, 2004; Carslaw, 2006). An annual mean concentration of $40\mu\text{g}/\text{m}^3$ has been proposed as a limit value within the European Union Air Quality Directives for 2010. A short term 99.8 percentile limit value has also been set at $200\mu\text{g}/\text{m}^3$.

While current international policies will greatly reduce emissions of oxides of nitrogen in near future, maps of estimated annual mean NO_2 concentrations at both background and roadside locations will remain a valuable resource for the development of air quality policy and the identification of locations at which local air quality management measures are required.

An individual's exposure to NO_2 from outdoor sources will depend largely on their proximity to vehicular traffic in space and time; given that mobile sources are the chief contributors to ambient NO_2 in contemporary European cities. Ambient NO_2 concentrations measured at fixed urban sites may not accurately reflect personal exposure to NO_2 from outdoor sources, because ambient NO_2 concentrations vary widely in most locales due to traffic patterns, the characteristics of the built environment, and meteorological conditions (WHO, 2003). Fixed monitors are not necessarily sited with the intent of reflecting the population average exposure, and therefore, the accuracy with which their measurements reflect population exposures may vary. This may be particularly pronounced with regard to short-term exposure in the order of days (WHO, 2003).

NO_2 measurements from fixed-site monitors may provide better indices of exposure over longer time periods depending on where the monitors are located. For example, good relationships between personal and ambient NO_2 concentrations have been observed in areas

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with high traffic densities as reported by WHO (WHO, 2003). Such measurements, including concentrations measured at fixed residential locations (“front door” concentrations) may be particularly useful indicators of exposure to traffic-related pollution, especially when combined with data on individual time-activity patterns, traffic patterns, and other geographical information. The cost of continuous monitoring particularly in large, heavily industrialised and trafficked cities is enormous. However, Models are a cheap relatively suitable alternative recognised by regulatory bodies (European Commission, 1998). They can be suitably evaluated with monitored data (short or long term) to prove the models ability.

For any assessment of air quality impacts of road traffic much emphasis is placed on the application of appropriate air quality models. These models predict the dispersion and dilution of primary pollutants using data on emissions and appropriate meteorological conditions to determine road traffic concentrations. These road traffic concentrations are added to the local background concentrations to give the total concentrations, which decline as a function of the distance of the road. However, certain pollutants like NO_x pose a problem, as they undergo chemical transformations in atmosphere. For NO_x , the emission occurs primarily as NO but this is transformed in the atmosphere to NO_2 due to reaction with ozone. It is further compounded due to the free mixing of background NO and NO_2 with freshly emitted NO and NO_2 .

When NO_x concentrations are assessed from road traffic the primary interest lies in determining the effect of NO_2 concentrations as because they are mainly related to health problems rather than NO_x itself, hence the importance in determining the transformation of NO to NO_2 .

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2.2.2.2 Sources of oxides of nitrogen

Jacob (1999) outlined the major sources of NO_x emissions. They are (a) fossil fuel combustion (b) biomass burning (c) soils (d) lightning (e) NH₃ oxidation (f) aircraft emissions and (g) transport from the stratosphere. Table 2.2 presents estimated amounts from each source expressed as nitrogen (N) per year, (Jacob, 1999).

The table shows that the strongest source is fossil fuel combustion. The production of NO_x via fossil fuel combustion generally occurs through two processes, namely fuel NO_x which results from oxidation of nitrogen containing compounds in the fuel and thermal NO_x which results from the oxidation of the atmospheric nitrogen at high temperatures in presence of oxygen (Kiely, 1997). Vehicular exhaust generally emits NO, with a smaller non-negligible portion in the form of NO₂. Studies have shown that diesel engine vehicles emit higher concentrations of NO₂ than petrol engine vehicles, and emission rates vary with vehicle speeds (Alloway, 1997).

Sources	Range of estimates (Tg N/year)
Fossil Fuel combustion	21
Biomass Burning	12
Soils	6
Lightning	3
NH ₃ oxidation	3
Aircraft emissions	0.5
Transport from the stratosphere	0.1

Table 2.2 NO_x emission estimates.

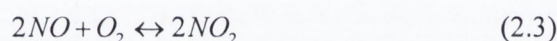
Intensive research activities have been carried out on the control and abatement of NO_x emissions from vehicles. Some of the suggested methods include lowering the combustion

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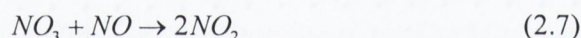
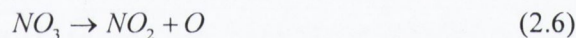
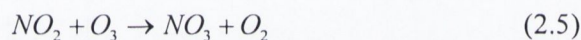
temperature, enhancing the fuel mixture to make the post combustion levels low and use of catalytic converters (Alloway, 1997).

2.2.2.3 Atmospheric chemistry of oxides of nitrogen

Kiely (1997) showed the mechanisms by which oxidation of NO to NO₂ occurs. They are highlighted by equations 2.3 and 2.4 as shown below:



The oxidized nitrogen dioxide takes part in a series of photochemical reactions including ozone. The series of reactions that occur can be summarised by the following sequences:



Reaction (2.5) plays a dominant role during the evening and night times. This is because the hydroxyl ion concentration that plays a dominating role during the daytime becomes almost inactive at night. Reaction (2.6) highlights the daytime chemistry with photolysis reactions occurring at wavelengths (λ) less than 630nm. Reaction (2.7) displays the reduction of NO₃ formed in reaction (2.5) by reacting with NO to form NO₂. During night time, nitrate can reduce methane as shown in reaction (2.8) in similar fashion to daytime hydroxyl reduction but at a much slower rate (Brimblecombe, 1986).

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2.2.3 Hydrocarbons

2.2.3.1 Introduction

Recent advances in technology have enhanced our ability to study the composition of trace substances in atmosphere. The most studied compounds of this kind are the volatile organic compounds (VOCs). A major area of study is in the field of environmental chemistry, particularly effects on stratospheric ozone depletion, tropospheric ozone formation, toxic and carcinogenic human health effects and their potential to act as greenhouse gases (Dewulf et al., 2002). The European Union defines VOCs as organic compounds with vapour pressure greater than 10Pa at 20 °C (CEC, 1999a). HCs represent about 50% of all VOCs, and are composed of solely carbon and hydrogen. Methane is one of the most abundant of hydrocarbons found in the atmosphere and is derived from decaying vegetation and livestock (Peavy, 1985). The background concentration of methane in atmosphere ranges from 1-7 ppm (Peavy, 1985). The vast majority of the HC's are sourced from anthropogenic activities, particularly as by-products of the petroleum industry, (Kiely, 1997) and are generally referred to as non-methane hydrocarbons (NMCH's). HC's are highly reactive and as such take part in numerous photochemical reactions in the atmosphere.

If a HC is constituted with a single bond it is called a saturated hydrocarbon, prime examples being alkanes and cyclo-alkanes. Unsaturated hydrocarbons consist of double or triple bonds and are such classified in three categories: alkenes, alkynes and aromatic hydrocarbons.

An important example of the air quality impacts of transport related emission is photochemical smog. This type of pollution event is associated with the secondary pollution formation of nitrous oxides and VOC's, generally emitted from vehicles. HCs have profound health effects on humans depending upon the type of pollutant, the magnitude, duration and frequency of exposure and the relevant toxicity of the pollutant (WHO, 1995). From a human health

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perspective, the HC's of major concern are benzene, toluene, ethyl benzene, and ortho/para/meta xylene which are collectively called (BTEX's) and 1, 3-butadiene. Amongst the BTEX group it is widely known that benzene is a human carcinogen, (Bond et al, 1986). Short term exposure may cause drowsiness, headache, and irritation to skin, eyes and respiratory tracts while long term exposure can decrease the amount of red blood cells (EPA, 2004). The other compounds in the BTEX group have a pronounced effect on central nervous system. The limit value regarding benzene as laid down by the CEC directive (CEC, 2000) is an annual mean of $5\mu\text{g}/\text{m}^3$.

WHO classifies 1, 3-butadiene as a suspected carcinogen and it is known to have adverse health effects on humans. Acute exposure to 1, 3-butadiene to humans may result in irritation of the eyes, nasal passages, throat and lungs. The EU annual average limit value for benzene is $5\mu\text{g}/\text{m}^3$ and the UK limit value for 1, 3 butadiene is $2.25\mu\text{g}/\text{m}^3$. The limit values for other HC's with the exception of benzene has not yet been set throughout EU.

2.2.3.2 Sources of hydrocarbons

The major sources for HC are anthropogenic and biogenic sources. Anthropogenic sources are further categorized in two parts: mobile and stationary sources. An in depth analysis of the sources of HCs has been described by O'Donoghue, (2004). Some of these include, domestic/industrial fossil fuel combustion, fuel evaporation, solvent use and chemical manufacturing, mobile source HC's emissions from transport and area source emissions from terrestrial vegetation (Clarke, 1996; Jacob, 1999; Barletta, 2002).

2.2.3.3 Atmospheric chemistry of hydrocarbons

The atmospheric chemistry of hydrocarbons is primarily dependant on the molecular chemistry of the associated subgroups. Hydrocarbons are generally sub-divided into four

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subgroups depending upon the bonding arrangement that exists between carbon atoms. They can be classified as: alkanes, alkenes, alkynes and aromatic hydrocarbons.

2.3 Modelling traffic impacts on air quality

This section describes the impact that certain meteorological and topographical conditions have on air pollutant concentrations. The temporal and spatial variation of pollutants is also discussed.

2.3.1 Meteorological Impacts on air pollution.

2.3.1.1 Wind

The predominant driving force behind atmospheric dispersion is the wind. Mass movements of air according to the geographic range of influence may be designated as macroscale (global), mesoscale (regional), or microscale (local). Air movements on the mesoscale and micro scale have the greatest impacts on locally observed air quality, (Peavy, 1985). Mesoscale wind flow is affected predominantly by regional topography, e.g. location of mountains, oceanic bodies, forestation and urban developments. Examples of well known wind effects on a mesoscale include sea breezes, mountain and valley winds and urban heat islands. Microscale wind flow occurs over areas of less than 10 kms, and is mainly affected by what is known as the friction layer. The friction layer is the turbulent zone that exists when wind flow is altered from its usual pattern by obstacles such as buildings on the Earth's surface. Also thermal effects due to localised heating of tarmac and concrete causes thermal turbulence that affects air flow.

2.3.1.2 Heat

Heat is a critical atmospheric variable determining climatic conditions. Within the troposphere, four heating processes exist:

(1) Greenhouse effect: In this case, direct radiation from the sun travels unabated to the Earth's surface. The rays are then reradiated back into the atmosphere. The wavelength of the

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reradiated solar energy however is longer, and is subsequently absorbed by CO₂ and water vapour in the atmosphere, leading to an increase in temperature.

(2) Evaporation- Condensation Cycle: Evaporation of water takes place at the earth's surface. This process requires energy input as the vaporised water rises into the troposphere, it condenses, releasing the stored energy. This process is concerned with moving heat from lower regions to higher regions.

(3) Conduction: Conduction is the process that results from physical contact" between air and the Earth's surface. Parcels of buoyant air move downwards and take heat from the earth into the atmosphere.

(4) Convection: Convection is the natural process initiated by the rising of warm air and the sinking of cold air. It is the major process in transferring heat from the earth to the troposphere, (Peavy, 1985).

2.3.1.3 Ambient and Adiabatic Lapse Rates

The temperature of ambient air usually decreases with respect to increasing altitude. This temperature gradient is known as the ambient lapse rate. The ambient lapse rate in the atmosphere can be recorded with a balloon that is equipped with a thermometer. When the balloon is released, it will move upwards through the atmosphere and record a temperature profile with respect to altitude. The profile of the ambient lapse rate will vary from day to day, day to night and season to season, (Kiely, 1997). Usually the lapse rate decreases with altitude, but given certain meteorological conditions, the opposite can occur. The ambient lapse rate can be compared to the dry adiabatic lapse rate. Under dry adiabatic conditions, a parcel of air will behave like a balloon, rising until it assumes the density of the air surrounding it. For a dry adiabatic parcel of air, the decrease in temperature with respect to altitude is 9.80 C/km or -1°C/100m. A variety of ambient lapse rates are compared to the adiabatic lapse rate. Figure

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2.1 presents a representative diagram about lapse rates.

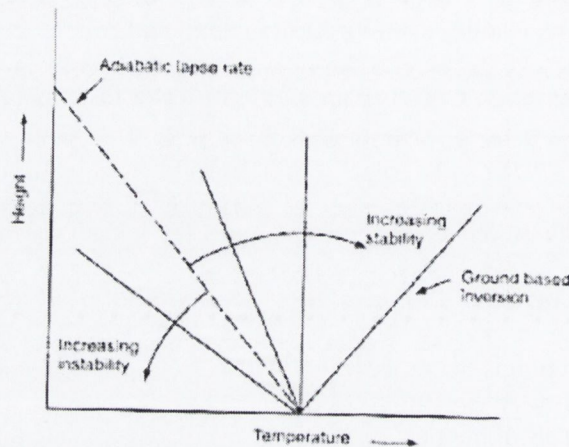


Figure 2.1 Lapse Rates

2.3.1.4 Atmospheric Stability

Ambient and adiabatic lapse- rates are a reflection of atmospheric stability and are concerned with the amount of vertical motion within the atmosphere. The atmosphere is said to be unstable so long as a parcel of air remains warmer (or descending parcel of air remains cooler) than the surrounding air and will continue to accelerate in the direction of displacement (Peavey, 1985). The lapse rate in this case is superadiabatic and the associated Pasquill stability classes is either A, B, or C. An unstable atmosphere is conducive to good vertical dispersion of pollutants. In a stable atmosphere (Pasquill stability class E, F or G), the parcel of air is cooler than its surroundings, and is pushed towards the Earth's surface. Poor vertical pollutant dispersion is a feature of a stable atmosphere. The associated lapse rate is sub adiabatic.

A condition known as a temperature (thermal) inversion can also occur during stable conditions. Here the lapse rate profile is of increasing temperature with increasing altitude. A warm parcel of air will cool rapidly in this environment and be forced downward. From the

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standpoint of air pollution, both stable conditions and thermal inversions are undesirable because they minimize the rate of dilution of pollutants in atmosphere. Thermal inversions in this case act as a barrier to vertical mixing and contaminants will accumulate in the surface layer below inversion.

2.3.2 Temporal and spatial variation of pollutants.

Spatial factors usually reflect the background characteristics, while temporal variation represents the influence of meteorological conditions. Since the ambient monitoring data are usually based on daily measurements, the temporal variation is often represented by day-to-day concentration changes (Wight, 2000; Watson and Chow, 2001). Spatial factors, such as distance from a highway, topography, land surface roughness, and the presence of other pollution sources affect the pollutant concentration and composition (Martuzevicius et al, 2004). Time-related factors, such as local meteorology (wind speed and direction, stability of the atmosphere boundary layer, precipitation, etc.), as well as traffic intensity are known to essentially affect the pollutant dispersion and consequently human exposure (Martuzevicius et al, 2004). In general, low spatial variation is generally associated with high temporal variation.

2.4 Street Canyon theory

A street canyon is a relatively narrow street between buildings that line up continuously along both sides. The combination of vehicle emissions and reduced dispersion in these circumstances can lead to high levels of pollution (Buckland and Middleton, 1999) which in turn pose a substantial health risk to pedestrians and others. When the wind blows across a street canyon, a vortex is typically generated, with the wind flow at street level in the opposite direction to that at roof level (Figure 2.2), resulting in higher concentrations of pollutants on the leeward side of the street compared with the windward side (Manning *et al.*, 2000). The windward side is here defined as the side of the street to which the wind blows whilst the

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leeward side is the side from which the wind blows (Figure 2.2). The formation of a stable vortex is much less likely at lower wind speeds, i.e. winds speed below 2 m/s (Kukkonen *et al.*, 2003).

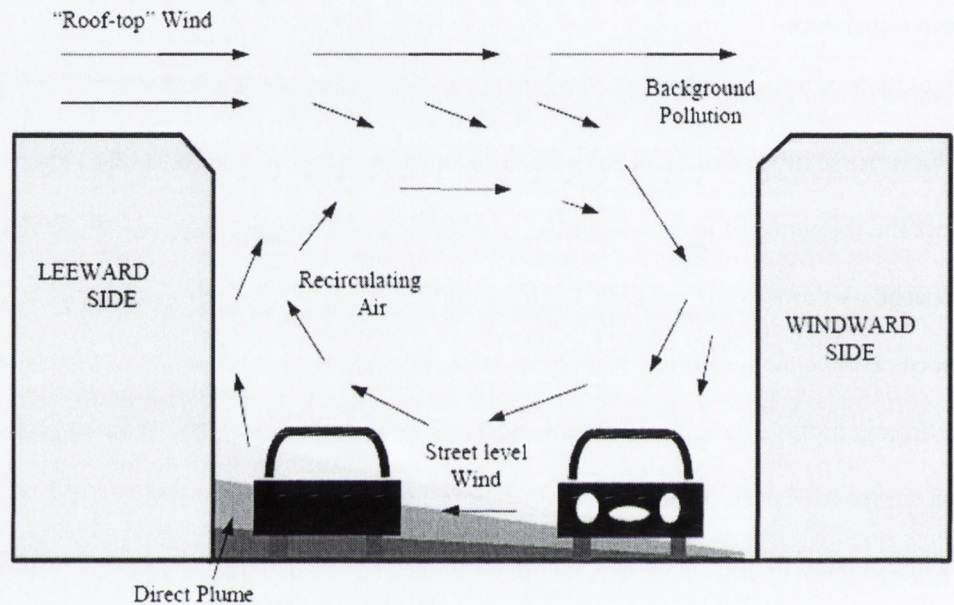


Figure 2.2: Schematic diagram of flow and dispersion of pollutants in a street canyon showing the formation of a vortex (Manning *et al.*, 2000)

Testing the formation of a street canyon vortex is difficult as field monitoring of wind flows is normally only carried out at a few discrete points within a street canyon, and measurements can be influenced by local structures (Berkowicz *et al.*, 1997). DePaul and Sheih (1986) used tracer balloons to produce a three dimensional flow visualisation within the street canyon. Mean wind velocities within a street canyon were determined by analysis of trajectories of the tracer balloons that were photographed in rapid sequence once released in the canyon. Formation of a vortex within the canyon occurred at an ambient wind velocity above 1.5-2.0 m/s (DePaul and Sheih, 1986). One important conclusion from their work is the vertical extent of the vortex cell did not seem to extend beyond roof level.

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Wind measurements in an urban canyon were carried out by Nakamura and Oke (1989) who measured horizontal wind speed and direction above and within the canyon using instruments placed 3.6m above roof level and another located 1m above street level at mid-width inside the canyon (Nakamura and Oke, 1989). They concluded that a street canyon vortex formed for wind flows perpendicular to the street axis and the wind direction at street level was approximately "a mirror reflection" of the roof level wind direction. Nakamura and Oke (1989) also examined the relationship between the street level and roof level wind speeds and found that for roof level wind speeds above 2m/s, the street level wind speed was approximately two - thirds of the wind speed at roof level. This is in broad agreement with the observations of DePaul and Sheih (1986).

Research using wind tunnels has provided much of the current data on flow and dispersion characteristics in street canyons (Berkowicz *et al.*, 1997). Hussain and Lee (1980), Hosker (1985), and Oke (1988) analysed wind tunnel data to provide systematic classification of flow regimes in street canyons. Flow regimes in urban street canyons can be classified under three headings depending on the canyon geometry: isolated roughness flow, wake interference flow, and skimming flow (Figure 2.3). The geometry of street canyons is defined by the aspect ratio (H/W) defined as the ratio of the building height (H) to the width of the canyon (W). Isolated roughness flow (Figure 2.3 (a)) occurs in street canyons where the buildings are widely spaced ($H/W < 0.3$). Canyons where buildings are spaced closer together ($0.3 < H/W < 0.7$) result in wake interference flow (Figure 2.3 (b)) where the wake created by the upwind building is disturbed by the downwind building creating a downward flow along the windward building façade (Berkowicz *et al.*, 1997). Closer spacing between buildings ($H/W \geq 0.7$) results in a skimming flow regime (Figure 2.3 (c)) where a stable circulatory vortex is established in the

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canyon and the ambient flow is decoupled from the street flow (Oke, 1988). Despite these scenarios, Berkowicz *et al* (1997) have cautioned against extrapolating wind tunnel results to real atmospheric conditions.

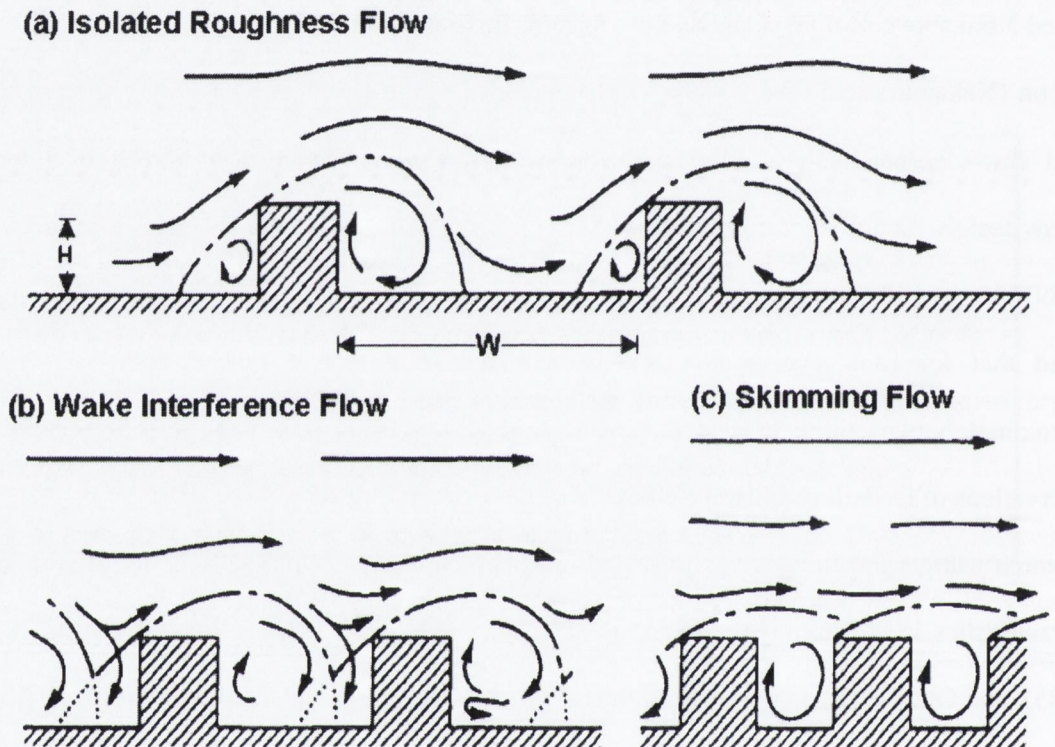


Figure 2.3: Flow regimes associated with street canyons of different aspect (H/W) ratios (Nakamura and Oke, 1989).

Wind speed and direction are the two major driving factors behind dispersion of pollutants within a street canyon and it is generally accepted that a street canyon vortex will not occur at low wind speeds. Vardoulakis *et al*, (2005) found evidence for vortex formation within a street canyon at synoptic winds above 2m/s and also found that modelled concentrations of CO and NO_x demonstrated a clear dependence on wind direction (Vardoulakis *et al.*, 2005). Winds parallel, or near parallel to the street axis, favoured pollution build-up along the footpaths, while winds

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perpendicular to the street axis provided better dispersion conditions. These findings support the idea that in relatively long street canyons without major intersecting streets, accumulation of emissions outweighs the ventilation induced by parallel winds. A street canyon vortex is formed with wind directions perpendicular to the street canyon (within $\pm 30^\circ$) and as the angle of the wind approaches that of the street axis, the vortex disappears (Kukkonen *et al.*, 2001). Therefore, a street vortex will only form when there is significant wind speed and the wind direction is near perpendicular to the street axis. Low wind speed and winds parallel to the street axis result in the worst dispersion conditions (Vardoulakis *et al.*, 2002a).

2.5 Statistical Parameters.

For the purpose of comparing monitored and predicted data, the statistical parameters used are the mean, the standard deviation, the index of agreement (IA) (Wilmott, 1981), the normalised mean square error (NMSE), Pearson's correlation coefficient (R), the fractional bias (FB) and the factor of two (F_2), which are defined as follows :

$$IA = 1 - \frac{\overline{(c_{pred} - c_{obs})^2}}{\left(\left| \overline{c_{pred}} - \overline{c_{obs}} \right| + \left| \overline{c_{obs}} - \overline{c_{obs}} \right| \right)^2}, \quad (2.9)$$

$$NMSE = \frac{\overline{(c_{obs} - c_{pred})^2}}{\overline{c_{obs}} \overline{c_{pred}}}, \quad (2.10)$$

$$R = \frac{\overline{(c_{obs} - \overline{c_{obs}})} \overline{(c_{pred} - \overline{c_{pred}})}}{\sigma_{obs} \sigma_{pred}}, \quad (2.11)$$

$$FB = \frac{2(\overline{c_{pred}} - \overline{c_{obs}})}{\overline{c_{pred}} + \overline{c_{obs}}} \quad (2.12)$$

and

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$$F_2 \text{ is the fraction of data for which } 0.5 < \frac{c_{pred}}{c_{obs}} < 2 \quad (2.13)$$

Where c_{pred} and c_{obs} are the predicted and observed concentrations respectively, $\bar{c}$ is the mean of all hourly concentration values, and σ_{pred} and σ_{obs} are the standard deviations of the predicted and measured data, respectively. The index of agreement determines the level to which the model predictions agree with measured concentrations, with an IA value of 1 implying that the monitored and predicted data are in complete agreement. The NMSE is a fundamental statistical performance parameter, as it gives actual information on the error produced by the model. The normalisation assures that in most applications the NMSE does not bias towards models that overpredict or underpredict. An NMSE value of 0.5 on average implies a factor of two between predicted and monitored values. The Pearson's correlation coefficient describes the proportional change with respect to the means of two quantities in question, but it cannot distinguish the type or magnitude of possible covariance. The above three parameters described are measures of the agreement between the predicted and monitored time series of concentrations. The fractional bias is a measure of the agreement between the mean concentrations and its values range between +2 and -2, where a value of +2 indicates an extreme underprediction, and a value of -2 is an extreme overprediction. The factor of two statistically is a coarse but easily understood measure of the likelihood that an individual model result will agree reasonably well with its equivalent measured value.

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2.6 Statistical distribution model.

For urban environments, air pollution ‘episodes’ are caused due to extreme pollutant concentrations, which are governed by meteorological fluctuations and changes in emission characteristics which result in ‘stochastic variability’ (Gokhale and Khare, 2006). Air pollutant concentration can therefore be treated as a random variable. As per Jakeman et al, (1988) the particular type of fitting distribution and the values of the associated parameters are influenced by a number of factors including pollutant and source types, averaging times, emission characteristics, meteorology and topography. Several statistical distribution models have proven to be useful tools for representing air pollutant concentration data (Jakeman and Taylor, 1989), with previous studies showing that most atmospheric dispersion data are lognormally distributed (Gokhale and Patil, 2003; Ott, 1995; Surman et al, 1982) irrespective of the source. However, other forms of probability distribution fits have also been reported by Maffei (1998) and Genikhovich et al. (2005). In this regard, Maffei (1998) used the Weibull distribution to predict the exceedance probability of a fixed threshold of CO concentration in the Lombardy region. Genikhovich et al. (2005) applied different statistical techniques to the annual mean concentrations of NO₂, NO_x, benzene and ozone and found that Weibull distribution fits were more appropriate than lognormal fits for the datasets.

To identify the best distribution form, graphical and analytical tests on the atmospheric data sets were performed. For small sample sizes, graphical analysis techniques have been used (Gokhale and Khare, 2006). In contrast, quantitative techniques such as goodness of fit tests including the Kolmogorov-Smirnov (KS) test, the chi-square test and the Anderson Darling (AD) test were preferred (Gokhale and Khare, 2006) and are usually the first step in identifying the statistical distribution model. The KS and AD statistics identify the appropriate

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model corresponding to the minimum values (Gokhale and Khare, 2006). The KS test compares the observed cumulative distribution function (CDF) for a variable with a specified theoretical distribution, which may be normal, lognormal, gamma, exponential, Weibull, etc. The KS statistic is computed from the largest absolute difference between the observed and theoretical cumulative distribution functions (Gokhale and Khare, 2006). The Anderson-Darling procedure is a general test to compare the observed fit of a cumulative distribution function to an expected cumulative distribution function. This test gives more weight to the tails than the KS test.

In this thesis, Kolmogorov-Smirnov and Anderson Darling tests were performed to identify the distributions of the monitored and modelled CO data at M4 to determine how well the range of concentrations calculated with the GFLSM model and CALINE4 models agreed with that of measured data.

Three types of probability distribution were considered, namely the lognormal, Weibull and gamma distributions.

Lognormal distribution

The probability density function (PDF) of the lognormal distribution, $p_l(x_i)$, as given by Lu (2002), is:

$$p_l(x_i) = \frac{1}{\sqrt{2\pi x_i \ln(\sigma_g)}} \exp\left[-(\ln x_i - \ln \mu_g)^2 / 2(\ln \sigma_g)^2\right], \quad (2.14)$$

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Where x_i is the pollutant concentration of species i and μ_g and σ_g are the parameters of the distribution representing the geometric mean and the standard geometric deviation respectively. The cumulative distribution function (CDF) is given by the following equation:

$$F_1(x) = \Pr(x_i < x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\eta} e^{-t^2/2} dt, \quad \eta = \frac{\ln x - \ln \mu_g}{\ln \mu_g} \quad (2.15)$$

The probability of variable x_i exceeding the value of x is given by the complementary distribution function:

$$\overline{F}_1 = \Pr(x_i > x) = 1 - F_1 \quad (2.16)$$

Weibull distribution.

The PDF of the Weibull distribution, $p_w(x_i)$, as given by Lu (2002), is:

$$p_w(x_i) = \frac{\lambda}{\sigma} (x_i / \sigma)^{\lambda-1} \exp\left[-(x_i / \sigma)^\lambda\right], \quad x_i \geq 0, \sigma, \lambda > 0 \quad (2.17)$$

Where λ and σ are parameters of the Weibull distribution. The probability of the variable x_i exceeding the value of x is given by the complementary distribution function:

$$\overline{F}_w(x) = \Pr(x_i \geq x) = \exp\left[-(x / \sigma)^\lambda\right] \quad (2.18)$$

Gamma distribution.

The PDF of a gamma distribution with shape parameter α and scale parameter β is given by (Jakeman et al, 1986; Nadarajah and Gupta, 2006):

$$p_g(x_i) = \frac{\beta^\alpha x_i^{\alpha-1}}{\Gamma(\alpha)} \exp(-\beta x_i), \quad (2.19)$$

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The probability of variable x_i exceeding the value of x is given by the complementary distribution function:

$$P(X \leq x) = F(x; \alpha, \beta) = F\left(\frac{x}{\beta}, \alpha\right) \text{ where } F(x; \alpha) = \int_0^x \frac{y^{\alpha-1} e^{-y}}{\Gamma(\alpha)} dy \quad (2.20)$$

The probability distribution curves were examined using for the pollutant CO.

2.7 Atmospheric Dispersion Modelling.

2.7.1 Introduction:

A model is basically a scaled down version of reality. It can never fully depict real life situations but it may contain certain features of interest for management issues or of a scientific problem. The uses of models are widely prevalent and are often used to make predictions/scientific calculations for specific environmental problems. Models may be:

- Physical - a reduced version of reality.
- Mathematical - a description of systems using mathematical relationships and equations.

As per Benarie (1980), modelling means to look for mathematical formulae apparently fitting the real situation, to introduce into this formula adequate experimental data and to compute a result.

An atmospheric dispersion model is a:

- mathematical simulation of the physics and chemistry governing the transport, dispersion and transformation of pollutants in the atmosphere.
- means of estimating downwind air pollution concentrations given information about pollutant emissions and the nature of atmosphere.

Dispersion models can represent data in various forms. The simplest provide data in the form of graphs, tables or formulae on paper. Modern dispersion models take the form of computer

programmes which are user friendly and run on desk PC. The latest air pollution dispersion models that compute pollutant concentration downwind of the source tend to use the following information (ME522, 2004):

- contaminant emission rate;
- characteristics of the emission source;
- information on chemical/physical transformation of pollutants;
- local topography;
- meteorology of the area;
- ambient or background concentration of pollutant;

The input values for the above mentioned factors greatly affect the model performance as inferior model input can drastically reduce the efficiency of the model.

A generic overview of how this information is used in a computer-based air pollution model is shown in figure 2.4 (ME522, 2004)

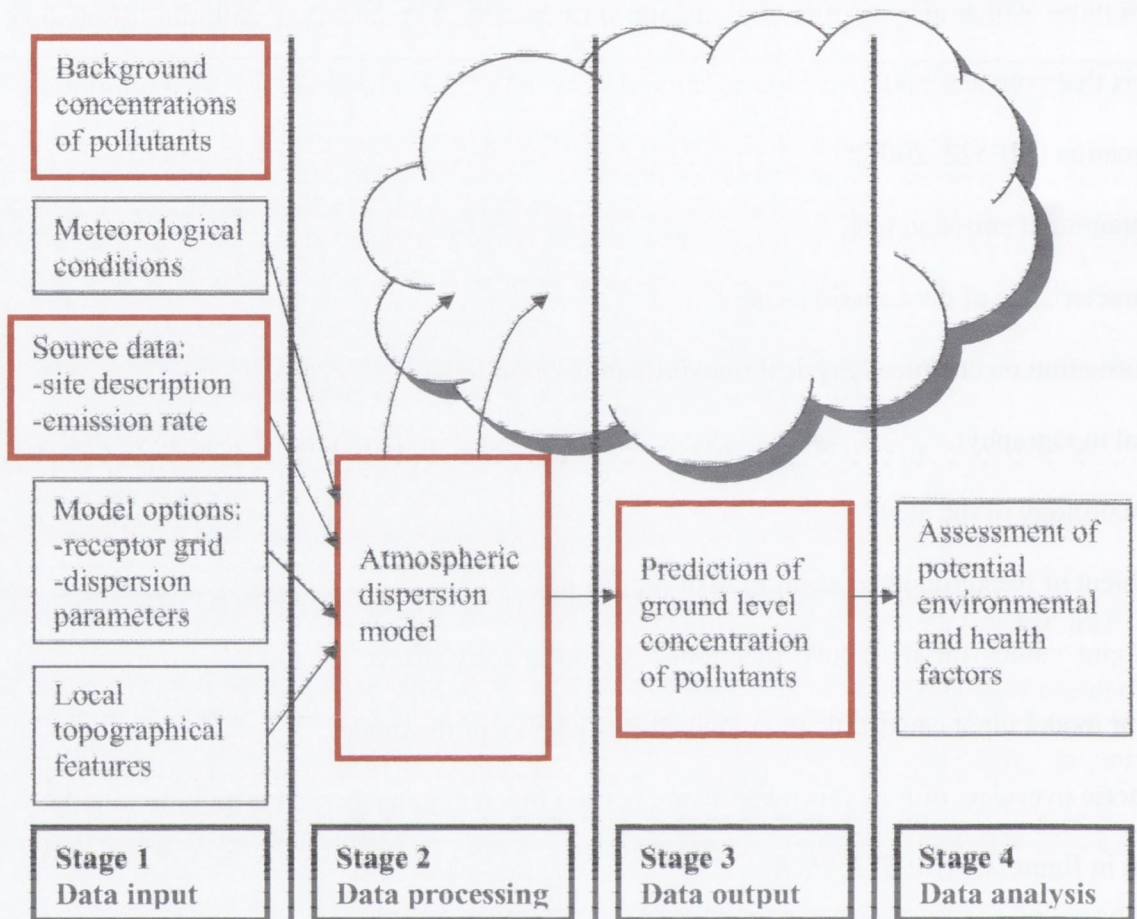


Figure 2.4 Overview of the air pollution modelling procedure

2.7.2 Characteristics of an Ideal Model

The following are the characteristics of an ideal air pollution model (Stern, 1984):

1. Physically realistic and accurate.
2. Universal, suitable for various:
 - temporal and spatial scale;
 - meteorological and topographical conditions;
 - emission sources (point, area, line);
 - air pollution species.

3. Supported by readily available input data
4. Easy to understand and use
5. Easy to adopt for running on simple computer
6. Computationally fast
7. Interactive with users
8. Integratable with other software based modelling systems.
9. Well documented
10. Well evaluated against observations.
11. Fully verified on real data.

2.7.3 Use of Dispersion Models

Dispersion modelling can be used to estimate downwind concentrations of pollutants over varying averaging periods which may range from three minutes to one year. The most common use of dispersion modelling is to assess the potential environmental and health effects of discharges to air from industrial or trade premises. They are of importance in assessing impact emission of new pollutants and to determine changes due to process modifications. Models can be used for the following purposes (ME 522, 2004):

- assessing compliance of emissions with air quality guidelines, criteria and standards;
- planning new facilities;
- determining appropriate stack heights;
- managing existing emissions;
- designing ambient air monitoring networks;
- identifying the main contributors to existing air pollution problems;
- evaluating policy and mitigation strategies;
- forecasting pollution episodes;

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- assessing the risks of and planning for the management of rare events such as accidental hazardous substance releases;
- estimating the influence of geophysical factors (terrain elevation, land use and presence of water bodies);
- saving cost and time over monitoring.

The EU Daughter Directives (CEC, 1999, 2000, 2002) allow 50% uncertainty in modelling of the eight hour average concentration of CO, 50% to 60% uncertainty in modelling of the hourly average concentration of NO₂ and NO_x and 30% uncertainty in modelling of the annual average concentrations of NO₂ and NO_x and 50% uncertainty in modelling of the annual average concentration of PM₁₀.

2.7.4 Drawbacks of Dispersion Modelling

The most sophisticated dispersion model fails in predicting the location, magnitude and ground level concentration with one hundred percent accuracy. In general, most of the models used today have undergone model evaluation processes and are fairly accurate provided that the correct model is chosen and that correct input data is provided. The major factors which determine the reliability and the accuracy of a model are (ME 522, 2004):

- the suitability of the model for the task;
- the availability of accurate source information;
- the availability of accurate meteorological data.

2.7.5 Selection of Dispersion Model

As pointed out before, the accuracy of the chosen model is determined by its suitability for that purpose. For selection of a model, the major issues to be considered are the complexity of dispersion (terrain and meteorological effects) and the potential scale and its effect. For

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regulatory purposes there are generally two types of model that are prevalent i.e, Gaussian Plume model (GPM) and advanced dispersion models such as CALPUFF.

It has been observed in general that for medium-complex atmospheric and topographical conditions with relatively simple effects the GPM is best suited. For more complex atmospheric and topographical conditions, advanced puff or particle models and meteorological modelling may be required to obtain the same level of accuracy. In the selection of a model it is important to understand the model's limitations and apply it to conditions which match its capabilities.

In situations dealing with complex terrain or coastal boundary regions, significant changes of meteorological conditions occur over short distances. In such cases, use of advanced modelling systems is more suited for simulating their effects than GPM. For proper functioning of an advanced model, detailed meteorological data input is a must. Figure 2.5 illustrates the type of models applied to particular scenarios, depending on their scale and complexity.

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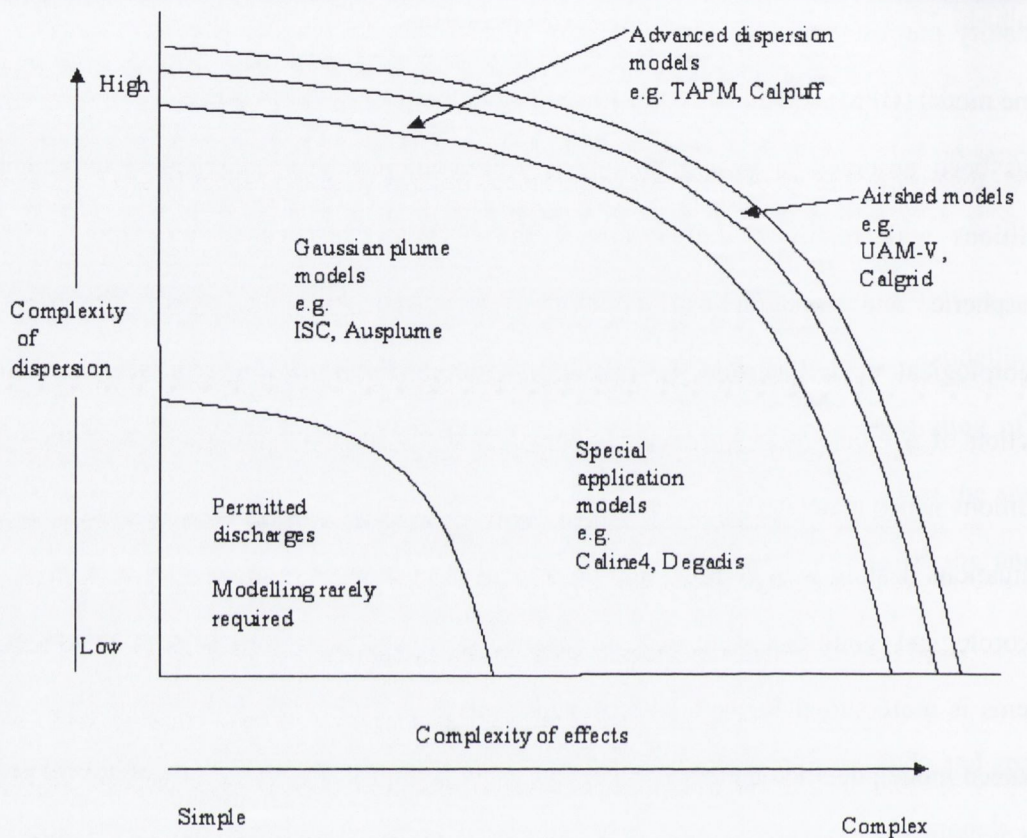


Figure 2.5 Type of model typically applied according to the complexity of the problem (ME 522, 2004)

2.7.6 Gaussian Plume Modelling.

The Gaussian plume model is the most prevalent, and user friendly form of atmospheric dispersion model. They are primarily used for regulatory purposes. Meteorological conditions are assumed stationary during dispersion from source to receptor. Though emission and meteorological conditions may vary from hour to hour, the model calculations are independent for each hour; hence they are referred as steady state dispersion models. In real life situations, plume characteristics keep on changing as they depend on actual emission and meteorological conditions. Steady state models compute concentrations based on hourly average emission rates and assuming no variation in meteorological conditions, hence they simulate hourly

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average concentrations. The Gaussian plume model is therefore most suited for use where there is no rapid change in conditions. Gaussian dispersion models require dispersion coefficients dependant upon atmospheric convective and mechanical turbulence. For elevated point source problems, these coefficients are largely dependant on meteorological conditions, primarily solar insolation and wind speed. However, the dispersion of vehicular emissions from roadway is more heavily influenced by mechanical turbulence and variations in the local wind field due to the motion of vehicles on the road. Exhaust emissions also have an influence on convective turbulence.

2.7.7 Assumptions of Gaussian Plume Modelling.

The main assumptions implicit in Gaussian plume modelling are described below (ME 522, 2004):

1. Steady state conditions are assumed. All variables and parameters remain constant with time. This assumption implies that the Gaussian model is applicable for relatively short travel times and distances
2. Flow is homogeneous, implying no spatial variability in the meteorological parameters. In particular wind shear is not considered.
3. The pollutant is inert and passive. The pollutant is not lost by decay, chemical reaction and gravity deposition.
4. There is no ground absorption of pollutants emitted.
5. Turbulent diffusion in the x-direction is neglected relative to advection in the transport direction, which implies that the model should be applied for average wind speeds of more than 1m/s.

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2.7.8 Characteristic Features of Gaussian Plume Modelling.

Gaussian plume models enjoy certain advantages over more complex numerical models, as listed below (ME 522, 2004):

1. They do not require significant computer resources. They can be run on desk PC and have the capability of processing a year's data in couple of minutes.
2. They are very user friendly and require less input variables.
3. They are widely used. The process of operating is well known due to large number of users and comparison of the results of different studies is fairly easy.
4. The model input has simple meteorological data requirements, which are easily available from standard meteorological recordings.

2.7.9 Limitations of Gaussian Plume Modelling.

The limitations of Gaussian plume modelling are pointed out below (ME 522, 2004):

1. Causality effects- GPM's assume that pollutant material is dispersed in a straight line manner instantly although it may take some time to reach the receptor locations. This is because it does not take into account the effect of wind shear; hence it does not take into consideration causality effects. This effect is pronounced if the receptor is located at a far distance from the source.
2. Low wind speed- GPM's are unable to operate for wind speeds less than 1m/s or in calm conditions due to the inverse wind speed dependence of steady state plume equations. It has been observed that the worst case dispersion results occur during these conditions.
3. Spatially uniform meteorological conditions- Gaussian steady state models assume that meteorological conditions are stable for the entire modelling domain and that they do not change during the transport and dispersion of pollutant from source to receptor. In real practice

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truly uniform conditions are a rarity. However, this is not a serious problem for short range roadside modelling.

4. In calculating each hour's ambient concentration the plume model has no memory of the contaminants released during previous hours. This limitation is especially important for the proper simulation of morning inversion breakup, fumigation and diurnal recycling of pollutants over cities.

2.8 Roadway Emission Modelling.

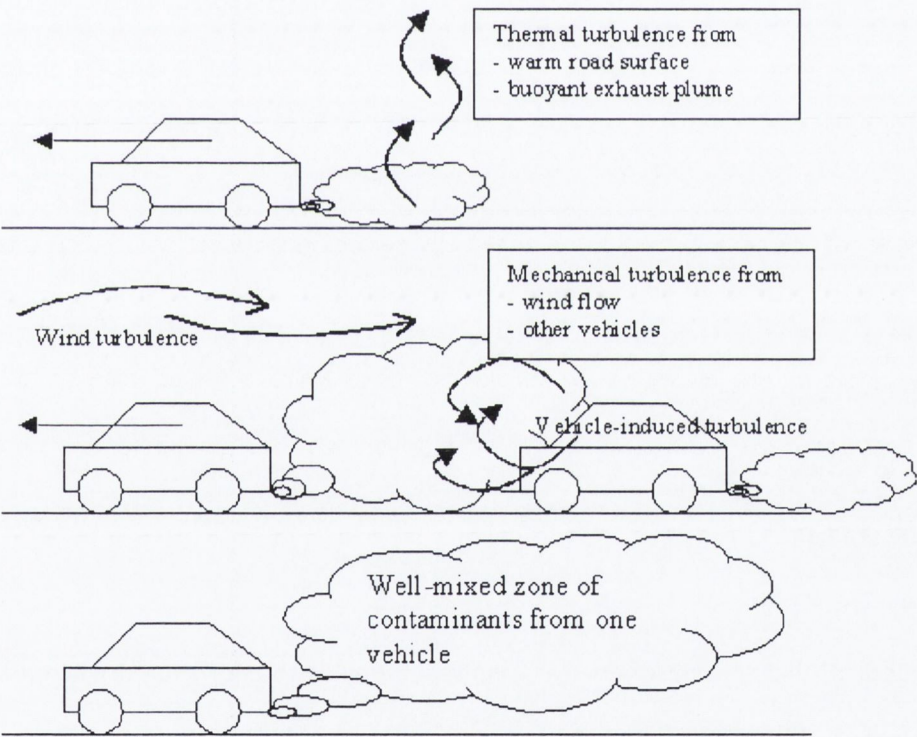


Figure 2.6 The effect of thermal and mechanical turbulence combining to form a well mixed zone of contaminants (ME 522, 2004).

Figure 2.6 represents a schematic diagram of the mixing processes associated with vehicle emissions. In the top picture, emissions from a car are dispersed behind and upwards being influenced only by thermal turbulence. In the middle picture, wind turbulence and mechanical

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turbulence from a following car also interact with the front vehicle emissions. The bottom picture shows how these combine to create a well mixed zone of contaminants in the plume behind a vehicle.

It can be easily understood from Figure 2.6 that thermal and mechanical turbulence occurring behind a vehicle contributes to mixing the emissions, so that the air behind the vehicle is relatively well mixed. If the situation depicted in figure 2.6 is extended to fleet of vehicles traveling both ways along a road a 'line source' of pollutants is developed. Modelling of roadway emissions is carried out using GPM's that are configured to emulate the dispersion of contaminants from this type of line source. The emissions from the vehicles on the roadway depend on a number of factors and estimating the type and concentration of pollutants can be complex. Certain factors which affect the rates of emission are (ME 522, 2004);

- The driving cycle (acceleration, steady speed, braking).
- Roadway conditions (free flow or congested).
- Vehicle fleet composition
- Vehicle speed
- Traffic volume

2.8.1 Roadway Emission Models.

It is suggested that specialised roadway emission models should be used when assessing the effects of contaminants discharged from transport corridors. The emission factor models considered in this study were COPERT III and MEET. A brief description about them is presented below:

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2.8.1.1 COPERT III

The Computer Programme to calculate Emissions from Road Traffic (COPERT) is an emission model developed by the European Environmental Agency (Marmur, 2003). It estimates emission factors for a range of pollutants including CO, NO_x, HC's, particulate matter and heavy metals. Cars are classified into three subsectors depending on engine size i.e. <1.4l, 1.4-2.0l and > 2.0l. Each subsector is then further subdivided into 10-12 technology classes reflecting the various stages of EU exhaust regulations (Ekstrom, 2004). Diesel cars are classified into two subsectors, < 2.0l and >2.0l both containing six different technology class. Emission factors can then be derived using knowledge of the fleet profile and driving speed. The fleet characteristics and driving speed are major criteria in determining the emission factor. The fleet characteristics generally describe the vehicle flow as per their year range and generally older the car, more the emission. Further to this speed of the vehicle also plays an important part as because different speeds lead to different emission rates. This has been studied in more details in section 3.4.3, Chapter 3. Marmur *et al*, (2003) reviewed a number of emission models and concluded that COPERT was the most consistent generating low NMSE values.

2.8.1.2 MEET

The MEET programme was designed following the COST 319 initiatives. The COST program ("European Co-operation in the Field of Scientific Research") was a Europe-wide program for the co-ordination of national research, managed by 25 signatory countries and the European Commission. The COST program typically addressed areas of research, where concerted action could bring benefit to the participating countries. With its emphasis on open participation, COST actively promotes the concept of "bottom-up working", the research areas

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being defined by the participants themselves. COST open and adaptable approach brings many advantages. It enables avoiding the duplication of effort, the sharing of results by all participating countries, the building of a scientific consensus and the efficient coverage of the complex field of European research, while allowing the individual countries to focus on problems of particular interest (<http://www.cordis.europa.eu/transport/home.html>).

The three main objectives of the project, called Methodologies for Estimating Air Pollutant Emissions from Transport (MEET), were:

- To provide a set of data and models, allowing various users to calculate the pollutant emissions and the fuel or energy consumption of the various transport modes at strategic level.
- To provide a comprehensive method of calculation using the set of data and models.
- To make sure that this comprehensive method corresponds to the requirements of the potential users in terms of accuracy, simplicity and input data availability.

The outcomes obtained from the COST 319 project allows the development of a set of methodologies accepted by most European researchers. The use of common methods to evaluate emissions and energy consumption levels all over Europe and possibly more widely will make different studies and assessments comparable. Simultaneously, the undertaken actions allowed the participating laboratories to compare and co-ordinate their research methods, and the European countries to co-ordinate their research programs. In the frame of the COST 319 action and the MEET project - which is a part of it - a great number of reports were made, each being a synthesis of the European knowledge available,

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expressing a common opinion of the involved scientific circles. The outcomes of the COST 319 project varied but can be summarised as:

- The final inventory methodologies with all the necessary data concerning the emission factors and the traffic characteristics are presented in the final MEET report. The corresponding data are transferable from a specific file. The report and the data file allow any user calculate an emission inventory of traffic emissions.
- The final COST report discusses the available data, their accuracy; it presents the synthesis methods and the assumptions. It is especially useful for researchers interested in the building of methods of estimating pollutant emissions from transport, rather than for users.

2.9 Atmospheric Dispersion Models for traffic emissions.

A range of atmospheric dispersion models have been developed to calculate the impacts of traffic emissions. The models can be classified as screening models, highway models street canyon models and general models.

2.9.1 Screening Models.

2.9.1.1 DESIGN MANUAL FOR ROADS AND BRIDGES (DMRB)

This screening method was formulated by the former Department of Transport, UK. The method gives a preliminary indication of air quality near roads, and is more suited to rural motorways and trunk roads than city centre traffic conditions. It is a simple procedure based on tables and nomograms; originally published in August 1994, a revision was made at the end of 1997 and 1999, which included features also applicable to urban situations. The DMRB method requires information on vehicle flow, vehicle speed and receptor-road distances. It contains a useful database of vehicular emission factors for future years.

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The method assumes a fixed set of meteorological conditions (a low wind speed and neutral atmospheric stability; the wind direction is assumed to be evenly distributed around the compass). Assumptions about background pollutant levels are included in the calculations. However modelling of links and roundabouts and its modifications were made in the latest versions (Version 1.02, November 2003).

2.9.1.2 CAR

This is a screening model formulated to support the implementation of air quality legislation in the Netherlands and is a parameterisation of the Gaussian TNO traffic model proposed by Eerens *et al*, (1993). It predicts annual average and 98th percentile concentrations of pollutants from road traffic at 1.5m height. The formulae are based on wind tunnel experiments, theoretical considerations and monitoring; these formulae have been published for use with a hand calculator, though a computer version is also available. CAR takes into account the configuration of buildings and trees along the road and photochemistry. Emission factors and the wind speed are defined by the user.

2.9.1.3 US models

The website (<http://envfor.nic.in/divisions/iass/eia/Annex5.htm>) lists the models used for Guidance of assessment relevance and reliability of analytical methods for prediction of air environment. It lists PTMAX and PTDIS as the screening models used for dispersion modelling.

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2.9.2 Highway models

2.9.2.1 Csanady Equation

Csanady (1972) proposed an equation for calculating dispersion from finite line sources where the line source may be considered to be a superposition of point sources. It assumes a hypothetical line source with the wind is perpendicular to it. The concentration at a receptor due to this line source is given by the equation 2.4.

$$C' = \frac{Q}{2\pi\sigma_y'\sigma_z'\bar{u}} \left[\exp\left\{-\frac{1}{2}\left(\frac{z-H}{\sigma_z'}\right)^2\right\} + \exp\left\{-\frac{1}{2}\left(\frac{z+H}{\sigma_z'}\right)^2\right\} \right] X \int_{-L/2}^{L/2} \exp\left[-\frac{1}{2}\left(\frac{y_1'-y_1}{\sigma_y'}\right)^2\right] dy_1' \quad (2.4)$$

Where, Q is the source emission rate per unit length, z is the height of the receptor above ground, H is height of line source, $\bar{u}$ is the mean ambient wind speed at source height H , σ_y' and σ_z' are the horizontal and vertical dispersion coefficients respectively (wind coordinate system) and are functions of downwind distance and stability class.

2.9.2.2 CALINE

This model was developed by the California Department of Transportation and the US Federal Highways' Agency (FHA). It is a Gaussian model designed for the assessment of traffic emissions from roads. It can model junctions, street canyons, parking lots, bridges and underpasses; it includes a photochemistry model to predict downwind concentrations of NO_2 from NO emitted by vehicle exhausts. CALINE predicts 1-hour mean concentrations and is therefore useful for investigating episodes of high NO_2 and CO concentrations. Hourly meteorological conditions are user-defined, and line source emission rates must be calculated independently by the user based on vehicle speeds, traffic flows and published emission

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factors. CALINE requires details on the site configuration, and of the ambient NO₂, NO and ozone levels for the photochemistry simulations. The model can handle up to 20 road links and 20 receptors.

2.9.2.3 CAL3QHC (*CALINE3 with queuing and hot spot calculations*).

This US Environmental Protection Agency (EPA) model is designed to handle near-saturated and/or over capacity traffic conditions and complex intersections. It predicts 1 hour mean concentrations, for up to 120 road links and 120 receptors.

2.9.2.4 CALINE4

This section illustrates some of the important generic issues associated with roadway modelling using the California Line Source Model (CALINE4) as an example. This model is commonly used in New Zealand, the USA and England, is quite user-friendly and is freely available. CALINE4 was developed by the California Department of Transportation and the US Federal Highways Agency for assessing roadway traffic emissions. It is based on the Gaussian diffusion equation and employs a mixing zone concept to characterise dispersion over the roadway. CALINE4 is a Gaussian-plume model and as such is subject to the same limitations as other steady-state Gaussian-plume models. CALINE4 can model roadways, intersections, street canyons, parking areas, bridges and underpasses. Each CALINE run allows the prediction of up to eight one-hour mean concentrations. Therefore it is useful for investigating one-hour concentrations of NO₂ and CO and eight-hour concentrations of CO.

The US EPA lists CALINE4 as the preferred/recommended roadway model (US EPA, 1999). The UK Department of the Environment, Transport and the Regions lists CALINE4 as an

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advanced model (UK DETR, 2000) but does not indicate any form of approval or endorsement.

Further details of CALINE4 model has been made in Section 3.5.2 of Chapter 3 of the thesis.

2.9.2.5 HIWAY and HIWAY2

HIWAY (Zimmerman and Thompson, 1975) developed by the USEPA, divides the roadway into an equivalent set of finite line sources. HIWAY2 (Peterson, 1980) represents an improved version of HIWAY and gives more accurate predictions under stable atmospheric conditions, during parallel and low wind speeds due to an updated dispersion algorithm.

2.9.2.6 GRAL

Rebolj and Sturm (1999) designed a graphical interface model including GIS for use in combination with an emissions model. The emission model, which includes a dispersion model, has been developed at the Technical University in Graz (Sturm et al, 1997) based on German/Austrian/Swiss emission factor handbook and on the real world driving patterns. The Graz dispersion model is not named but was based on the GM model experiments as described by Chock (1977). The results of modelling were stated to be applicable up to 500m from the road side.

2.9.2.7 GFLSM

The General Finite Line Source model (GFLSM) model for vehicular prediction (Luhar and Patil, 1989) is so formulated that it can be used for any wind direction relative to the roadway. The mathematical approach is based on a coordinate transformation which reconciles the local highway alignment with the wind direction. The main advantage of this model lies in the simplicity of its application as it is an analytical solution of the Gaussian equation. The main disadvantage of the model is the limited receptor co-ordinates for which concentrations can be calculated. The GFLSM requires the receptor to be located at 90 degrees to the segment of the

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road considered and the length of line source should be at least three times the distance between the receptor location and road. (Gokhale and Khare, 2004). Further details of this model have been presented in Section 3.5.1 of Chapter 3 of the thesis.

2.9.2.8 IITLS

Goyal and Ramakrishna (1999) developed the IITLS model to predict concentrations of gaseous pollutants CO, SO₂, NO_x and particulates for various types of roads. The model uses separate equations for calculating pollutant concentrations under cross wind and parallel wind conditions. For the other wind angles, the concentrations are determined by weighted average of the crosswind and parallel concentrations. Further details of this model have been presented in Section 7.3.2 of Chapter 7.

2.9.3 Street Canyon Models

2.9.3.1 AEOLIUS

In this model hourly mean concentrations of NO_x, NO₂, CO, SO₂ PM₁₀, benzene and 1,3-butadiene are calculated within a street canyon at kerbside level. Further calculations are made for the 98th percentile of NO₂, and the maximum 8-hour mean CO level. This model is useful as it is recognized that the highest exposures to traffic emitted pollutants can often occur in street canyons, where the presence of buildings can cause a re-circulating flow; pollutant concentrations being higher on one side of the street than the other according to wind direction. AEOLIUS can make use of hour-by-hour traffic data over a week. Emission factors must be user-defined. It requires sequential hourly meteorological data, and can process up to one month at a time.

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2.9.3.2 IMM

The Intersection Midblock Model (IMM) is an operational regulatory model in US that accounts for influence of modal traffic behaviour (acceleration, queuing etc.) at intersections and is used to model CO concentrations only. It uses dispersion parameters from the GM model (Sharma and Khare, 2001).

2.9.3.3 TEXIN

Hlavinka *et al*, (1987) described TEXIN2, an updated version of TEXIN, the Texas Intersection Model for air quality near street junctions. TEXIN was improved to include T-junctions, one way streets, four way junctions, inspection and maintenance capabilities, and shortcut emission algorithm using MOBILE3 emission factors. The model performance was found to be better than IMM for street canyon studies (Nagendra and Khare, 2002)

2.9.3.4 AURORA

Mensink *et al*, (2003) used the AURORA model to assess pollutant concentration in street canyons, showing variation in CO, NO₂ and PM₁₀ throughout the city of Antwerp. The model predictions were close enough to observations to satisfy the EU directive guidelines for all pollutants except NO₂.

2.9.3.5 Matzoros's model

Matzoros (1990) developed a model to predict air pollution concentrations from road networks at any receptor. It consists of three parts: a queuing model, an emission model and a dispersion model. It was designed especially for urban areas, to take into account the spatial variability in emissions by allowing that due to queuing, emissions are highest near junctions. Matzoros states that conventional models such as MOBILE/HIWAY2 consider roads to be line sources with constant emissions, but this is inaccurate near junctions where vehicles spend time

queuing, accelerating and retardation (Taylor, 1982). Emissions are generally higher for these transient operating modes.

Gaussian dispersion modelling of CO, HC, NO_x and PB concentrations was applied to both signalised and prioritised/roundabout junctions. CO emissions and concentrations showed the highest spatial variation. Maximum emissions generally occurred before the stop line for signalised intersections but at stop lines for the roundabout junctions. Emissions and concentrations were lower for signalised junctions than for roundabouts with equal flow and capacity.

2.9.3.6 STREET

The STREET (Johnson et al, 1973) model was one of the earliest street pollution models. It uses two different expressions to calculate concentrations on the windward and the leeward side of the street and assumes that the leeward side concentrations are higher than the windward side (Berkowicz, 2000). For a parallel wind direction the concentration is assumed as half of the combined concentrations obtained from leeward and windward sides. The STREET model is widely still in practise today.

2.9.3.7 OSPM

The Operation Street Pollution Model (OSPM) was developed by the National Environmental research institute in Denmark. OSPM is a parameterised semi-empirical model that makes prior assumptions about wind flow and dispersions in street canyons (Berkowicz, 2000). Concentrations are calculated using a Gaussian plume model to describe the effects of direct vehicle emissions in the street, while recirculation in the street is modelled by the box model. The model assumes that concentrations on either side of the street are similar for wind speeds < 2m/s or when winds are parallel to street orientation, otherwise separate concentrations are calculated either side of the street.

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2.9.4 General Models

2.9.4.1 ADMS-Urban

ADMS-Urban is basically an extension of the ADMS2 industrial model, combining a line and area source model with street canyon model, a chemistry model for nitrogen, sulphur and ozone and a traffic emissions database (McHugh et al, 1997). For urban areas major roads are modelled as line sources whereas minor roads are modelled as area sources. Traffic sources are defined using the following parameters: location of the road, road width, height of building along the road, vehicle type, number of vehicles, vehicle speed and monthly/hourly variation of emissions. The nitrogen dioxide formation is calculated using a semi empirical model formulated as a series of seven chemical reactions. The street canyon analysis is based on OSPM. For improved predictions, the model takes into account advanced algorithms for height dependence of wind speed, turbulence and stability. A validation study has been reported by McHugh et al (1997).

2.9.4.2 CAR-FMI

The CAR-FMI (Contaminants in the Air from a Road – Finnish Meteorological Institute) model was developed for regulatory purposes, and consists of an emission module, treatment of meteorological time series, an atmospheric dispersion module and statistical analysis of the computed concentrations (Harkonen et al, 1997). The dispersion model is based on the GFLSM approach (Luhar and Patil, 1989) which prevents need of numerical solutions as required in HIWAY and CALINE4 (Kukkonen et al, 2000). The chemical transformation of oxides of nitrogen is modelled using a version of the discrete parcel method employed in CALINE4, revised so that the size of the reaction volume is dependant on receptor location. It employs a meteorological pre-processing model MPP-FMI.

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2.10 Previous model investigation research

2.10.1 *HIWAY and CALINE*

Noll et al. (1978) compared the HIWAY, CLS and CALINE2 models by performing sensitivity analysis. The sensitivity analysis showed that the dependence of normalised concentrations depended on a variety of input parameters. HIWAY was found to predict higher pollution concentrations during oblique and crosswinds than the other two models. CLS was found to predict the highest concentration for parallel winds amongst all three models. The validation showed common differences between measured CO concentrations and those predicted by the models: that all the three models overestimated concentrations for parallel winds and underestimated concentrations for oblique and crosswinds.

Rao and Visalli (1981) identified a lack of both field data and well defined measures of performance, especially when models are used for regulations. They investigated four models HIWAY1, AIRPOL4, HIWAY2 and CALINE3 and found that arbitrary screening of data could adversely affect model performance; that if the extreme values were not associated with worst case scenarios it was not advisable to remove the model estimates for worst case scenario. They also suggested that the meteorological and emissions data should be screened to find the frequency of the combinations of the meteorological and emissions characteristics which led to the combination of the high observed and predicted concentration. Rao later evaluated HIWAY2, ROADWAY and CALINE3 and found all three models successfully predicted extreme concentrations of tracer gas to within 30% of observations (Rao et al, 1986). Kono and Ito (1990) compared the HIWAY2 model with two Japanese models using SF₆ tracer concentrations measured at three locations in Japan. The model was found to have a bias for overprediction in calm conditions.

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In Australia, Shenouda (1994) compared concentrations of CO₂, CO, NO_x and HC predicted by HIWAY and CALINE with measured air quality alongside arterial roads and highways. The monitoring was carried out at locations of up to 60m downwind and at heights up to 10m above ground. Traffic flow, speed, and profile were taken by camera. No conclusions on the validation were in the abstract examined, however in a paper with Schmidt, (Shenouda and Schmidt ,1997) compared roadside CO₂ concentration predictions by CALINE4 and HIWAY2 with concentrations measured over eight days at locations upto 60m downwind of roadside and 10m above ground. A power based emission model was used for both models and they concluded that CALINE4 and HIWAY2 are potentially useful models for regulatory purposes. Dabberdt et al, (1995) compared HIWAY2, CALINE4 and a hybrid Lagrangian model with measurements from a wind tunnel tracer gas flows at an urban intersection between uniform, low rise, rectangular blocks. The Gaussian models (HIWAY2 and CALINE4) were judged to be less suited to urban intersection modelling due to the lack of explicit consideration of the effects of buildings on dispersion.

In Japan, Okamoto et al, (1999) studied dispersion for various highway conditions: flat, viaduct, cutting, embankment and with noise barriers. They concluded that most roadside vertical dispersion could be considered as Gaussian and the noise barriers cause the initial σ_z to be higher and less dependant on atmospheric stability. They rated the effect of road structure to be more significant for dispersion than the traffic conditions. Their experimental data was used to validate CALINE3 and HIWAY2.

Ionel et al, (1999) used CALINE3 to quantify the effects of traffic sources modelled as CO emissions, as opposed to the effects of other sources of pollution. Real meteorological and topographical data were determined from the city of Timisoara, Romania. The background pollution due to non traffic sources such as power plants and industrial units was measured.

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CO concentrations were calculated at two receptors located at an intersection. CO emissions were measured to be approximately three times the Romanian standard of 1.67ppm. The monitoring period was adjudged to be short but the CALINE3 was found to be useful modelling tool.

2.10.2 CAL3QHC

The USEPA evaluated the performance of eight intersection models in simulating CO concentrations at six intersections in New York City. The eight models evaluated involved the CAL3QHC, CALINE4, TEXIN2 and IMM models already described. Meteorological and CO air quality data were collected at two background sites and at each of the six intersections. The meteorological data collected at each intersection included wind direction, wind speed, temperature and fluctuation of the wind direction. These data were measured at two towers per intersection at a height of $10\text{m} \pm 1\text{m}$. A series of video cameras were also used to record three months of continuous traffic data at the site. The videotapes from the top 50 hours of CO concentrations were examined to obtain detailed information about road traffic.

CAL3QHC was seen to perform better than any other intersection model. The average difference between the top ten observations and their time paired predicted values were as low as 6%, but as high as 65% depending on the site. Comparing individual and observed predicted values, differences as low as 10% but as high as 150% occurred.

2.10.3 CALINE4

Benson (1992) described five independent studies employed in the validation of CALINE4:

- the GM Sulphate dispersion experiment;
- the Illinois Freeway/Intersection study (CO measurements adjacent to a freeway and a major intersection close to Chicago);

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- the EPA NO₂/O₃ Sampler Siting Study (NO_x and O₃ samples collected at six sites close to major freeway in California);
- the Caltrans Intersection study (CO concentrations averaged over 1 hour measured at 15 locations in the vicinity of intersection at Sacramento);
- the Caltrans Highway 99 tracer experiments (SF₆ tracer concentration sampled at 50, 100 and 200m from a highway in Sacramento).

Benson (1992) employed six separate statistical measures to compare the performance of CALINE3 and CALINE4 in the above studies; an overall figure of merit based on the weighted sum of these six statistics was also defined. Of the highway studies, CALINE4 was seen to perform better than CALINE3 and in the GM and the Caltrans experiments, while the Illinois experiment results were inconclusive. In the Caltrans experiment, less than 15% of the CALINE4 predictions fell outside the factor of two envelope, with majority of these occurring when the wind speed was less than 1m/s or the wind road angle was less than 15°. Both models seemed to predict the spatial distribution of pollutants better than the temporal variation. The performance of CALINE4 at intersection sites was similar to that at highway sites, but the higher winds in these studies probably masked inaccuracies in the model emissions factors. CALINE4 also performed well in the NO₂ study during favourable meteorological conditions.

2.10.4 TEXIN and IMM

Nelli et al (1983) compared four models for two sites in Texas and one in California. The models were TEXIN, IMM, MICRO and ISG. TEXIN, which the authors had developed, was found to perform the best. IMM performed almost as well as TEXIN but required more input data and computer time. The accuracy of both TEXIN and IMM was independent of the wind angle and receptor location.

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Hlavinka et al, (1987) compared TEXIN2 with the TEXIN, IMM and MICRO models at two sites. One site had scattered single story buildings, the other was surrounded by buildings, which were up to 24 stories high. The effects of changes in the receptor height, the wind speed and direction was evaluated. TEXIN2 was found to perform somewhat better than the other models.

2.10.5 GFLSM

The General Finite Line Source Model (GFLSM) for vehicular pollution prediction was evaluated by Luhar and Patil (1989) using statistical analysis of predicted and observed CO concentrations in Mumbai, and particulate concentrations in New York. In the CO evaluation, the GFLSM was seen to perform better than the GM, CALINE3 and HIWAY2 models. In the particulate evaluation, the GFLSM model out performed the GM model. Khare and Sharma (1999) assessed the performance of the GFLSM by comparing predicted CO concentrations with measured values at different traffic intersections in Delhi. Khare and Sharma (1999) modified the GFLSM model to create the DFLSM by removing the error function term and obtained improved results. Nagendra et al (2004) applied the GFLSM at busy traffic intersections at Bangalore, India and found that model performance was good when compared with monitored data. Gokhale and Patil (2004) used the GFLSM model to predict concentrations of size separated particular matter below 10 μ m size from vehicular exhausts using a modified GFLSM model for particulates and obtained a good correlation between observed and predicted values for size ranges below 4.7 μ m.

2.10.6 CAR-FMI

Harkonen et al, (1997) compared the predictions of CAR FMI with measurements obtained in a suburban part of the city of Espoo, Finland. Concentrations of five gaseous pollutants (CO, NO_x, NO₂, O₃, and SO₂) were measured at three heights together with traffic flow and

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meteorological parameters. Vertical concentration profiles were determined by varying the sampling height at ten minute intervals. Good agreement was observed for NO_x , NO_2 and O_3 although NO_2 and O_3 concentrations were slightly underestimated. This study was hampered by significant but uncertain background concentrations. Details of the results of CO were not given.

Kukkonen et al, (2001b) performed a second validation study of CAR-FMI beside a rural highway. Air quality (NO_x , NO_2 and O_3), traffic and meteorological data were obtained over a six week period at three sites, 17m, 34m, 57m from road way at heights of 3.5m, 6m, 10m. Mean traffic flows of 300 vehicles per hour were observed. Due to these relatively low flows and high vehicle speeds on the road, the measured CO concentrations of CO were too low to be useful. Kukkonen also collaborated with Oettl et al, (2001) to evaluate CAR-FMI and the road side data set against GRAL, a Lagrangian dispersion model specifically adjusted to allow for enhanced horizontal dispersion in low wind speed conditions. GRAL was found to be able to better simulate for low wind speeds and parallel wind conditions than CAR-FMI. The comparison of predicted and measured data were carried out using five statistical parameters: index of agreement (IA), normalised mean square error (NMSE), Pearson's correlation coefficient (R), fractional bias (FB) and factor of two (F2).

2.10.7 STREET

The STREET model is an empirical model which predicts concentrations on both the windward and leeward sides of the road. It includes an empirical parameter constant 'K' which should be validated for each individual application site. Qin and Kot (1993) estimated the value of K to be 6 for their work in an asymmetric street canyon in China whereas Bogo et al. (2001) reportedly used a K value of 8 for a similar study in Buenos Aires. Vardoulakis et al., 2002 used a K value of 7 for application in a street canyon in Paris.

2.10.8 OSPM

Berkowicz *et al*, (1996, 1997) found strong correlations between measured and modelled NO_x results during initial OSPM tests on data from three streets in Copenhagen. The strongest correlation was found with measured data from Jagtvej (a street canyon with $H/W = 0.72$, angled at 30° with respect to North) with a correlation coefficient of $R^2 = 0.85$ for 1993 data and $R^2 = 0.89$ for 1994 data. In tests against data from monitoring stations in the street Albanigade in Odense, Denmark and Schildhortrasse in Berlin, Germany, Berkowicz (2000) found good correlation between measured and modelled NO_x results with correlation coefficients $R^2 = 0.71$ for Albanigade and $R^2 = 0.71$ for Schildhortrasse (Berkowicz, 2000). It should be noted that these results were for daytime hours only (07:00-18:00) and for wind speeds between 4m/s and 7m/s. A large scatter of data was evident at low wind speeds ($< 1\text{m/s}$), when traffic induced turbulence is assumed to dominate, indicating that the modelling of traffic induced turbulence may need to be improved within OSPM (Berkowicz, 2000). The agreement between measured and modelled NO_2 concentrations, for daytime hours only, was strong for Albanigade ($R^2 = 0.90$), yet quite weak for Schildhortrasse ($R^2 = 0.52$). The relatively poor result for correlation for Schildhortrasse was attributed to urban background ozone (O_3) concentrations used in the calculations, (which OSPM requires to model the chemical transformation between NO_x and NO_2), which came from a sub-urban monitoring location rather than an urban site close to the measurement point. This finding highlights the need for accurate and representative background concentration data as an input to OSPM.

Kukkonen *et al* (2001) assessed the performance of OSPM against measured data for 1997 from Runeberg Street in Helsinki and found good overall agreement between the measured and modelled concentrations of CO, NO_x , and NO_2 . The fractional bias between measured and modelled concentrations of CO (- 4.2%) and NO_x (+ 4.5%) indicated a slight under-prediction

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and over-prediction of modelled concentrations respectively. OSPM seemed to over-predict the concentrations of NO_2 (FB = + 22.5%) which was attributed to overestimation of background ozone levels (Kukkonen *et al.*, 2001).

2.10.9 ADMS

McCrae *et al.*, (2000) reports results of comparison of PM_{10} and NO_2 measurements at two sites in Birmingham with predictions using ADMS-Urban. Good agreement was achieved with the predicted mean and the 99th percentile concentrations being within 20% to 30% of those observed. Summary results were also given from an investigation in which the ability of the ADMS to predict measured concentrations at roadside locations adjacent to the M25 was evaluated. The maximum 8 hour mean CO concentration was measured as 17ppm but modelled as only 8.5ppm. CALINE4 modelling predicted an even lower value of 4.4ppm. GRAL (a model developed by University of Greenwich) performed best, predicting a value of 14.3ppm. ADMS overpredicted the observed PM_{10} concentration: the annual mean concentration was predicted as $52\mu\text{g}/\text{m}^3$, but measured as only $11\mu\text{g}/\text{m}^3$; the 99th percentile of the 24 hour means was predicted as $113\mu\text{g}/\text{m}^3$, but measured as only $52\mu\text{g}/\text{m}^3$.

2.11 Research carried out in context to Ireland.

A number of recent studies into transported related air pollution in Ireland have been conducted, which are summarised in this section.

Reynolds (2000) developed an air quality modelling systems (AQMS) for metropolitan areas in Europe and applied to Dublin. The primary objective of the AQMS was to incorporate traffic, size and air quality data at temporal and spatial distribution. It consisted of three modules: a traffic module, an emission module and dispersion module and integrated it into a GIS system. Reynolds (2000) also compiled an emission inventory for the greater Dublin area for base year (1991) and their relative changes in 1996, 2006, 2016.

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Budd (2004) assessed the concentrations of CO, NO_x and PM₁₀ at the M4 motorways at Leixlip and (in association with researchers in NUI Galway) at a busy roundabout in intersection in Galway. DMRB and CALINE4 model was used to predict pollutant concentrations at both sites. The background concentrations were taken to be the average of hourly pollutant concentrations when the traffic flow had least influence. Background concentrations used were 0.23 ppm for CO, 10ppb NO₂ and 11.9µg/m³ PM₁₀ for the motorway site and 0.18ppm CO, 10ppb NO₂ and 13µg/m³ PM₁₀ at the roundabout. Composite emission factors of 4.14g/km and 1.4g/km for CO and NO_x respectively were used for both, the motorway and roundabout site and emission factors of 0.12g/km and 0.06g/km were used for motorway and roundabout sites respectively for PM₁₀. The diurnal variation profiles followed the traffic profile at the motorway site. DMRB modelling usually overpredicted pollutant concentrations at both sites. This was expected as the DMRB model uses worst case meteorological situation. Ganguly and Broderick. (2006) used an updated version of the DMRB model and observed that this version of the screen DMRB model was successful in predicting reduced concentrations for NO_x and particulate matter at the motorway and gives close results for the other pollutants when compared to the previous version. In the roundabout problem, certain modifications were made in relation to the earlier version suggested in the DMRB manual. This led to improved but still overpredicted model estimates. Ganguly and Broderick (2006, 2008) further modelled the CO concentrations using GFLSM and showed that it was a better modelling option than CALINE4. O'Donoghue. (2004) carried out a hydrocarbon monitoring campaign at the M50 site in Dublin. This campaign was conducted for approximately eight months. Hydrocarbon peak concentrations were shown to be higher in winter than in summer and heavily dependant on wind speeds. Traffic related compounds such as acetylene, ethene and aromatic hydrocarbons showed strong diurnal profiles associated with M50 traffic flow. Highest concentrations were

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shown to occur with parallel or near parallel wind directions relative to the motorway orientation. High traffic flow and lower speeds contributed to this observation. Analysis of concentrations obtained from non motorway directional winds showed no obvious source effects, confirming that hydrocarbon concentration in the area was are primarily sourced from M50 road. O'Donoghue (2004) used the CALINE4 model to predict the observed concentrations and reported that CALINE4 modelled results were a good match for the observed hydrocarbon concentrations. Further details regarding the CALINE4 modelled results and its comparison with the GFLSM model has been presented in Section 4.3.1 in Chapter 4. Ganguly and Broderick. (2006, 2007) showed that the use of GFLSM model was better suited for predicting hydrocarbon concentration than CALINE4.

Delaney. (2006) carried out an assessment study at a rural site (Monasterevin, Co. Kildare) from October 2004 to January 2005 with the prime objective of assessing the change in traffic impacts due to opening of a new town bypass. The pollutants studied were CO, NO_x HC's and PM₁₀. The Gaussian model CALINE4 was used to assess the observed changes in pollutant concentrations was examined. Ganguly and Broderick. (2006) used the GFLSM model to determine the changes. Ganguly and Broderick. (2007) also carried out urban street canyon modelling for CO and NO_x for an eight months data set and showed that the performance of OSPM was better than STREET.

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2.12 Study Summary

The chapter presents comprehensive detail of the pollutants and the suitability and applicability of a variety of Gaussian based atmospheric dispersion models. In general, the transport sector is responsible for 50% of total NO_x emissions and 80% of total CO emissions in Ireland. One of the ways to counteract these high rates would be proper planning of future roadway projects, which would involve the use of an integrated transport environment model to give an estimate of the pollutant concentrations released based on the design traffic flow. In this context, simple analytical Gaussian based dispersion models are handy enough to be incorporated in the detailed traffic models. The use of GFLSM (for motorway) and STREET and OSPM (for street canyon) are hereby selected and evaluated to check for its suitability to be incorporated in an integrated transport environment model.

3.1 Introduction.

This chapter addresses highway dispersion modelling. First, a screening model is employed at motorway and roundabout sites. The aim of the screening model is to determine whether further detailed modelling practice is required or not. A detailed modelling exercise is then carried out at a highway site using the GFLSM model for predicting CO and NO_x concentrations. Statistical and graphical analyses are used to compare the monitored and modelled results. The CO modelled results are compared with CALINE4 modelled results, and a thorough treatment of effect of background concentrations on the final modelled concentrations of NO_x is also presented. The use of hourly emission factors as an alternative to a constant composite emission factor is also proposed and studied.

3.2 Study Sites:

Two study sites were considered by Budd (2004): a motorway and a roundabout. The site description details are given below:

3.2.1 Motorway Site

The site chosen for the motorway was adjacent to the M4 motorway at about 15 km from Dublin city centre and was within the grounds of Leixlip Water Treatment Plant. The M4 motorway at Leixlip consists of two lanes in each direction and is orientated East-West. The mean peak traffic flow recorded on weekdays was 2690 vehicles per hour as measured by automatic traffic counters and the average vehicle speed observed was 60-70 miles/hour. From measurements taken at Dublin airport, the general wind direction was from the southwesterly. The monitoring unit was set up at a distance of 20 m from the roadside. The road alignment is straight for a distance of 1.25 km East and West of the monitoring location. A small aerodrome is located south of the M4 and Leixlip town is 1 km to the north of the site. A layout of the monitoring station at the motorway site is shown in Figure 3.1. A schematic

diagram of the monitoring location at M4 site at Leixlip is shown in Figure 3.2. The importance of the selection of this site lies in the fact that a huge quantity of requisite data required for evaluation of the models was available at this site. The presence of the building in the close vicinity of the monitoring site suggests that parallel winds blowing from the east would lead to low monitored concentration of the pollutants. For NE winds, the wind speeds and direction could be affected.



Figure 3.1 Monitoring site by the M4 motorway at Leixlip.

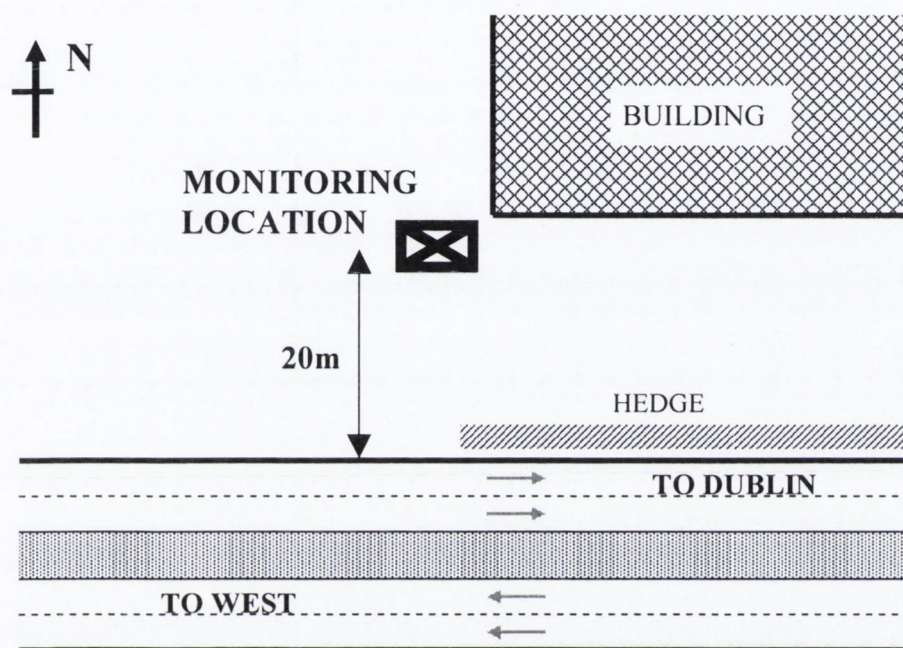


Figure 3.2 A schematic diagram of location of monitoring unit by the M4 site at Leixlip.

Meteorological data at the motorway site.

The major meteorological parameters of wind speed, wind direction, temperature and relative humidity were continuously recorded by Budd (2004) at the monitoring site. The sensors were located at a height of 6 m from the ground. Data was collected at every fifteen minutes intervals and was combined to give hourly averages. Atmospheric stability and cloud cover were recorded hourly at the aerodrome.

3.2.2 The Roundabout Site

The roundabout site selected by Budd. (2004) for the study was located on the N6 in Galway, named the Headford Road roundabout. It is considered to be the second busiest roundabout in Galway city. The roundabout connects five roads, signifying it as a five arm junction. The

three major road links are the N6 Dublin Road to the east, the N84 Headford Road to the north-northeast and the N6 road towards Galway city centre. Both N6 links are dual carriageways. The roundabout has a peak traffic flow of about 3900 vehicles/hour. The monitoring unit was located at 15 m from southern kerb of the Dublin Road arm, about 25m from the roundabout. The sensor height was 5m.

Figure 3.3 gives the schematic sketch of the roundabout site.

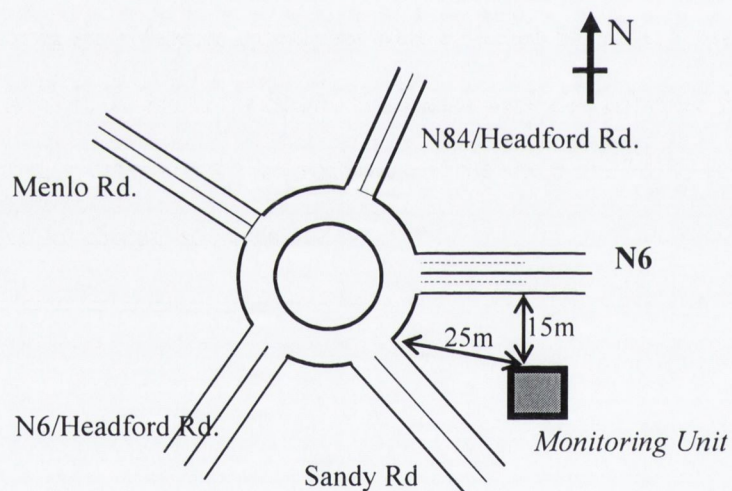


Figure 3.3 Schematic sketch of the Galway roundabout site, showing the junction layout.

Meteorological data at the roundabout site

As mentioned by Budd. (2004), the wind speed and wind direction was continuously measured at the monitoring site. Meteorological data were collected from Met Eireann's synoptic station at Shannon Airport, 70 km to the South. Some data were also collected from the roof of a 15 m high building, located about 2 km southwest of the site in the NUIG campus, and these data were also used for comparison with site data.

3.3 Screen Model (DMRB).

In general, a screening model is first applied to estimate concentrations at the study sites and then a more detailed model is applied for in depth study. Applications of screening models are one of the most common methods for estimating the effects of vehicle emissions, but they employ large simplifications of the physical processes involved in pollution dispersion and the effects of such simplifications on the accuracy of the result is often unknown.

The screening model applied here is the DMRB model. The model was developed by UK Transport Research Laboratory and is generally used for the initial assessment of any existing or planned road programmes. It includes a method for the estimation of vehicular emissions from light and heavy duty vehicles up to year 2020. Sharma and Khare (2001) reported that the primary objective of this model was to assess whether further air quality assessments were required, that the model was primarily designed for CO and that it was assumed that the dispersion characteristics of all other pollutants were equivalent to those of CO. In this context Budd (2004) applied the DMRB model at both the motorway and roundabout sites and checked whether the DMRB modelling results were within the limit values as specified by the EU daughter directives (CEC 1999, 2000). An updated version of the DMRB model (version 1.02, November 2003) subsequently became available and was applied at the study sites to:

- observe whether there was an improvement using the updated version of the DMRB model over the previous one at the selected sites for the same data sets.
- set a benchmark for detailed modelling studies.

The model in its simplest form employs a series of look up tables based on outputs from a Gaussian dispersion model. The previous version (1999) referred to in this study employs the following as input data:

- Hourly vehicle flow

- Proportion of light and heavy good vehicles
- Vehicular speed
- Year
- Distance to receptor
- Background Concentrations.

The updated version of the DMRB model (version 1.02, Nov 2003) uses the same input parameters with slight alterations. The Annual Average Daily Traffic (AADT) values are expressed in terms of vehicles per day rather than in vehicles per hour. In addition a road type parameter is introduced as explained in the Design Manual for Roads and Bridges (DMRB). Road type A signifies all motorways, whereas Road type B identifies all urban roads which are not motorways. Road type C classifies any other type of road. In addition to this Road type parameter D exists which is used to designate any other type of road employed by the user.

The screening model (DMRB) was initially employed to predict the concentration of certain pollutants at motorway and roundabout sites in Ireland. The pollutants considered in the study were CO, benzene, NO_x and PM₁₀. The present study involves the comparison of a previous version of the DMRB model (version 1999) with the updated DMRB model version (version 1.02, November 2003), including inter comparisons of modelled and monitored data. The performance of the model for motorway emissions was assessed for a free flowing straight stretch of the M4 close to Dublin. The roundabout situation was studied at a junction on the N6 in Galway. The modification of the roundabout problem from the original modelling approach was investigated, along with the variation of concentration with vehicle speed, by applying the latest version of the DMRB model to the actual 5 link and modified 3 link problem suggested by the DMRB.

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Highway Modelling – Part 1.

3.3.1 Model Input Data for Motorway.

The input parameters as determined by Budd (receptor and link data) and shown in Table 3.1 were utilized with the older version of the DMRB model. The same data set with some input modifications were also utilized with the latest version of the model. Application of the input data to the updated version of the DMRB model involved the input of AADT in vehicles/day, the road type (type A) and the distance of receptor from the centre of the road along with other input data (receptor name, year, link number, % HDV and average speed) already described.

Receptor and link	Receptor name	Leixlip WTW
	Year to be modelled	2001
	Link no (1-20)	1
	Link description	M4, Leixlip
	Distance to receptor (from centre of road) m	30
	Distance to receptor (from kerbside) m	20
	Annual average vehicle flow (veh/hr)	1400
	% HDV	20
	Average speed (km/hr)	90
Background concentrations (year adjusted)	CO (mg/m ³)	0.27
	Benzene (µg/m ³)	0.40
	NOx (µg/m ³)	11.73
	PM ₁₀ (µg/m ³)	11.90

Table3.1. DMRB input data for motorway

3.3.2 Model Input Data for Roundabout.

The input parameters recommended by Budd (2004) are shown in Table 3.2 and (receptor and link data) were utilized for the previous version of the DMRB model. The same data set has been used for in the updated version of the DMRB model. This is shown in Table 3.2

As mentioned before, while describing the data entry for motorway in DMRB model, a similar procedure is followed. The DMRB model predicts only the annual mean concentration; the

other equivalent values are obtained by performing mathematical calculations on the annual mean concentration as described later.

Receptor and link	Receptor name	Roundabout
	Year to be modelled	2001
	Link no (1-20)	5
	Link description	N6 Dublin Road Sandy Road N6 Headford Road Menlo N84
	Distance to receptor (from centre of road) m	15
		15
		35
		45
		45
	Distance to receptor (from kerbside) m	10
		10
		30
		40
		40
Background concentrations (year adjusted)	Annual average vehicle flow (veh/hr)	2480
		1070
		2760
		1200
		1790
	% HDV	7
	Average speed (km/hr)	15
	CO (mg/m ³)	0.21
	Benzene (µg/m ³)	0.40
	NO _x (µg/m ³)	11.73
	PM ₁₀ (µg/m ³)	12.90

Table 3.2 DMRB input data for roundabout

Modification of the roundabout problem.

In the previous investigation of the DMRB model, the 5 link road network was modelled explicitly. As per the latest guidelines issued by DMRB manual (February 2003) the 5 link problem can be transformed to a three link problem on the basis of traffic flows. In this study, the road links that were combined are links 1 and 3 and links 2 and 4 while link 5 remains as

the third link. Based on this modification the concentrations are obtained. Table 3.4 presents the results obtained using these 5 link and 3 link approaches with the 2003 version of the DMRB model and compares these with the results obtained using the 1999 version and with the measured values.

3.4 DMRB Model Results.

The results for the DMRB modelling exercise carried out at the motorway and roundabout sites are presented in this section. A speed versus emission characteristic study is also reported.

3.4.1 DMRB Model Results for Motorway.

Table 3.3 presents the model results and equivalent monitoring data. These results can be considered in three ways: by comparing the predicted values from DMRB using the old and the updated versions, by comparing equivalent statistical parameters obtained from the measured and monitored values and by applying certain numerical relations to the annual mean values of the pollutants that were measured and comparing these with model results.

If we compare the annual mean CO values from both versions of the model, it will be seen that there is no substantial difference in the concentrations. On the other hand the new version of the DMRB model gives a large reduction (46%) in the annual mean concentration of benzene. The predicted values for annual mean concentration of NO_x using the 2003 version of the DMRB model are also much lower (44%) than the concentration with the 1999 version. The comparison of the modelled concentrations of particulate matter shows a slight increment in the concentration with the new version of the DMRB screen model. It is to be stated that the new version of the DMRB model only gives the annual mean concentration of the pollutants.

Both versions of the DMRB model overpredicted the measured annual average concentration of CO by 20-30%. The 2003 version predicted a maximum running annual mean

concentration of benzene that is much closer to the measured value than did the 1999 version while both models grossly overpredicted the annual mean concentrations of NO_x . Use of the 2003 version led to good agreement between modelled and measured annual mean NO_2 concentrations. Both versions of the model predict annual PM_{10} concentrations that are close to the measured values, with the 1999 version result agreeing particularly well

For the different pollutants, certain mathematical relationships have been proposed that convert annual average concentrations to other statistical variables that agree with those specified as limit values. For example, the CO 8 hr mean concentration can be obtained by multiplying the CO annual mean concentration by a factor of 10, and the 90th percentile of the daily mean PM_{10} is 1.79 times the annual mean concentration of PM_{10} (Wealden Council, 2000). A similar relation has been proposed by Stedman and Dore (1998) to obtain the maximum annual running mean concentration of benzene from the annual mean concentration of benzene:

$$\text{Maximum annual running mean} = 1.102 \text{ annual calendar mean} - 0.004. (R^2 = 0.960) \quad (3.1)$$

These calculations have been applied to both the measured annual mean concentrations and the results of both versions of DMRB model. For the determination of the annual mean roadside concentration of NO_2 from the model predictions of the annual mean roadside concentration of NO_x , a more complex procedure was followed which involves the following steps :

1. Obtain the annual mean background concentrations of NO_2 and NO_x in the area – $\text{NO}_2(\text{background})$ and $\text{NO}_x(\text{background})$, respectively;
2. From model outputs, determine the contribution of emissions from the road to the annual mean concentration of NO_x at the location of interest - $\text{NO}_x(\text{road})$;

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3. Convert $NO_x(\text{road})$ to $NO_2(\text{road})$ using the equation

$$NO_2(\text{road}) = ((-0.068 \ln(NO_x(\text{total}))) + 0.53 NO_x(\text{road})) \quad (3.2)$$

where, $NO_x(\text{total}) = NO_x(\text{background}) + NO_x(\text{road})$;

4. Add $NO_2(\text{road})$ to $NO_2(\text{background})$ to obtain the total concentration of NO_2 at the location of interest.

Lastly, a comparison is made between all the statistical equivalent parameters for all the pollutants for which the values are obtained. For example, considering the CO 8 hr mean values it can be seen that the actual measured concentration were 2.56 mg/m^3 , as predicted from the old version of DMRB was 3.69 mg/m^3 , from the new version 3.9 mg/m^3 and as obtained by using mathematical relationship is 3.2 mg/m^3 . This shows that there still is significant overprediction by both versions of DMRB and as calculated from annual mean, to a lesser extent. Similarly the actual benzene maximum running annual mean was $0.53 \mu\text{g/m}^3$ while values obtained by the DMRB model are $1.09 \mu\text{g/m}^3$ and $0.59 \mu\text{g/m}^3$, using the old and new versions, respectively. Similarly for NO_2 , the annual mean concentration was $19.37 \mu\text{g/m}^3$ and as obtained by the DMRB model were $58.27 \mu\text{g/m}^3$ and $15.86 \mu\text{g/m}^3$ using the old and the new versions respectively, and that obtained from the annual NO_x concentration was $17.09 \mu\text{g/m}^3$. This shows that the new version of DMRB model and the calculated value from annual mean are in close proximity to the actual measured value, whereas the older version of DMRB overpredicts by a factor of 3. For particulate matter it is seen that the values for 90th percentile of daily means are close to the actual value, with a general tendency of overprediction.

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	Measured concentrations		DMRB model Prediction	
	Actual	Calculated from annual mean	1999 version	2003 version
CO annual average (mg/m ³)	0.32	0.32	0.37	0.39
CO 8 hr mean (mg/m ³)	2.56	3.20	3.69	3.90
benzene annual mean (µg/m ³)	-	-	0.99	0.54
benzene maximum running annual mean (µg/m ³)	0.53	-	1.09	0.59
NO _x annual mean (µg/m ³)	32.29	32.29	142.05	80.13
NO ₂ annual mean (µg/m ³)	19.37	17.09	58.27	15.86
PM ₁₀ annual mean (µg/m ³)	15.50	15.50	15.83	17.99
PM ₁₀ 90percentile daily mean (µg/m ³)	22.83	27.75	28.34	32.2

Table 3.3 DMRB model results at motorway site.

3.4.2 DMRB Model Results for Roundabout.

It is to be noted that same procedure was followed for the roundabout as for the motorway when calculating equivalent statistical values. The mean annual concentration of all the pollutants considered was measured at the roundabout site by Budd (2004). By using the numerical relationships as described before, the equivalent statistical parameters were calculated based on the values of annual average mean. In a similar fashion, the entire statistical equivalent parameters of all the pollutants were measured at the monitoring site by Budd. The actual measured values of the statistical equivalents and the equivalent values calculated from the measured annual means are presented Table 3.4

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Pollutant	DMRB model results			Measured Concentration	
	1999 5 links	2003 5 links	2003 3 links	Actual	Calculation from annual mean
CO annual average (mg/m ³)	2.09	2.25	1.36	0.54	0.54
CO 8 hr mean (mg/m ³)	20.93	3.9	13.6	2.86	5.4
benzene annual mean (µg/m ³)	12.54	4.39	2.53	-	-
benzene maximum running annual mean (µg/m ³)	13.79	4.83	2.78	-	-
NO _x annual mean (µg/m ³)	774.95	283.2	165.04	39.42	39.42
NO ₂ annual mean (µg/m ³)	193.95	39.65	31.84	19.79	13.09
PM ₁₀ annual mean (µg/m ³)	44.91	54.68	36.49	25.50	25.50
PM ₁₀ 90percentile daily mean (µg/m ³)	80.38	97.88	65.32	39.61	45.62

Table 3.4 DMRB model results at the roundabout site.

From the comparison Table 3.4, it is clearly evident that the 2003 version of DMRB screen model, to a very large extent predicts much lower concentrations for benzene and NO_x when compared to the 1999 version. The percentage decrease is 65% and 64% for benzene and NO_x respectively. It is also observed that there is no significant difference in the CO concentration prediction given by the two versions of the model as in the motorway case. The PM₁₀ values predicted using the new version lie in close proximity to the value obtained using the older version, but it is observed that there is a slight increase in the concentration predicted by the newer version. These observations agree with those at motorway site. It is seen from the

results that using the updated version of the DMRB model that for benzene and NO₂ yields predicted results which lie within the EU limit values using both as 5 link and 3 link problem. The limit values for CO and PM₁₀ are satisfied using the 3 link approach but exceeds the limit values using 5 link approaches.

The results obtained by modifying the five link arm to the three link arm problem show a significant decrease in the concentrations of all pollutants. The reduction in CO concentration is about 40%, while the reduction in benzene concentration is 42%. A similar reduction in the concentration of NO_x of 41% is observed. The PM₁₀ concentration reduces by 33%.

The annual mean values for all pollutants were recorded at the roundabout monitoring site as were the statistical equivalent parameters for all pollutants were also measured at the roundabout site. By using the mathematical relations, reference of which has been mentioned previously, statistical equivalent parameters for the pollutants calculated and compared with the actual measured data. It will be observed that while for CO the actual maximum 8 hour mean concentration measurement was much lower than the value predicted from the annual mean concentration, the comparison results for NO₂ show better agreement with a slight underprediction. In a similar fashion, the results for particulate matter show that the actual measured values and those predicted from the annual mean are in close proximity to each other with a slight tendency of overprediction. No monitoring data was available for benzene at the roundabout site.

Lastly if all the equivalent statistical parameters for the respective pollutants are compared it can be seen that irrespective of the modelling approach (3 or 5 links) or model version (1999 or 2003) employed the predicted values heavily overpredict the measured concentration. The only indicative point is that by applying the newer version of DMRB model the modification

of the five arm roundabout to the three arm roundabout the levels of overprediction decrease considerably.

3.4.3 Study of speed versus emission characteristics for new version of DMRB model (5 links and 3 links).

The vehicle speeds on the approaches and through the roundabout are highly variable.

Speeds versus concentration curves were plotted for both the 5 link and 3 link problems using the 2003 model version. This was done for all pollutants by varying the average vehicle speed value of 15km/hr given in Table 3.2. Figures 3.4 -3.7 present these curves.

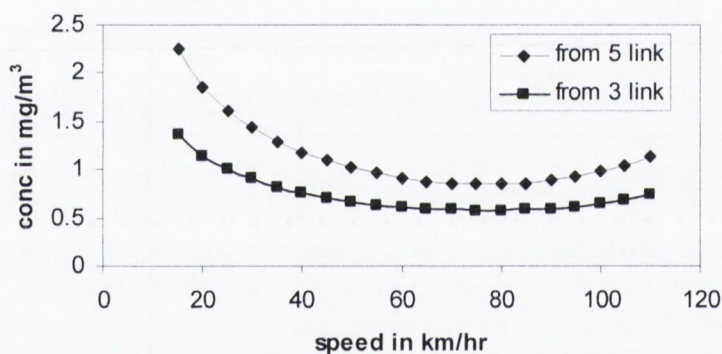


Figure 3.4 Comparison of speed versus concentration for CO for 5 link and 3 links.

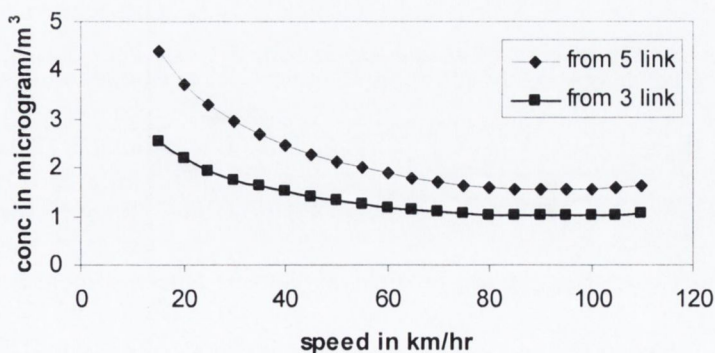


Figure 3.5 Comparison of speed versus concentration for Benzene for 5 link and 3 links

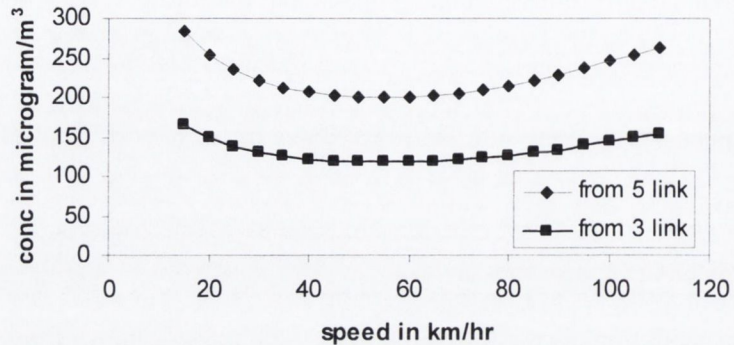


Figure 3.6 Comparison of speed versus Concentration for NO_x for 5 link and 3 links

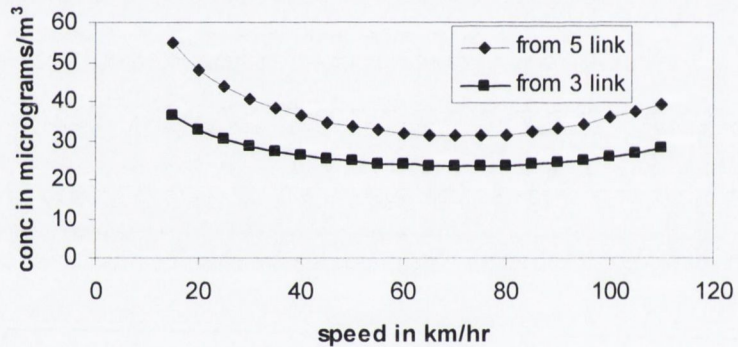


Figure 3.7 Comparison of speed versus Concentration for PM_{10} for 5 link and 3 links.

Similar patterns are displayed for all pollutants, although the differences in concentration obtained by using the original 5 link and modified 3 link approaches are significant. As average vehicle speed increases above 15km/hr the model predictions all reduce until they reach a minimum at certain speed that varies from pollutant to pollutant. These speeds for both the versions were found to be 60km/hr, 75km/hr, 85km/hr, and 100km/hr for NO_x , PM_{10} , CO and benzene respectively. Clearly the level of agreement between measured and modelled concentrations will depend strongly on the average vehicle speed assumed. Traffic conditions at the roundabout varied and 15km/hr was a reasonable value for times when flow through the

junction is congested. At other times, higher speeds up to 60km/hr would be appropriate. The DMRB model cannot represent this level of complexity; however it is worth noting that using an average vehicle speed of 30km/hr in with the 3 link model recommended in the 2003 DMRB version leads to very good agreement between the modelled and measured annual average concentrations of CO and PM₁₀.

3.4.4 Study Conclusions.

It was seen that from the comparison results that the newer version of the screen DMRB model is successful in predicting reduced concentrations for NO_x and particulate matter at the motorway and gives close results for the other pollutants when compared to the old version. For the same site a comparison of statistical equivalent parameters for the respective pollutants were made, based on actual measurements of those parameters and values calculated from the measured annual mean concentrations by applying previously proposed numerical relations.

A similar approach was followed in the study of the roundabout. Here, certain modification to the actual conditions was applied as suggested in the DMRB manual. This led to improved but still overpredicted model estimates. The level of overprediction was seen to depend on assumed average vehicle speed. Overall, it can be concluded that the DMRB model gives conservative estimates of traffic emission impact.

After analyzing the results obtained using the screen model, it is clear that more detailed modelling analysis is necessary if accurate predictions are required. In this context, a detailed modelling analysis was carried out for the motorway site using the GFLSM and CALINE4 models. The description of these models along with the modelling results is described in the following sections. The pollutants selected for the purpose of this study were CO and NO_x and separate hourly concentrations are predicted for each hour of the study period.

3.5 Detailed Highway Modelling.

This work builds upon that of Budd (2004) who examined the accuracy of the CALINE4 model, by assessing the relative performance of a simpler analytical model, the GFLSM and examining key issues of emission factors and background concentrations in more detail.

3.5.1 The roadside dispersion model GFLSM.

The General Finite Length Source Model (GFLSM) is based on the Gaussian diffusion equation and is formulated so that it can be applied for any wind direction and any length of line source. Its solution is based on the modification of an equation derived by Csanady (1972) that allowed receptor concentrations due to emissions from a finite length line source to be calculated for perpendicular winds. The modification by Luhar and Patil (1989) extended this solution to include all possible wind road angles. The main advantage of this model lies in the simplicity of its application. The main disadvantage of the model is the limited receptor co-ordinates for which concentrations can be calculated. The GFLSM requires the receptor to be located at 90 degrees to the segment of road considered, and the length of the line source should be at least three times the distance between the receptor location and road. (Gokhale and Khare, 2004). The GFLSM uses the following equation to calculate the contribution of a line source to ambient concentrations (Luhar and Patil, 1989):

$$C = \frac{Q_l}{2\sqrt{2\pi}\sigma_z(u\sin\theta + u_0)} \left[\exp\left(-\frac{(z-h)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z+h)^2}{2\sigma_z^2}\right) \right] \times \left[\operatorname{erf}\left(\frac{\sin\theta(p-y) - x\cos\theta}{\sqrt{2}\sigma_y}\right) + \operatorname{erf}\left(\frac{\sin\theta(p+y) + x\cos\theta}{\sqrt{2}\sigma_y}\right) \right] \quad (3.3)$$

where C is the receptor concentration, Q_l is the source strength per unit length, u is the average wind speed, θ is the angle between the wind direction and the road varying between 0-180 degrees, x , y and z are the receptor co-ordinates relative to an origin located at the

midpoint of the line source, h is the effective source height, p is the half length of the line source, erf is the error function and σ_z and σ_y are the vertical and horizontal dispersion coefficients. The term u_0 is a wind speed correction to account for the effects of traffic wake and assumes different values for different stability classes as suggested in the GM model (Chock, 1978). The vertical and horizontal dispersion coefficients are dependent on the downwind distance ' x ' and the Pasquill (1974) stability class. The Briggs urban dispersion coefficients are employed for σ_z and σ_y (Zannetti, 1990).

Measured traffic and meteorological data, and roadway geometry were used as the input parameters to the model. The emission rate, Q_l was determined from composite vehicle emission factors calculated using the COPERT methodology (Kouridis et al, 2000); as described later. A schematic representation of the GFLSM is shown in Figure 3.8

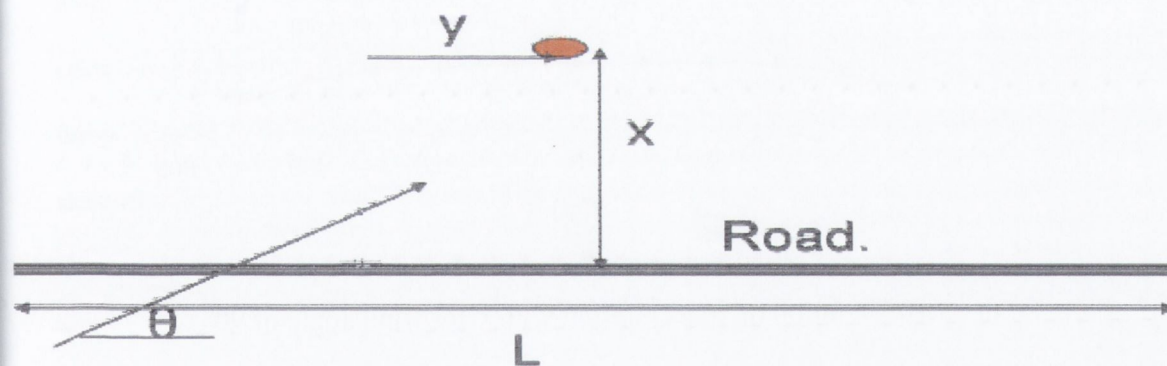


Figure 3.8 Schematic representation of the GFLSM model.

From equation 3.3 it is clearly evident that the concentration values predicted using the GFLSM model are heavily influenced by the ' y ' coordinate of the receptor. Figures 3.9 and 3.10 show the variation of concentration with ' y ' for wind directions corresponding to 45° and 90° .

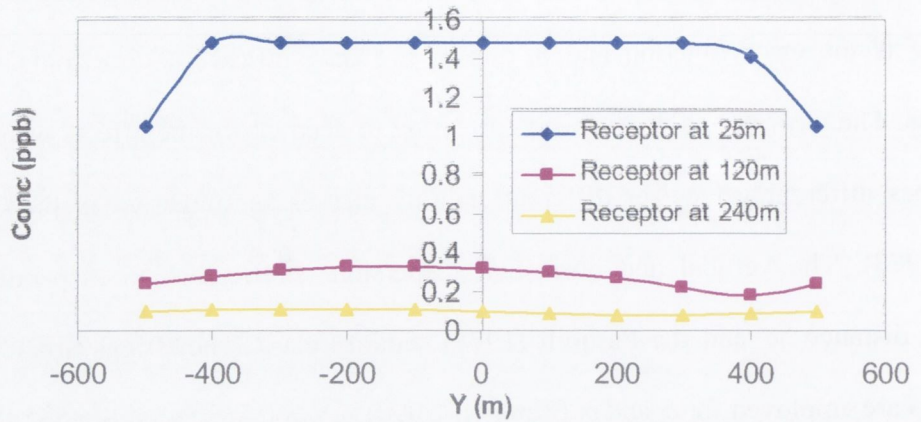


Figure 3.9 Variation of concentration with y for wind angle of 45° .

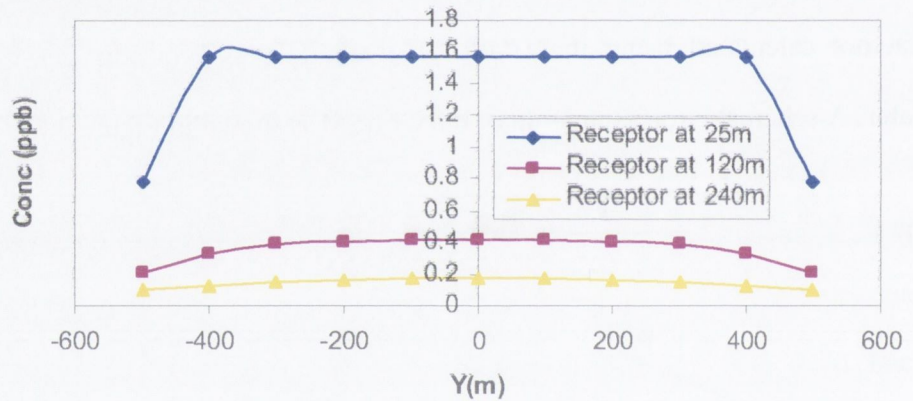


Figure 3.10 Variation of concentration with y for wind angle of 90° .

GFLSM modelling at the M4 motorway site.

For the Leixlip (M4) motorway site, the road length modelled was 1250m; hence a p value of 625m was employed. The values of 'x' 'y' and 'z' coordinates used for the study were 30m, 0m, 4m respectively. The value of the 'y' coordinate was zero as the receptor was placed at the centre of the road link. The 'h' value used was 0.5m. Recorded meteorological parameters of wind speed and wind direction were used. The dispersion coefficients were calculated using Briggs equation for the particular stability class in each particular hour (Zannetti, 1990).

3.5.2 The roadside dispersion model CALINE4

CALINE4 is a computer-based line source Gaussian dispersion model that uses semi-empirical solutions to the Gaussian dispersion equation (Benson, 1992; Sharma and Khare, 2001). It was developed to calculate CO concentrations but it can be used to predict the concentrations of various other pollutants (other inert gases, NO₂, and particulates) in a variety of road networks (Marmur and Mamane, 2003). The input parameters required for the model involve roadway geometry, meteorological parameters, traffic flow and composite emission factors.

The road modelling approach followed by CALINE4 is to divide highway links into a series of elements from which incremental concentrations are computed and then summed to obtain the total concentration estimate at a particular receptor location. Each element is further subdivided into three sub-elements and each sub-element is orientated at right angles to the wind direction, allowing the analytical solution of Csanady (1972) to be applied. This is shown in Figure 3.11.

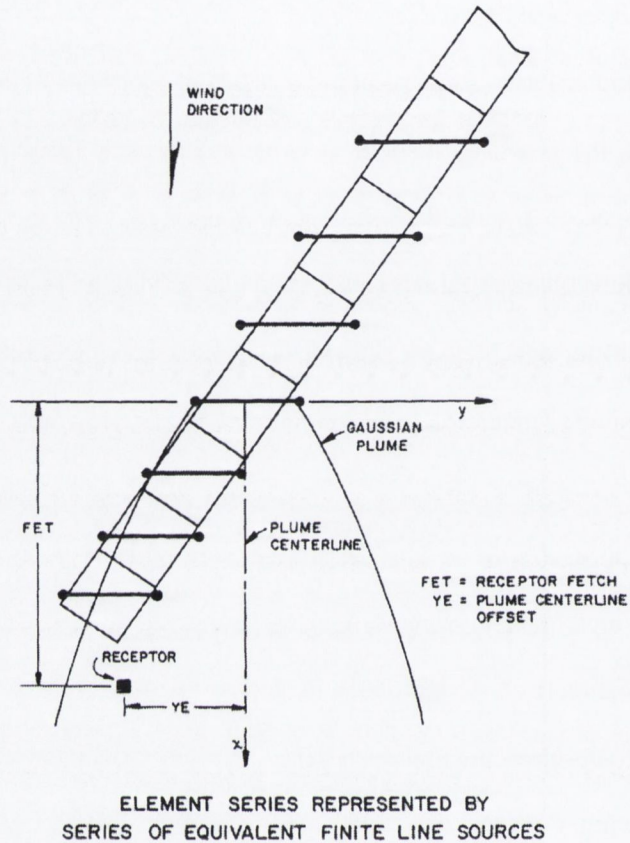


Figure 3.11 Element series represented as finite series of equivalent line sources in CALINE4

Central to the CALINE4 model is the concept of a ‘mixing zone’ that exists above the roadway where the intense mechanical turbulence, augmented by buoyancy, results in enhanced mixing of pollutants (Held et al, 2003). The primary role of the mixing zone is to establish initial Gaussian dispersion parameters at a reference distance near the edge of the roadway. Hence, the initial vertical dispersion parameter σ_{zi} at the edge of the mixing zone is evaluated using an empirical equation (Cadle et al, 1977):

$$\sigma_{zi} = 1.5 + t_r / 10 \quad (3.4)$$

where: t_r is the pollutant residence time in the mixing zone. This is shown in Figure 3.12.

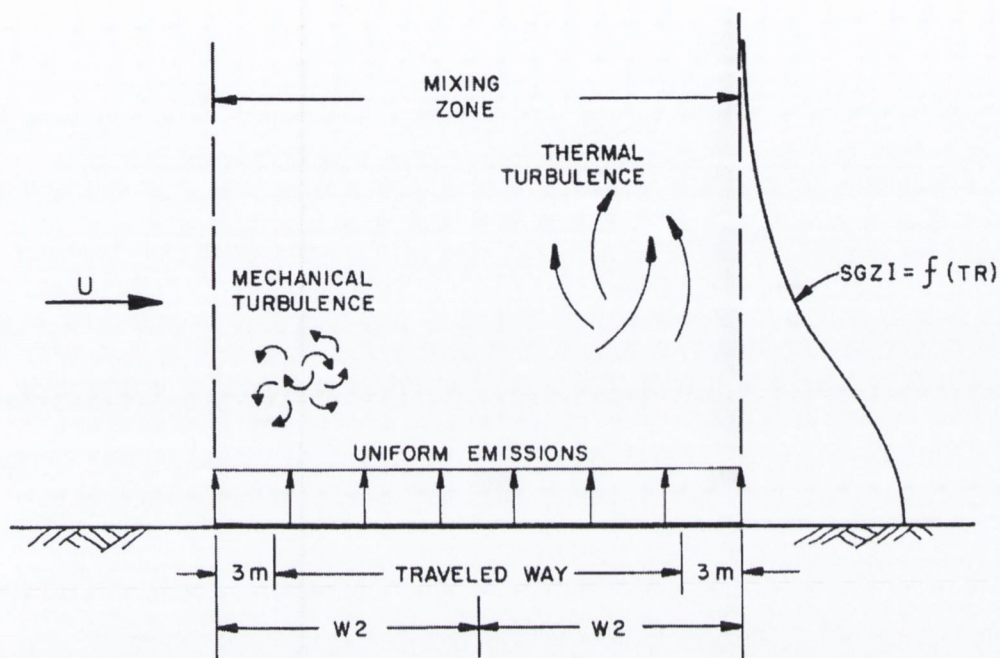


Figure 3.12 Mixing zone concept used in CALINE4

Between the edge of the mixing cell and the reference distance, the vertical dispersion coefficient, σ_z , is estimated using a modified power curve approximation, which takes the functional form (Benson, 1989):

$$\sigma_z = P_{z_1} \cdot R_{FET}^{P_{z_2}} \quad (3.5)$$

Where: P_{z_1} and P_{z_2} are power curve coefficients; and R_{FET} is the element fetch, which is the downwind distance to a receptor from a cross wind line drawn through the centre of the element.

3.5.3 Evaluation of vehicular emissions.

Atmospheric dispersion modelling requires information on the emissions of pollutants from the target source. COPERT III (Computer Programme to calculate Emissions from Road Traffic) is an emission model developed by the European Environment Agency (Kouridis et al, 2000), to estimate emissions of a wide range of pollutants from road transport. The emission equations and methodology embedded in this programme were employed to estimate composite CO emission factors for the traffic conditions encountered in this study. The COPERT methodology covers a wide range of vehicles, divided into five primary categories, and sub-divided by model year, emission-reduction technology, engine volume, weight and fuel type. Methods to calculate hot (exhaust), cold start and evaporative emissions are set out. To calculate representative composite emissions factors, up to date vehicle fleet statistics are required. To this end, information on the composition of the 2003 Irish car fleet was employed (CSO, 2004), which reflected the considerable renewal of the fleet in the years immediately preceding the field study.

Separate COPERT III equations are used to estimate hot (exhaust) emissions for uncontrolled (pre-Euro 1) and controlled (Euro 1 and later) passenger cars and goods vehicles, while emission reduction percentages are applied for post-Euro1 passenger cars and post-conventional HGVs. For each particular vehicle category, these were used to calculate total hot exhaust emissions for an average speed of 100km/hr. By using this information with the characteristics of the 2003 traffic fleet, and the estimated annual kilometres travelled by each vehicle type (Reynolds, 2000), a weighted emission factor was estimated.

Heeb et al. (2003), outlines that 90% of cold start emissions from Euro 1 and Euro 2 cars are emitted within the initial 1.6 km travelled, and within 0.5 km for Euro 3 cars. These three

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vehicle types make up the vast majority of the 2003 fleet. Heeb et al (2003), also states that cold start emissions are not significant during motorway driving, while Ntziachristos and Samaras (2000) outline in the COPERT III methodology that cold start emission is in the main confined to urban driving conditions. As a result, the equations in COPERT III do not cater for cold start emissions from vehicles on motorways, and the highest speed for which cold start emissions can be estimated is 45km/hr. For these reasons cold start emissions are assumed to be low and are not considered further in this study. Emission factors of 1.75g/km and 0.50g/km computed assuming a mean vehicle speed of 100km/hr were used for CO and NO_x respectively. Hourly emission factors (HEF) were also computed using the COPERT III methodology as an alternative to these composite emission factors so as to assess the performance of GFLSM. The HEFs for the Leixlip highway study were obtained by plotting the percentage of HGV against the emission factor. Since the percentage of HGV was known for each hour of the monitoring period, an individual HEF could be calculated for each hour. The graphs for calculating HEFs for CO and NO_x are shown in Figures 3.13 and Figures 3.14 respectively.

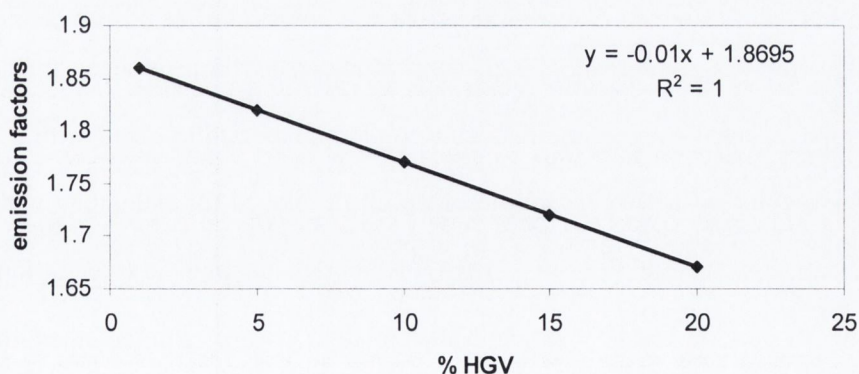


Figure 3.13 Hourly emission factors for CO

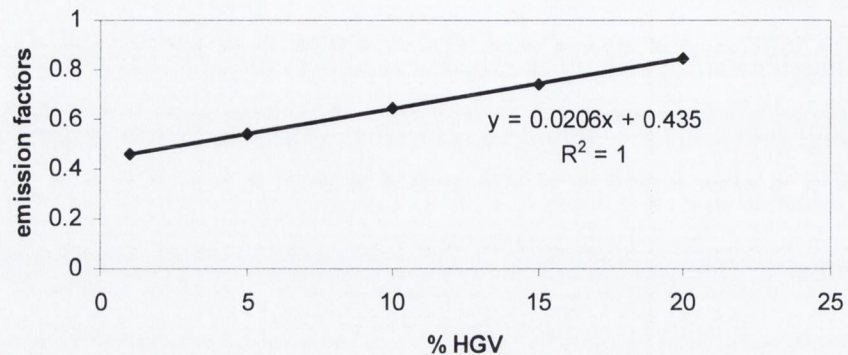


Figure 3.14 Hourly emission factors for NO_x

3.6 Modelling Results for CO.

3.6.1 Measured and modelled concentrations.

Figure 3.15 represents a graph showing a sample of the hour-by-hour monitored and predicted data obtained using GFLSM and CALINE4 at the study site for January 2002. It is observed from Figure 3.15 that there are certain high peaks of monitored data and that some zero concentrations of monitored data. One of the reasons for the high peaks of monitored data could be due to thermal inversions associated with high pressure systems that do not break up during the daytime. Figure 3.15 also highlights the fact that the Gaussian based dispersion models are unable to predict these high concentrations as these models are deterministic models that calculates the mean pollutant concentration expected to occur with a given set of input parameters. Its predictive capabilities are well developed for estimating both short- and long-term average concentrations, but it is not able to predict extreme concentrations that occur due to stochastic variability. If extreme value predictions are required, then these can be determined by fitting an appropriate statistical distribution, identified from a goodness of fit test, to the modelled data. This approach fits within the general concept of hybrid modelling,

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which involves fitting an appropriate statistical distribution to modelling results obtained using deterministic models such as GFLSM and CALINE4.

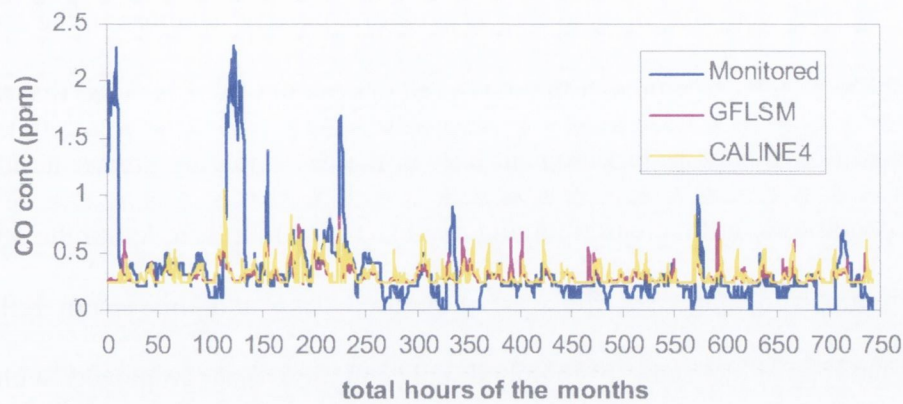


Figure 3.15 Plot of hour by hour values of measured and modelled data for January 2002.

The average diurnal variations in the measured and modelled CO concentrations are shown in Figure 3.16.

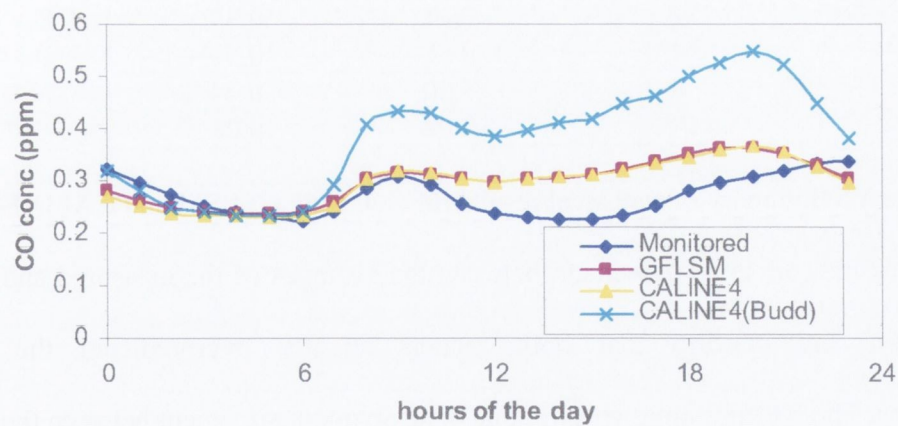


Figure 3.16 Average diurnal variations in CO concentration at the M4 motorway site

All the modelled values include a background concentration of 0.23ppm, identified as the average CO concentration observed when the traffic source was at a minimum in the early hours of the morning. The measured peak annual average hourly CO concentration is 0.33ppm

at 23:00, whereas the modelled peaks at 20:00 hours are 0.36ppm and 0.37ppm obtained using GFLSM and CALINE4 respectively. It was observed from the figure that both models are able to predict the peak concentrations in the early part of the day, whereas in the latter part both models tend to slightly overpredict the measured concentration. It is noted that the ‘unstable’ stability condition was more predominant later in the day implying greater turbulence during low wind conditions, and increased mixing depths. This could have led to the afternoon drop in the diurnal profile obtained from the monitored data, and this is not reflected in the predicted data as a constant background concentration was employed with the model calculations. More importantly for this study, the diurnal profiles obtained with the GFLSM and CALINE4 models show very close agreement.

To further compare the GFLSM and CALINE4 models with the monitored data, statistical analysis of the entire data set was performed, the results of which are shown in Table 3.5.

Model/Parameters	GFLSM	CALINE4
IA	0.41	0.39
NMSE	0.60	0.59
R	0.20	0.24
FB	0.09	0.08
F2(%)	60	60

Table 3.5 Summary of statistical results for CO using GFLSM and CALINE4.

The FB values indicate good agreement between the averages of the measured and modelled concentrations, and confirm that both models slightly overpredicted the observed concentrations. The NMSE values confirm that a not so good agreement between the modelled and measured data sets was observed on an hour by hour basis. About sixty percent of the predicted datasets obtained using both GFLSM and CALINE4 lay within a factor of two of their correspondingly hourly measurements. The R- values indicate that the degree of correlation between the monitored and predicted data obtained with either model is not high;

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however this statistic is strongly influenced by short term variations in background concentrations, which affect both set of model results equally. On an overall basis, the statistical results obtained from GFLSM model are marginally better than those obtained with the CALINE4 model. However, it is clear that the statistical results obtained by comparing the monitored and predicted data from both models are consistent.

This is highlighted by the scatter plot in Figure 3.17 comparing the hourly concentrations calculated with either model for the period January 2002. A high degree of correlation between the predicted data obtained with either model is observed. The similarity between the performances of the two models suggests that the GFLSM is a suitable basis for wider studies on modelling practice and sensitivity.

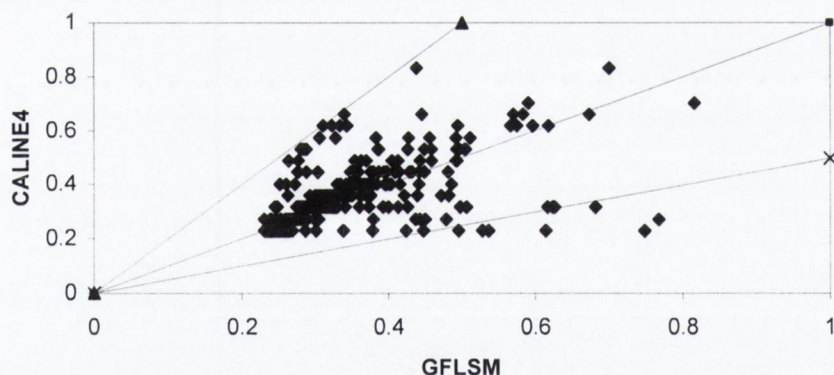


Figure 3.17 Scatter plots of predicted data at Leixlip site for January 2002.

The GFLSM model was further tested with hourly emission factors (HEF) derived from COPERT III methodology (Kouridis et al, 2000). Statistical analysis of the predicted data, so obtained was compared with the statistical analysis of the predicted data obtained using constant composite emission factors (CEF). These results are presented in Table 3.6 and indicate no improvement when HEFs rather than constant CEFs were used at this particular site.

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Model/Parameters	GFLSM (CEF)	GFLSM (HEF)
IA	0.41	0.40
NMSE	0.60	0.61
R	0.20	0.20
FB	0.09	0.09
F2	60	60

Table 3.6. Summary of statistical results for CO using GFLSM for CEF and HEF.

However, the use of HEFs is considered to be a better logical approach then constant CEFs and could yield better results for different pollutants or at different study sites, especially where traffic and emission characteristics vary greatly during the course of the day. This is further investigated in section 5.3.3 of chapter 5.

3.6.2 Sensitivity analysis of GFLSM model.

Sensitivity analysis of the GFLSM model was carried out by performing statistical computations on the predicted data obtained under different stability categories and wind speed conditions. The results are shown in Tables 3.7 and 3.8.

Parameters/Stability class	Unstable	Stable	Neutral
IA	0.39	0.47	0.53
NMSE	0.40	0.43	0.10
R	0.30	0.14	0.49
FB	-0.16	-0.34	0.26

Table 3.7 Stability class analysis of CO data.

Parameters/Wind speed	<0.5m/s	0.5-2m/s	>2m/s
IA	0.35	0.39	0.50
NMSE	0.68	0.23	0.12
R	-0.09	0.11	0.50
FB	-0.40	0.10	0.30

Table 3.8 Wind Sensitivity analysis of the CO data.

For the stability class analysis, the entire monitored and predicted data sets were sorted according to the stability conditions pertaining for each hour. Three classifications were considered: unstable, stable and neutral. It was observed that the model performed best under

neutral conditions. The relatively large underprediction of mean concentration during stable conditions, indicated by the FB value of -0.34 is attributable to the use of a constant background concentration, rather than reflecting the GFLSM calculations themselves.

In a similar fashion, for the wind sensitivity analysis study the monitored and modelled data were sorted for three different wind speed classes (defined as less than 0.5m/s, between 0.5 and 2m/s and greater than 2 m/s) and were statistically analysed. It was observed that the GFLSM model performed best for wind speeds above 2m/s (for this particular study) and performed least well for wind speeds less than 0.5m/s (calm conditions). The low R value observed for the low wind concentration arises because under these conditions, wind direction is poorly defined which affects model reliability. The FB value displayed during low wind conditions is in line with that observed for stable conditions which are normally associated with low wind speeds. The effect of wind direction on model performance is addressed in Chapter 7.

3.6.3 Statistical distribution analysis

The results obtained from the goodness of fit tests on the monitored and modelled CO concentrations are presented in Table 3.9.

Statistical distribution	Monitored data		Modelled data			
			GFLSM		CALINE4	
	KS	AD	KS	AD	KS	AD
Weibull	0.13	0.72	0.10	0.45	0.12	0.51
Gamma	0.145	0.69	0.13	0.61	0.14	0.80
Lognormal	0.15	0.75	0.14	0.68	0.15	0.88

Table 3.9 Goodness of fit results.

The result of these tests show that the both sets of modelled data were best fit by the Weibull distribution, followed by the gamma distribution and thirdly by the lognormal distribution for the predicted data sets. However, for the monitored data, the AD test suggests that it is best fit

by the gamma distribution, while the KS test suggests the Weibull distribution. The individual parameter values obtained for each of the three fits are summarised in Table 3.10 and the probability distribution plots are shown in Figure 3.18 (a)-(c).

Statistical distribution	Monitored data	Modelled data	
		GFLSM	CALINE4
	Parameters	Parameters	
Weibull	$\lambda=7.83, \sigma=0.28$	$\lambda=7.98, \sigma=0.32$	$\lambda=7.28, \sigma=0.31$
Gamma	$\alpha=52.04, \beta=5.21 \times 10^{-3}$	$\alpha=54.72, \beta=5.47 \times 10^{-3}$	$\alpha=46.73, \beta=6.34 \times 10^{-3}$
Lognormal	$\mu=-1.32, \sigma=0.14$	$\mu=-1.22, \sigma=0.14$	$\mu=-1.23, \sigma=0.15$

Table 3.10 Parameter values of the various statistical distribution fits

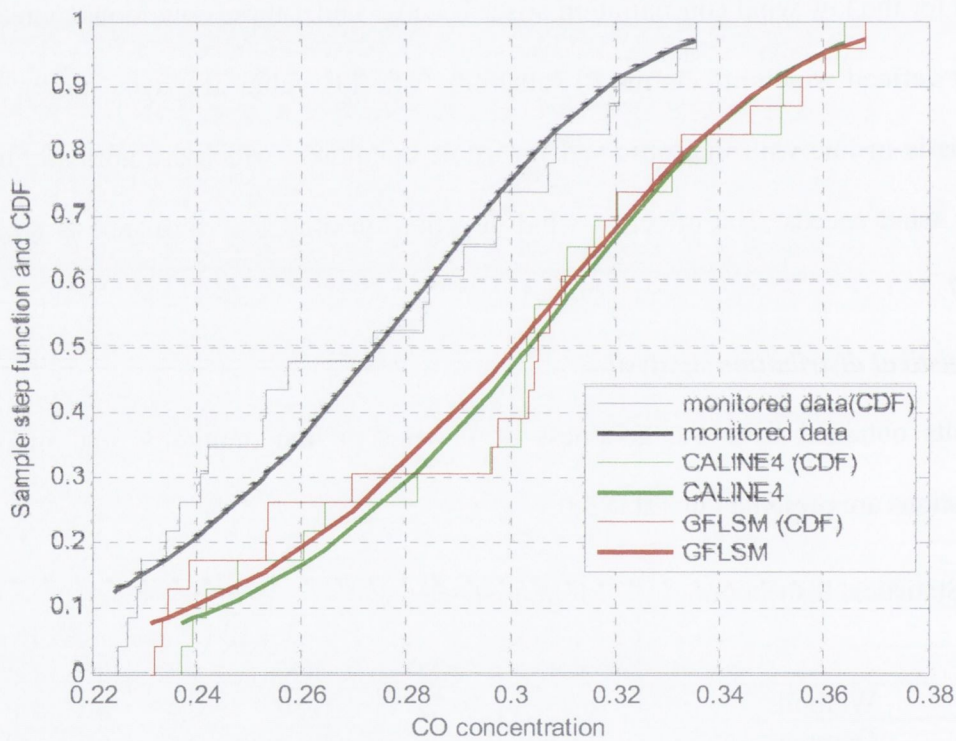


Figure 3.18(a) Probability distribution plots –Weibull.

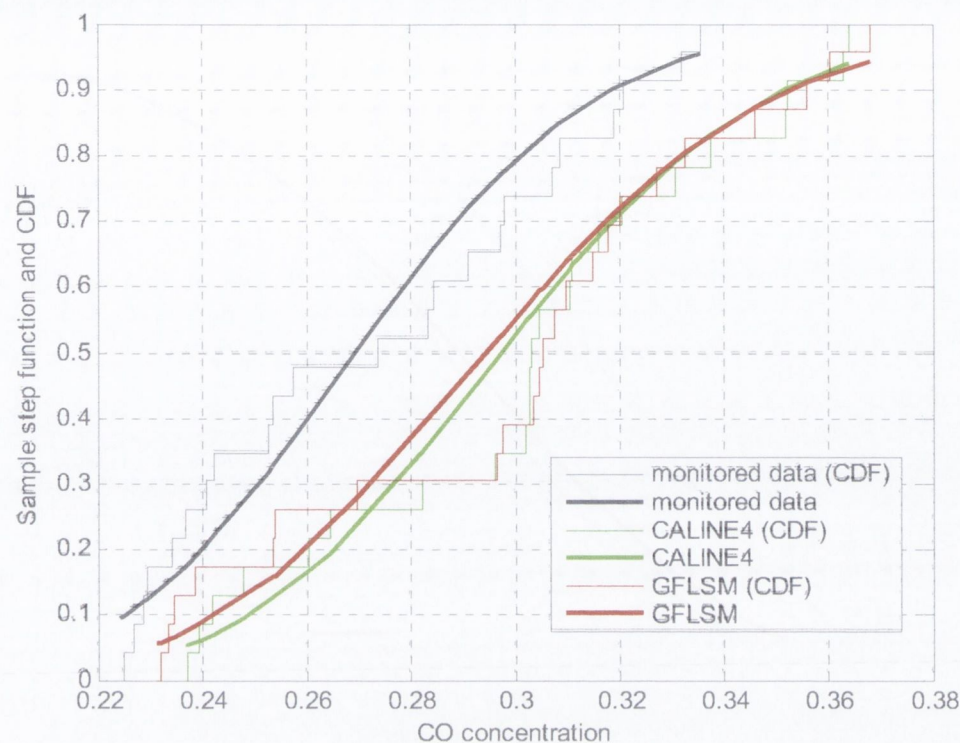


Figure 3.18(b) Probability distribution plots –Gamma.

These results suggest that while there are differences between the distributions of monitored and modelled data (depending upon the goodness of fit selected), neither the GFLSM nor the CALINE4 model results achieve a better match with the monitoring data.

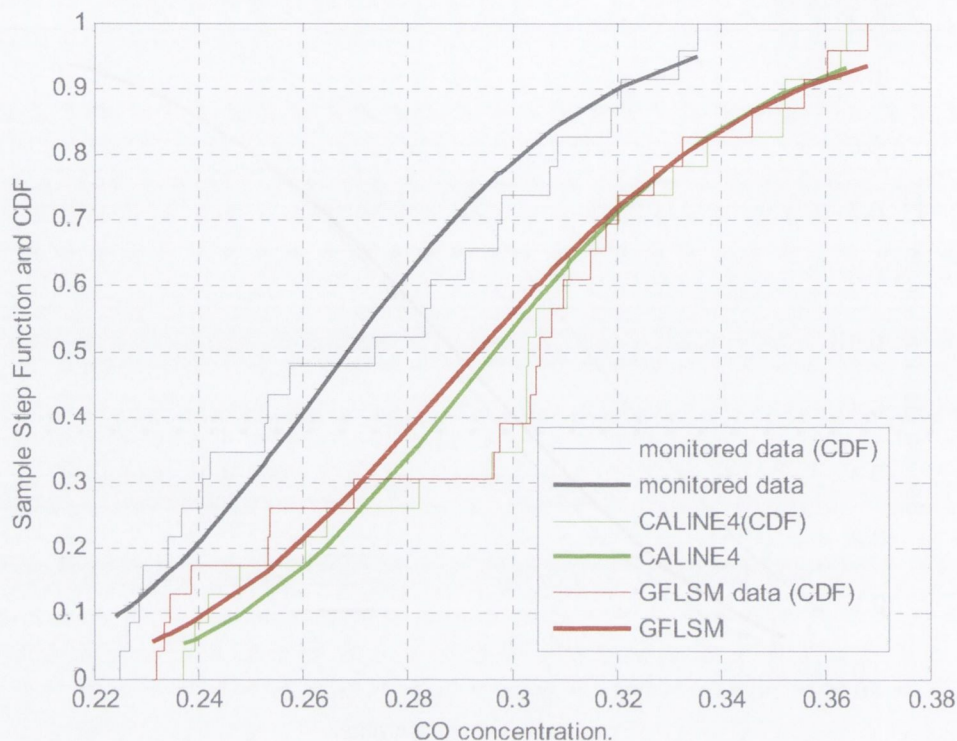


Figure 3.18(c) Probability distribution plots –Lognormal.

3.6.4 Study Conclusions

The modelling exercise carried out for the pollutant CO represents an inter-comparison of the GFLSM and CALINE4 atmospheric dispersion models against monitored data collected in an ambient CO measurement campaign conducted adjacent to a four-lane motorway. Graphical and statistical analyses revealed reasonable agreement between the measured and predicted datasets using both models. For the purpose of comparing the predicted data obtained with the two models, a constant emission factor was used. The alternative use of specific hourly emission factors was investigated using the GFLSM model, but improved model performance was not indicated.

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Sensitivity analysis of the GFLSM model data was performed by considering the influences of wind speed and atmospheric stability. This revealed that the model works best for neutral conditions and for wind speeds exceeding 0.5 m/s i.e., non-calm conditions.

A statistical probability plot was also fitted to the monitored and predicted data to characterise the statistical variation of the data. It was found that the Weibull distribution was generally best suited to both the monitored and predicted data at the particular site considered. The performance of the GFLSM and CALINE4 models was very similar in this regard.

This study shows that the performance of GFLSM, an analytical model, is similar to that of CALINE4, a more complex numerical and a computer based modelling system, and in fact marginally outperformed the CALINE4 in this study. These results indicate that the GFLSM offers a good basis for highway modelling studies, including parametric studies and sensitivity analyses aimed at improving dispersion modelling practice. The following section and chapters present studies of this kind.

3.7 Modelling Results for NO_x

The performances of the GFLSM and CALINE4 models examined in the previous section are partly obscured due to the varying contribution of regional air quality - or - background concentrations to the total ambient concentrations measured at the receptor.

Over the course of monitoring period, to record this background concentration, a second NO_x monitoring instrument placed approximately 200m south of the motorway recorded hourly NO_x concentrations for the last six months of the monitoring period. Using this data, the final modelled hourly NO_x concentration obtained from the application of the GFLSM model can be represented as:

$$(\text{NO}_x)_{\text{FP}} = (\text{NO}_x)_P + (\text{NO}_x)_{\text{BKG}} \quad (3.6)$$

Where $(NO_x)_{FP}$ is the final predicted hourly concentration, $(NO_x)_P$ is the GFLSM predicted hourly concentration and $(NO_x)_{BKG}$ is the measured hourly background concentration.

It will be observed from the above equation that the final predicted values are dependent on the assumed background concentrations. A detailed study was performed to analyse model performance with different background concentration assumptions. Five such cases were considered, which are briefly described here:

3.7.1 Background Concentration Assumptions

Case 1

In the first case, the mean of the entire six months of hourly background concentrations, irrespective of any hour to hour variation, was taken as the background concentration value. The mean background concentration value so obtained was $17.54\mu\text{g}/\text{m}^3$ i.e.

$$(NO_x)_{FP} = (NO_x)_P + 17.54\mu\text{g}/\text{m}^3 \quad (3.7)$$

This approach is the one most often followed in Environmental Impact Assessment.

A statistical evaluation of the concentrations predicted using equation (3.7) is presented in Table 3.11. This evaluation entails the comparison of hourly and average predictions with equivalent measured values.

Case 2

In the second case, the mean of all hourly concentrations recorded at 0500 hours were computed and the value obtained taken to represent the background concentration. This particular hour was chosen as because it was deemed that the effect of local vehicle emissions would be at a minimum at this time, and agreed by Budd (2004) and followed in the previous section on CO monitoring. The mean background value so determined was $11.57\mu\text{g}/\text{m}^3$ i.e.

$$(NO_x)_{FP} = (NO_x)_P + 11.57 \quad (3.8)$$

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A statistical comparison of the monitored and predicted data obtained using equation (3.8) is presented in Table 3.12.

Case 3

In case 3, use is made of the individual hourly NO_x concentrations measured at the background monitoring site during the second half of the study period (13/3/2002-15/9/2001). For this period, the individual hourly values can be used directly, i.e. for each hour

$$(\text{NO}_x)_{\text{FP}} = (\text{NO}_x)_{\text{P}} + (\text{NO}_x)_{\text{MB}} \quad (3.9)$$

Where $(\text{NO}_x)_{\text{MB}}$ is the measured hourly background concentration. For the first half of the study period (15/9/2001-12/3/2002) the background concentrations used are taken from the observed average diurnal variation of NO_x concentration at the background site, shown in Figure 3.19. For this period the predicted NO_x concentration is obtained from

$$(\text{NO}_x)_{\text{FP}} = (\text{NO}_x)_{\text{P}} + (\text{NO}_x)_{\text{DP}} \quad (3.10)$$

Where $(\text{NO}_x)_{\text{DP}}$ is the mean NO_x concentration at the background site for the hour of the day concerned, taken from calculated diurnal profile. The statistical evaluation of the predicted $(\text{NO}_x)_{\text{FP}}$ values calculated using equations (3.9) and (3.10) are shown in Table 3.13. Plots of the statistical values obtained using these three different cases of background concentration are shown in Figure 3.20(a) and 3.20(b) for the first and second six months respectively.

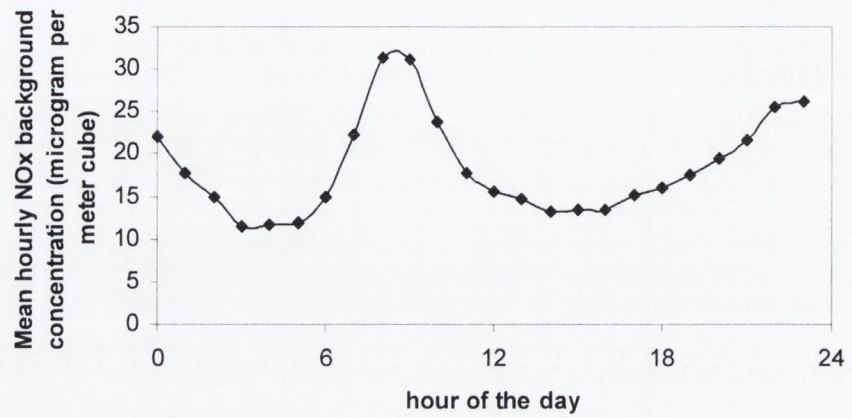


Figure 3.19 Average diurnal variation of NO_x concentration at the background site (13/3/2002-15/9/2002).

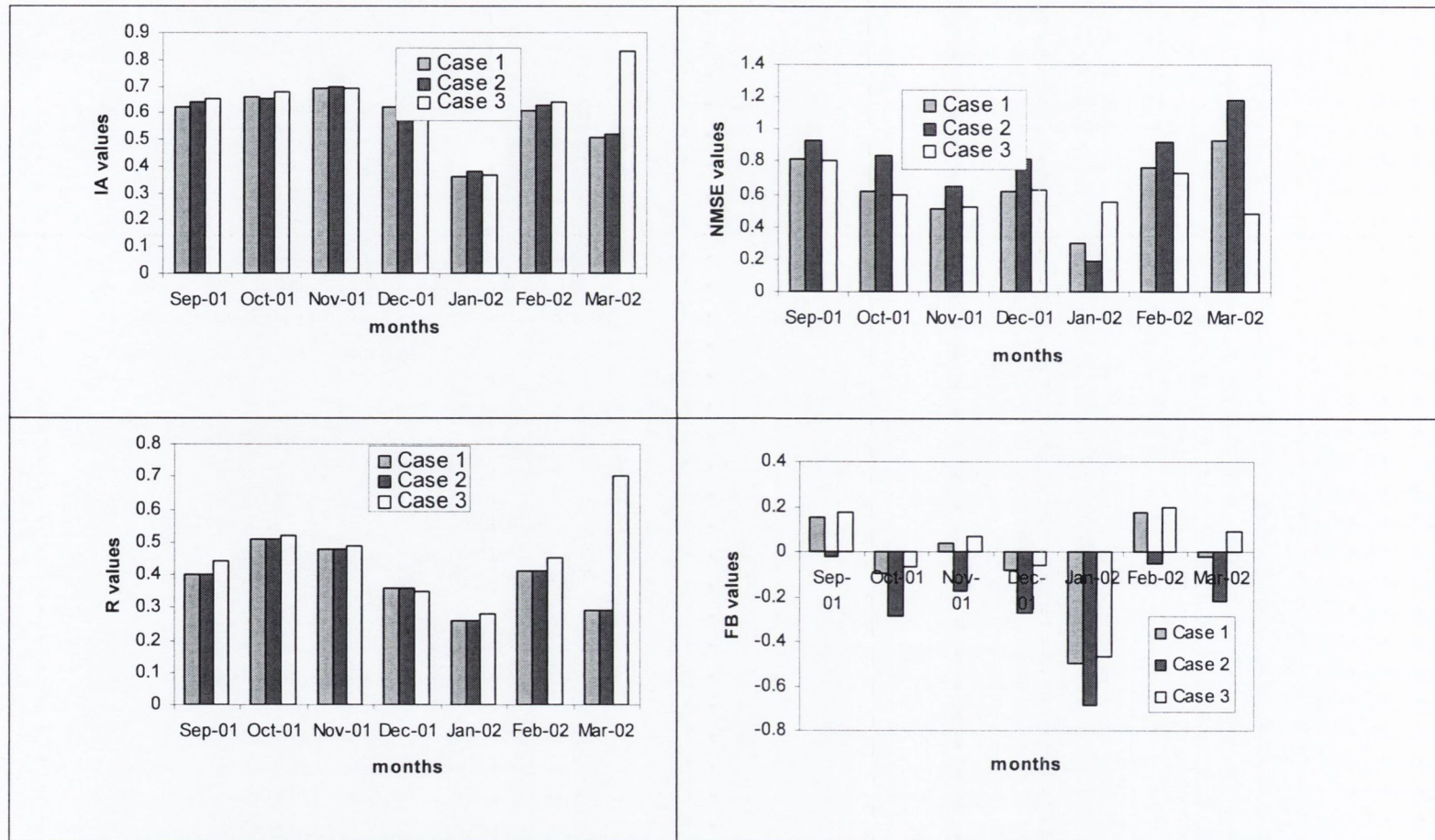


Figure 3.20(a). Graphical representation of statistical values for Case 1-Case 3 background concentrations for first six months

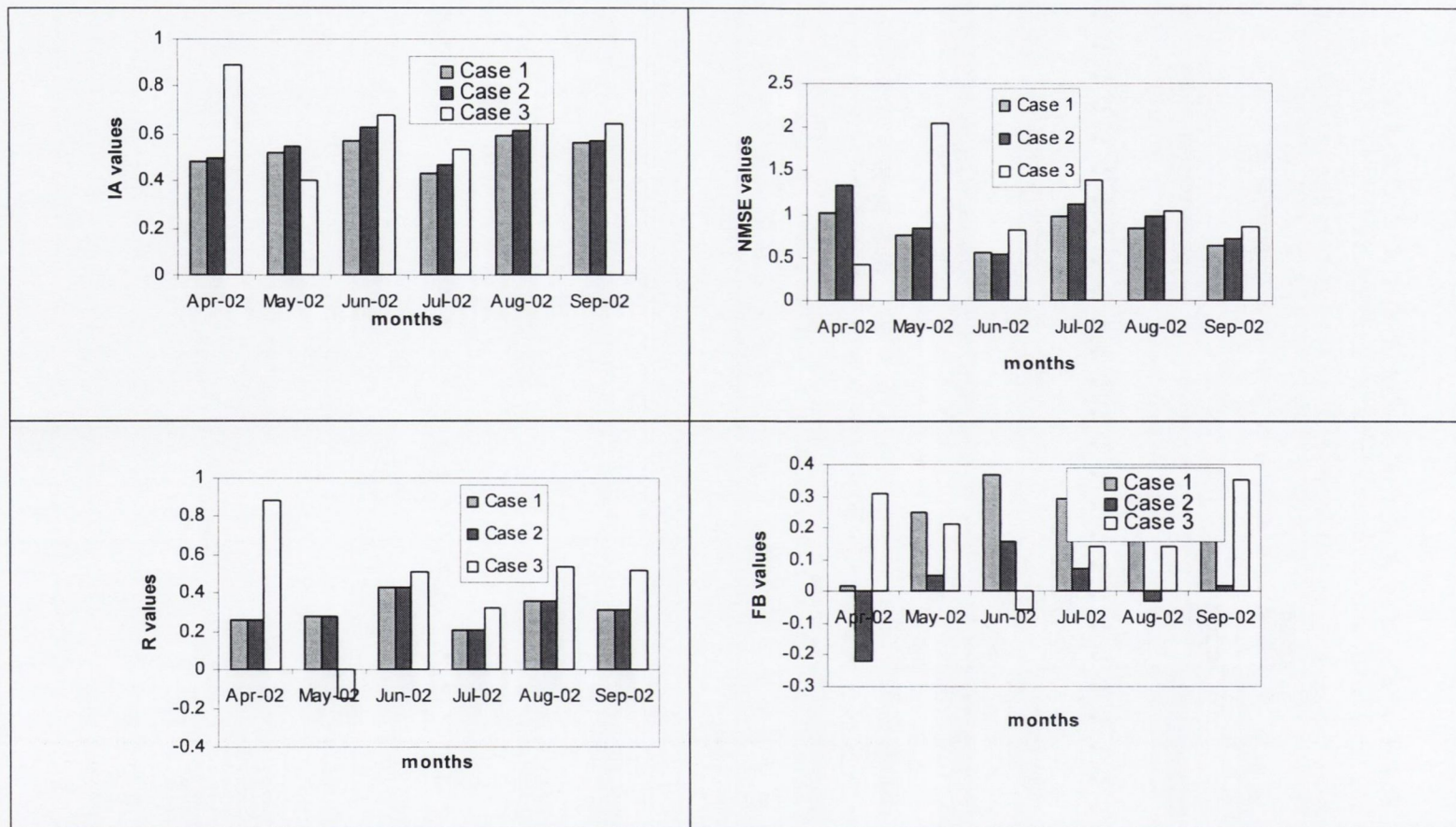


Figure 3.20(b). Graphical representation of statistical values for Case1-Case3 background concentrations for second six months.

Mon/par	Sep 01	Oct 01	Nov 01	Dec 01	Jan 02	Feb 02	Mar 02	Apr 02	May 02	Jun 02	July 02	Aug 02	Sep 02	overall
IA	0.62	0.66	0.69	0.62	0.36	0.61	0.51	0.48	0.52	0.57	0.43	0.59	0.56	0.62
NMSE	0.81	0.62	0.51	0.62	0.30	0.76	0.93	1.01	0.75	0.56	0.98	0.83	0.63	0.81
R	0.40	0.51	0.48	0.36	0.26	0.41	0.29	0.26	0.28	0.43	0.21	0.36	0.31	0.29
FB	0.15	-0.10	0.04	-0.08	-0.50	0.17	-0.02	0.02	0.25	0.37	0.29	0.17	0.18	0.04

Table 3.11 Statistical Results for Case 1 conditions.

Mon/par	Sep 01	Oct 01	Nov 01	Dec 01	Jan 02	Feb 02	Mar 02	Apr 02	May 02	Jun 02	July 02	Aug 02	Sep 02	overall
IA	0.64	0.65	0.70	0.61	0.38	0.63	0.52	0.50	0.55	0.63	0.47	0.61	0.57	0.51
NMSE	0.93	0.84	0.65	0.82	0.19	0.92	1.18	1.33	0.84	0.54	1.12	0.98	0.71	1.34
R	0.40	0.51	0.48	0.36	0.26	0.41	0.29	0.26	0.28	0.43	0.21	0.36	0.31	0.29
FB	-0.02	-0.29	-0.17	-0.27	-0.69	-0.05	-0.22	-0.22	0.05	0.16	0.07	-0.03	0.02	-0.16

Table 3.12 Statistical Results for Case 2 conditions

Mon/par	Sep 01	Oct 01	Nov 01	Dec 01	Jan 02	Feb 02	Mar 02	Apr 02	May 02	Jun 02	July 02	Aug 02	Sep 02	overall
IA	0.65	0.68	0.69	0.61	0.37	0.64	0.83	0.89	0.40	0.68	0.53	0.70	0.64	0.73
NMSE	0.80	0.60	0.52	0.63	0.55	0.73	0.48	0.42	2.04	0.81	1.38	1.04	0.86	1.03
R	0.44	0.52	0.49	0.35	0.28	0.45	0.70	0.88	-0.15	0.51	0.32	0.54	0.52	0.45
FB	0.17	-0.07	0.07	-0.06	-0.47	0.20	0.09	0.31	0.21	-0.06	0.14	0.14	0.35	0.05

Table 3.13. Statistical Results for Case 3 conditions.

Case 4

In this case, the individual hourly background concentrations measured during the second six months of the study period were sorted by stability classes i.e.; stable, unstable and neutral, and the means of the values observed in each class were computed for each hour of the day. The diurnal variations of these values are shown in Figure 3.21. These values were then employed as the background concentrations throughout the first six months of the study depending on the stability class that pertained during each particular hour. Statistical analyses of the results obtained with background cases 1 - 4 are shown in Tables 3.14 and 3.15 for the second and first six months respectively.

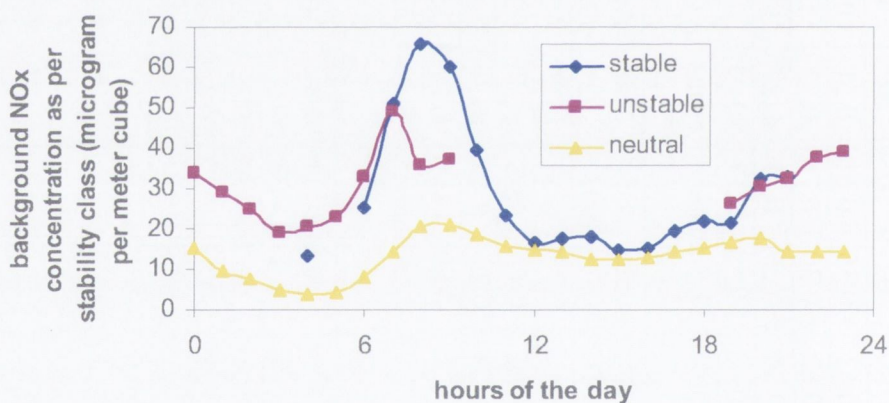


Figure 3.21 Background concentrations as per stability class (13/3/2002-15/9/2002).

Case/Parameters	Case 1	Case 2	Case 3 (individual hourly)	Case 4 (Stability class)
IA	0.53	0.55	0.76	0.72
NMSE	0.82	0.95	0.85	0.76
R	0.30	0.30	0.65	0.55
FB	0.21	0.01	0.19	0.23

Table 3.14. Statistical Results for last six months for Case 1-4

Chapter 3

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Case/Parameters	Case 1	Case 2	Case 3 (individual hourly)	Case 4 (Stability class)
IA	0.48	0.49	0.56	0.61
NMSE	1.26	1.62	1.15	1.12
R	0.30	0.30	0.38	0.44
FB	-0.09	-0.29	-0.05	-0.10

Table 3.15. Statistical Results for first six months for Case 1-4

Case 5

In the last case, the mean of the entire six months of background concentrations observed with the different stability classes, irrespective of any hour to hour variation, was taken as the background concentration value. The mean background concentration values so obtained were 29.74, 29.68 and 13.20µg/m³ for stable, unstable and neutral conditions respectively i.e.

(NO_x)_{FP} = (NO_x)_P + 29.74µg/m³ (Stable)

(3.11)

(NO_x)_{FP} = (NO_x)_P + 29.68µg/m³ (Unstable)

(3.12)

(NO_x)_{FP} = (NO_x)_P + 13.20µg/m³ (Neutral)

(3.13)

A statistical evaluation of the concentrations predicted using equations (3.11)-(3.13) is presented in Tables 3.16 and 3.17 for the first and second six months respectively for the different stability classes.

Case/Parameters	Stable	Unstable	Neutral	overall
IA	0.45	0.45	0.50	0.49
NMSE	0.96	0.96	1.50	1.37
R	0.30	0.30	0.31	0.31
FB	0.22	0.22	-0.24	-0.13

Table 3.16. Statistical Results for first six months for Case 5

Case/Parameters	Stable	Unstable	Neutral	overall
IA	0.48	0.48	0.55	0.53
NMSE	0.86	0.85	0.91	0.89
R	0.30	0.30	0.30	0.30
FB	0.51	0.51	0.05	0.18

Table 3.17 Statistical Results for last six months for Case 5

3.7.2 Discussion of NO_x modelling results

The FB statistic reflects the agreement between the averages of the measured and modelled concentrations, and confirms that the model slightly overpredicted (cases 1 and 3) or underpredicted (cases 2 and 4) at the motorway site depending upon the assumed background concentrations. However, the variation of the FB values between the different cases is small. Good correlation between the monitored and predicted hourly concentrations is generally not observed. The R value for the entire year is 0.29 for cases 1 and 2, but for case 3 reaches 0.45 for the entire year and 0.65 for the later six months. For case 4, an R value of 0.44 was obtained over the first six months and 0.55 for the last six months.

On comparing the results from Table 3.15 it is seen that there is a slight improvement in model performance over the second six months. This is because that the actual background concentrations were available for this period. The IA values are probably the most representative statistical parameters for as they assess the level of error in the model predictions. The IA values for case 3 are 0.73 (entire year), 0.56 (first six months), 0.76 (second six months) and for case 4 are 0.61 (first six months) and 0.72 (second six months) respectively. This suggests that relatively a high percentage of model predictions by GFLSM using case 3 and 4 are largely error free. On an overall basis, the statistical results obtained from GFLSM model in conjunction with the different background concentrations classifications suggest that when available, the use of measured hourly values of the

background concentration improves model performance substantially. Alternatively, the classification of background data by time - of - day and stability class is also appropriate method for increasing the efficiency of the model. The main drawback with case 3 is that a large quantity of data is required, and this data will not be available for future predictions. However, using case 4, even with a limited background data set the efficiency of the model can be increased. Consideration of case 5 shows that in the first six months assuming the mean concentration for the neutral stability class yields slightly better statistical results than does assuming the mean concentrations for stable and unstable conditions. Overall, while applying the mean values of the background concentrations as per stability class was slightly better for the last six months than the first six month of the study period; this method appears to achieve very similar model performance compared to Case 1 and Case 2 with very little additional data requirements. Figure 3.22 shows the diurnal profiles of the monitored and modelled concentrations obtained using different background case values.

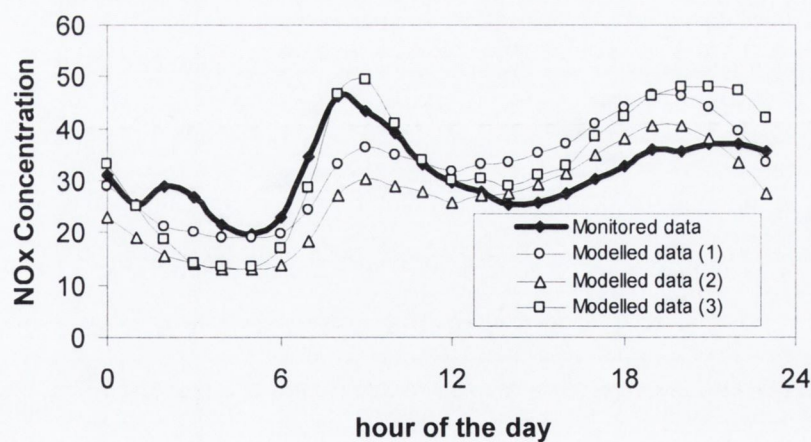


Figure 3.22 Diurnal profile variation considering three different background scenarios (15/9/2001-15/9/2002).

It will be observed that for case 3 the modelled data shows a marked resemblance to monitored data. It is observed from the figure that the model is able to predict the peak concentrations in the earlier part of the day, whereas in the later part of the day the model tends to slightly overpredict the measured concentration.

3.7.3 HEFs and Sensitivity analysis of GFLSM

The GFLSM model was further tested with hourly emission factors (HEF) derived using the COPERT III methodology (Kouridis et al, 2000). Statistical analysis of the predicted data obtained with these HEFs and with composite emission factors CEFs are compared in Table 3.18.

Model/Parameters	GFLSM (CEF)	GFLSM (HEF)
IA	0.73	0.72
NMSE	1.03	1.06
R	0.45	0.44
FB	0.05	0.10

Table 3.18. Summary of statistical results for NO_x using GFLSM for CEF and HEF.

It is seen from the result that as was the case for CO, there is no significant improvement in the statistical parameters obtained using HEFs, for the particular study site.

A sensitivity analysis of the GFLSM model was carried out by performing statistical computations of the monitored and predicted data (case 3 background values) under different stability categories and wind speed conditions. These are shown in Table 3.19 and Table 3.20 respectively.

Parameters/Stability class	Unstable	Stable	Neutral
IA	0.65	0.50	0.75
NMSE	0.62	0.65	0.18
R	0.50	0.23	0.66
FB	-0.09	-0.28	0.19

Table 3.19. Stability class analysis for NO_x.

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Parameters/Wind speed	<0.5m/s	0.5-2m/s	>2m/s
IA	0.39	0.70	0.77
NMSE	0.86	0.26	0.00
R	0.02	0.51	0.63
FB	-0.17	0.06	0.16

Table3.20. Wind sensitivity analysis for NO_x.

For the stability class analysis the entire monitored and predicted data set from GFLSM were sorted as per the stability conditions (unstable, stable and neutral) and statistically analysed. It was observed that the model performed best under neutral conditions.

In a similar fashion for the wind sensitivity analysis study the monitored and modelled data were sorted for three different wind speed conditions ranging from less than 0.5m/s, 0.5-2m/s and greater than 2 m/s and were statistically analysed. It was observed that the GFLSM model best performed for the wind speed conditions above 2m/s (for this study) and performed least well for wind speeds less than 0.5m/s (calm conditions). These results agree with those observed previously for CO.

3.7.4 Study Conclusions

This study evaluated the GFLSM model, a Gaussian type atmospheric dispersion model, using monitored data collected adjacent to a free flowing motorway. The effect of background concentration on the model efficiency has been studied in detail and the classification of background concentration by stability class proposed. Graphical and statistical analyses revealed reasonable agreement between measured and predicted datasets but emphasises the key role played by the modelled or assumed background concentrations. Model performance improved greatly when actual measured concentrations were employed. However, most of the improvement can be realised by taking the stability class into consideration when defining

mean background concentrations. This approach is applicable when model calculations are required to predict future ambient concentrations.

The use of Hourly emission factors (HEFs) as an alternative to Composite Emission factor (CEFs) was also used to assess the performance of the GFLSM model but little difference was observed. Sensitivity analysis of the model was also performed with regards to wind speed and stability conditions and the model performance was found to be best for neutral stability and medium to high wind speeds and worst for stable conditions and low wind speed conditions.

Chapter 4

Highway Modelling – Part 2.

Chapter 3 dealt with modelling of the pollutants emitted from vehicle exhausts (CO and NO_x) to calculate concentrations at single receptor adjacent to a free flowing motorway. Comparison with measured concentrations showed that dispersion models based on Gaussian techniques were able to model CO and NO_x with quite a high degree of accuracy but model performance was highly dependant on the assumed background concentration. To ascertain further the ability of the Gaussian models to predict pollutants with trace concentrations, both the CALINE4 and GFLSM were used to predict the spatial variation in background corrected concentrations of hydrocarbons observed in a highway study conducted by O'Donoghue, (2004). The HCs considered in this study were ethene, propene, acetylene, butadiene, n-pentane, isopentane and benzene. The first part of this chapter describes this modelling of hydrocarbon concentrations using CALINE4 and GFLSM. The second part of this chapter presents the application of these models to the prediction of the improvement in air quality due to the opening of town bypass.

4.1 Measurement Site and Experimental Setup.

4.1.1 *Monitoring site*

The M50 motorway is an orbital route for the city of Dublin. At the monitoring site employed by Donoghue (2004), the motorway has a straight alignment with carriageway bearings of 330° and 150°. Six sampling locations (receptors) were located on a line perpendicular to the motorway alignment, at distances of 25m, 120m and 240m from either roadside, as shown in Figure 4.1. By obtaining concentration measurements at all of these locations, both the variation in air quality downwind of the motorway and the background concentration upwind of the motorway could be determined, irrespective of the wind direction at the time of sampling. Furthermore, subtracting the background concentration from the values measured at

the downwind sampling points leads to a set of ‘background corrected’ concentrations attributable to emissions from the motorway alone. These data represent an ideal basis for model evaluation because the comparison of modelled and measured concentrations is not observed by varying and uncertain background contributions.

The area surrounding the receptors is mostly open parkland with some trees and playing fields. Measurements of traffic flow on the motorway were obtained through induction loops embedded under both carriageways, and hourly traffic flows in either direction were summed to obtain the total vehicle flows. Twenty one days of traffic data were obtained during the monitoring period. The average hourly traffic flow was 3936 vehicles per hour, with a relative standard deviation of 23%. Traffic on this part of the motorway is invariably free-flowing, with an average vehicle speed of 100 km/hr and a 12% HGV content.

The monitoring site is located 6 km south-west of the city centre, and 2 km east of the satellite town of Tallaght, which contains a large number of commercial and light industrial premises. A minor road serving a local residential area lies approximately 350m east of the motorway.

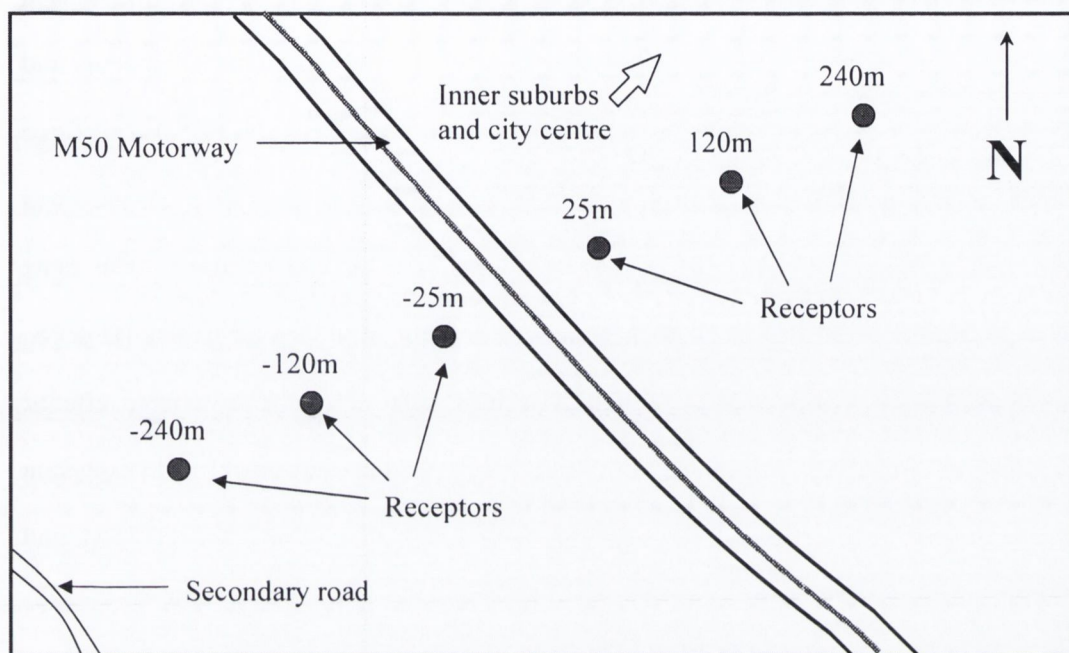


Figure 4.1 Schematic diagram of receptor locations.

4.1.2 Hydrocarbon measurements

Measurements of the concentrations of eleven C_2 - C_6 hydrocarbons were obtained using a recently evaluated sampling and analysis method (O'Donoghue, 2004) over a five week period during July and August of 2003. Whole air samples were collected using a 1 litre SKC Vac-u-chamber, SKC Universal Pump and 1 litre tedlar bags. Sampling was carried out between 07:00 and 10:00 on weekdays at each of the six receptors shown in Figure 4.1. A five minute pumped sampling duration was employed at each receptor, allowing the total sampling procedure for all six samples to be completed within 45 minutes. A five minute sampling interval is in line with the methodology employed by Harkonen et al, (1997) who used a ten minute sampling interval to determine vertical concentration profiles by varying the sampling height. The whole air samples were analysed using a Perkin-Elmer 'ozone precursor monitoring system'. Calibration was carried out on a weekly basis using a multi-component

calibration standard produced by the UK National Physical Laboratory. The monitoring system consists of an AutoSystem gas chromatograph fitted with two capillary columns and two flame ionization detectors (FIDs), an automatic thermal desorption unit (ATD 400) fitted with an air sampler accessory and controlling hardware and software. The carrier gas used was helium, while the combustion gases for the FIDs were zero air and hydrogen. The same monitoring system is used in US Photochemical Assessment Monitoring Stations (USEPA, 2000). Of the eleven hydrocarbons monitored, seven displayed motorway source effects: ethene, propene, n-pentane, isopentane, benzene, 1-3, butadiene and acetylene. Dispersion model assessment was performed for each of these compounds using the GFLSM and CALINE4 models.

4.1.3 Meteorological conditions

During each period of sampling, local meteorological conditions (wind speed, wind direction and temperature) were measured using portable instruments. Conditions were calm over the course of the entire monitoring period. On only one occasion was the local wind speed observed to rise to 2 m/s. The majority of observations were in the range 1.0-1.5 m/s or less, and the average wind speed was 1.06 m/s. These conditions have previously been observed to be the most challenging for Gaussian dispersion models, as shown in Section 3.7.3 in Chapter 3.

The observed wind directions were grouped into the two sectors expected to produce source effects on opposite sides of the motorway. These two wind sectors, namely 345-135° and 165-315°, can be considered as easterly and westerly wind directions relative to the M50. The single occasion on which parallel or near-parallel wind directions was observed is omitted in later analyses due to the difficulty in establishing a background concentration for these

Chapter 4

Highway Modelling – Part 2.

conditions, and to exclude the effects of emissions from a signal controlled roundabout located approximately 1km south-east of the sampling site. Both wind direction sectors are evenly represented in the remaining twenty days. The atmospheric stability during the entire monitoring period remained neutral (Class D).

In the previous chapter, the Gaussian based atmospheric dispersion models CALINE4 and GFLSM were discussed. The method of calculating emission factors using COPERT and the statistical parameters used for comparing the monitored and predicted data have also been described in Chapter 3. A composite emission factor for each of the HCs studied was computed and the values for each of the HCs under consideration are presented in Table 4.1 (O'Donoghue, 2004).

Hydrocarbons	Emission Factors(g/km)
Ethene	0.0073
Propene	0.0034
1,3-Butadiene	0.0014
N-pentane	0.0013
Isopentane	0.0039
Acetylene	0.0031
Benzene	0.0044

Table 4.1 Emission factors for hydrocarbons.

4.2 Results

4.2.1 Predicted versus measured concentrations

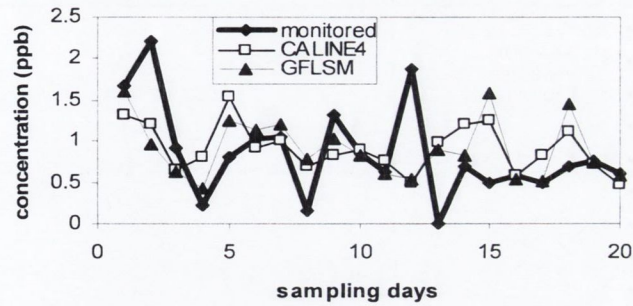
The variations in monitored and modelled data over the entire sampling period for all the hydrocarbons at receptor distances of 25m and 120m are presented in Figure 4.2.

It is observed that the both models effectively predict **the ranges of** the observed variations in monitored concentrations. It is further noted that both models fail to predict the magnitude of the larger day to day changes in measured values for all of the HCs under consideration.

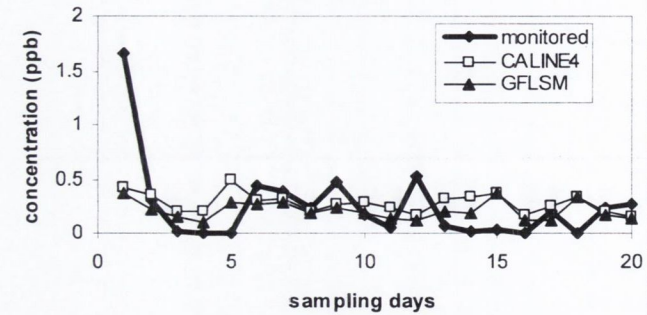
Scatter plots of measured and modelled data from CALINE4 and GFLSM were also plotted for all the hydrocarbons for the receptors at 25m and 120m, as shown in Figure 4.3.

It is observed that at 25m most of the predicted data lie within a factor of two of the measured data. In cases where the predicted data lie outside the factor of two, the predicted values are higher than monitored values. Overall, the results highlight that the performance of the GFLSM is similar to that of CALINE4. At a receptor distance of 120m, the majority of the predicted values lie outside the factor of two range, especially when the monitored background-corrected concentrations are zero. This occurs when difference between the upwind and the downwind concentrations is less than the accuracy of the measurement technique. However the models always yield a non-zero concentration value on one side of the road or other, which causes the predicted values to lie outside the factor of two range.

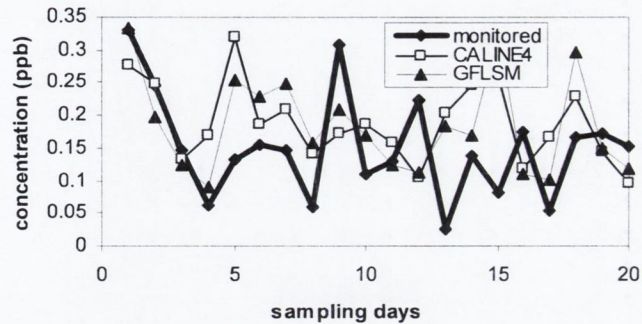
The spatial variations of the mean predicted and measured hydrocarbon concentrations are compared in Figure 4.4



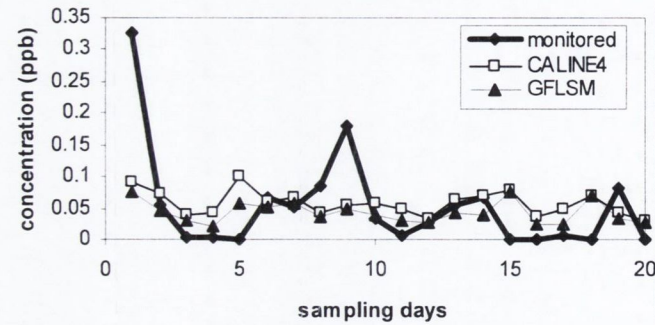
(a) Ethene at 25m



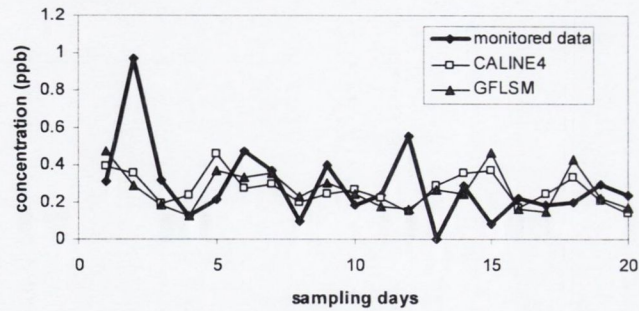
(b) Ethene at 120m



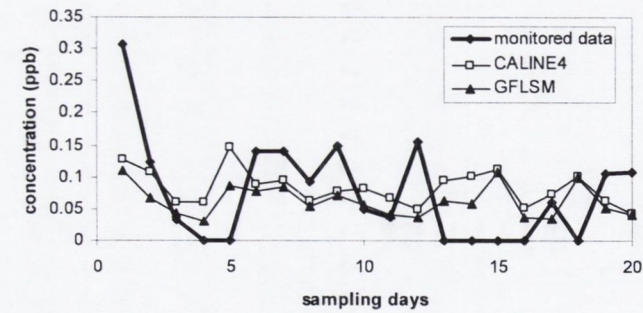
(c) Benzene at 25m



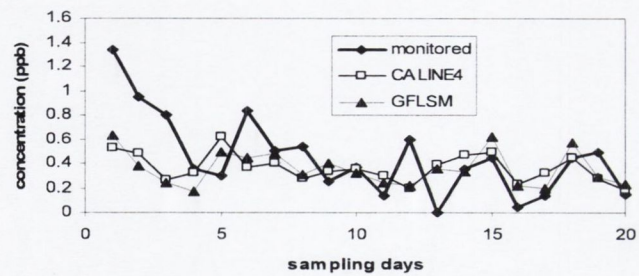
(d) Benzene at 120m



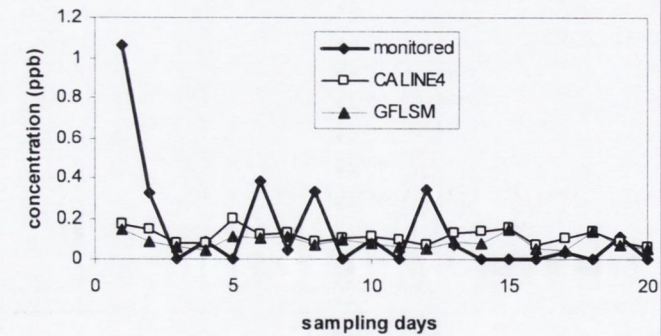
(e) Propene at 25m



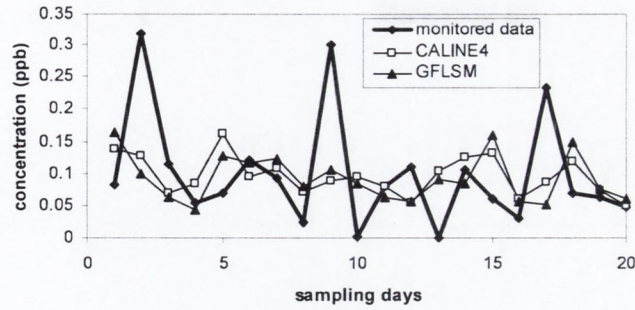
(f) Propene at 120m



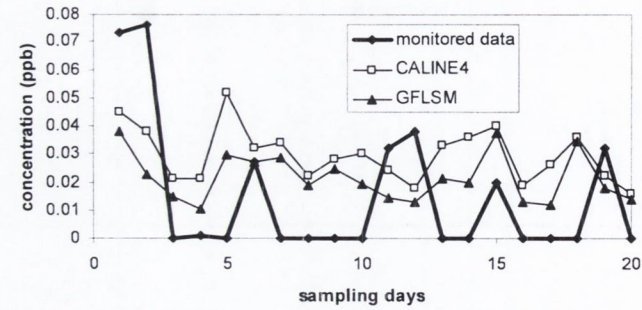
(g) Acetylene at 25m



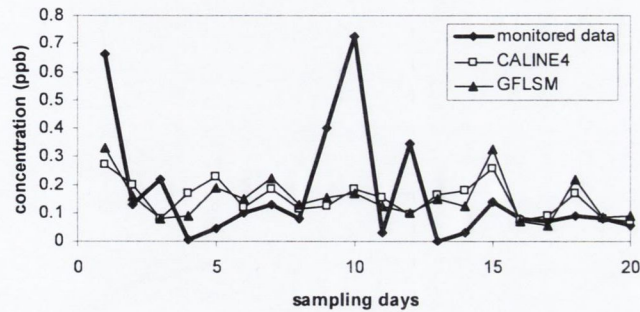
(h) Acetylene at 120m



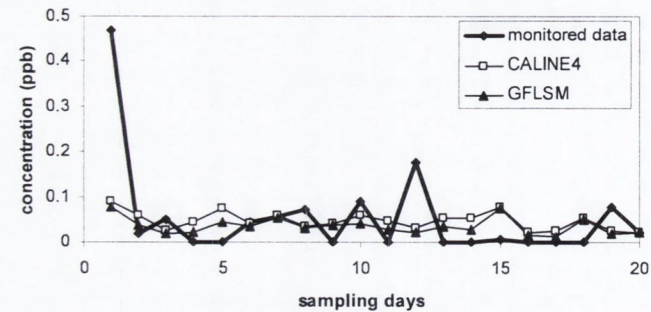
(i) Butadiene at 25m



(j) Butadiene at 120m



(k) N-pentane at 25m



(l) N-pentane at 120m

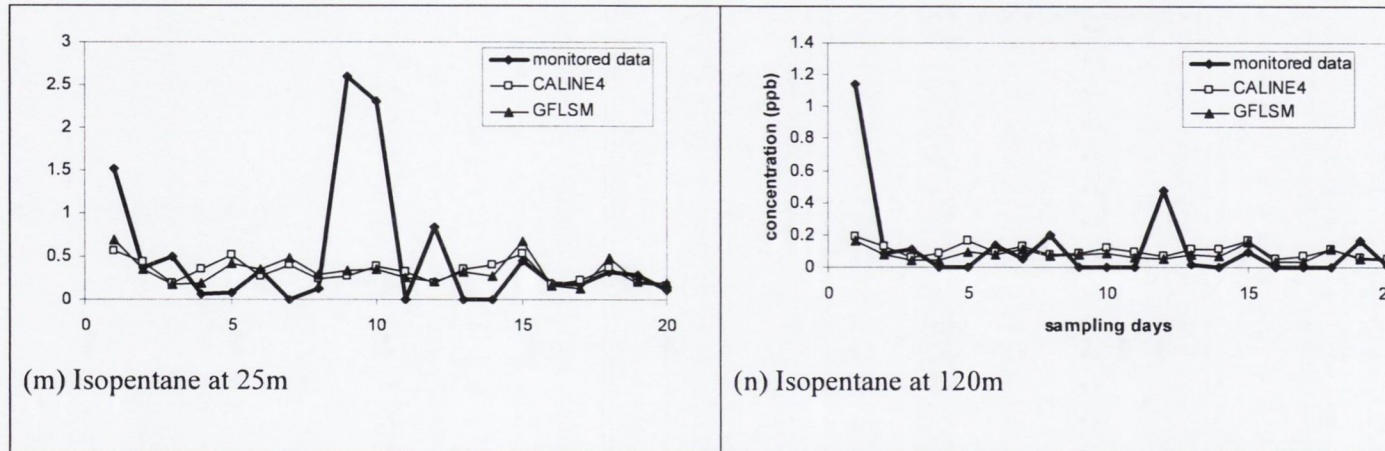
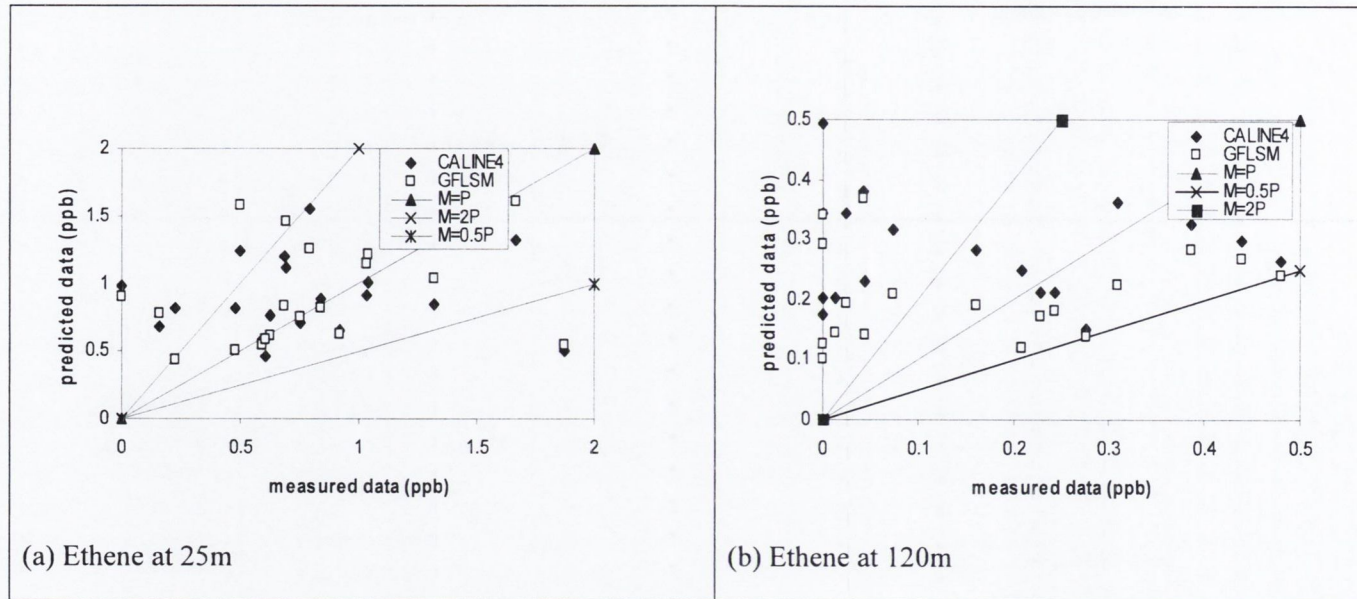
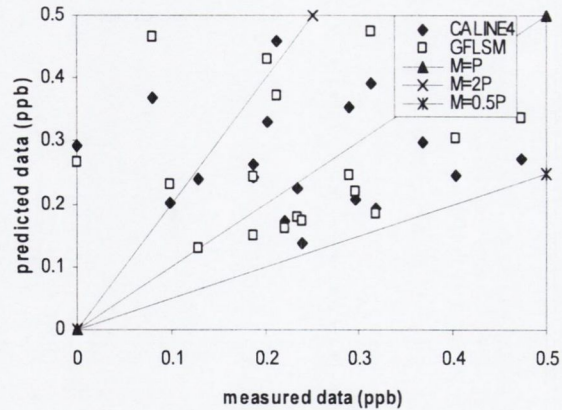
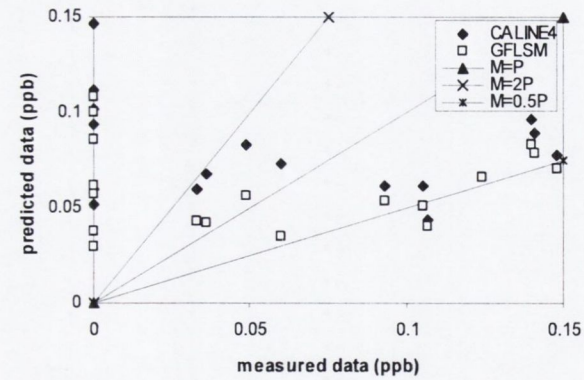


Figure 4.2 Variation of monitored and modelled concentration over the sampling period

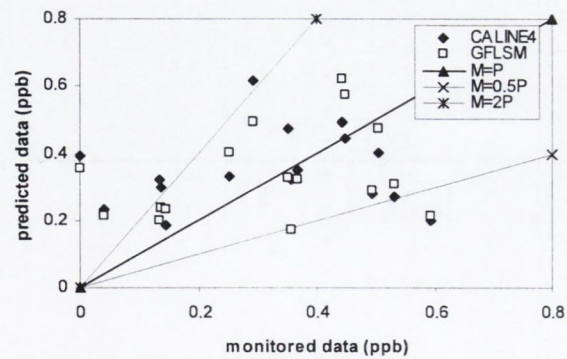




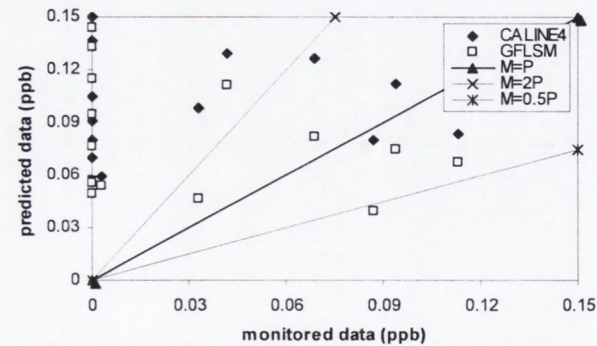
(c) Propene at 25m



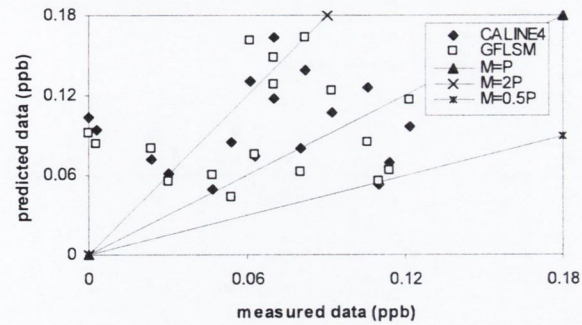
(d) Propene at 120m



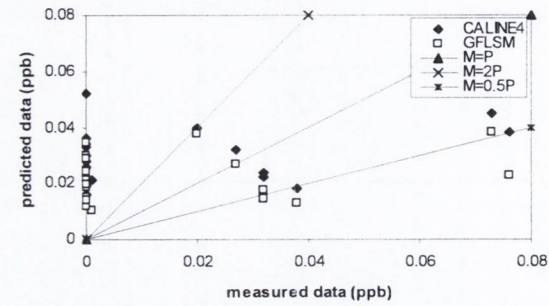
(e) Acetylene at 25m



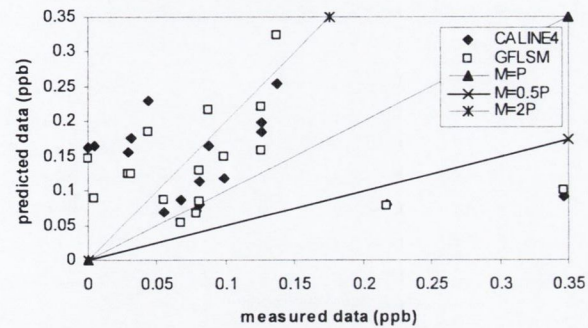
(f) Acetylene at 120m



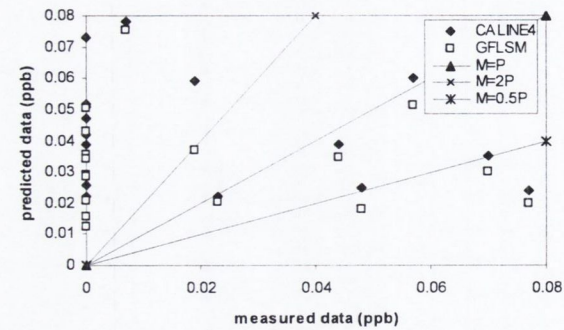
(g) Butadiene at 25m



(h) Butadiene at 120m



(h) N-pentane at 25m



(i) N-pentane at 120m

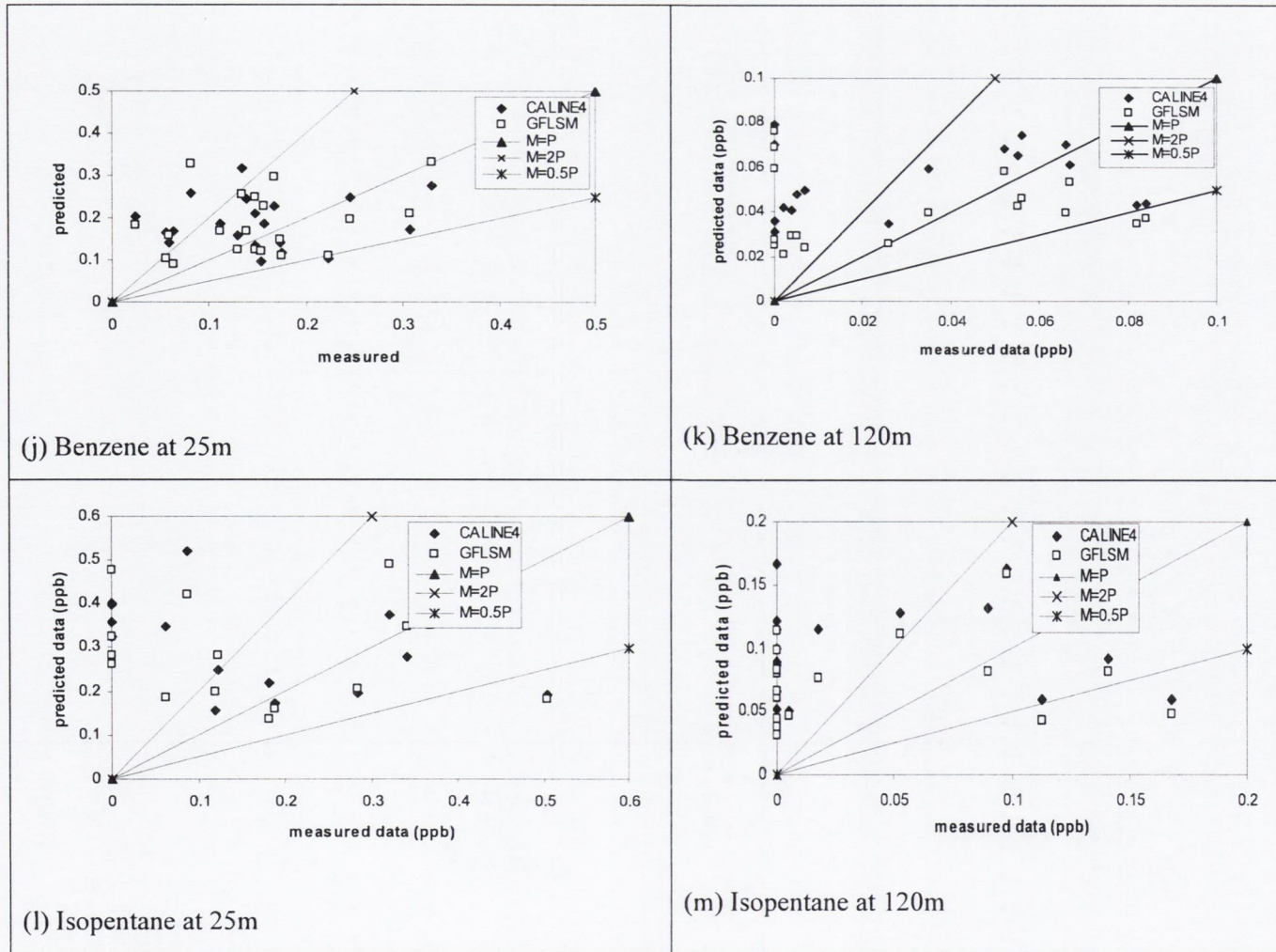
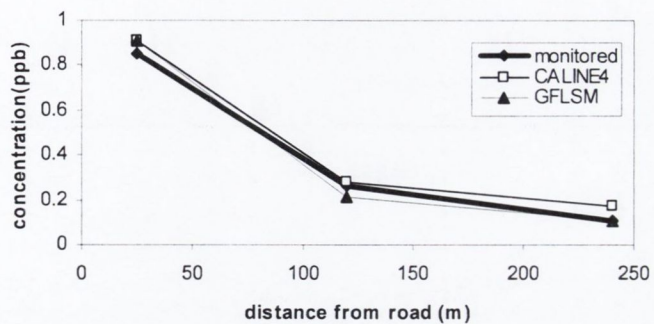
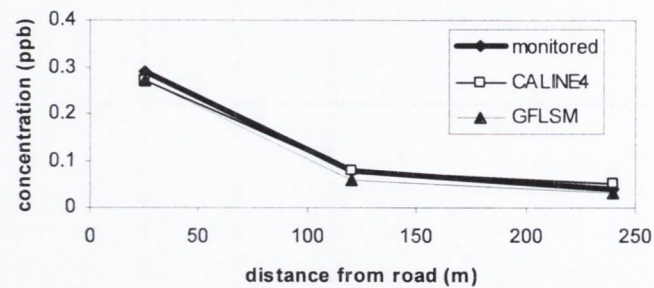


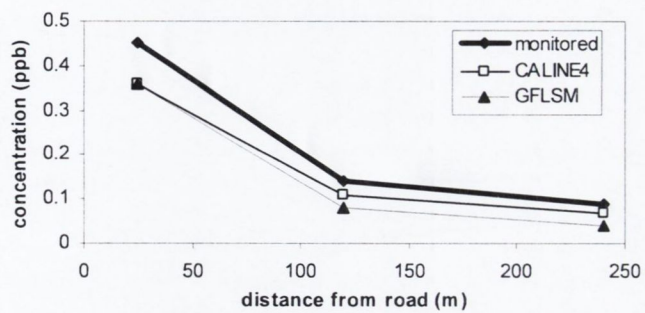
Figure 4.3 Scatter plots for monitored and modelled data at 25m and 120m



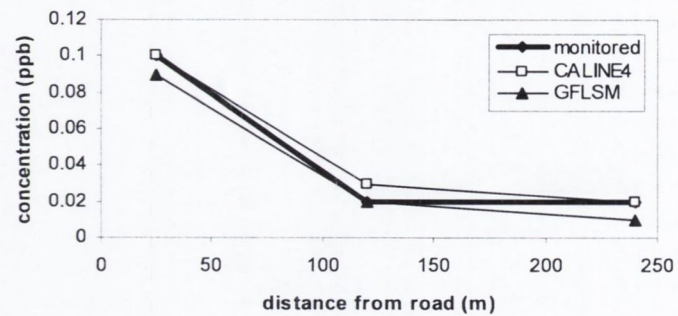
(a) Ethene



(b) Propene



(c) Acetylene



(d) Butadiene

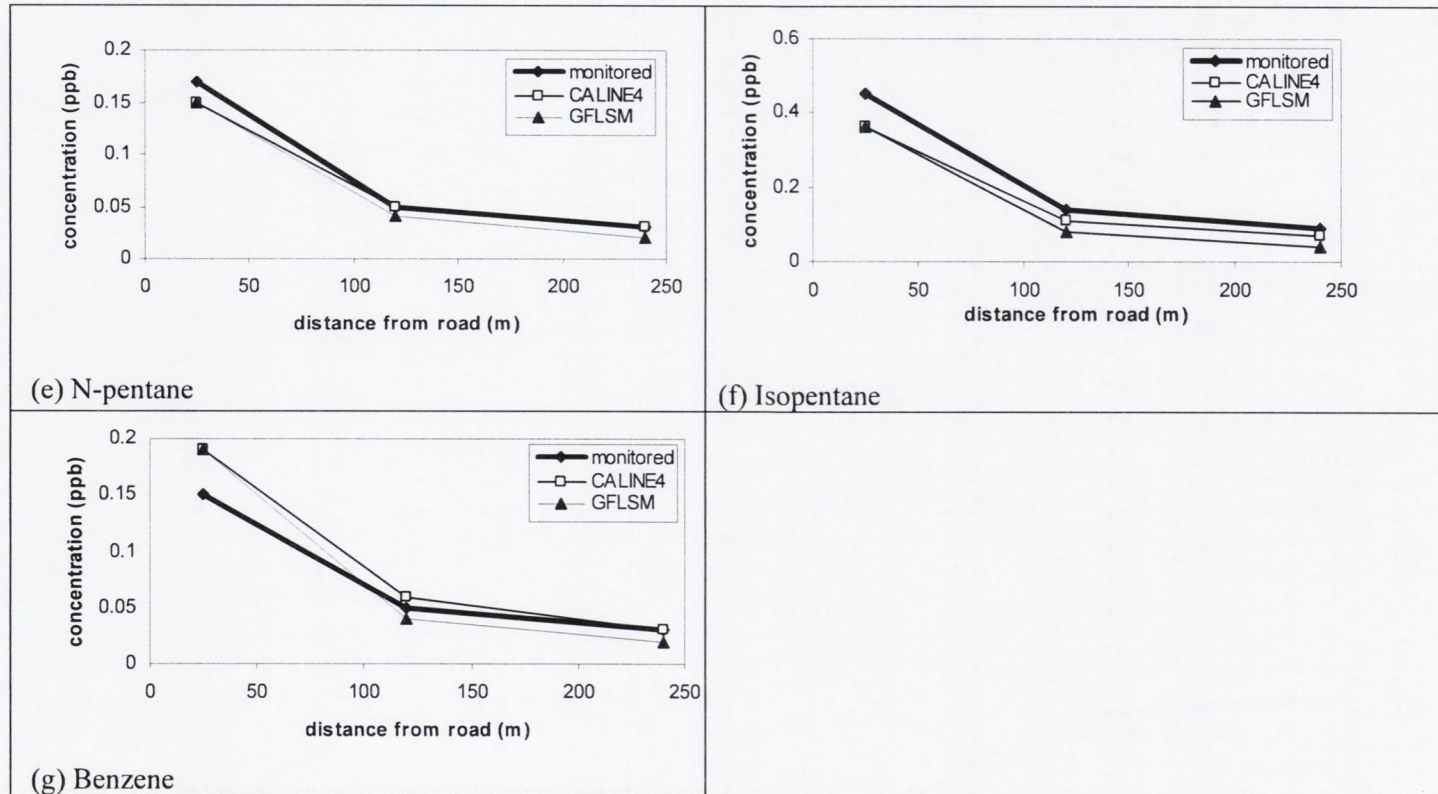


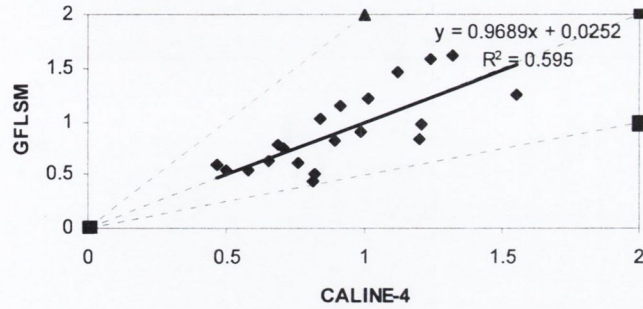
Figure 4.4 Spatial distributions of monitored and modelled data.

These indicate the agreement between the measured and modelled long term average concentrations of all the hydrocarbons over the three different receptor distances of 25m, 120m and 240m. The patterns of the spatial plots computed with both models are similar to the monitored data, and a similar pattern is displayed by all the hydrocarbons. At 25m the mean concentrations predicted by the models are nearly identical. At 120m and 240m the GFLSM data tends to be slightly lower than the CALINE4 data. In most, but not all of these cases the CALINE4 data show closer agreement with monitored result.

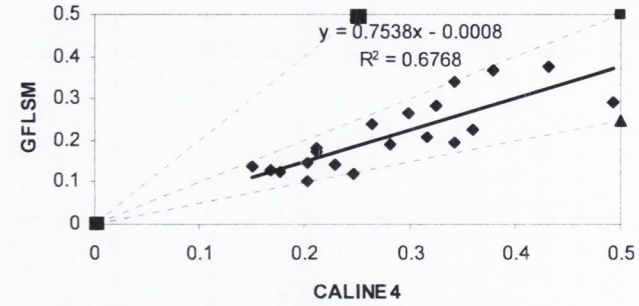
4.2.2 Inter –comparison of model predictions.

Scatter plots of GFLSM versus CALINE4 predictions for all seven hydrocarbons and at different downwind distances of 25m, 120m and 240m were plotted and the corresponding results are presented in Figure 4.5. The lines shown in the figure represent exact agreement between the models and the band for which the model predictions are within a factor of two of each other. The bold line in these graphs is a linear fit to the data points. It is clear that the predictions of the two models are in good agreement with each other for all hydrocarbons and at all downwind distances. It is observed that the slopes of the linear fits of the scatter plots deviate almost negligibly from ideal agreement at downwind distances of 25m, deviate by about -25% at the downwind distance of 120m and deviate by about -35% at 240m. These results suggest that as downwind distance increases the GFLSM tends to predict lower concentrations than CALINE4. It is also noted that for all the hydrocarbons considered, the R^2 value increases with the increase in downwind distances. This can be attributed to the fact that whereas the concentration for receptors closest to the source is highest and hence there is a more variation in the predictions, at the receptor location furthest from the source, the

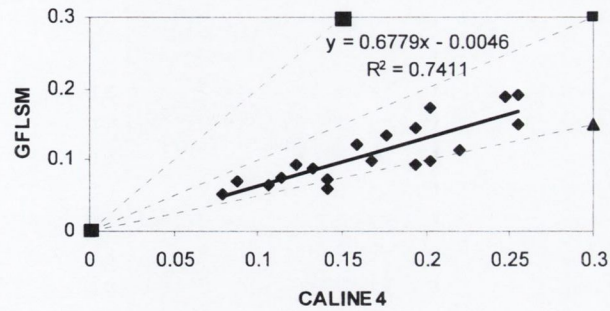
predicted concentrations are quite small and the variation amongst predicted data is low, leading to an improvement in the R^2 value.



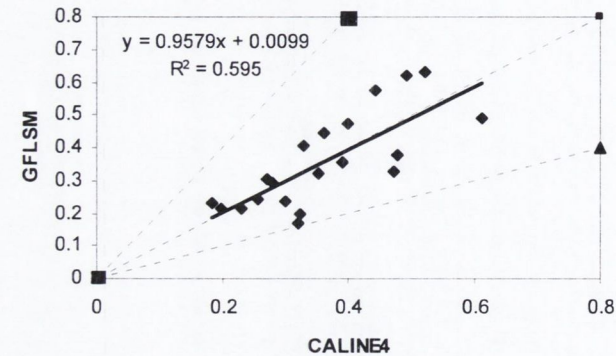
(a) Ethene at 25m



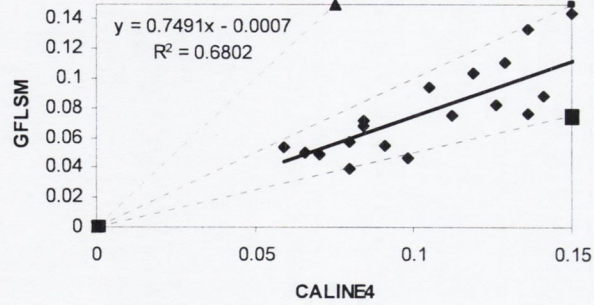
(b) Ethene at 120m



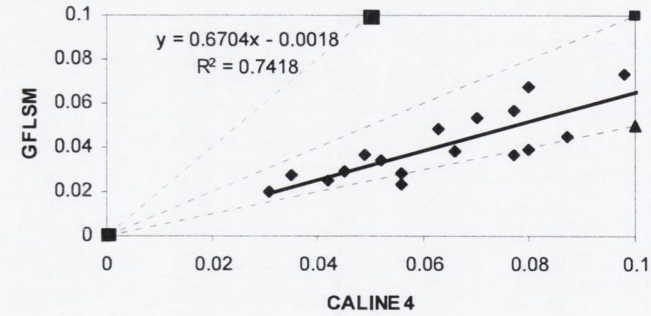
(c) Ethene at 240m



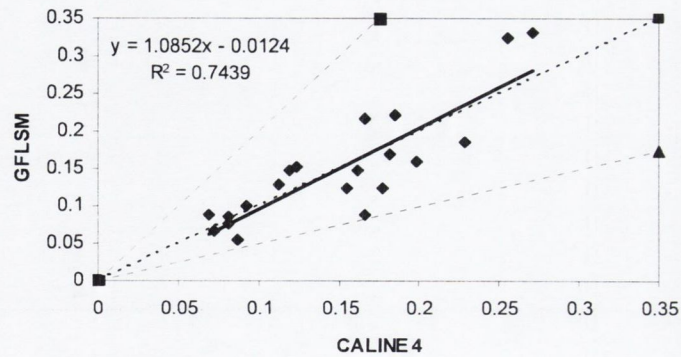
(d) Acetylene at 25m



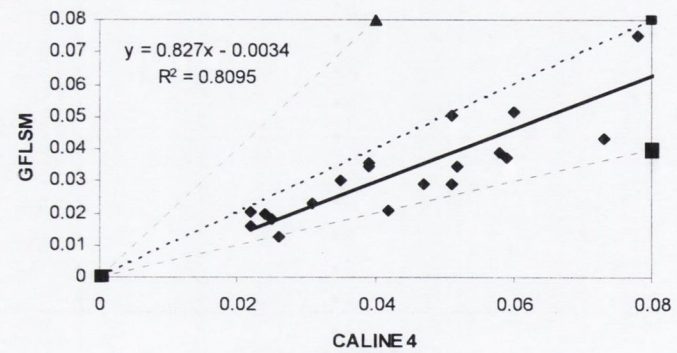
(e) Acetylene at 120m



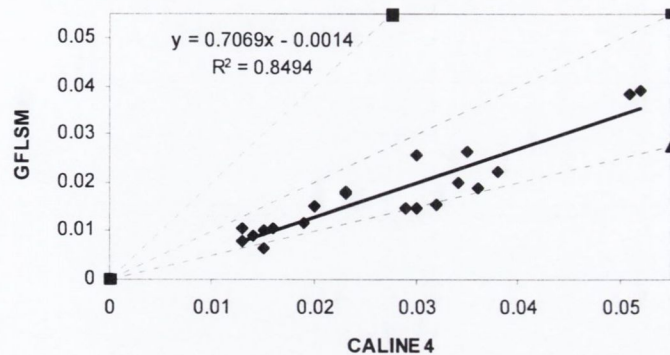
(f) Acetylene at 240m



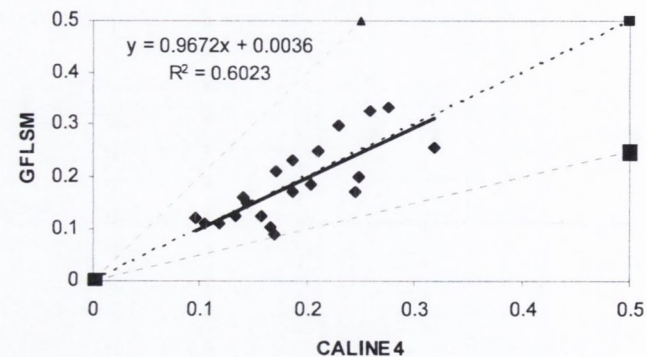
(g) N-pentane at 25m



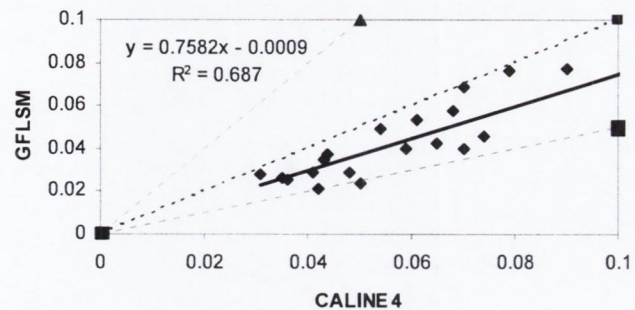
(h) N-pentane at 120m



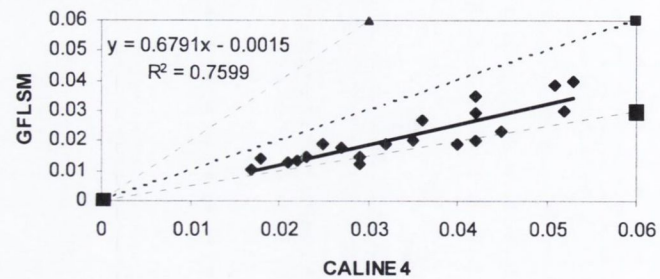
(i) N-pentane at 240m



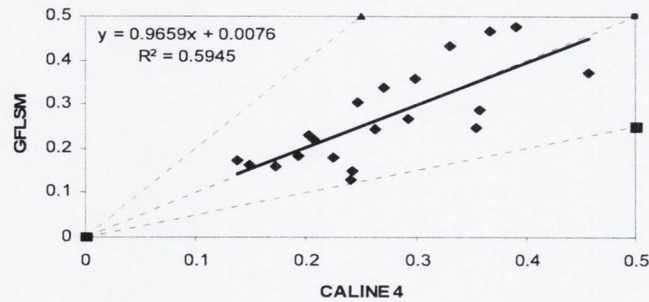
(j) Benzene at 25m



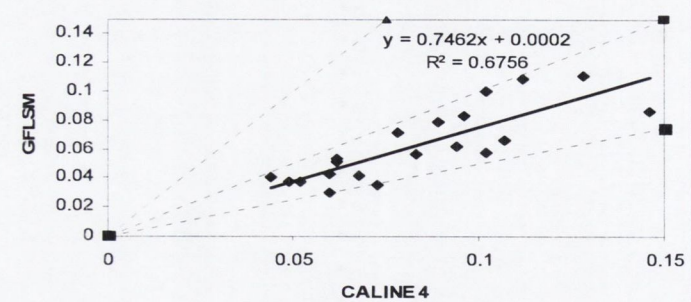
(k) Benzene at 120m



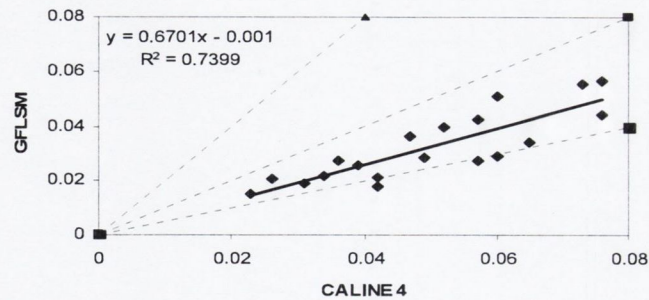
(l) Benzene at 240m



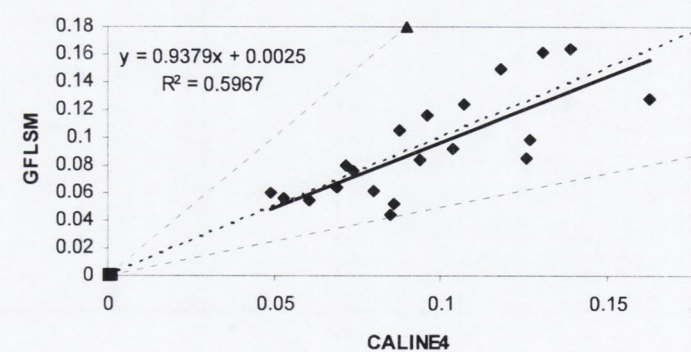
(m) Propene at 25m



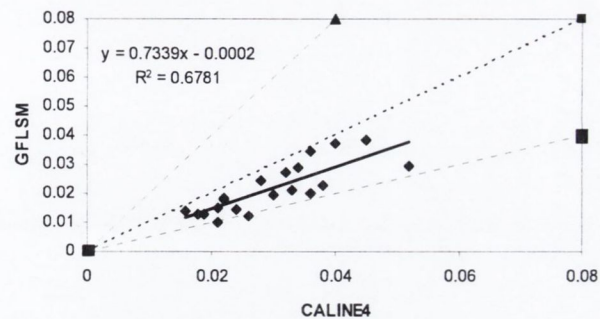
(n) Propene at 120m



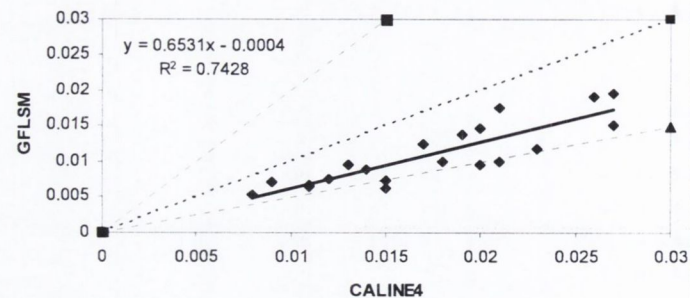
(o) Propene at 240m



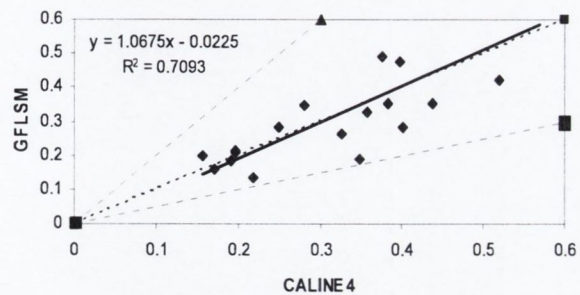
(p) Butadiene at 25m



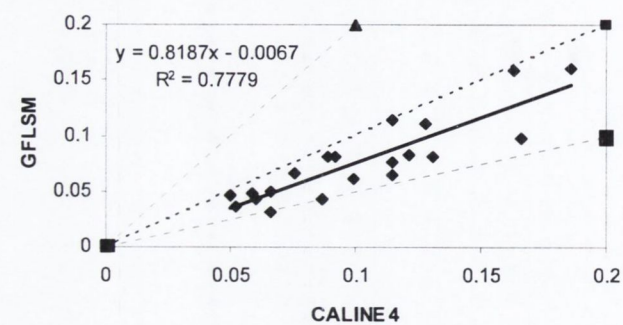
(q) Butadiene at 120m



(r) Butadiene at 240m



(s) Isopentane at 25m



(t) Isopentane at 120m

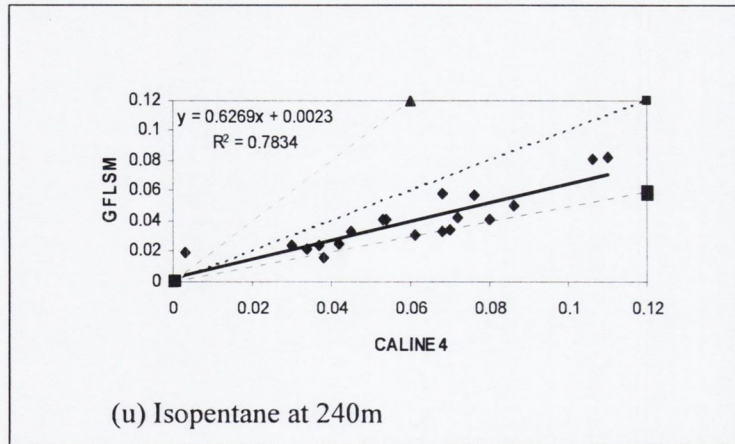


Figure 4.5 Scatter plots for predicted data.

4.3.3 Statistical analysis of the measured and predicted concentrations.

Tables 4.2 and 4.3 present statistical evaluation parameters that quantify the performance of both the models, GFLSM and CALINE4.

The Index of Agreement (IA) between the modelled and monitored data shows that with the increase in downwind receptor distances, both the models were prone to producing less accurate results. It is also to be noted that while the IA values obtained using GFLSM and CALINE4 are very similar to each other, in nearly all cases the GFLSM displays a higher IA value than CALINE4, indicating better agreement with measured values. This trend is observed for all pollutants, with the exception of butadiene at 25m and 120m.

The majority of the FB values shown in Tables 1 and 2 are close to zero, which reflects the substantial agreement between mean measured and predicted values observed with both models. The FB statistics are better for compounds with negligible evaporative emissions closer to the source, whereas for evaporative compounds they improve as distance from source increases.

Compound	D ^a	$\overline{C}_O$ ^b	$\overline{C}_P$ ^c	IA ^d	FB ^e	R ^f	NMSE ^g	F2 ^h
n-pentane	25	0.17	0.15	0.36	-0.13	0.27	1.5	50%
	120	0.05	0.05	0.30	-0.16	0.39	3.9	30%
	240	0.03	0.03	0.17	-0.04	-0.02	2.6	20%
Iso-pentane	25	0.51	0.33	0.27	-0.44	0.12	3.2	40%
	120	0.13	0.10	0.25	-0.21	0.35	4.8	20%
	240	0.06	0.06	0.20	-0.04	0.03	2.1	25%
Ethene	25	0.85	0.91	0.43	0.07	0.16	0.4	80%
	120	0.26	0.28	0.34	0.10	0.24	1.7	45%
	240	0.11	0.17	0.27	0.41	-0.15	1.1	40%
Propene	25	0.29	0.27	0.30	-0.07	0.05	0.6	70%
	120	0.08	0.08	0.38	0.11	0.06	1.1	50%
	240	0.04	0.05	0.11	0.16	-0.31	1.7	25%
1,3 butadiene	25	0.10	0.10	0.29	-0.03	0.12	0.8	55%
	120	0.02	0.03	0.50	0.66	0.26	1.7	30%
	240	0.02	0.02	0.23	0.12	0.01	1.6	20%
Acetylene	25	0.45	0.36	0.44	-0.22	0.29	0.6	55%
	120	0.14	0.11	0.23	-0.25	0.26	3.7	20%
	240	0.09	0.07	0.29	-0.26	0.05	1.6	25%
Benzene	25	0.15	0.19	0.43	0.22	0.11	0.3	65%
	120	0.05	0.06	0.36	0.10	0.33	1.7	45%
	240	0.03	0.03	0.20	0.07	-0.04	1.4	20%

^a downwind receptor distance (m), ^b observed (measured) average background corrected concentration (ppb), ^c predicted (modeled) average background corrected concentration (ppb), ^d Index of Agreement, ^e Fractional bias, ^f Pearson's correlation coefficient, ^g Normalized mean square error, ^h Percentage of data in range $0.5 \leq C_O/C_P \leq 2$

Table 4.2 Statistical comparison of measured and modelled data from CALINE4.

Compound	D ^a	$\overline{C_o}^b$	$\overline{C_p}^c$	IA ^d	FB ^e	R ^f	NMSE ^g	F2 ^h
n-pentane	25	0.17	0.15	0.47	-0.13	0.39	1.4	45%
	120	0.05	0.04	0.31	-0.43	0.46	5.3	20%
	240	0.03	0.02	0.25	-0.46	-0.03	4.1	25%
Iso-pentane	25	0.51	0.33	0.33	-0.44	0.25	3.2	40%
	120	0.13	0.08	0.28	-0.48	0.45	6.5	15%
	240	0.06	0.04	0.26	-0.43	-0.03	3.3	15%
Ethene	25	0.90	0.91	0.49	0.06	0.23	0.4	80%
	120	0.26	0.21	0.36	-0.19	0.39	2.1	45%
	240	0.11	0.11	0.28	-0.02	0.06	1.3	25%
Propene	25	0.29	0.27	0.29	-0.07	0.02	0.7	70%
	120	0.08	0.06	0.42	-0.18	0.26	0.8	40%
	240	0.04	0.03	0.23	-0.27	-0.03	2.0	35%
1,3 butadiene	25	0.10	0.09	0.25	-0.07	0.02	0.9	60%
	120	0.02	0.02	0.45	0.36	0.27	1.7	20%
	240	0.02	0.01	0.29	-0.34	0.09	2.5	20%
Acetylene	25	0.45	0.36	0.55	-0.23	0.45	0.6	65%
	120	0.14	0.08	0.26	-0.54	0.35	5.1	20%
	240	0.09	0.04	0.39	-0.67	0.04	2.8	10%
Benzene	25	0.15	0.19	0.57	0.20	0.31	0.3	90%
	120	0.05	0.04	0.38	-0.193	0.44	2.2	35%
	240	0.03	0.02	0.33	-0.38	0.02	2.2	20%

^a downwind receptor distance (m), ^b observed (measured) average background corrected concentration (ppb), ^c predicted (modeled) average background corrected concentration (ppb), ^d Index of Agreement, ^e Fractional bias, ^f Pearson's correlation coefficient, ^g Normalized mean square error, ^h Percentage of data in range $0.5 \leq C_o/C_p \leq 2$

Table 4.3 Statistical comparison of measured and modelled data from GFLSM.

The Pearson's correlation coefficients obtained with both models are fairly low for all hydrocarbons, but would improve substantially if total rather than background corrected concentrations were examined. The highest R- values tend to occur at the distance 120m whereas there seems to be hardly any correlation between the monitored and predicted datasets at 240m downwind of the road. It is to be noted that the R values obtained from both the models are quite close to each other, even at a downwind distance of 240m. However it is also observed that the GFLSM usually displays a higher R value than CALINE4, which suggests that the prediction values from GFLSM are more in sync with the monitored data than CALINE4.

With both models, NMSE values less than 0.5 were obtained for ethene and benzene at 25m receptor, while for receptors located at 120m and 240m, the NMSE values are nearly all greater than 0.5. The lowest NMSE values were obtained at the receptor nearest the M50 with exhaust emitted hydrocarbons, for which all values are less than 0.8. On the contrary, compounds with evaporative emissions display high NMSE values even at the receptor closest to the source. Overall the NMSE values obtained with CALINE4 tend to be slightly lower than those obtained with GFLSM.

The percentage of F_2 values decreases with receptor distance. This can be attributed to the fact that the receptor near the source has a higher concentration whereas for receptor locations further downwind, the frequency of background corrected concentrations of zero increases. This tends to reduce the F_2 values further downwind.

4.3 Study summary.

An inter-comparison of the GFLSM and CALINE4 against monitored data collected during an ambient hydrocarbon measurement campaign conducted near a motorway has been presented.

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Graphical and statistical analyses reveal reasonable agreement between measured and predicted datasets using both models for all hydrocarbons. Agreement is best close to the road, however, and for both models model performance decreases with the increase in downwind distances. Model results were compared with background- corrected concentrations measurements which it is suggested represents the best basis for model assessment.

An inter-comparison study of the models themselves was also performed. On most measures the performance of CALINE4 was exceeded by that of GFLSM. Predicted values obtained with both models when compared with monitored data reveal good long term model accuracy. This is especially relevant as the limit values of certain hydrocarbons are expressed as long term (annual) averages.

Short term model performance was not as good. On an overall basis the range of predicted values was lower than the range of the monitored values, which implies that short term modelling will underestimate higher percentile concentrations. Overall, the short term model performance was best at receptor nearest to the source.

This study showed that the performance of the GFLSM, an analytical model, was quite impressive when compared with that of the more computationally complex CALINE4 and that the GFLSM often outperformed the CALINE4 on some measures.

4.4 Monasterevin Bypass Study.

A monitoring campaign was carried out at Monasterevin, Co. Kildare from October 2004 to January 2005, which covered the immediate periods before and after the opening of a new bypass of the town. A modelling assignment was carried out to determine whether the subsequent change in the air quality could be predicted using highway modelling and for this purpose the GFLSM as previously described was used. The relevant details of the modelling exercise are described in the next few sections. The pollutants chosen for the study were CO and NO_x.

4.4.1 Site Description.

Monasterevin lies 80km south of Dublin, near the Laois/Kildare county border. Kildare County Council classifies Monasterevin as a moderate growth town with a population of roughly 3000. Figure 4.6 shows a map showing the location of Monasterevin and the new M7 motorway. The monitoring unit was located at the edge of the town adjacent to the N7 in the grounds of the Garda station. The N7 is aligned at $110^{\circ} - 290^{\circ}$ at this location. The monitoring unit was located 10 meters from the center line of the road and behind a 0.5m high wall. Figure 4.7 presents a schematic sketch of the site and Figure 4.8 shows a photograph of the Garda station. The same instruments and their operational techniques as described in Chapter 3 were used for recording monitored concentrations of CO and NO_x at the M4 site.

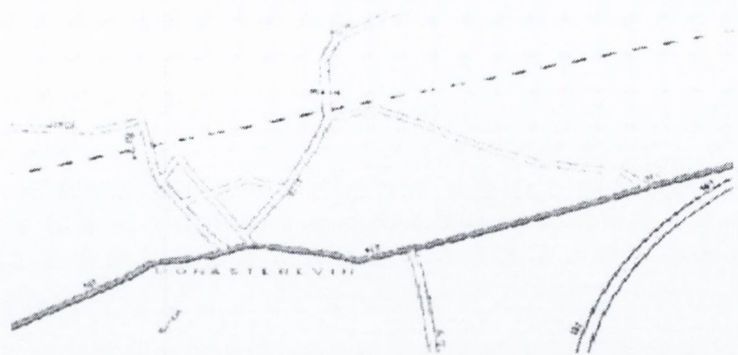


Figure 4.6 Map of N7 through Monasterevin.

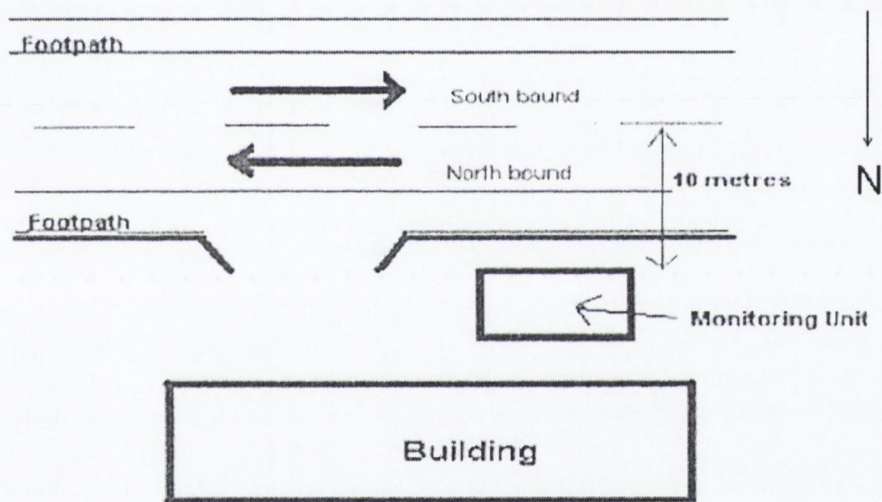


Figure 4.7 Schematic diagram of the site.

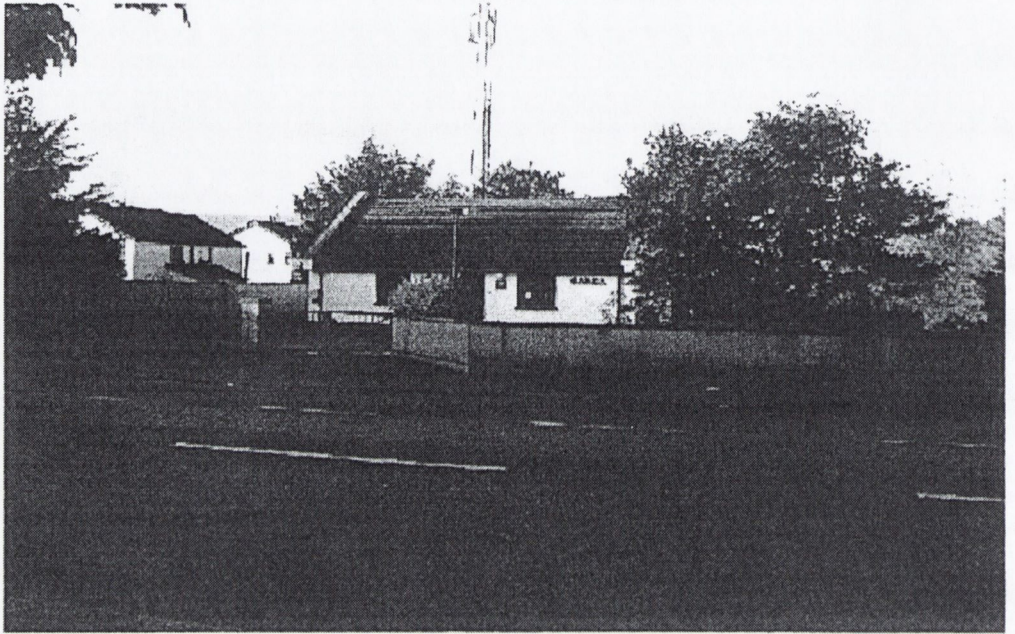


Figure 4.8 Garda station at Monasterevin.

4.4.2 Traffic data.

The initial traffic flow for the Monasterevin site was obtained from the National Roads Authority (NRA) website (www.nra.ie). It reported that an annual average daily traffic (AADT) of 17450 vehicles was passing through the town. At the time of study this data set was not assumed to be entirely correct as it represented the data for the year 2003. Consequently, the flow through the town before the opening of the bypass was estimated from the M7 traffic recorded after opening by assuming that all the traffic on the bypass had previously no option but to use the N7 through Monasterevin. A series of manual counts were conducted in the town centre to calculate residual flows in each case. Traffic data were recorded hourly and the percentage HGVs noted. The AADT data for the before case was calculated as 24106 for the weekdays with about 17% HGVs while the AADT values after opening was 11982 with 6% being HGVs.

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4.4.3 Meteorological data.

The requisite meteorological data comprising of wind speed, wind direction and temperature were recorded on site. Met Eireann data of wind speed, wind direction, temperature and Pasquill stability classes were also obtained. These were measured at Casement Aerodrome 50km northeast of the site giving a good account of the regional meteorological conditions.

4.5 Results.

4.5.1 Monitoring Results

The monitoring results for the two pollutants CO and NO_x are discussed below. A significant change in pollutant concentrations was observed upon the opening of the bypass, as is clearly evident in the monitoring results.

4.5.1.1 Monitoring Results for CO

The average CO concentration monitored before the opening of the bypass was 0.39ppm whereas the average monitored CO concentration after the opening of the bypass was 0.27ppm which confirms the improvement of air quality. Figure 4.9 shows the diurnal profiles for the before and after cases for CO.

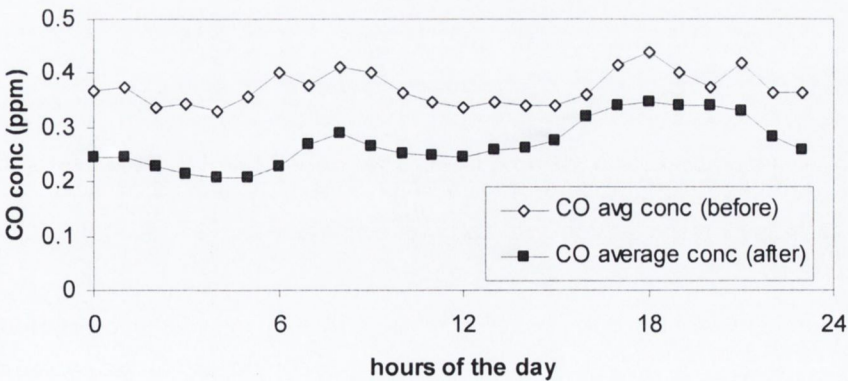


Figure 4.9 Diurnal profiles for CO for before and after cases.

The maximum difference in concentrations occurs at 0700 hours (0.17ppm) whereas the minimum difference occurs at 1700 and 2100 hours (0.04ppm). The presence of two peaks in both the profiles at 0900 and 1900 hours are attributed to the peak traffic flows, which confirms that local air quality is significantly affected by vehicular emissions.

4.5.1.2 Monitoring Results for NO_x .

The average monitored NO_x concentration before the opening of the bypass was observed to be 41.83 ppb whereas the average concentration observed after opening of the bypass was 18.39 ppb implying an average reduction of 23.44 ppb. Figure 4.10 presents the diurnal profiles for NO_x for both cases. The maximum reduction occurs at 0600 hours (44.62 ppb) and the minimum reduction occurs at 1500 hours (6.30 ppb). Clear traffic related peaks are observed in both cases.

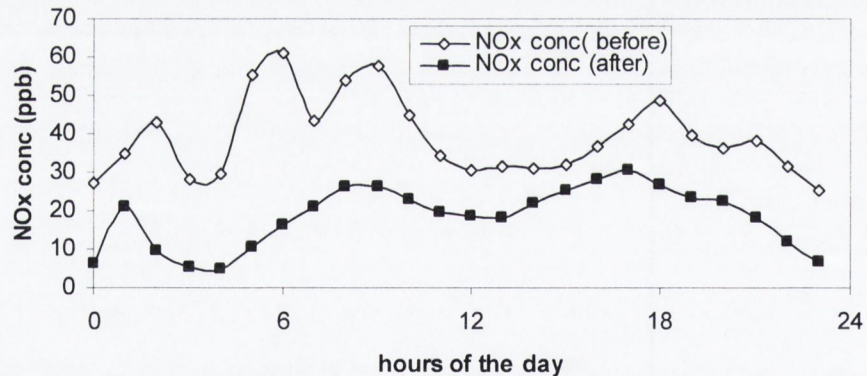


Figure 4.10 Diurnal profiles for NO_x for before and after cases.

4.5.2 Modelling Results

The GFLSM model was applied to predict the change in NO_x and CO concentrations due to the opening of the bypass. The details of the model have already been explained in the last chapter. The modelling of the pollutants was carried out for two different conditions, before

opening of the bypass and after the opening of the bypass. The difference between these results represents the predicted change in air quality due to the opening of the bypass Table 4.4 presents the CEF values used for CO and NO_x modelling of the before and after cases. The modelling results for the pollutants CO and NO_x are described below.

Composite Emission Factor	CO (g/km)	NO _x (g/km)
Before (25km/hr)	2.06	0.52
After (45km/hr)	1.27	0.42

Table 4.4 CEF values for CO and NO_x.

4.5.2.1 Modelling Results for CO.

Figure 4.11 – 4.13 present the diurnal profiles of the monitored and modelled CO concentrations for the before case, the after case and the change in air quality due to the opening of the bypass.

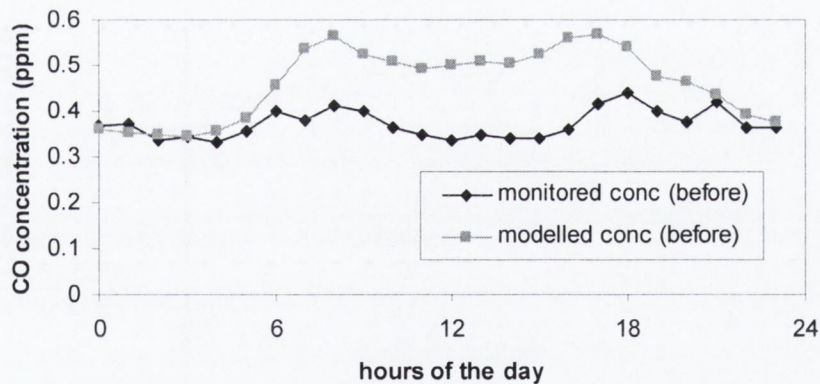


Figure 4.11 Diurnal profiles for CO before opening of the bypass.

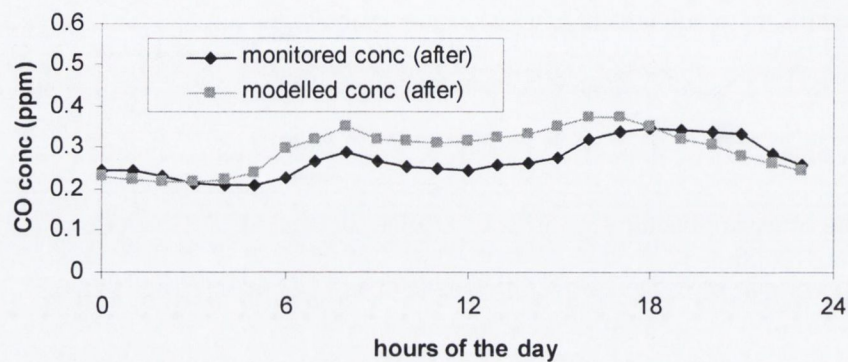


Figure 4.12 Diurnal profiles for CO after opening of the bypass.

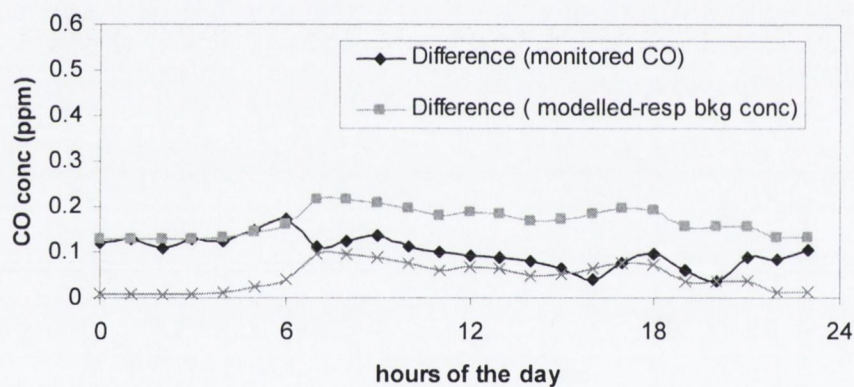


Figure 4.13 Diurnal profiles for CO due to change in air quality due to opening of bypass.

The model evaluation parameters determined for the different modelling scenarios are summarised in Tables 4.5 and 4.6. In Table 4.5, the statistical parameters are calculated using the hourly averages whereas in Table 4.6, they are calculated using the diurnal profile approach.

Parameters	Measured CO (before)	Predicted CO (before)	Measured CO (after)	Predicted CO (after)
Mean	0.39	0.48	0.27	0.30
SD	0.05	0.07	0.04	0.05
IA	1.00	0.49	1.00	0.61
NMSE	0.00	0.19	0.00	0.20
R	1.00	0.23	1.00	0.49
FB	0.00	0.20	0.00	0.10

Table 4.5 Statistical analysis for before and after cases at Monasterevin for CO (hourly approach).

Parameters	Mon CO (before)	Mod CO (before)	Mon CO (after)	Mod CO (after)	Observed change	Predicted change	
						Act bkg	Bkg corrected
Mean	0.37	0.46	0.27	0.30	0.10	0.17	0.05
SD	0.03	0.08	0.04	0.05	0.03	0.03	0.03
IA	1.00	0.36	1.00	0.74	1.00	0.32	0.32
NMSE	0.00	0.08	0.00	0.03	0.00	0.38	1.12
R	1.00	0.40	1.00	0.64	1.00	-0.15	-0.15
FB	0.00	0.22	0.00	0.09	0.00	0.49	-0.75
F2	100.00	78	100.00	60	100.00	62.50	62.50

Table 4.6 Statistical analysis for three different cases at Monasterevin for CO (diurnal profile approach).

It is important to point out that there existed no adequate background data for the particular study. It was assumed that the background value of the CO concentration was the average concentration observed at 0400 hours when it is assumed that the traffic influence at this site would be the least. Consequently the CO background values used were 0.33ppm and 0.21ppm for the before and after opening scenarios of the bypass. A ‘background corrected’ condition was also considered. The difference between the two background values (in the before and after cases) is 0.12ppm. This difference (0.12ppm) was subtracted from the difference between the modelled concentrations for the before and after cases to obtain a set of ‘background corrected’ values.

It is seen from the diurnal profiles that the modelled data generally follows the trend of the monitored data. However, the model results overpredict the measured concentrations in both the before and after cases. The statistical analysis tests carried out seem to confirm this fact. This is particularly highlighted by the low IA and R values. In an overall sense, the model seems to perform best in the after case. One reason for this could be that a longer monitoring period was employed in the after case. There seems to be no improvement when considering the ‘background corrected’ conditions. Delaney (2006), studied the linear relationship between the modelled data obtained using CALINE4 and monitored data at the same study site and obtained an R^2 value of 0.2 and 0.4 for the before case and the after cases respectively. In a likewise comparison the R^2 value obtained using GFLSM was 0.16 and 0.4 (diurnal profile approach) for the before and after cases respectively. It can be seen from the comparison that the performance of GFLSM is similar to CALINE4 and that performance of both models in predicting the change in air quality is poor.

4.5.2.2 Modelling Results for NO_x

A similar study was carried out for NO_x . Figures 4.14 – 4.16 represent the diurnal profiles for NO_x concentration for the before case, the after case and the change in air quality scenarios.

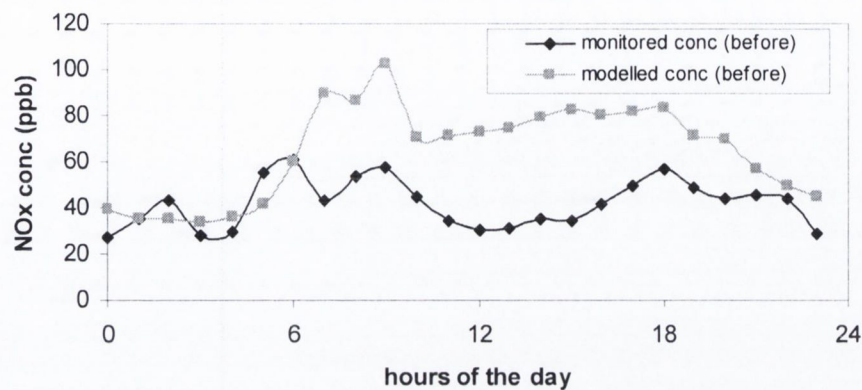


Figure 4.14 Diurnal profiles for NO_x before opening of the bypass.

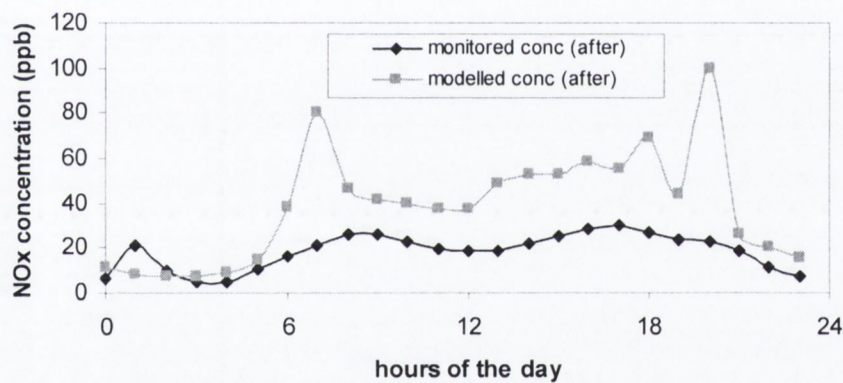


Figure 4.15 Diurnal profiles for NO_x after opening of the bypass.

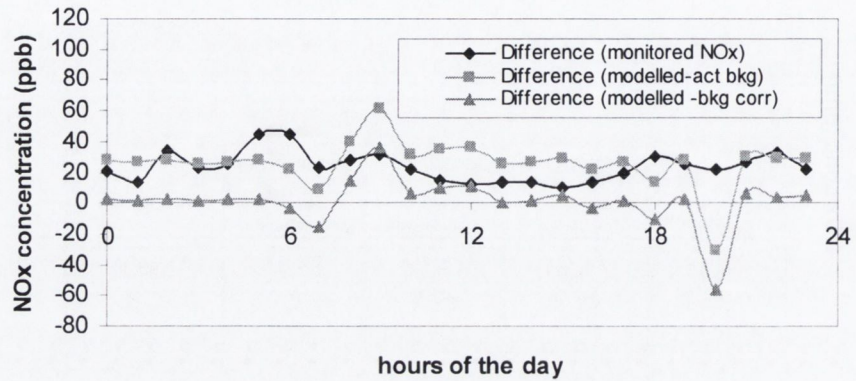


Figure 4.16 Diurnal profiles for NO_x due to change in air quality due to opening of bypass.

Tables 4.7 and 4.8 gives the statistical analysis of the results for all the three different scenarios using monitored and modelled NO_x data using the same approach as used for calculating CO concentrations.

Parameters	Measured NO_x (before)	Predicted NO_x (before)	Measured NO_x (after)	Predicted NO_x (after)
Mean	41.83	60.47	18.23	31.17
SD	7.28	9.95	6.55	16.69
IA	1.00	0.54	1.00	0.72
NMSE	0.00	0.82	0.00	1.26
R	1.00	0.30	1.00	0.60
FB	0.00	0.36	0.00	0.52
F2	100.00	50.00	100.00	50.00

Table 4.7 Statistical analysis for before and after cases at Monasterevin for NO_x (hourly approach).

Parameters	Measured NO _x (before)	Predicted NO _x (before)	Measured NO _x (after)	Predicted NO _x (after)	Observed change	Predicted change	
						Act bkg	Bkg corrected
Mean	41.81	60.36	18.40	38.38	23.40	26.04	1.13
SD	10.35	20.48	7.77	24.48	9.46	15.26	15.26
IA	1.00	0.41	1.00	0.41	1.00	0.27	0.29
NMSE	0.00	0.31	0.00	1.09	0.00	0.50	29.95
R	1.00	0.42	1.00	0.72	1.00	0.04	0.04
FB	0.00	0.43	0.00	0.70	0.00	0.11	-1.82
F2	100.00	75.00	100.00	54.00	100.00	62.50	62.50

Table 4.8 Statistical analysis for three different cases at Monasterevin for NO_x (diurnal profile approach).

As seen in the CO the modelled data tends to overpredict the monitored data. The background concentrations used for NO_x were based on the similar assumptions as mentioned for the CO and the background concentrations used were 29.62ppb and 4.71ppb for the before and after cases respectively. Statistical analysis of the modelled data sets and monitored data sets indicate that the model performance is poor. This is particularly highlighted by the low IA and R values. Delaney 2006, reported that the R² value for the before and after cases for NO_x was 0.25 and 0.21 for the before and after cases respectively using CALINE4 modelling technique. The R² value using GFLSM were found to be 0.18 and 0.52 (diurnal profile approach) for before and after cases respectively. It can be said that the performance of both models in predicting the dataset is poor however the performance of the GFLSM model in predicting the after case gives a much better result for R² than obtained using CALINE4. Another reason for relative prediction of NO_x concentrations could be due to the models inability to account for the NO_x/ozone reactions that are common during the daytime period. A wrong usage of the background concentration can also alter the model results heavily and could also be an important criterion that leads to poor modelling results. However with the lack of proper

information, the usage of the average value at 0400 hours as the background concentration is reasonably justified.

4.6 An Overall Summary of Highway Modelling.

Chapter 3 and 4 of this thesis describes the modelling of air quality adjacent to highways using two Gaussian based dispersion models, GFLSM and CALINE4. Three separate study sites were selected having different monitoring scenarios, available data and pollutants for study.

The first site selected was the M4 site. A screening model DMRB was first employed followed by a detailed modelling assessment. This is an almost ideal site used for such a study. A detailed monitoring campaign had provided a lot of necessary data (traffic and meteorological and background) for modelling and model assessment. Recorded hourly background concentrations were available for the last six months of the study and a diurnal average of those was used as the background concentrations for the first six months. Also, a new proposal regarding the use of background concentrations as per stability class was proposed and it was shown to give good model efficiency. Generally, in modelling a CEF is often used, however the proposed new concept of an Hourly Emission Factor was investigated. Though not much significant changes occurred in the results, this represents a more logical approach for modelling emission factors. Whereas the GFLSM model is an analytical model the CALINE4 model is a computer based numerical model, however the model predictions obtained from the GFLSM model were as good as that obtained from CALINE4, and even outperformed it sometimes. This is of particular interest as because it seems that the GFLSM model could be easily incorporated in an existing traffic model to determine pollution effects and support policy and planning decisions. Further to this a sensitivity analysis of the GFLSM and CALINE4 models were carried out for different wind speed conditions and stability class

conditions and the results again confirmed the inherent weakness of the Gaussian models, namely their underperformance in calm conditions and stable stability conditions.

The second site selected for the study was adjacent to the M50 motorway. Here the monitoring was carried out for hydrocarbons with receptors placed at 25m, 120m and 240m from either kerbside, allowing for 'background corrected' concentrations to be determined. As a result of the modelling exercise carried out it was observed that both models were able to particularly model trace concentrations of hydrocarbons reasonably well particularly at the receptor location close to the motorway. Both the selected models were more effective in predicting the long term modelling results. Short term modelling results was not that good. The performance of modelled values decreased with the increase of receptor locations and also the performance of GFLSM was similar or better to CALINE4 modelling results.

Lastly the GFLSM model was applied to the Monasterevin site to predict the change in air quality due to the opening of the bypass. The dataset available here was the least of all cases and this probably actually represents a real life modelling scenario. Monitoring and modelled data showed that there indeed existed a change in air quality due to the opening of the bypass; however the change was not accurately depicted in the modelling results. The modelling results though seem to follow the trend for before and after cases and give an improved result for the after case. The non availability of the proper background data may have also impeded the modelling results at the Monasterevin site. Further to this Delaney (2006) performed the CALINE4 modelling using three different links, whereas the GFLSM modelling results were obtained using a single link approach due to application limitations. Despite this, the GFLSM

model performed well particularly when compared to CALINE4 modelling results for the after case. On an overall basis the GFLSM model seems to perform well when compared with monitored data and with modelled data using CALINE4 and the use of HEF and background concentrations as per stability class can lead to improved modelling results. In general, the accuracy of these models seems low but considering the variables they consider and variables they leave out, they do well satisfy the EU 50% prediction criteria for the M4 and Monasterevin.

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5.1 Introduction.

Chapter 3 and 4 of the thesis described in detail the application of the GFLSM and CALINE4 models to the agreement of air quality in the vicinity of the highways. This chapter deals with the modelling of CO and NO_x concentrations on Pearse Street, an urban street canyon in the heart of Dublin city centre. The models are specifically designed for evaluating air quality in street canyons, where the existence of a recirculating vortex leads to unique pollutant transport and dispersion conditions.

In this context, two urban street canyon models, namely STREET and OSPM, were investigated. STREET (Johnson et al., 1973) is a simple semi-empirical model that calculates series of hourly concentrations at different receptor locations within a street canyon. The OSPM (Berkowicz, 2000) is also a semi-empirical model and calculates on-street concentrations as the sum of three separate components, i.e., (1) direct transport of pollutants from source to receptor, (2) recirculation due to flow of pollutants around the vortex generated within and (3) background concentrations. Model performance is assessed by comparison with measured CO and NO_x concentrations. Modelling analysis was carried out for weekdays during the monitoring period, which extends over an eight-month period for which measured traffic flows and background pollutant concentrations were available. Both models considered are semi empirical in nature, but STREET can be considered an analytical model (similar to GFLSM) whereas OSPM is more numerically intensive, albeit not to the same extent as CALINE4. Both models are described in detail in later sections of this chapter.

One of the objectives of the work was to investigate the STREET model as a suitable alternative for the prediction of CO and NO_x concentrations in an urban street canyon, with a view to its later use in integrated transport air quality modelling. Emission factor modelling

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was also studied. Composite emission factors (CEFs) and hourly emission factors (HEFs) were both used to assess their effect on prediction of CO and NO_x concentrations, with separate CEFs being used for the daytime and nighttime periods. The dependency of model predictions on the assumed background concentrations was also studied for the pollutant NO_x. Of particular interest was the relative accuracy of these models with the GFLSM and CALINE4 highway models assessed in Chapters 3 and 4.

5.2 Application to a Street Canyon Site (Pearse Street junction).

Pearse Street is a four-lane one-way route in the centre of Dublin City, with an approximately East-West orientation and an average daily traffic flow of 60,000 vehicles, of which 10% are HGVs. The height of the canyon is 16m and width is 21m. An overall layout of the Pearse Street canyon is shown in Figure 5.1.

Continuous monitoring of hourly CO and NO_x concentrations is performed by Trinity College Dublin at a long-term air quality monitoring station on the southern side of the street using the same monitoring equipment as described in Chapter 3. The sampling point is located 4.48m from the bus lane and 1.91m above street level. Hourly meteorological conditions were recorded at Dublin Airport. Hourly traffic flows on the street were measured by the traffic control system operated by Dublin City Council



Figure 5.1 An overall view of the Pearse Street Canyon.

Hourly background concentrations were obtained from an urban air quality monitoring station operated by Dublin City Council at Winetavern Street, which is located approximately 1 km west of Pearse St, and approximately 100m from the nearest trafficked street. A location map outlining both the streets is shown in figure 5.2.

All these recorded parameters were used in computing the modelled CO concentrations. These were then compared with measured CO concentrations. Background concentrations computed using different assumptions and their influence on modelling results have also been shown and will be described in details in later sections of this chapter for the pollutant NO_x . These were then compared with measured NO_x concentrations. Comparison was carried out based on an eight months data set from May 2006 to December 2006.

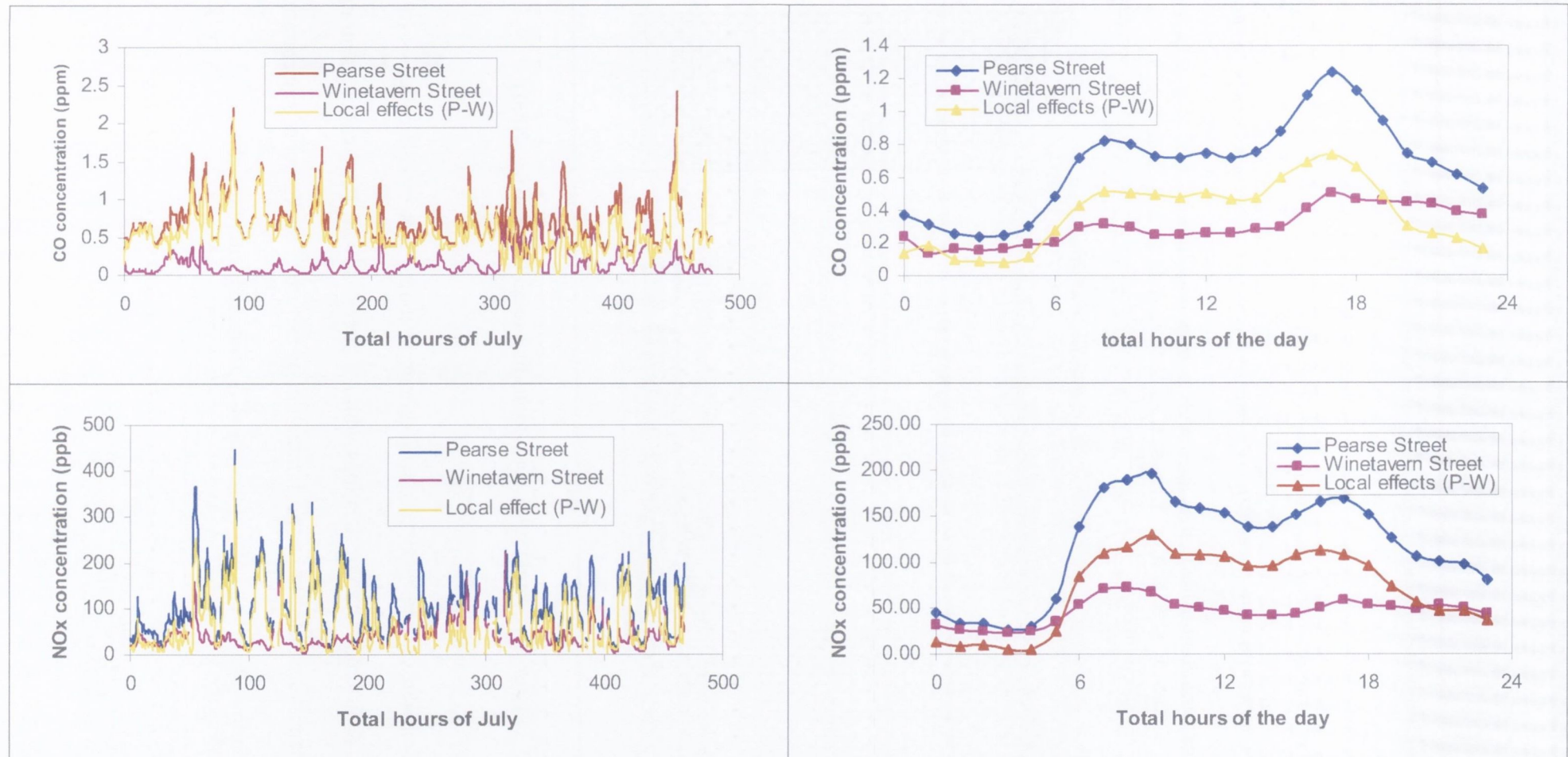
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Figure 5.2 Location details of background and monitoring site.

Evaluating the local effects of CO and NO_x concentration.

As mentioned previously, continuous monitoring data from Pearse Street and the relevant background concentrations from Winetavern Street were available to determine and compare the final modelled values using STREET and OSPM. In this context the monitored and background data, so available, were used for determining the local effects of CO and NO_x which primarily consists of subtracting the background data from the monitored data to determine the local effects of CO and NO_x concentration. The average monitored and background concentrations were 118.36ppb and 46.91ppb respectively for NO_x and 0.67ppm and 0.30ppm for CO. Hence the background concentrations constitute about 40% of the monitored concentrations for NO_x and 45% for CO with the remaining being constituted due to local effects of NO_x primarily being traffic. Figure 5.3 represents a graphical overview of the local traffic impacts.

Figure 5.3 Local effects of CO and NO_x

5.3 Computational Methods.

5.3.1 STREET.

The principal assumption when using street pollution models is the formation of a wind vortex with respect to air flow in street canyon. The formation of this vortex leads to an uneven pollutant concentration profile across the street, as shown in Figure 5.4

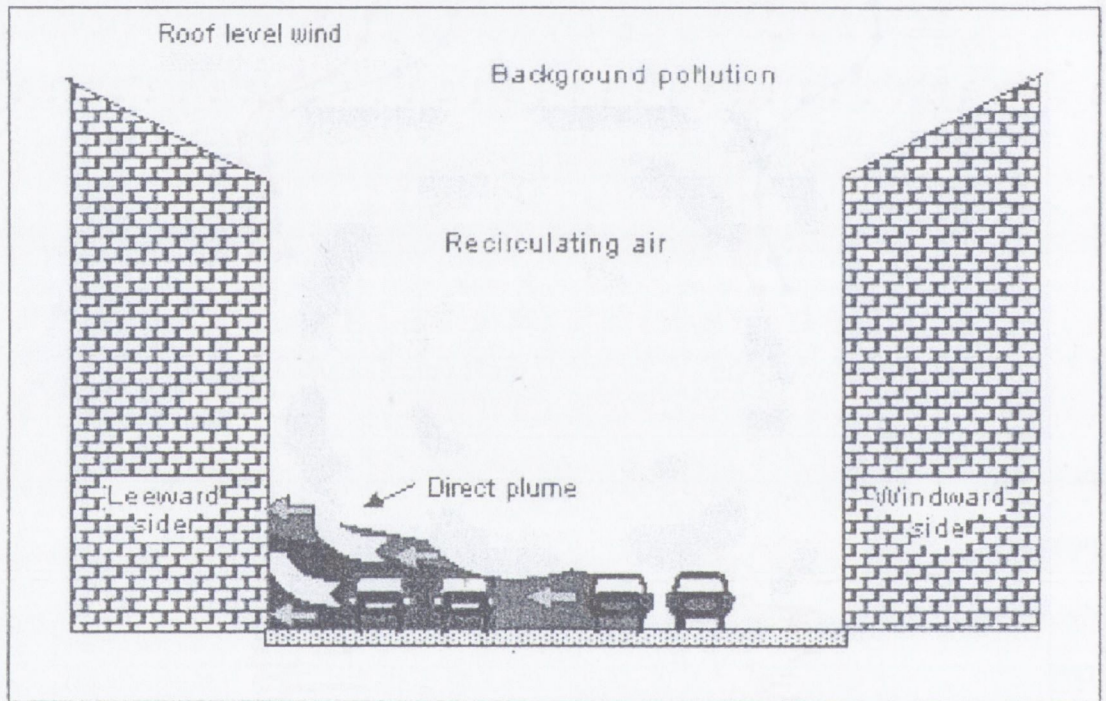


Figure 5.4 Wind vortex formations in a street (Berkowicz, 2000).

STREET (Johnson et al., 1973) is a semi-empirical model that calculates series of hourly calculations at different receptor locations within a street canyon. The total concentration (C) of the pollutant is assumed to be the summation of the urban background concentration (C_b) and concentration due to vehicular emissions (C_s) generated within the canyon.

$$C = C_s + C_b \quad (5.1)$$

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The C_s concentration component is derived from a simple box model (Johnson et al., 1973) that gives the concentrations of the pollutant on the leeward and windward sides of the street. The windward side is defined as the side of the street to which the wind blows at roof level, while the leeward side is the side of the street from which the roof wind blows. The concentration on the leeward side of the street is computed using equation (5.2)

$$C_s^L = \frac{KQ}{(U + U_s)(\sqrt{x^2 + z^2} + h_o)} \quad (5.2)$$

where K is an empirical constant parameter, Q is the rate of release of emissions in the street, x is the horizontal distance between the receptor and the centre of the nearest traffic lane, z is the height of the receptor, h_o is a constant that accounts for height of initial pollution dispersion (empirical value of 2 m). In this context Johnson et al. (1973) mentioned that the motion of the cars mix the pollutants into an initial volume of dimension (h_o) comparable to the vehicle size of 2 m. U is the roof level wind speed and U_s is a constant that accounts for the additional air movement induced by vehicle traffic (empirical value of 0.5m/s). In this study, the value of $K = 7$ was determined and the procedure for determination is explained below. Previous studies on the STREET model have used K values of 7 (Vardoulakis et al., 2002b), Qin and Kot (1993) estimated the value of K to be 6 for their work in an asymmetric street canyon in China whereas Bogo et al. (2001) reportedly used a K value of 8 for a similar study in Buenos Aires. On the windward side, the initial expression for C_s given by Johnson et al. (1973) was revised by Dabberdt et al. (1973) to take into consideration the decrease in concentrations due to entrainment of fresh air through the top of the canyon. The resulting equation for calculating concentrations on the windward side of the street is given in equation (5.3)

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$$C_s^w = \frac{KQ}{W(U + U_s)} \left(\frac{H - z}{H} \right) \quad (5.3)$$

Where H is the height and W is the width of the canyon. For parallel or near parallel winds, the average of the windward and leeward concentrations calculated using equations (5.2) and (5.3) was adopted for both sides of the street. The concentrations obtained on the leeward side represent the build-up of the pollutant concentration whereas the windward side accounts for the background pollutant concentration and pollutant concentration obtained due to recirculation in the street.

5.3.2 OSPM

The OSPM model (Berkowicz, 2000) is based on principles that are similar to the CPB model proposed by Yamartino and Wiegand (1986). Concentrations of exhaust gases are calculated using a combination of a plume model for the direct contribution and a box model for the recirculating component of the pollutants in the street.

Berkowicz, (2000) states six main assumptions that are incorporated in the model:

- A vortex is formed in the street whenever a wind component perpendicular to the street exists. Vortex length is dependant on upwind (leeward) building height. The length of the vortex is also dependent on the wind speed and wind direction.
- The upwind receptor receives contributions from traffic emissions within the recirculation zone (i.e., the vortex area), the recirculation pollution and a portion of the emissions outside the recirculation zone. These contributions are wind speed and wind direction dependant.
- The downwind receptor receives the contribution mainly from the recirculation zone and if the vortex does not occupy the entire street, traffic emissions from outside the recirculation zone.

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- As wind speed approaches calm conditions, or wind direction is parallel to the street, concentrations on both sides are equal.
- The direct contribution in the recirculation zone is calculated by a plume model that assumes linear dispersion of pollutants with distance. Emissions are assumed to be uniformly distributed across the street.
- A box model describes the recirculation component. Concentrations are calculated assuming equality of the incoming and out going pollution fluxes.

Turbulence within the street is composed of two parts- (1) ambient turbulence, which is a function of wind speed and (2) vehicle induced turbulence. Vehicle induced turbulence is dominant at low wind speeds, and is dependent on traffic intensity, average vehicle speeds and average vehicle dimensions. The effects of thermal stratification on turbulence are not considered and the stability class is assumed to be always neutral. The main argument for such an assumption is that atmospheric stability is determined by both mechanical stresses and buoyant forcing but, for a typical urban setting with a given thermal stability or sensible heat flux, building induced mechanical stresses can become so dominant to drive the resulting stability toward nearly neutral

The total concentration of pollutant at a receptor on the street is given by equation (5.4)

$$C_s = C_d + C_r + C_b \quad (5.4)$$

Where C_s is the total concentration, C_d is the direct contribution, i.e., the direct flow of pollutants from vehicles to monitor, C_r is the recirculation component due to the wind vortex and C_b is the urban background concentration of the pollutant. C_d is calculated using a plume model and taken to be zero on the windward side. As a consequence, the concentrations obtained on the windward side are lower than those on leeward side. Emissions are assumed to

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be constant throughout the street and are modelled as a number of infinitesimal line sources aligned perpendicular to wind direction at street level. The dispersion of the plume is assumed to represent both to convective and mechanical turbulence in vehicle wakes. C_r is computed using a box model in which the underlying principle is that the inflow rate of the pollutants in the recirculation equals the outflow rate, and that the pollutants are thoroughly mixed in the zone. Figure 5.5 depicts the assumed recirculation process. The value of C_b is determined by the modeller. Figure 5.6 gives a schematic diagram of the model input parameters required for proper evaluation of the OSPM model.

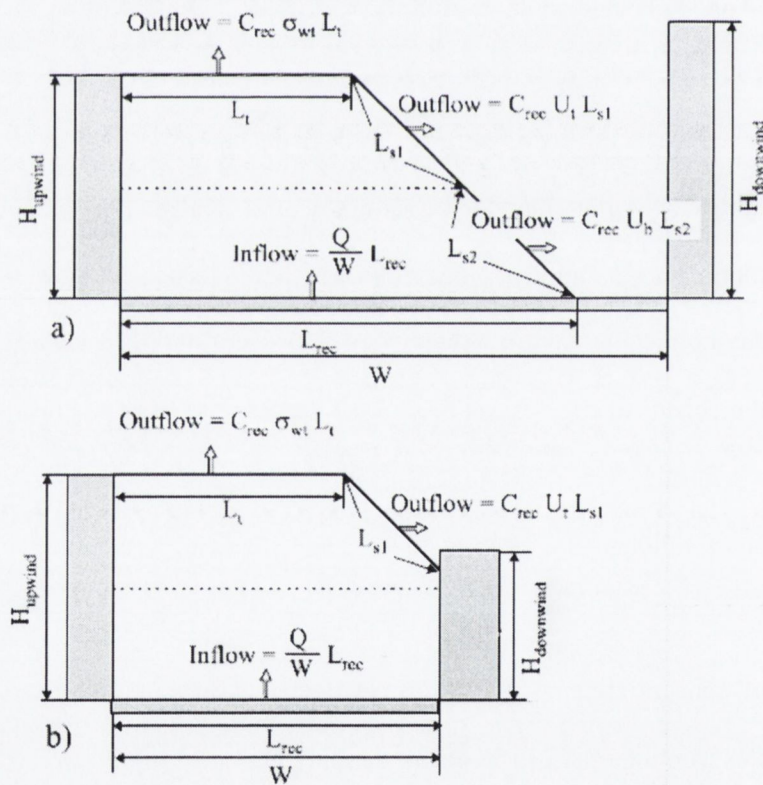


Figure 5.5 The geometry of the recirculation zone; (a) the recirculation zone totally inside the canyon and (b) the downwind building intercepting the recirculation zone

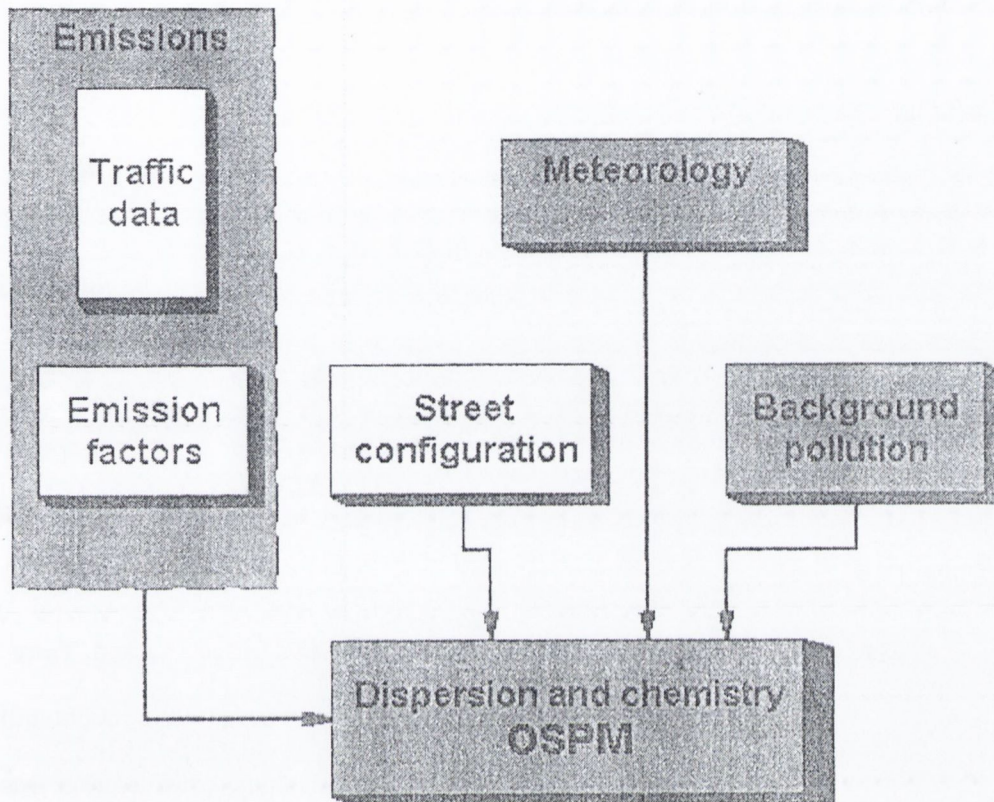


Figure 5.6 OSPM model inputs.

The relevant mathematical formulation of the OSPM has been reported by Buckland (1998) and Vardoulakis et al (2002) and is presented below in an algorithm for determining pollutant concentration using a series of equations. This algorithm has been implemented on a computational platform (MS excel) to allow full investigation of model accuracy

Step 1: Calculate the length of the street vortex (L_v) using the following expression:

$$L_v = 2rH_b \quad (5.5)$$

Where r indicates the strength of the vortex and is dependent on the wind speeds. The value of ' r ' is 1 for wind speed $U \geq 2\text{m/s}$ and 0.5 for $U < 2\text{m/s}$. H_b denotes the height of the building.

Step 2: Calculate the length of the recirculation zone (L_{rec})

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The L_{rec} is calculated using the following expression:

$$L_{rec} = \text{Min}(L, L_v \sin \phi) \quad (5.6)$$

Where ' ϕ ' represents the wind angle and L represents the width of the street.

Step 3: The traffic turbulence and combined turbulence are calculated using the following expressions:

$$\sigma_{wo} = b \left(\frac{V_c N_c S_c^2 + V_h N_h S_h^2}{l} \right)^{0.5} \quad (5.7)$$

$$\sigma_w = \sqrt{(0.1U_b)^2 + \sigma_{wo}^2} \quad (5.8)$$

Where, ' b ' is the aerodynamic drag coefficient and a value of 0.3 is used, V_c and V_h are average driving speeds for cars and heavy vehicles and values of 4.17m/s (0900-1800hours) and value of 9.72m/s was used for period 1700-0800hours. Heavy vehicle consideration was not assumed at this site. N_c and N_h are traffic intensities for cars and heavy vehicles and S_c^2 and S_h^2 are average horizontal areas and a value of 2.41m² was utilised for the former. σ_{wo} is the traffic created turbulence and σ_w is the total mechanical turbulence calculated. U_b represents the wind at street level and is a logarithmic function of the roof level wind speed given by the expression:

$$U_b = U \left(\frac{\ln \left(\frac{h_0}{z_0} \right)}{\ln \left(\frac{H}{z_0} \right)} \right) (1 - 0.2 \sin \phi) \quad (5.9)$$

Step 4: The length of the slant edge and the vent velocity is calculated using the following expressions:

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$$L_s = \left((0.5L_{rec})^2 + H_b \right)^2$$

(5.10)

$$U_d = \sqrt{(U_b)^2 + \sigma_{wo}^2} \quad (5.11)$$

Step 5: The C_d and C_r are calculated using the following expressions:

$$C_d = \sqrt{\frac{2}{\pi}} \frac{1}{U_b} \sum_i \left[\frac{Q}{h_0 + \left(\frac{\sigma_w}{u_b} \right) x_i} \right] \quad (5.12)$$

Where x_i is the distance between source and receptor.

$$C_r = \left(\frac{QL_{rec}}{L\sigma_{wi}(0.5L + U_dL_s)} \right) \quad (5.13)$$

Step 5 marks the end of process for calculating C_d and C_r and if the background concentrations C_b is known, the final pollutant concentration can be calculated using equation 4.

5.3.3 Evaluation of vehicular emissions.

To assess the STREET and OSPM models at the Pearse street study sites composite emission factors were calculated using vehicle fleet characteristics data for the study year of 2005. For the purpose of computing of these CEFs, the vehicle fleet data was substituted in a MEET excel spreadsheet and the composite emission factor computed. Separate daytime and nighttime emission factors were employed to allow for the varying effect of congestion on vehicle speeds. The average speed of the vehicles during the daytime was approximately 20km/hr, but this rose to approximately 35km/hr at night, resulting in daytime (0900-1800) emission factors of 2.59g/km and 0.75g/km and nighttime emission factors of 1.30g/km and 0.52g/km for CO and

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NO_x respectively. The speed versus emission characteristic for CO and NO_x is shown in Figure 5.7 and 5.8 respectively.

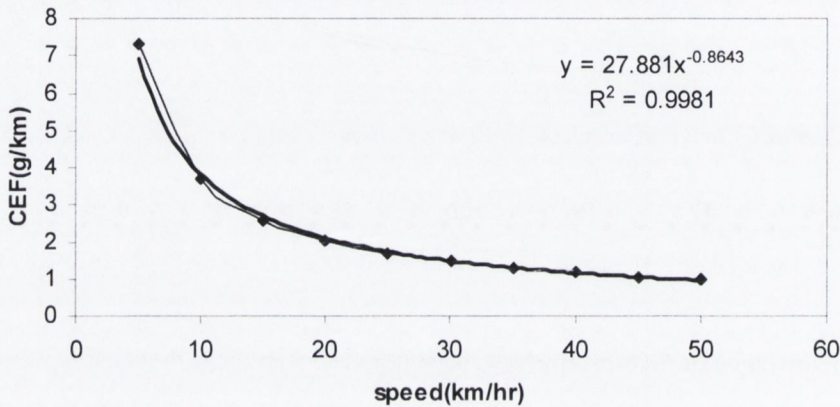


Figure 5.7 Speed versus emission characteristics for CO

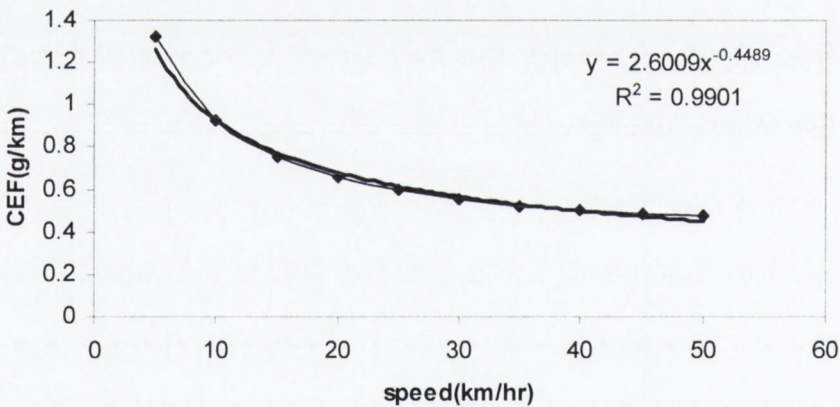


Figure 5.8 Speed versus emission characteristics for NO_x

A power series was observed to provide the best fit to the data for both pollutants, and this is later used to determine hourly emission factors (HEFs). HEFs were calculated for the period 0700-1800 and the average diurnal profiles of the CO and NO_x emission factors are presented in Figure 5.9 and 5.10 respectively. The main criteria considered for calculating HEFs was the

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speed of vehicle. Since there were no HGVs passing through the study site (as per local traffic management plan) the dependency of hourly emission factors on HGVs was not considered. In this context a speed measurement campaign was carried out on the Pearse Street over for two consecutive days wherein the time taken for individual cars was allowed to travel a specified distance and the time it took was noted on a stop watch. This identified to obtain the speed profile for 0700-1800 hours. The maximum speed on Pearse Street is 35km/hr, which is generally observed during nighttime (Dublin City Council) and was assumed to be valid for the period 1900-0600 hours.

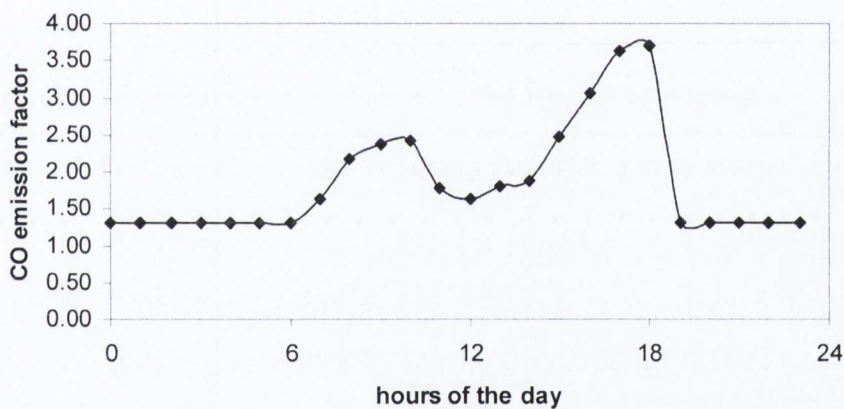


Figure 5.9 Diurnal profile of CO emission factor.

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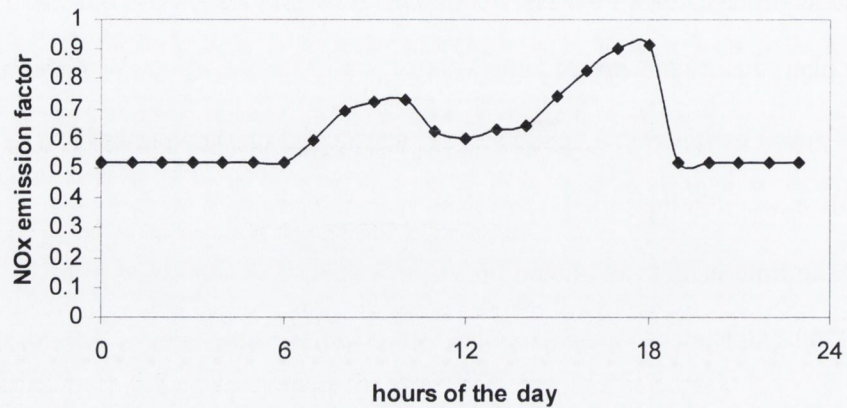


Figure 5.10 Diurnal profile of NO_x emission factor.

5.3.4 Model Evaluation.

The statistical parameters used for evaluating the model performances have already been described in Chapter 2. All the parameters that were described there were also used to evaluate the STREET and OSPM models

5.4 Comparison of Modelled and measured concentrations.

5.4.1 Evaluation of parameter K for STREET model.

It has been mentioned that the K values in the STREET model is an empirical value and its value has varied from 6-8 on an average for street canyons. In this context it was deemed fit to determine the value of K for the Pearse street canyon. The principle involved for the determination of the appropriate K value involves modelling the pollutant concentration (CO or/and NO_x) using different values of K and comparing the modelled and monitored results. Three values of K (6, 7 and 8) were chosen for the purpose of this evaluation and graphical

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and statistical analysis of the results obtained is shown in Figures 5.11 and Figures 5.12 and tables 5.1 and 5.2 respectively for CO and NO_x.

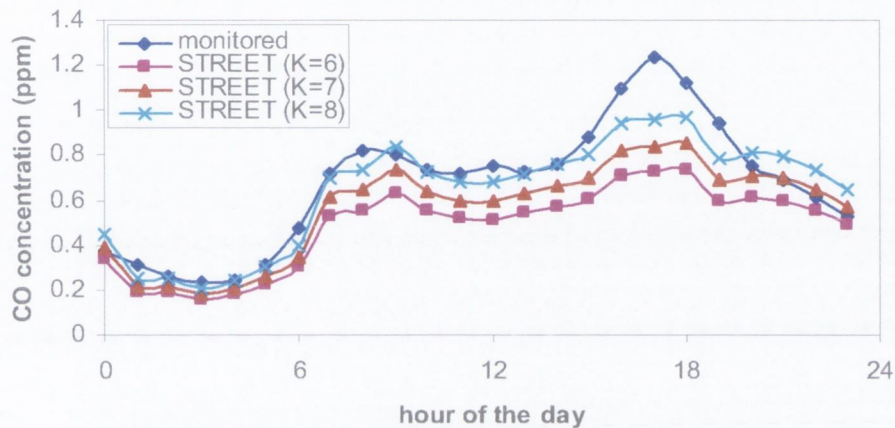


Figure 5.11 Monitored and modelled diurnal profiles for CO using different values of K

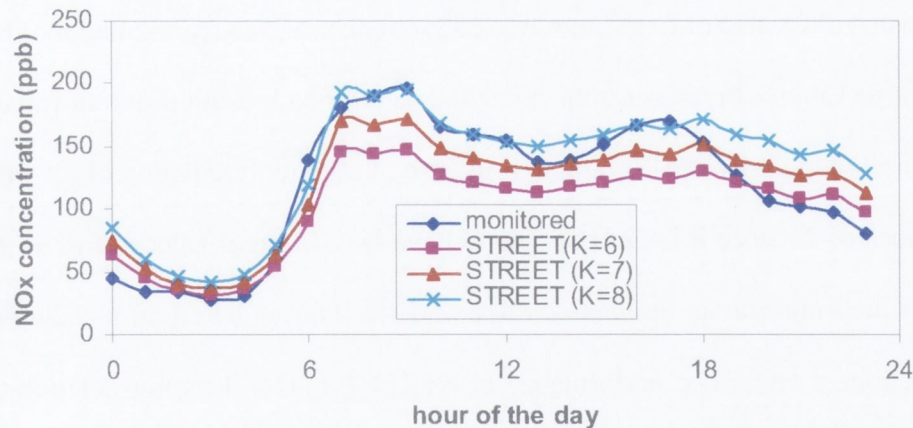


Figure 5.12 Monitored and modelled diurnal profiles for NO_x using different values of K

		STREET (K=6)	STREET (K=7)	STREET (K=8)
Parameters	Mon	CO	CO	CO
Mean (ppm)	0.67	0.48	0.56	0.64
SD	0.47	0.57	0.67	0.76
IA	1.00	0.65	0.64	0.62
NMSE	0.00	1.06	1.05	1.11
R	1.00	0.45	0.45	0.45
FB	0.00	-0.32	-0.18	-0.05
F2	100	78	78	75

Table 5.1 Statistical evaluation of monitored and modelled data for different K values for CO

		STREET (K=6)	STREET (K=7)	STREET (K=8)
Parameters	Mon	NO _x	NO _x	NO _x
Mean (ppb)	117.91	101.32	117.81	134.30
SD	88.54	98.22	114.21	130.20
IA	1.00	0.73	0.74	0.70
NMSE	0.00	0.68	0.69	0.77
R	1.00	0.56	0.56	0.56
FB	0.00	-0.15	0.00	0.13
F2	100	86	86	83

Table 5.2 Statistical evaluation of monitored and modelled data for different K values for NO_x.

From Table 5.1 it is seen that for the pollutant CO, the short term parameters IA and NMSE are best using a K value of 6 or 7, but the long term average as represented by FB is best with K value of 8. Table 5.2 represents the modelled data for NO_x using different values of K and it will be observed that IA, NMSE and FB suggest a better representation of the monitored data for K values of 7. Since it is not possible to have two different values of K for the STREET model for the same site an optimal K value of 7 was chosen based on its better performance for prediction of NO_x. The performance of STREET model does not deteriorate drastically when using a K value of 7 neither for CO nor for NO_x with a K value of 6. Hence a K value of 7 was deemed as an optimal value for usage at the Pearse street canyon. The choice of K as 7

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favours NO_x modelling accuracy over CO modelling accuracy. This is appropriate because the most likely exceedance of limit values in urban areas for NO₂ and as described in Chapter 6. Accurate NO₂ modelling requires accurate NO_x predictions.

5.4.2 Results for CO.

Tables 5.3 and 5.4 present a statistical comparison of modelled and monitored CO concentrations using CEFs and HEFs respectively for both models.

The mean and NMSE values show that the mean concentrations predicted by the STREET model tend to slightly underpredict the monitored results, as would be expected with K as 7.

The OSPM predicted the mean monitored concentration with a greater degree of accuracy.

Parameter	Monitored	STREET	OSPM
Mean	0.67	0.56	0.68
SD	0.47	0.67	0.62
IA	1.00	0.64	0.70
NMSE	0.00	1.05	0.67
R	1.00	0.45	0.52
FB	0.00	-0.18	0.01
F2	100	78	81

Table5.3 Statistical evaluation of CO using CEF (STREET& OSPM)

Parameter	Monitored	STREET	OSPM
Mean	0.67	0.57	0.68
SD	0.47	0.70	0.66
IA	1.00	0.63	0.71
NMSE	0.00	1.11	0.69
R	1.00	0.46	0.55
FB	0.00	-0.17	0.02
F2	100	78	82

Table5.4 Statistical evaluation of CO using HEF (STREET& OSPM)

The FB values suggest that there is substantial agreement between measured and predicted values with both models, with the OSPM performing better. It is observed from the statistical analysis that relatively high IA values were obtained using both the models, with the OSPM

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values again suggesting better model performance than the STREET model with both CEFs and HEFs. The use of HEFs lead to there was a slight increase in the IA values for OSPM. These results imply that relatively a high percentage of the modelled results were substantially error-free, indicating that a proper modelling approach was followed. The Pearson's correlation coefficients obtained with both models are relatively high, but the OSPM model performed marginally better than the STREET model in this regard. This suggests that more of the factors affecting short-term concentration variations are correctly represented in the OSPM formulation, given that the same meteorological, traffic and background concentration datasets were used in both cases.

Overall, the model evaluation parameters for the OSPM are better than those for STREET. A statistical evaluation of an intra-model performance using CEFs and HEFs were carried out for both models for the daytime period in which traffic conditions and hence emission rates vary most. The results are presented in Table 5.5 and Table 5.6 for STREET and OSPM respectively.

Parameter	Monitored	STREET(CEF)	STREET(HEF)
Mean	0.86	0.70	0.70
SD	0.44	0.65	0.72
IA	1.00	0.54	0.54
NMSE	0.00	0.79	0.86
R	1.00	0.31	0.33
FB	0.00	-0.21	-0.20
F2	100	82	82

Table5.5 Statistical evaluation of CEF and HEF results for STREET (0700-1800)

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Parameter	Monitored	OSPM(CEF)	OSPM(HEF)
Mean	0.86	0.89	0.90
SD	0.44	0.60	0.67
IA	1.00	0.56	0.61
NMSE	0.00	0.51	0.52
R	1.00	0.33	0.41
FB	0.00	0.03	0.04
F2	100	84	84

Table5.6 Statistical evaluation of CEF and HEF results for OSPM (0700-1800)

It is seen for the period for which the comparison is made (0700-1800hrs) that STREET model using CEF and HEF tends to underpredict measured concentrations (although this is again partly function of the K value used). The IA value for OSPM HEF is higher than that for OSPM CEF suggesting it to be a better approach, however no such change is observed for the STREET model. However it is observed that there is also a slight improvement in the Pearson’s correlation coefficient for both models when using HEFs. The statistical analysis presented in Table 5.6 suggests that the OSPM model with (both CEF and HEF) tended to only marginally overpredict daytime concentrations. There is a substantial improvement in IA and Pearson’s correlation coefficient when OSPM (HEF) is used in comparison to OSPM (CEF).

Figures 5.13 and 5.14 present the average diurnal variations of the measured and modelled concentrations of CO for both the models using CEFs and HEFs respectively.

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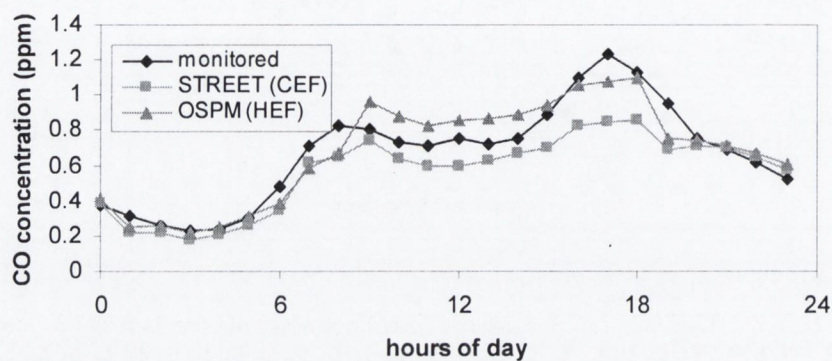


Figure5.13 Diurnal profile variation for CO using CEF (STREET& OSPM)

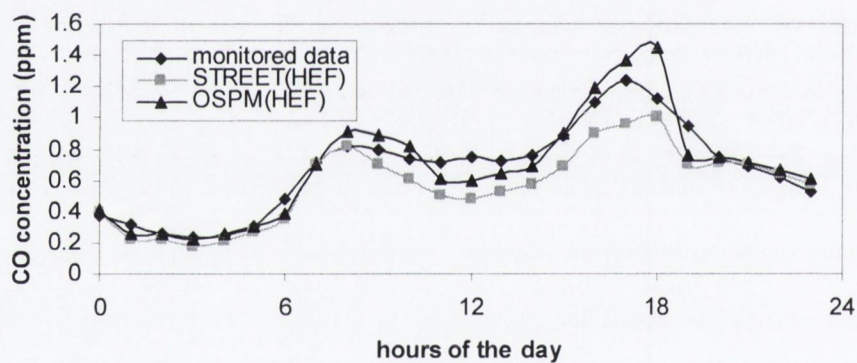


Figure5.14 Diurnal profile variation for CO using HEF (STREET&OSPM)

The monitored CO profile displays morning and evening peaks coinciding with periods of maximum travel demand. The evening peak is higher than the morning peak because traffic congestion on Pease Street is worst at this time of day, causing average vehicle velocities to fall and unit emissions to rise. This variation is successfully captured by both models, particularly the OSPM which produces a diurnal concentration profile very similar to that monitored. Figure 5.15 and 5.16 compare the diurnal variations of monitored and predicted

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data using STREET (CEF & HEF) and OSPM (CEF & HEF) respectively. It is seen that the use of HEFs better represents the measured diurnal profile for both models.

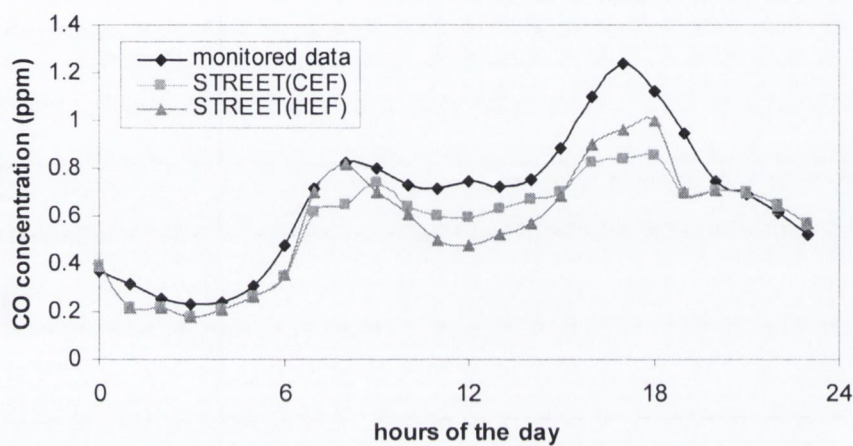


Figure5.15 Comparison of CEF and HEF results for STREET

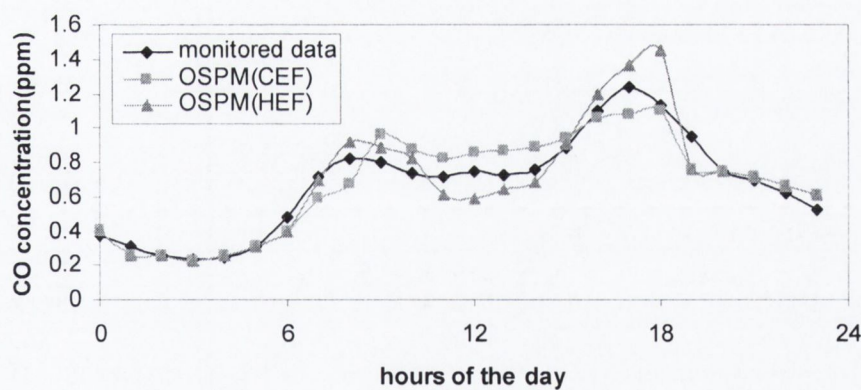


Figure5.16 Comparison of CEF and HEF results for OSPM

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5.4.3 Results for NO_x.

As performed for CO, a statistical analyses of NO_x modelling results was carried out for both CEFs and HEFs using the models STREET and OSPM.

The mean and NMSE values in Tables 5.7 and 5.8 shows that with CEFs, and HEFs the mean concentrations predicted by the STREET model tended to vary slightly underpredict or overpredict the monitored results, however a slight rise was observed in NMSE values when using STREET model with HEFs. The OSPM tended to slightly overpredict the mean measured concentrations with both CEFs and HEFs.

Parameter	Monitored	STREET	OSPM
Mean	117.91	117.81	140.96
SD	88.54	114.21	97.07
IA	1.00	0.74	0.80
NMSE	0.00	0.69	0.39
R	1.00	0.56	0.65
FB	0.00	0.00	0.18
F2	100	86	86

Table 5.7 Statistical evaluation of NO_x using CEF (STREET& OSPM)

Parameter	Monitored	STREET	OSPM
Mean	117.91	118.47	141.40
SD	88.54	118.21	101.38
IA	1.00	0.72	0.79
NMSE	0.00	0.74	0.42
R	1.00	0.55	0.65
FB	0.00	0.00	0.18
F2	100	86	86

Table 5.8 Statistical evaluation of NO_x using HEF (STREET& OSPM)

The FB values suggest that there is substantial agreement between measured and predicted values with both models and particularly for the STREET model using CEFs and HEFs an exact value of zero is observed. It is observed from the statistical analysis that relatively high IA values were obtained using both the models, and as expected the OSPM model values

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suggested better model performance than the STREET model for both CEFs and HEFs. The Pearson's correlation coefficients obtained with both models are not very high, with similar levels of performance for both models with both CEFs and HEFs, though the performance of OSPM is relatively better. Overall, the model evaluation parameters for both the models are similar but the results clearly indicate that the OSPM model performance is better. A statistical evaluation of the daytime performance of the models with CEFs and HEFs is presented in Table 5.9 and Table 5.10.

Parameter	Monitored	STREET(CEF)	STREET(HEF)
Mean	163.39	148.20	149.48
SD	83.56	115.67	123.31
IA	1.00	0.59	0.58
NMSE	0.00	0.56	0.61
R	1.00	0.36	0.36
FB	0.00	-0.10	-0.09
F2	100	88	88

Table5.9 Statistical evaluation of CEF and HEF results for STREET (0700-1800)

Parameter	Monitored	OSPM(CEF)	OSPM(HEF)
Mean	163.39	186.75	187.69
SD	83.56	85.61	94.65
IA	1.00	0.61	0.62
NMSE	0.00	0.32	0.34
R	1.00	0.36	0.38
FB	0.00	0.13	0.14
F2	100	88	88

Table 5.10 Statistical evaluation of CEF and HEF results for OSPM (0700-1800)

It is seen for the period for which the comparison is made (0700-1800hrs) that the STREET model using CEFs and HEFs tends to underpredict the measured concentrations but not to the extent observed with CO. The IA value fort STREET HEF is slightly lower than that for STREET CEF, suggesting similar model performance. However it is observed that there is no change in the Pearson's correlation coefficient when using HEF for STREET model. The statistical analysis presented in Table 5.8 shows that the OSPM model with (both CEFs and

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HEFs) tended to overpredict the daytime measured NO_x concentrations. There is a marginal improvement in IA and Pearson's correlation coefficient when OSPM (HEF) is used in comparison to OSPM (CEF) even though the values are marginally higher than those obtained with STREET.

Figures 5.17 and 5.18 present the average diurnal variations of the measured and modelled concentrations of NO_x for both models using CEFs and HEFs respectively.

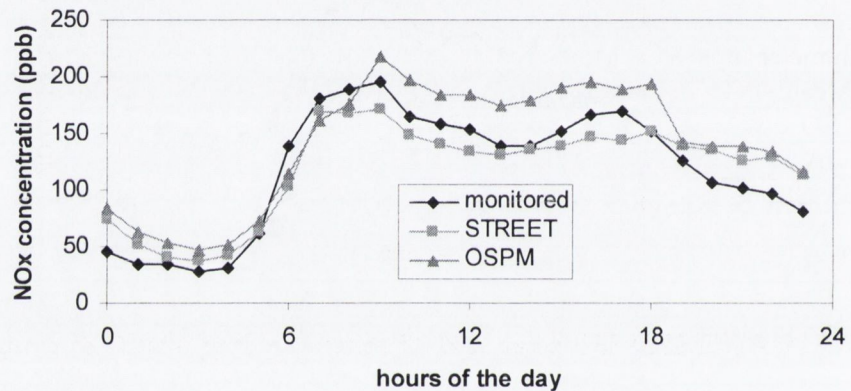


Figure 5.17 Diurnal profile variation for NO_x using CEF (STREET & OSPM)

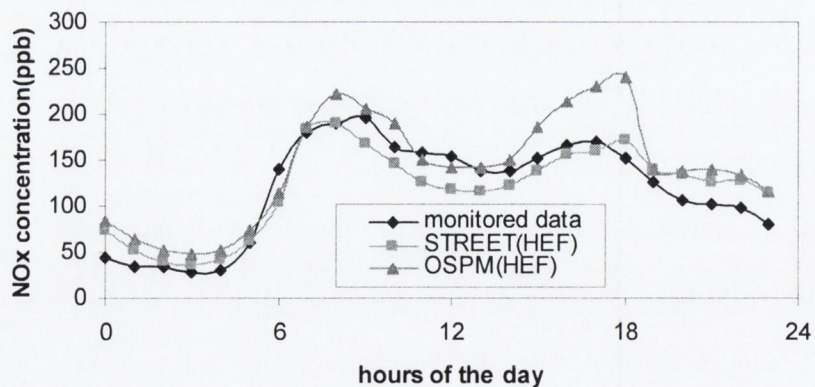


Figure 5.18 Diurnal profile variation for NO_x using HEF (STREET & OSPM)

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The monitored NO_x profile displays morning and evening peaks coinciding with periods of maximum travel demand. The evening peak is slightly lower than the morning peak and this variation is successfully captured by both models, particularly the STREET which produces a diurnal concentration profile very similar to that monitored. Similar levels of agreement are observed in the modelled and measured NO_x results, with the STREET model again tending to replicate the impact of increased daytime traffic flows. For this pollutant, maximum concentrations occur during the rush-hour, and this is better predicted by the STREET model. Figure 5.19 and 5.20 represent the diurnal variations of monitored and predicted data using STREET (CEF&HEF) and OSPM (CEF&HEF) respectively.

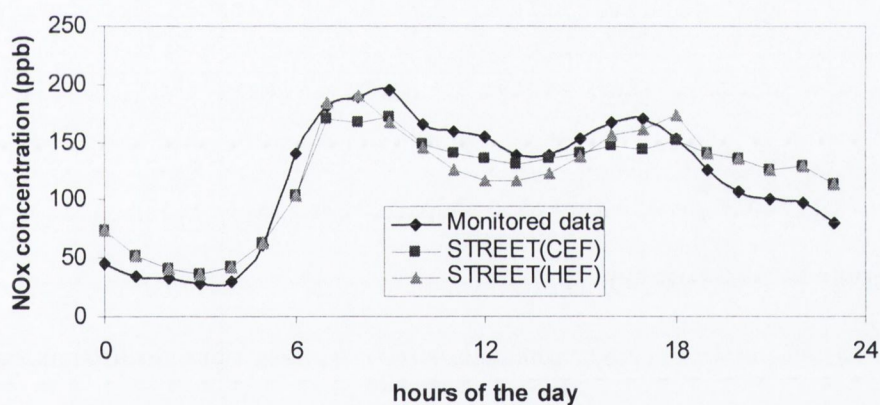


Figure5.19 Comparison of CEF and HEF results for STREET

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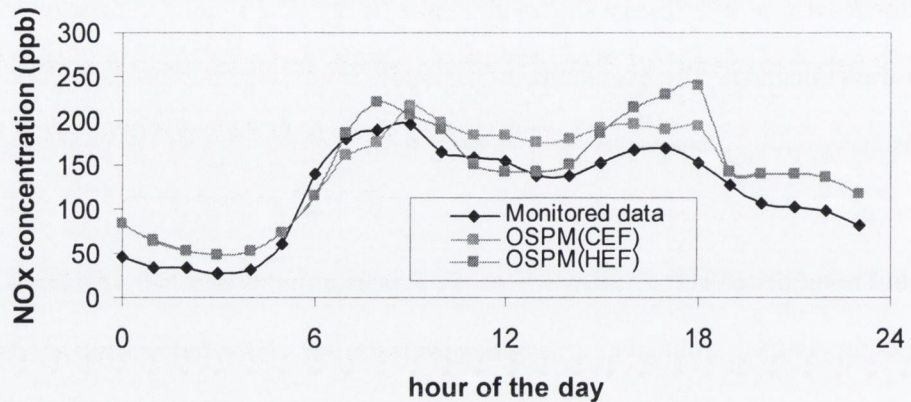


Figure 5.20 Comparison of CEF and HEF results for OSPM

It is seen that the use of HEFs represents the actual diurnal profile in progress for both models. In this context it can be mentioned that the HEFs seem to have a more pronounced effect than that as observed before. In comparing the OSPM and STREET values for HEF a steep fall in the OSPM value is observed in the diurnal profile (Figure 5.20) when compared to STREET (Figure 5.19) at 1800 hours which shows a gradual change.

5.5 Background Concentration Modelling

A study similar to that presented in chapter 3 on the effect of using different background concentrations was carried out for the street canyon site.

As mentioned before, a continuous monitoring assessment was carried out, and modelling results computed for a period of eight months, from May to December 2006. Over the course of this monitoring period, hourly urban background concentrations were also monitored by Dublin City Council at Winetavern Street. The final modelled NO_x concentration as obtained from the application of the models can be represented as an equation as:

$$(\text{NO}_x)_{\text{FP}} = (\text{NO}_x)_{\text{P}} + (\text{NO}_x)_{\text{BKG}} \quad (5.19)$$

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Where; $(NO_x)_{FP}$ is the final predicted concentration, $(NO_x)_P$ is the predicted concentration and $(NO_x)_{BKG}$ is the background concentration.

It will be observed from the above equation that the final predicted values are dependent on the background concentration employed and hence a comprehensive detailed study was performed to analyse model accuracy with different background concentrations. Four cases were considered which are briefly described:

Case 1

In the first case the overall mean of the eight months background concentration measurements was considered were used as the background concentration value, irrespective of any hourly variation. The mean background concentration value, so obtained was 34.93 ppb

i.e.

$$(NO_x)_{FP} = (NO_x)_P + 34.93 \quad (5.20)$$

Case 2

In the second case, the mean of all the concentrations recorded at 0500 hours was computed and the value obtained was considered to be the background concentration. This particular hour was chosen as because it was deemed that the effect of vehicles at this time would be minimum. The mean background value so determined was 46.29 ppb i.e.

$$(NO_x)_{FP} = (NO_x)_P + 46.29 \quad (5.21)$$

Case 3

Each individual hourly background value was added directly to the corresponding predicted concentration on an hour-by-hour basis.

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Case4

In this case, the individual hourly background data were sorted by stability classes i.e., stable, unstable and neutral and the mean value in each class was computed for each hour of the day. A plot of the background concentrations so obtained is shown in Figure 5.21.

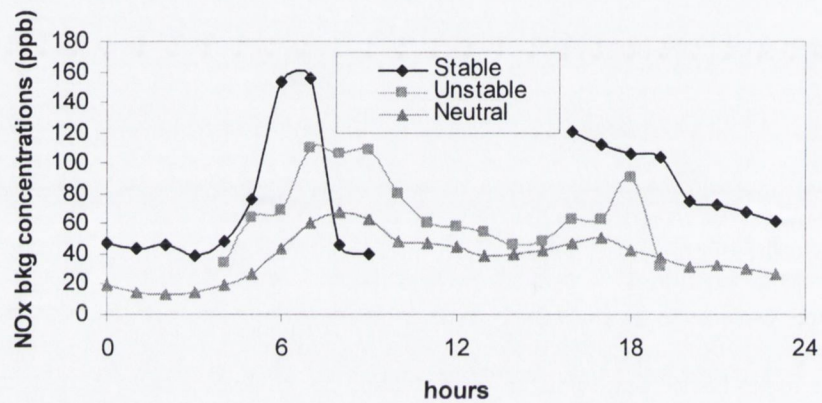


Figure5.21 Diurnal variation of background concentrations depending on stability class

Figures 5.22 and 5.23 present the diurnal profiles of the final predicted NOx concentrations obtained with the cases for STREET and OSPM, respectively with CEFs.

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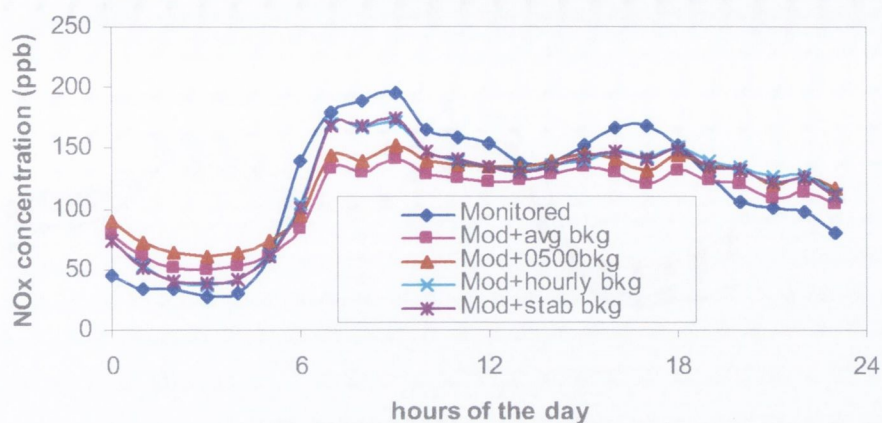


Figure5.22 Modelled data and different background values using STREET (CEF).

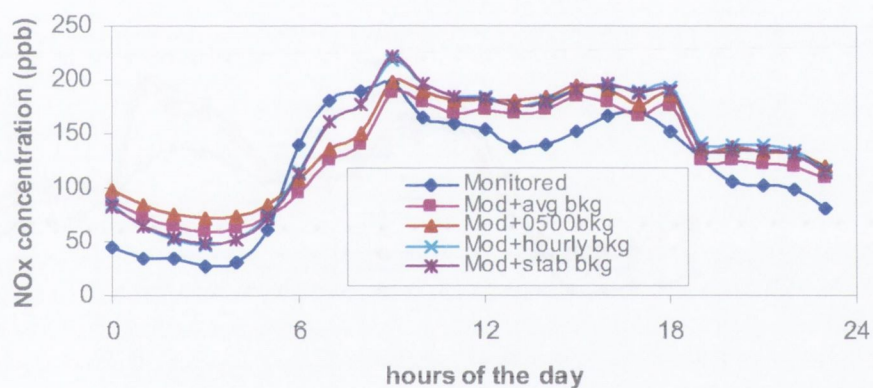


Figure5.23 Modelled data and different background values using OSPM (CEF).

Similarly figures 5.24 and 5.25 represent the diurnal profiles of the modelled concentrations obtained using the different background cases for STREET and OSPM, respectively with HEFs.

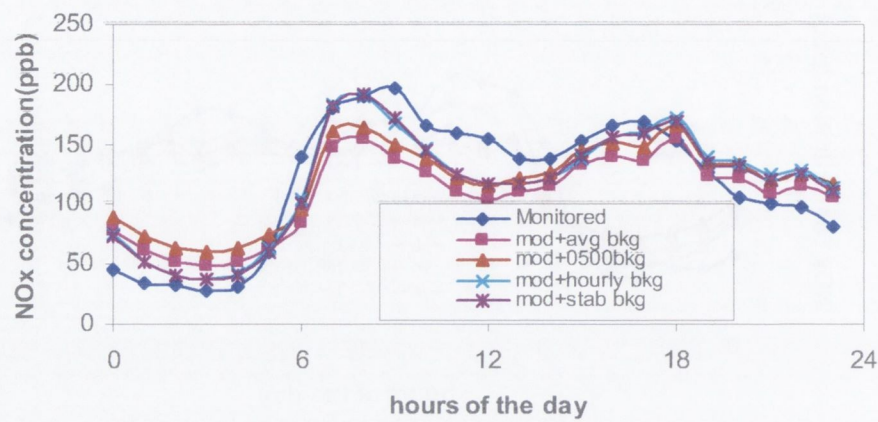


Figure5.24 Modelled data and different background values using STREET (HEF)

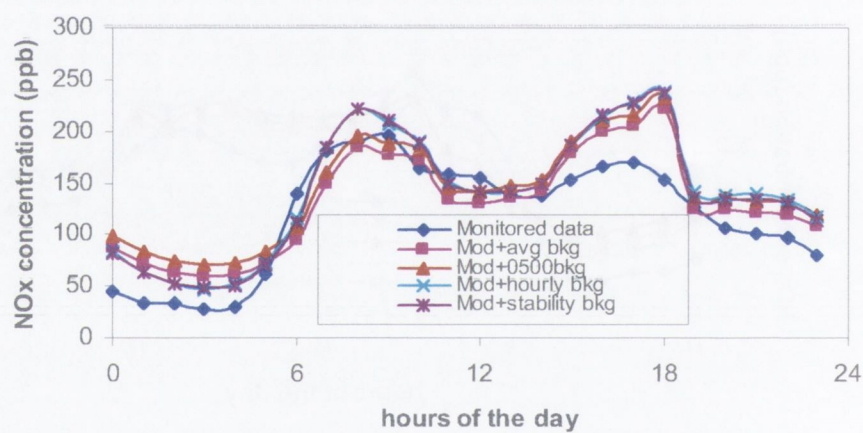


Figure5.25 Modelled data and different background values using OSPM (HEF)

From the diurnal profiles presented above considering both the models CEF and HEF and the different cases of background, it is difficult to distinguish the performance of modelling performance. In the case of STREET CEFs, (Figure 5.19) the values seems to underpredict the monitored concentrations for the period 0900-0500 whereas the use of OSPM CEFs (Figure 5.20) tend to overpredict for the same time scale using all the different cases of background

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concentrations. Similar trends are observed for the HEFs also, however the OSPM HEFs show a steep rise and fall in the diurnal profile values for the period 0300-0700 hours whereas the diurnal profile obtained using STREET CEFs shows a more gradual change in the same time frame for all cases of background concentrations.

Statistical analysis of the modelled results using different background concentrations was carried out. Table 5.11 presents the model evaluation parameters obtained with the different background scenarios for both STREET and OSPM using CEF values.

It is seen from the table that all the suggested techniques achieved reasonable agreement with the monitored data. Of particular importance is the results obtained using stability background values which seem to give very good modelled data when compared to monitored data using both models. The importance of this particular approach lies in the fact that hourly background data will not normally be available but defining the available background data as per stability class leads to modelled results that perform nearly as well on the ideal hourly background case. Table 5.12a describes the overall statistical evaluation of both models using HEF and all possible background scenarios. Table 5.12b describes the statistical evaluation for the period when actual HEF was applied (0700-1800hrs).

It is observed that the statistical results displayed in Table 5.12b are not particularly impressive. However the use of the hourly and the stability background values does seem to improve the prediction results for both models. An intra-comparison of the STREET model was done using CEF and HEF and all possible background scenarios. Table 5.13a represents the overall comparison and table 5.13b represents the comparison for the period's 0700-1800hours.

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It is observed that good level of agreements with monitored data is reached using all possible scenarios, however the alternative application of background concentration as per stability class rather than hourly background concentration values if not available is suitably highlighted. This is also indicated in tables 5.14a and tables 5.14b which presents the intra-comparison of OSPM model using CEF and HEF for overall and particular (0700-1800hours) respectively.

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Parameter	Monitor	STREET Avg bkg	OSPM Avg bkg	STREET 0500 bkg	OSPM 0500 bkg	STREET hr bkg	OSPM hr bkg	STREET Stab bkg	OSPM Stab bkg
Mean	117.91	106.55	129.67	117.84	141.03	117.81	140.96	116.84	139.86
SD	88.54	81.84	63.70	81.68	63.70	114.21	97.07	91.57	74.09
IA	1.00	0.62	0.67	0.61	0.66	0.74	0.80	0.70	0.73
NMSE	0.00	0.72	0.42	0.64	0.41	0.69	0.39	0.64	0.39
R	1.00	0.39	0.50	0.39	0.50	0.56	0.65	0.46	0.56
FB	0.00	-0.10	0.10	0.00	0.18	0.00	0.18	-0.01	0.17
F2	100	75	78	78	83	86	86	82	85

Table5.11 Statistical evaluation of modelled data and different background cases using CEF.

Parameter	Monitor	STREET Avg bkg	OSPM Avg bkg	STREET 0500 bkg	OSPM 0500 bkg	STREET hr bkg	OSPM hr bkg	STREET Stab bkg	OSPM Stab bkg
Mean	117.91	107.40	130.09	118.70	141.45	118.47	141.40	117.48	140.26
SD	88.54	86.17	67.55	86.31	67.55	118.21	101.38	96.00	79.04
IA	1.00	0.62	0.69	0.61	0.67	0.72	0.79	0.69	0.73
NMSE	0.00	0.75	0.42	0.67	0.41	0.74	0.42	0.67	0.41
R	1.00	0.39	0.51	0.39	0.51	0.55	0.65	0.45	0.56
FB	0.00	-0.09	0.10	0.01	0.18	0.00	0.18	0.00	0.17
F2	100	75	78	80	83	86	86	82	85

Table5.12a. Statistical evaluation of modelled data and different background cases using HEF.

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Parameter	Monitor	STREET Avg bkg	OSPM Avg bkg	STREET 0500 bkg	OSPM 0500 bkg	STREET hrl bkg	OSPM hrl bkg	STREET Stab bkg	OSPM Stab bkg
Mean	163.39	130.57	168.45	141.90	179.81	149.48	187.69	149.57	187.50
SD	83.56	98.02	68.90	98.25	68.90	123.31	94.65	104.14	74.67
IA	1.00	0.51	0.51	0.51	0.50	0.58	0.62	0.53	0.57
NMSE	0.00	0.64	0.34	0.56	0.32	0.61	0.34	0.55	0.33
R	1.00	0.25	0.21	0.25	0.21	0.36	0.38	0.27	0.25
FB	0.00	-0.22	0.03	-0.14	0.10	-0.09	0.14	-0.09	0.14
F2	100	78	82	85	88	88	88	83	88

Table5.12b.Statistical evaluation of modelled data and different background cases using HEF (0700-1800hrs).

Parameter	Monitor	STREET (CEF) Avg bkg	STREET (HEF) Avg bkg	STREET (CEF) 0500 bkg	STREET (HEF) 0500 bkg	STREET (CEF) hr bkg	STREET (HEF) hr bkg	STREET (CEF) Stab bkg	STREET (HEF) Stab bkg
Mean	117.91	106.55	107.40	117.84	118.70	117.81	118.47	116.84	117.48
SD	88.54	81.84	86.17	81.68	86.31	114.21	118.21	91.57	96.00
IA	1.00	0.62	0.62	0.61	0.61	0.74	0.72	0.70	0.69
NMSE	0.00	0.72	0.75	0.64	0.67	0.69	0.74	0.64	0.67
R	1.00	0.39	0.39	0.39	0.39	0.56	0.55	0.46	0.45
FB	0.00	-0.10	-0.09	0.00	0.01	0.00	0.00	-0.01	0.00
F2	100	75	75	78	80	86	86	82	82

Table5.13a. Statistical comparison of CEF and HEF for STREET and all background cases (overall)

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Parameter	Monitor	STREET (CEF) Avg bkg	STREET (HEF) Avg bkg	STREET (CEF) 0500 bkg	STREET (HEF) 0500 bkg	STREET (CEF) hrl bkg	STREET (HEF) hrl bkg	STREET (CEF) Stab bkg	STREET (HEF) Stab bkg
Mean	163.39	129.02	130.57	140.19	141.90	148.20	149.48	148.18	149.57
SD	83.56	90.61	98.02	90.38	98.25	115.67	123.31	95.99	104.14
IA	1.00	0.51	0.51	0.51	0.51	0.59	0.58	0.53	0.53
NMSE	0.00	0.61	0.64	0.53	0.56	0.56	0.61	0.50	0.55
R	1.00	0.23	0.25	0.23	0.25	0.36	0.36	0.26	0.27
FB	0.00	-0.24	-0.22	-0.15	-0.14	-0.10	-0.09	-0.10	-0.09
F2	100	78	78	85	85	88	88	83	83

Table5.13b. Statistical comparison of CEF and HEF for STREET and all background cases (07-1800hr)

Parameter	Monitor	OSPM (CEF) Avg bkg	OSPM (HEF) Avg bkg	OSPM (CEF) 0500 bkg	OSPM (HEF) 0500 bkg	OSPM (CEF) hr bkg	OSPM (HEF) hr bkg	OSPM (CEF) Stab bkg	OSPM (HEF) Stab bkg
Mean	117.91	129.67	130.09	141.03	141.45	140.96	141.40	139.86	140.26
SD	88.54	63.70	67.55	63.70	67.55	97.07	101.38	74.09	79.04
IA	1.00	0.67	0.69	0.66	0.67	0.80	0.79	0.73	0.73
NMSE	0.00	0.42	0.42	0.41	0.41	0.39	0.42	0.39	0.41
R	1.00	0.50	0.51	0.50	0.51	0.65	0.65	0.56	0.56
FB	0.00	0.10	0.10	0.18	0.18	0.18	0.18	0.17	0.17
F2	100.00	78	78	83	83	86	86	85	85

Table5.14a. Statistical comparison of CEF and HEF for OSPM and all background cases (overall)

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Parameter	Monitor	OSPM (CEF) Avg bkg	OSPM (HEF) Avg bkg	OSPM (CEF) 0500 bkg	OSPM (HEF) 0500 bkg	OSPM (CEF) hr bkg	OSPM (HEF) hr bkg	OSPM (CEF) Stab bkg	OSPM (HEF) Stab bkg
Mean	163.39	167.52	168.45	178.88	179.81	186.75	187.69	186.61	187.50
SD	83.56	61.68	68.90	61.68	68.90	85.61	94.65	64.35	74.67
IA	1.00	0.47	0.51	0.46	0.50	0.61	0.62	0.50	0.57
NMSE	0.00	0.33	0.34	0.32	0.32	0.32	0.34	0.31	0.33
R	1.00	0.16	0.21	0.16	0.21	0.36	0.38	0.21	0.25
FB	0.00	0.02	0.03	0.09	0.10	0.13	0.14	0.13	0.14
F2	100	82	82	88	88	86	88	88	88

Table5.14b. Statistical comparison of CEF and HEF for OSPM and all background cases (0700-1800hr)

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5.6 Overall summary of CO and NO_x modelling results at Pearse Street.

When compared with monitored data, concentrations calculated using STREET and OSPM both successfully predict observed variations in air quality. From the statistical parameters presented it is quite evident that both models are successful in predicting long-term average concentrations. It is also seen that the hourly OSPM results correlate better with the monitored data than the STREET values for CO. However, the STREET model remains reasonably accurate, in spite of its simplicity which allows it to be more readily incorporated into transport network models of urban areas. The best possible modelled data arises with the combination of OSPM using HEF and hourly background concentrations.

The OSPM results also correlate slightly better with the monitored data than the STREET values for NO_x. In this study, very good data were available for background air quality. The use of different NO_x background conditions based on certain assumptions, as considered in Chapter 3 for motorway conditions was also studied at the street canyon. It can be concluded that use of background concentrations dependent on stability class may be a very good alternative to individual hourly background concentration values when these are not available. In practice, model performance can be expected to deteriorate when inferior input data are employed.

The variation of emission factors and the different cases of background concentrations has been studied in detail at highway (Chapter 3) and street canyon (Chapter 5) sites. It is seen from both the studies that a proper selection of CEFs can give an equally good modelling result compared to those obtained with HEFs. The influence of the background concentrations is more pronounced than the variation of emission factors. Both studies (Chapter 3 and 5) have shown that the modelling performance is highly dependant on the background concentration

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assumption employed. In this context, summary tables regarding modelling results of highway and street canyon for CO and NO_x are given in table 5.15 and 5.16 for CO and NO_x respectively. A synthetic data set is generated for the CO comparison at Pearse Street using the mean concentrations recorded at 0500 hours on Pearse Street as the background concentration and the statistical analyses are compared to those as previously presented in Table 3.5 in Chapter 3. Coincidentally a mean background value of 0.23ppm was observed at Pearse Street which is same as that obtained at Leixlip site.

To carry the NO_x comparison, the statistical results for *Case 3* conditions (described in Chapter 3) for the last six months of the motorway studied period (Table 3.14) are compared with the STREET and OSPM results (Table 5.7) using CEFs.

Parameter	GFLSM (case 2 bkg)	STREET	OSPM
IA	0.41	0.54	0.65
NMSE	0.60	0.84	0.43
R	0.20	0.32	0.49
FB	0.09	-0.30	-0.09

Table 5.15 Statistical comparison of highway and street canyon results for CO

Parameter	GFLSM (case 3 bkg)	STREET	OSPM
IA	0.76	0.74	0.80
NMSE	0.85	0.69	0.39
R	0.65	0.56	0.65
FB	0.19	0.00	0.18

Table 5.16 Statistical comparison of highway and street canyon results for NO_x

From the tables it is clearly evident that the OSPM model achieved a significantly better result at the Pearse street site than did the STREET model at the same site, or the GFLSM model at the highway site. It can be recalled that the performances of the GFLSM and CALINE4 models were nearly identical. The NO_x modelling results also show a similar trend, however

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the variation is not as great as observed in the case of CO. Of the two less complex models, the GFLSM performed better than STREET.

From the study carried out in Chapters 3, 4 and 5 it is observed that the street canyon modelling gives a much better agreement with measured data than those that of highway modelling, this is mainly due to using two different CEF values (daytime and nighttime), availability of background concentrations for the entire study period and also probably a better location of the background unit in the street canyon modelling case.

6.1 Introduction

A variety of approaches have been used to model ambient NO₂ concentrations in urban locations, involving application of simple and complex chemical models, to empirically based models. In this context two empirical models as proposed by Stedman (2001) and Wilson and Laxen (2002) have been modified for use in Irish road conditions. Their formulation techniques and a comparison with the original methods are presented here. It is important to state that the relationships used in the derivation of NO₂ concentrations from NO_x are often based on observations from monitored data for both pollutants. In practice, where assessment of future air quality is required, monitored data is generally unavailable and NO_x data obtained using an appropriate dispersion model is used to predict the required NO₂ concentrations. In this study, a new model based on the power law is developed to take into consideration a better decay of the ratio of (NO₂/NO_x)_{road} with total NO_x concentrations rather than the logarithmic relationship initially followed in the Wilson and Laxen method. The formulations so derived are applied at motorway and street canyon sites.

6.2. Study Sites**6.2.1 Application to a Street Canyon Site (Pearse Street junction).**

The Pearse street site, along with all its important features and photographs, has been described in detail in Chapter 5. The modelling of the NO₂ concentrations are based on the monitored and modelled NO_x concentrations at this site.

6.2.2 Application to a Motorway Site (M4 Leixlip).

The details of the M4 site at Leixlip have already been presented in Chapter 3. Similar to above, the modelling of NO₂ concentrations are based on monitored and modelled NO_x concentrations at this site.

6.3. Computational Methods.

6.3.1 Stedman's Method.

The empirical approach described here has been developed using the Stedman's approach. The principle followed by Stedman (2001) involved splitting roadside NO₂ into two components.

(1) A component related to fresh emissions of NO_x from road and (2) a background component brought into the area from outside. Stedman's empirical analysis suggested that the former could be represented as a fixed proportion of the road traffic NO_{x(road)}, this proportion being 16% (Stedman et al, 2001) . The approach was thus to add background NO_{2(bkg)} to the road traffic NO_{2(road)}, to give the total NO₂. The detailed formulation has been described by Stedman (2001). The final mathematical representation of the Stedman equation is:

$$0.16NO_{x(road)} + NO_{2(bkg)} = NO_{2(total)} \quad (6.1)$$

6.3.1.1 Modified Stedman's method for Dublin

Nitrogen dioxide is often described as a secondary pollutant because the majority of ambient NO₂ is formed by oxidation of NO emitted by atmosphere. A detailed understanding of the principles that lead to measured concentrations of NO₂, and how the processes will vary due to changes in future emissions, are therefore essential for predicting future concentrations of NO₂. As mentioned before, ozone plays an important part in converting NO to NO₂. If NO_x emissions are reduced and ozone concentrations remain unchanged, this will lead to a rapid increase in NO₂.

Figure 6.1 shows the scatter plot of the diurnals of the annual mean NO_x and NO₂ concentrations for Pearse Street collected over a period of eight months from May to December 2006.

The regression coefficient and the intercept for the overall relationship are as follows:

$$NO_2(ppb) = 0.22NO_x + 11.64 \quad (r^2=0.92)$$

(a)

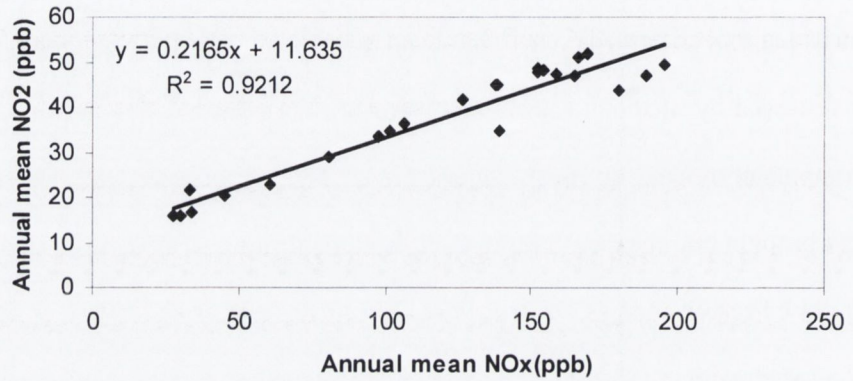


Figure 6.1 Comparison of annual mean NO_x and NO₂ concentrations at Pearse Street

A linear trend line has been drawn in Figure 6.1. This is recommended because this gives a better fit at higher measured NO_x concentrations. Non linear relationships have also been studied by Steadman (1999) and Carslaw and Beevers (1999). The advantage of this method is that future NO₂ concentrations can be directly predicted from NO_x predictions assuming that the relationship will remain the same in future years.

The measured NO₂ concentrations at the roadside depend on the relative contributions to measured NO_x concentrations from background sources and road itself. Figure 6.2 shows the relationship between the roadside increments of NO₂ and NO_x observed at Pearse Street.

The plotted values have been calculated using:

$$NO_{x(RI)} = NO_{x(mon)} - NO_{x(bkg)} \quad (b)$$

$$NO_{2(RI)} = NO_{2(mon)} - NO_{2(bkg \text{ calculated using eqn(a)})} \quad (c)$$

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where NO_{x(RI)} is the roadside increment of NO_x, NO_{x(mon)} is the monitored concentration of NO_x, NO_{x(bkg)} is the background concentration of NO_x, NO_{2(RI)} is the roadside increment of NO₂, NO_{2(mon)} is the monitored NO₂ and NO_{2(bkg calculated using eqn (a))} is the estimated background from NO_x using equation (a).

From Figure 6.2 it is evident that,

$$NO_{2(RI)} = 0.22NO_{x(RI)} \quad (r^2=0.88) \tag{d}$$

The final modified Steadman’s equation for Irish conditions is given equation 6.2 and is hereafter referred as the Modified Stedman’s equation.

$$0.22NO_{x(road)} + NO_{2(bkg)} = NO_{2(total)} \tag{6.2}$$

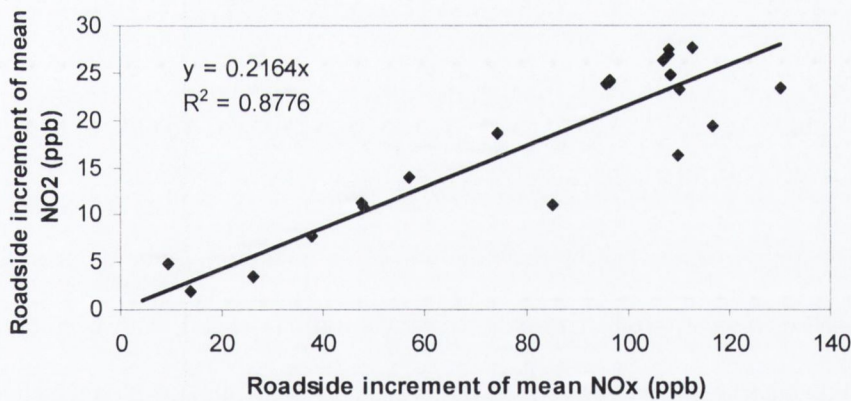


Figure 6.2 Relation between roadside increments of NO₂ and NO_x

6.3.1.2 Application and Validation of Modified Stedman’s equation for Dublin.

Urban Street Canyon

While formulating the above equation it is to be noted that the NO₂ background concentrations were computed using the relationship obtained from expression (a) from actual measured NO_x concentrations at the background site. However during the same study period, actual NO₂

background concentrations were also monitored at Winetavern Street. These values now serve as the actual background values for expression (2). A comparative study is carried out using the original Stedman equation and the Modified Stedman's equation. Statistical and graphical analysis of the results was carried out. They are illustrated in Table 6.1 and Figure 6.3 respectively. This is basically a partial validation of the equations (6.1) and (6.2).

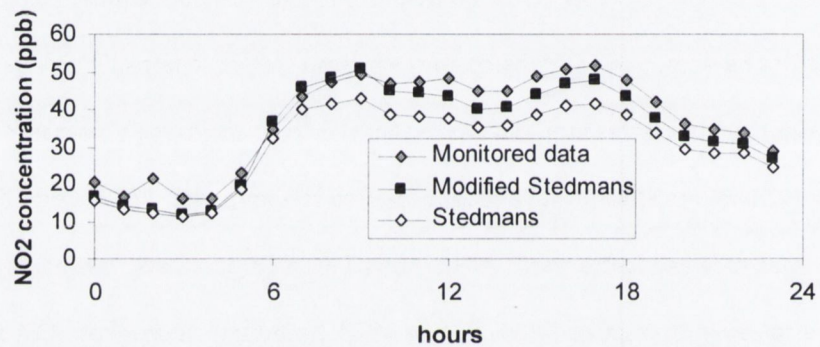


Figure 6.3 Diurnal profile variation using actual NO₂ background values

The models are further tested for an actually likely application scenario where there is no monitored NO_x concentrations but modelled concentrations of NO_x have been obtained using a suitable atmospheric dispersion model, (in this case STREET and OSPM) which have been described in detail in Chapter 5. In this case, the monitored data are compared to Stedman's and Modified Stedman's equations in which modelled NO₂ concentrations have been used using STREET and OSPM. Two types of emission factors (composite and hourly) were used to determine the modelled data using STREET and OSPM. Their effect has also been studied by calculating the NO₂ concentrations from OSPM and STREET using both types of emission factors (CEFs & HEFs). The background concentrations remain the same, being based on

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monitoring data from May to December 2006. The statistical analysis results and the diurnal profile variations are presented in Tables 6.2(a), 6.3(a), 6.4(a) and 6.5(a) for STREET (CEF), STREET (HEF), OSPM (CEF), OSPM (HEF) and Figures 6.6 to 6.9 for STREET (CEF), STREET (HEF), OSPM (CEF), OSPM (HEF) respectively. Statistical analysis for the time frame 0700hrs and 1800hrs were also carried out to determine the effect of using CEF and HEF on the modelling results. These results are presented in Tables 6.2(b), 6.3(b), 6.4(b) and 6.5(b) for STREET (CEF), STREET (HEF), OSPM (CEF) and OSPM (HEF) respectively.

Motorway

Further to this the Stedman's and the modified Stedman analysis were applied to the motorway site. In this case the comparison analyses were carried out for three cases: an overall comparison, a comparison for the period when constant hourly averaging background concentrations for NO_x were used and lastly for the period when hourly individual background values were used. The analyses were performed on modelled NO_x concentrations predicted using GFLSM and CEF. The statistical analysis for the three above cases are shown in Tables 6.6, 6.7 and 6.8 respectively and the diurnal profile variation for the cases are shown in Figures 6.10, 6.11 and 6.12.

6.3.2 DEFRA (Wilson and Laxen) method.

The DEFRA method is a further improvement to the Stedman method. Whereas in the Stedman method a fixed value is assigned for the NO_{x(road)} / NO_{2(road)} ratio, the DEFRA method modifies this ratios to allow for the variable contribution made by road traffic NO_x to road traffic NO₂. This is done to take into consideration the decreasing amount of ozone available for converting NO to NO₂ at higher NO_x concentrations. The variable proportion of NO_{2(road)} in fresh NO_{x(road)}

is determined by analysing the ratio of NO_{2(road)}/ NO_{x(road)} against total NO_x at roadside sites.

The final form of the Wilson and Laxen (2002) method is:

$$NO_{2(total)} = NO_{2(bkg)} + NO_{2(road)} \quad (6.3)$$

where NO_{2(road)} is given by

$$NO_{2(road)} = NO_{x(road)} [(-0.068 \ln(NO_{x(total)})) + 0.53] \quad (6.4)$$

6.3.2.1 Modified DEFRA (Wilson and Laxen) method for Dublin.

Following the procedure described above, the following equation for Dublin conditions was derived, which is illustrated in Figure 6.4

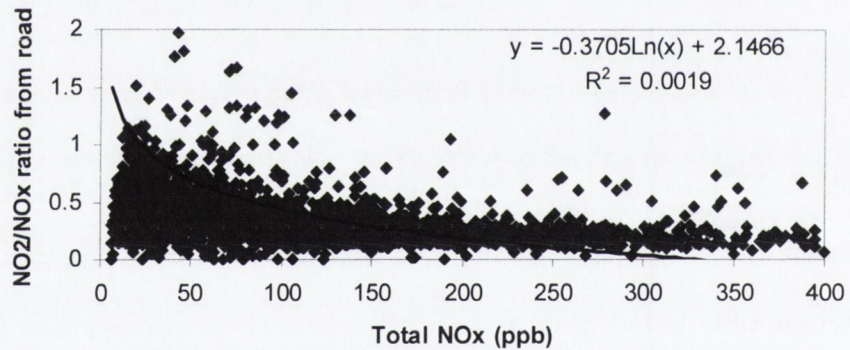


Figure 6.4 Plot of NO₂/NO_x from road vs total NO_x (all points)

The relevant expression was developed using all points for Pearse Street for the period May to December 2008.

The appropriate equation in this case is:

$$NO_{2(road)} = NO_{x(road)} [(-0.37 \ln(NO_{x(total)})) + 2.14] \quad (6.5)$$

For the case considered in Figure 6.4, a logarithmic pattern was followed as per the Wilson and Laxen (2001) method. However the best fitting option to the data as obtained in Dublin conditions was a power relation amongst the data set. This is shown in Figure 6.5.

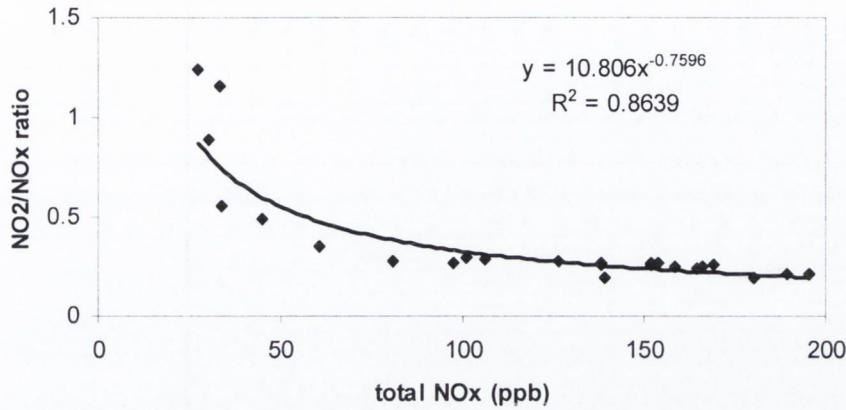


Figure 6.5 Plot of NO_2/NO_x from road vs total NO_x (average)-power fit.

The relevant expression when using the power fit for calculating $NO_{2(road)}$ from $NO_{x(road)}$ is given as follows:

$$NO_{2(road)} = NO_{x(road)} (10.806 [NO_{x(total)}]^{-0.7596}) \quad (6.6)$$

Equation 6.5 is hereafter referred to as the modified DEFRA method and equation 6.6 is referred as the *power method*.

6.3.2.2 Application and Validation of modified DEFRA and Power methods for Dublin.

Urban Street Canyon

In a similar fashion as followed for the Stedman method the modelled NO_2 concentrations obtained using the original DEFRA method, modified DEFRA method and the *power method* were compared with the monitored results. The statistical results so obtained are described in Table 6.1. The final $NO_{2(total)}$ is computed by using equation 3 where $NO_{2(bkg)}$ is the actual monitored background and $NO_{2(road)}$ is computed using equations (6.4), (6.5) and (6.6) using the original DEFRA, modified DEFRA and the power method equations respectively.

From the statistical results it is seen that the performance of the original DEFRA (Wilson and Laxen 2002) method yields a marginally better result than the Modified DEFRA equations when using monitored NO_x concentrations and actual NO₂ background values.

However the statistical tests show that the relationship between NO_{2(road)} and NO_{x(road)} follows a power relation rather than a logarithmic relation for Pearse Street junction.

Further to this, the three methods were compared using modelled NO_x data where NO_{x(total)} is the sum of NO_{x(road-modelled)} and NO_{x(bkg)}. The NO_{x(road-modelled)} concentrations were derived using STREET and OSPM models with different emission factors as described before. The statistical analysis results and the diurnal profile variations are presented in Tables 6.2 (a), 6.3(a), 6.4(a) and 6.5(a) for STREET (CEF), STREET (HEF), OSPM (CEF), OSPM (HEF) and Figure 6.6, 6.7, 6.8 and 6.9 for STREET (CEF), STREET (HEF), OSPM (CEF), OSPM (HEF) respectively. Statistical analysis for the time frame 0700hrs and 1800hrs were also carried out to determine the effect of using CEF and HEF on the modelling results. These results are presented in Tables 6.2(b), 6.3(b), 6.4(b) and 6.5(b) for STREET (CEF), STREET (HEF), OSPM (CEF) and OSPM (HEF) respectively.

The performance of the power model is commendable even when using the modelled data; followed closely by the original Wilson and Laxen method. The statistical parameters used for comparison purposes have already been described earlier in the thesis.

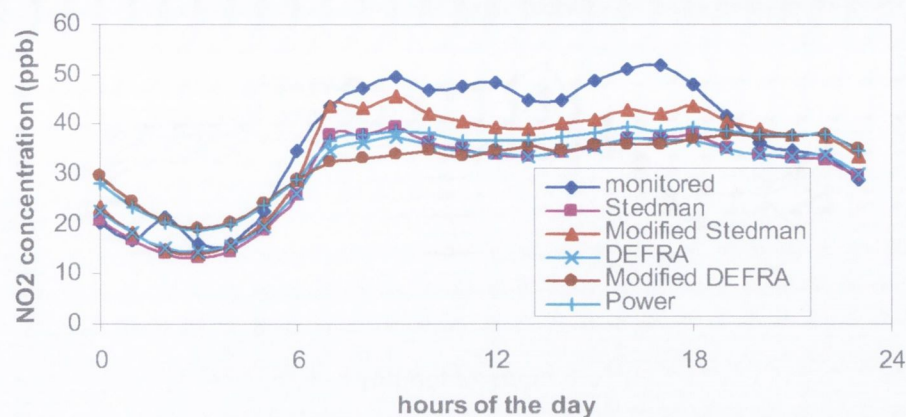


Figure 6.6 Performance evaluations for NO₂ concentration at Pearse Street using STREET (CEF)

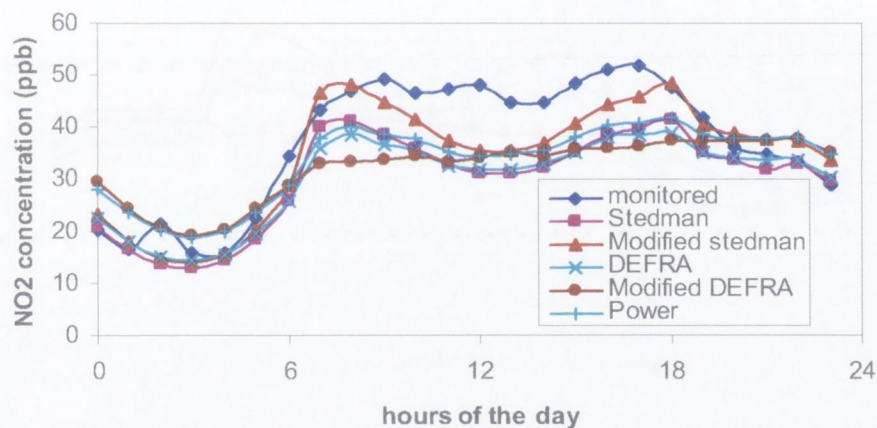


Figure 6.7 Performance evaluations for NO₂ concentration at Pearse Street using STREET (HEF)

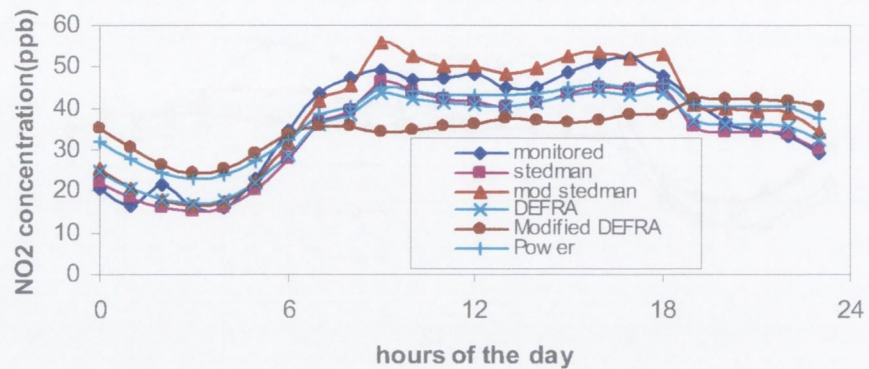


Figure 6.8 Performance evaluations for NO₂ concentration at Pearse Street using OSPM (CEF)

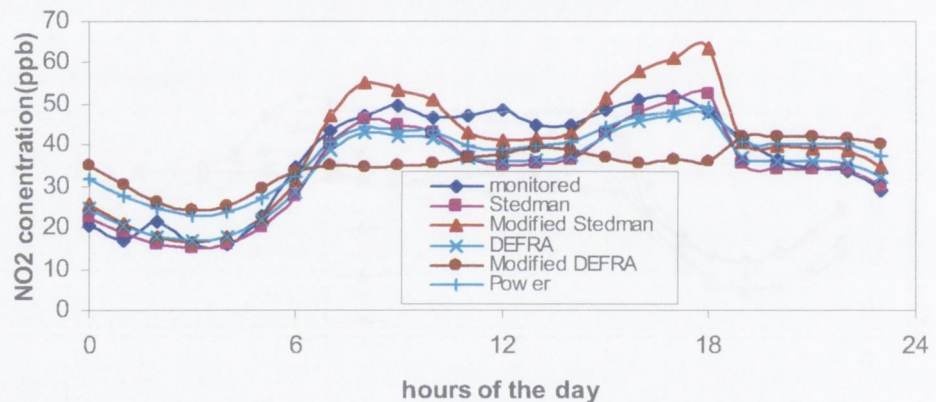


Figure 6.9. Performance evaluation for NO₂ concentration at Pearse Street using OSPM (HEF).

The diurnal profiles of modelled NO_x concentrations in Chapter 5 (Figures 5.17 and 5.18) had showed that that the STREET model underpredicted the concentrations using both CEF and HEF whereas the OSPM model had a slight tendency to overpredict. The modelled concentrations obtained from STREET NO_x calculations also show a tendency to underpredict, as observed in the diurnal profiles in Figures 6.6 and 6.7

However the modelled concentrations which were obtained using OSPM NO_x results which were observed to overpredict measured NO_x concentrations now show a slight underprediction

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Modelling of NO₂ Concentrations

of NO₂ measured concentrations. Only the modified Stedman method shows a slight overprediction during peak hours (Figures 6.8 and 6.9).

Parameter	Monitored	Stedman	Modified Stedman	DEFRA	Modified DEFRA	Power
Mean	37.26	30.31	34.29	33.39	37.94	37.48
SD	18.18	16.98	19.69	18.40	16.89	13.19
IA	1.00	0.91	0.95	0.81	0.69	0.92
NMSE	0.00	0.10	0.06	0.18	0.23	0.05
R	1.00	0.90	0.92	0.68	0.47	0.90
FB	0.00	-0.21	-0.08	-0.11	0.02	0.01
F2 (%)	100	99	99	97	94	99
99.8 percentile	114.10	98.21	111.13	160.43	160.43	88.85

Table 6.1 Statistical analysis using actual monitored NO_x and actual NO₂ background

Parameter	Monitored	Stedman	Modified Stedman	DEFRA	Modified DEFRA	Power
Mean	37.26	30.14	34.48	30.17	32.07	33.50
SD	18.18	20.87	25.35	16.27	11.05	14.34
IA	1.00	0.72	0.70	0.75	0.66	0.76
NMSE	0.00	0.35	0.38	0.25	0.23	0.20
R	1.00	0.56	0.53	0.61	0.51	0.58
FB	0.00	-0.21	-0.08	-0.21	-0.15	-0.11
F2	100	89	89	93	96	98
99.8 percentile	114.10	201.12	244.78	99.78	87.20	98.95

Table 6.2(a) Statistical evaluation (overall-CEF-STREET).

Parameter	Monitored	Stedman	Modified Stedman	DEFRA	Modified DEFRA	Power
Mean	47.55	36.29	41.95	35.53	34.79	37.88
SD	15.50	20.41	25.58	14.00	8.23	12.45
IA	1.00	0.52	0.49	0.53	0.45	0.54
NMSE	0.00	0.36	0.37	0.27	0.26	0.21
R	1.00	0.26	0.25	0.27	0.14	0.27
FB	0.00	-0.27	-0.13	-0.29	-0.31	-0.23
F2	100	87	87	89	93	95
99.8 percentile	114.10	201.12	244.78	90.97	77.59	91.56

Table 6.2(b) Statistical evaluation (7am-6pm-CEF-STREET).

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Parameter	Monitored	Stedman	Modified Stedman	DEFRA	Modified DEFRA	Power
Mean	37.26	30.19	34.61	30.18	32.05	33.51
SD	18.18	21.55	26.15	16.31	11.05	14.40
IA	1.00	0.71	0.69	0.75	0.66	0.76
NMSE	0.00	0.37	0.41	0.26	0.23	0.20
R	1.00	0.54	0.52	0.61	0.51	0.58
FB	0.00	-0.21	-0.07	-0.21	-0.15	-0.11
F2	100	92	93	96	96	97
99.8 percentile	114.10	182.34	218.96	99.78	87.20	97.60

Table 6.3(a) Statistical evaluation (overall-STREET-HEF).

Parameter	Monitored	Stedman	Modified Stedman	DEFRA	Modified DEFRA	Power
Mean	47.55	36.47	42.21	35.54	34.75	37.90
SD	15.50	21.46	27.09	14.11	8.27	12.59
IA	1.00	0.51	0.47	0.54	0.45	0.54
NMSE	0.00	0.37	0.40	0.27	0.26	0.22
R	1.00	0.26	0.24	0.28	0.14	0.27
FB	0.00	-0.26	-0.12	-0.29	-0.31	-0.23
F2	100	94	92	94	94	96
99.8 percentile	114.10	182.34	218.96	92.02	77.59	91.88

Table 6.3(b) Statistical evaluation (7am-6pm-HEF-STREET).

Parameter	Monitored	Stedman	Modified Stedman	DEFRA	Modified DEFRA	Power
Mean	37.26	33.88	39.62	34.28	35.42	37.97
SD	18.18	18.36	21.70	15.20	9.38	12.54
IA	1.00	0.80	0.79	0.81	0.58	0.79
NMSE	0.00	0.19	0.20	0.15	0.21	0.13
R	1.00	0.66	0.66	0.68	0.41	0.69
FB	0.00	-0.10	0.06	-0.08	-0.05	0.02
F2	100	95	96	97	94	97
99.8 percentile	114.10	143.52	178.58	97.70	84.68	96.93

Table 6.4(a) Statistical evaluation (overall-CEF-OSPM).

Parameter	Monitored	Stedman	Modified Stedman	DEFRA	Modified DEFRA	Power
Mean	47.55	42.49	50.47	41.49	36.43	43.48
SD	15.50	15.98	19.25	11.89	7.35	10.01
IA	1.00	0.56	0.54	0.55	0.43	0.55
NMSE	0.00	0.19	0.19	0.16	0.23	0.13
R	1.00	0.28	0.27	0.28	0.09	0.28
FB	0.00	-0.11	0.06	-0.14	-0.26	-0.09
F2	100	94	95	95	92	95
99.8 percentile	114.10	143.52	178.58	96.19	77.59	95.13

Table 6.4 (b) Statistical evaluations (7am-6pm-CEF-OSPM).

Parameter	Monitored	Stedman	Modified Stedman	DEFRA	Modified DEFRA	Power
Mean	37.26	33.94	39.71	34.12	35.36	37.80
SD	18.18	18.91	22.48	15.37	9.56	12.74
IA	1.00	0.80	0.78	0.80	0.58	0.77
NMSE	0.00	0.20	0.21	0.16	0.22	0.14
R	1.00	0.65	0.64	0.67	0.40	0.64
FB	0.00	-0.09	0.06	-0.09	-0.05	0.01
F2	100.00	95.00	95.00	96.00	95.00	97.00
99.8 percentile	114.10	145.40	184.10	99.29	84.68	97.11

Table 6.5(a) Statistical evaluation (overall-OSPM-HEF).

Parameter	Monitored	Stedman	Modified Stedman	DEFRA	Modified DEFRA	Power
Mean	47.55	42.62	50.66	41.26	36.47	43.25
SD	15.50	17.13	20.87	12.37	7.61	10.47
IA	1.00	0.56	0.53	0.55	0.42	0.54
NMSE	0.00	0.20	0.21	0.17	0.23	0.14
R	1.00	0.29	0.27	0.28	0.07	0.27
FB	0.00	-0.11	0.06	-0.14	-0.26	-0.09
F2	100.00	96.00	96.00	95.00	94.00	98.00
99.8 percentile	114.10	145.40	184.10	99.29	77.59	95.87

Table 6.5(b) Statistical evaluation (7am-6pm-HEF-OSPM).

Motorway

Similarly for the motorway site the analysis was carried out using the above formulations and the resulting diurnal profile variations and statistical analyses are presented in Figures 6.10, 6.11 and 6.12 and in Tables 6.6, 6.7 and 6.8 depending on three comparison classifications: an

overall comparison, comparison for the period when constant hourly averaging background concentrations for NO_x were used and comparison for the period when hourly individual NO_x background values were used respectively. The modelled NO_x concentrations were calculated using GFLSM and CEF.

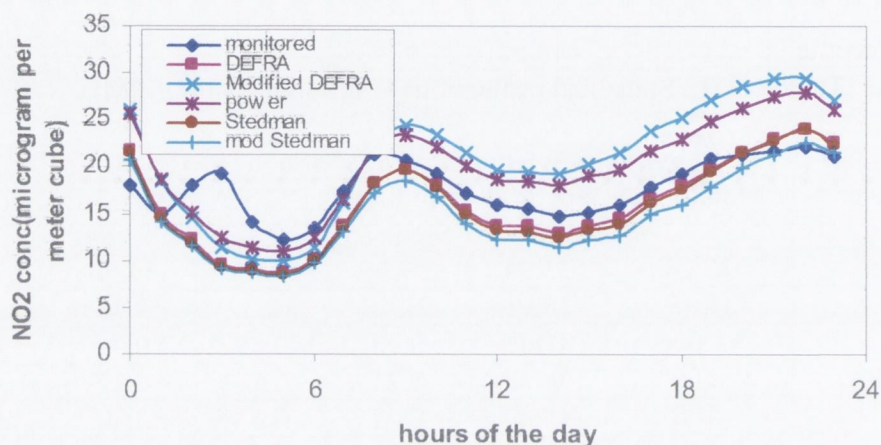


Figure 6.10 Performance evaluations for overall NO₂ concentration at Leixlip using GFLSM modelled data (CEF) and hourly background concentrations.

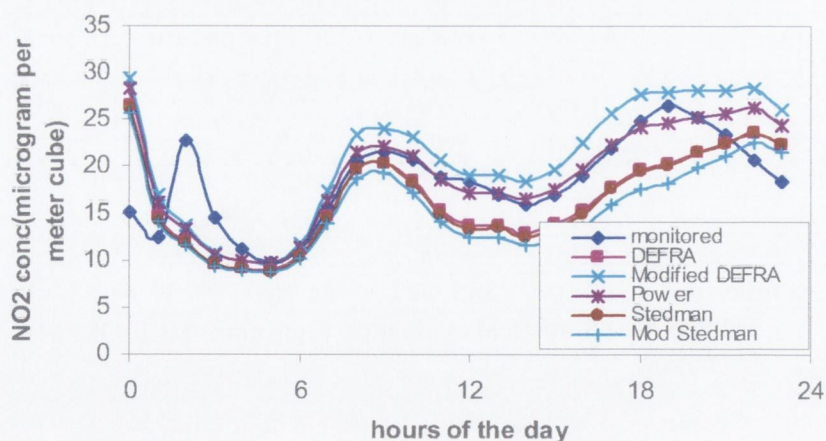


Figure 6.11. Performance evaluation for NO₂ concentration at Leixlip using GFLSM modelled data (CEF) and constant hourly average background concentrations for period 15/9/2001-13/3/2002.

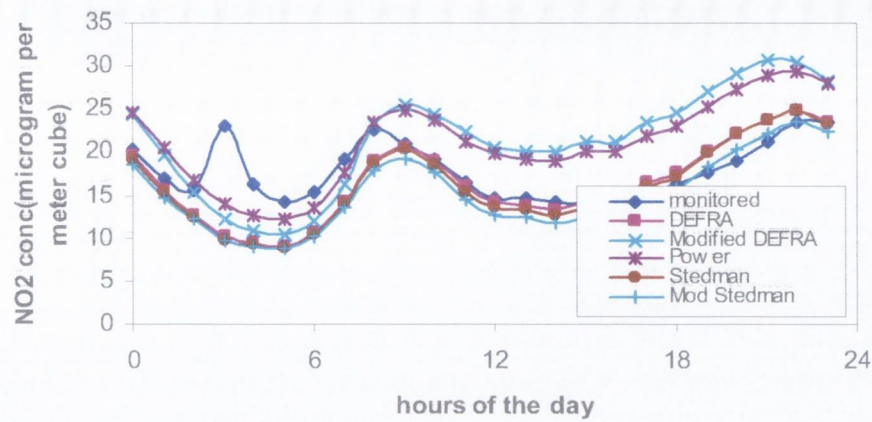


Figure 6.12.Performance evaluation for NO₂ concentration at Leixlip using GFLSM modelled data (CEF) and individual hourly average bkg concentrations for period 13/3/2002-15/9/2002.

Parameter	Monitored	Stedman	Modified Stedman	DEFRA	Modified DEFRA	Power
Mean	19.03	16.25	15.39	16.51	21.15	20.23
SD	14.19	12.74	12.08	12.21	13.73	12.32
IA	1.00	0.76	0.75	0.76	0.77	0.77
NMSE	0.00	0.50	0.54	0.47	0.40	0.38
R	1.00	0.60	0.59	0.61	0.60	0.60
FB	0.00	-0.16	-0.21	-0.14	0.11	0.06
F2	100	85	85	87	87	87
99.8 percentile	92.25	95.43	93	92.37	89.05	93.82

Table 6.6 Statistical evaluation for overall performance at motorway site.

Parameter	Monitored	Stedman	Modified Stedman	DEFRA	Modified DEFRA	Power
Mean	19.99	16.40	15.58	16.60	20.97	19.27
SD	14.83	6.61	5.76	6.39	10.06	8.19
IA	1.00	0.52	0.47	0.52	0.64	0.60
NMSE	0.00	0.63	0.70	0.61	0.46	0.49
R	1.00	0.36	0.31	0.37	0.43	0.41
FB	0.00	-0.20	-0.25	-0.19	0.05	-0.04
F2	100	81	81	82	85	86
99.8 percentile	92.06	47.44	44.60	45.55	51.38	49.54

Table 6.7 Statistical evaluation for NO₂ concentration at Leixlip using GFLSM modelled data (CEF) and constant hourly avg bkg concentrations for period 15/9/2001- 13/3/2002

Parameter	Monitored	Stedman	Modified Stedman	DEFRA	Modified DEFRA	Power
Mean	18.15	16.12	15.22	16.43	21.32	21.10
SD	13.53	16.44	15.76	15.74	16.36	15.08
IA	1.00	0.87	0.87	0.88	0.85	0.86
NMSE	0.00	0.37	0.37	0.32	0.34	0.28
R	1.00	0.79	0.79	0.79	0.75	0.77
FB	0.00	-0.12	-0.18	-0.10	0.16	0.15
F2	100	83	83	85	85	86
99.8 percentile	85.38	95.43	93	92.37	89.05	93.82

Table 6.8 Statistical evaluation for NO₂ concentration at Leixlip using GFLSM modelled data (CEF) and individual hourly average bkg concentrations for period -13/3/2002-15/9/2002

6.4 Discussion of Results.

The statistical results show that for the Stedman method, the modified Stedman method and the new formulation of a power method, good agreement is achieved between modelled and monitored NO₂ concentrations at the urban street canyon site. When actual monitored and background concentrations are used the IA value (Table 6.1) increases for the modified Stedman’s method and this is to be expected as it is calibrated for local conditions. When using modelled NO_x concentrations, a similar pattern is observed, although the original Stedman method gives slightly better short term model performance (IA, NMSE, and R) with both STREET and OSPM. The long term model performance as quantified by the mean and FB is better using the modified Stedman method.

The Wilson and Laxen approach when modified for Irish conditions yields an expression for $\overline{\text{NO}}_{2(\text{road})}$ derived from $\overline{\text{NO}}_{x(\text{total})}$. On inspection of the statistical analysis, it is observed that the modified DEFRA method do not adequately represent the transformation of NO₂ from NO_x and the original DEFRA (Wilson and Laxen method) gives better results. While computing the logarithmic variation as per Wilson and Laxen approach it was observed that it did not adequately represent the variation, which was fitted best using a power equation. The

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performance of the power method is very strong, even when using modelled NO_x concentrations. From Tables 6.2(a) and 6.2(b) it is clearly evident that the power model gives better estimates of both short term and long term model performances, followed closely by the original DEFRA method. Similar trends are observed from Tables 6.3(a) and 6.3(b). It can therefore be clearly stated that the power model is the appropriate technique when using the STREET model with either CEFs or HEFs. When the techniques are compared for OSPM CEF (Tables 6.4(a) and 6.4(b)) it is observed that the original DEFRA method gives a slightly higher value of IA than the power method (Table 6.4(a)). Other than this, all the other model evaluation parameters in Tables 6.4(a) and 6.4(b) are better for the power method. Similar trends are observed for Tables 6.5(a) and 6.5(b), except that the IA values in both tables are slightly lower for the power method compared to the DEFRA method.

The 99.8 percentile value seems to be heavily overpredicted by the Stedman and Modified Stedman methods, whereas it is slightly underpredicted by the DEFRA, modified DEFRA and power methods. Similar trends are observed in the statistical evaluations carried out for the 0700-1600 hours range. It is suggested that for Dublin city centre, the power equation should be used to represent local conditions and variations as it most accurately represents both short term and long term variations with for both the STREET and OSPM models using CEFs or HEFs.

As mentioned before, the motorway results were computed for two different background scenarios, one when hourly background NO_x concentration data was available and another when the average hourly background concentration was used. The overall statistical analysis show that all the models predict the NO₂ concentrations with a similar degree of accuracy, with

the power and modified DEFRA methods performing marginally better than the other ones. The best results are obtained with the power method when hourly background concentrations were available. The 99.8 percentile concentration values were well predicted by all the methods with the DEFRA method presenting the most accurate estimation.

However it is observed that when average constant hourly background values were used, the performance of all the models decreased drastically. The 99.8 percentile concentrations were heavily underpredicted by all the methods.

For the period in which individual hourly background concentrations were available there is no clear indication of which method gives the best results (Table 6.8). The power method gives the best results for the NMSE and F_2 values and close to the best for IA and R values. The 99.8 percentile concentration is slightly overpredicted using all methods and is best represented using the modified DEFRA method. The statistical comparison also highlights the fact that when the constant average hourly background concentration is considered (Table 6.7) the modified DEFRA and the power method (local calibrations) give overall better results with respect to the standard methods. When actual individual hourly background concentrations were available (Table 6.8) all the methods were similar in performance with no clear indication of which method performs best. The power method though gives the best NMSE and F_2 values for this case.

6.5. Study Summary

The above study presented modified Stedman's and DEFRA methods for predicting roadside NO₂ concentrations from roadside NO_x concentrations. The methods so obtained are compared with the original methods. Further to this a new model based on the power law was developed to take into consideration a better decay of the ratio of (NO₂/NO_x)_{road} with total NO_x rather than the logarithmic law initially followed by Wilson and Laxen (DEFRA,2003). In the first case, the modified Stedman method improves the prediction result when actual monitored data and background concentrations are used though the Stedman method in itself gives also good short term model performance when using modelled NO_x concentrations when applied for the street canyon. Long term model performance is better using the Modified Stedman method.

The original DEFRA method performs well in predicting NO₂ concentrations. However a modified DEFRA approach did not perform that well, and the proposed power method better represented the decay pattern.

At the motorway site the local calibration methods (modified DEFRA and power) give the best results when constant average background values were used, whereas it is not possible to conclude which method performed best when using individual hourly background concentrations. The power method performs well with both average and hourly background values, as shown by the evaluation analysis carried out for the entire year in which the power method performed best. It can therefore be safely stated that that the power method is a more accurate representation of the conversion of NO_x to NO₂ at the chosen street canyon and highway study site.

7.1 Introduction.

Previous chapters of the thesis (Chapters 3, 4 and 5) have dealt with the validation of dispersion models for highways and urban street canyons. It has been widely reported that one of the primary drawbacks of Gaussian based highway dispersion models is that their modelling abilities decrease under low wind speeds and parallel wind directions. In parallel wind conditions, Gaussian models are more sensitive to the assumption of steady state and homogeneous wind flow (Benson, 1992). Certain dispersion models like HIWAY2 have an inbuilt dispersion algorithm to particularly take care of such situations, but no such methods exist for *mathematical* Gaussian dispersion models like GFLSM. This chapter presents a step-by-step approach to the development and evaluation of a hybrid model (a combined ‘mathematical - numerical model’ in nature) to determine its suitability as an alternative to the existing Gaussian based models, particularly with reference to its accuracy in predicting concentrations during parallel wind conditions. The hybrid model was developed from two existing Gaussian based models, namely GFLSM and IITLSM, and its performance is tested over a period of one year at the M4 motorway site.

7.2 Development of Hybrid model.

7.2.1 The roadside dispersion model GFLSM.

The GFLSM model has been described in detail in Chapter 3 of the thesis. The proposed model was created by combining the GFLSM with part of the IITLS model.

$$C = \frac{Q_1}{2\sqrt{2\pi}\sigma_z(u\sin\theta + u_0)} \left[\exp\left(-\frac{(z-h)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z+h)^2}{2\sigma_z^2}\right) \right] \times \left[\operatorname{erf}\left(\frac{\sin\theta(p-y) - x\cos\theta}{\sqrt{2}\sigma_y}\right) + \operatorname{erf}\left(\frac{\sin\theta(p+y) + x\cos\theta}{\sqrt{2}\sigma_y}\right) \right] \quad (7.1)$$

7.2.2 The roadside dispersion model IITLS.

Goyal and Ramakrishna (1999) developed the Indian Institute of Technology Line Source (IITLS) model to predict concentrations of gaseous pollutants CO, SO₂, NO_x and particulates for various types of roads. The model formulations for finite and infinite line sources are developed from the standard point source Gaussian plume equation, given by

$$C_p = \frac{Q}{\pi u \sigma_y \sigma_z} \exp\left(\frac{-y^2}{2\sigma_y^2}\right) \exp\left(-\frac{(z-h)^2}{\sigma_z^2}\right) \exp\left(-\frac{(z-h)^2}{\sigma_z^2}\right) \quad (7.2)$$

Where Q is the source strength (g/s), u , wind speed (m/s), y , crosswind distance (m), z , vertical distance (m), h , source height (m), σ_y and σ_z are the horizontal and vertical dispersion parameters (m) respectively. The ground level concentrations of gaseous pollutants can be obtained by integration of equation (7.2) along the length of line source.

The model uses separate equations for calculating pollutant concentrations under cross wind and parallel wind conditions. In the crosswind case, the ground level concentration of the pollutants is given by the following equation (7.3):

$$C_{xwind} = \frac{2q}{(2\pi)^{0.5} \sigma_z u} \exp\left(-\frac{h^2}{2\sigma_z^2}\right) \quad (7.3)$$

Where C_{xwind} is the ground level concentration ($\mu\text{g}/\text{m}^3$) of the pollutants in crosswind, q the line source strength ($\text{gm}^{-1}\text{s}^{-1}$) and the remaining parameters hold the meanings given before.

For parallel wind conditions, concentrations are determined by dividing the roadway into a number of discrete line elements and applying the expression

$$C_{||wind} = \sum_{i=1}^{NEL} C_p \quad (7.4)$$

Where $C_{||wind}$ is the ground level concentration when wind is parallel to the road ($\mu\text{g}/\text{m}^3$), NEL is the number of line elements along the length of the roadway and C_p is obtained from

equation (7.2) considering all emission from an element to occur at a point in the centre of that element. This discretisation is shown in Figure 7.1

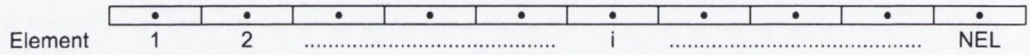


Figure 7.1 Representation of NEL

For other (oblique) wind angles ($15^\circ < \phi < 60^\circ$), concentrations are determined by weighted average of the crosswind and parallel concentrations using the expression

$$C_{obl} = \sin^2 \phi C_{xwind} + \cos^2 \phi C_{||wind} \quad (7.5)$$

The ' ϕ ' used in equation (7.5) is essentially the 'wind road angle'. The wind road angle is defined as the angle obtained by subtracting the road bearing from the observed wind direction. The road bearing at the M4 motorway study site is 85° .

7.2.3 A new Hybrid road dispersion model

The General Finite Length Source Model (GFLSM) is based on the Gaussian diffusion equation and is so formulated so that it can be applied for any wind direction and any length of line source (Luhar and Patil, 1989). The IITLS model as proposed by Goyal and Ramakrishna (1999) calculates concentrations of pollutants using different equations for crosswind, oblique and parallel concentrations as described above. The assumption made in formulating the new Hybrid model was that the GFLSM model was capable of accurately calculating concentrations during crosswind and oblique wind using equation (7.1) but that the performance of the GFLSM model could be enhanced by incorporating the 'parallel concentration' term (given in equation 7.4) arising from the IITLS model to achieve improved

predictions under parallel wind conditions. The wind road angle sectors considered by the models are geometrically represented in Figures 7.2 and 7.3

Figure 7.2

Figure 7.3

Figure 7.4

Figure 7.5

Figure 7.6

Figure 7.7

Figure 7.8

Figure 7.9

Figure 7.10

Figure 7.11

Figure 7.12

Figure 7.13

Figure 7.14

Figure 7.15

Figure 7.16

Figure 7.17

Figure 7.18

Figure 7.19

Figure 7.20

Figure 7.21

Figure 7.22

Figure 7.23

Figure 7.24

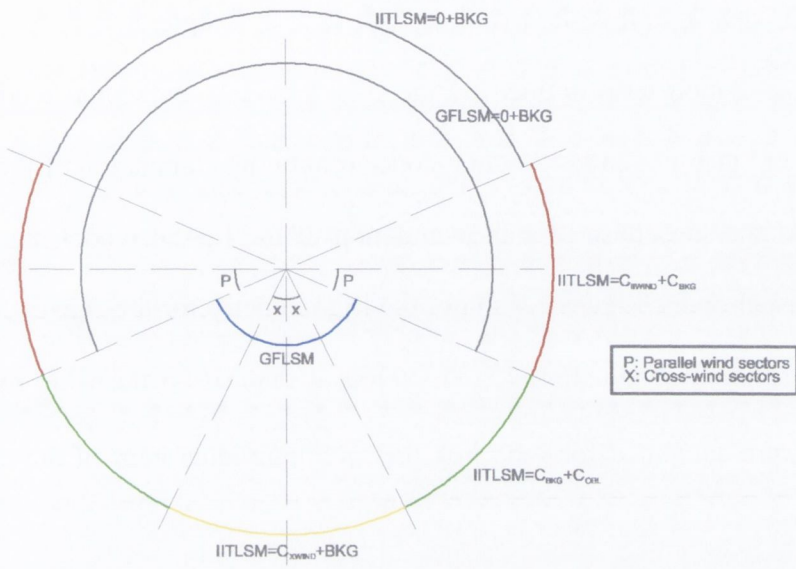


Figure 7.2 Geometric representations of GFLSM and IITLSM by sector

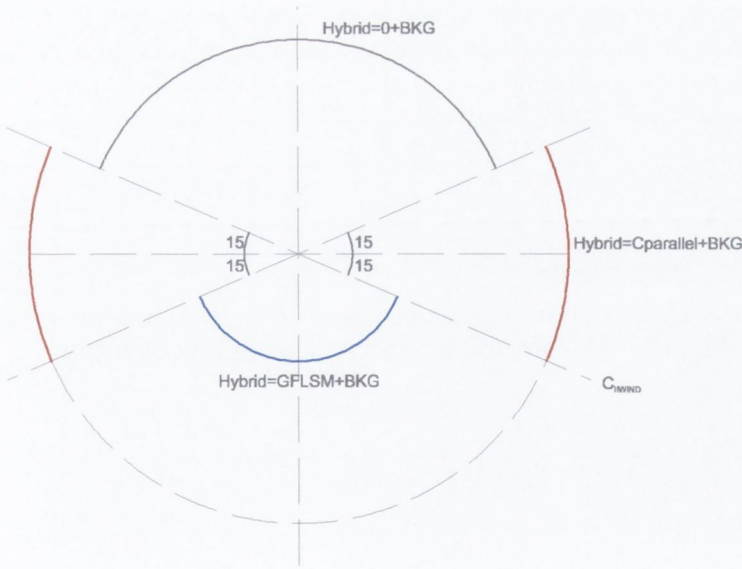


Figure 7.3 Geometric representation of Hybrid model by sector

7.3 Validation of Hybrid Model

7.3.1 Study Site

The evaluation and validation of the proposed hybrid model was performed at the M4 study site at Leixlip. Full details of this site have been provided in Chapter 3.

The parallel concentration term defined by the IITLS model divides the road length into a number of links and then computes the total concentration by summation of the contributions from all links. At the site chosen for the validation of the hybrid model, the roadway was divided into five such links. Figure 7.4 shows the trigonometry for the calculation of x_i and y_i required for the solution of equation 7.2. As x_i and y_i depend on the wind road angle ' ϕ ', separate values were computed for each link for each individual hour of the entire one year data set.

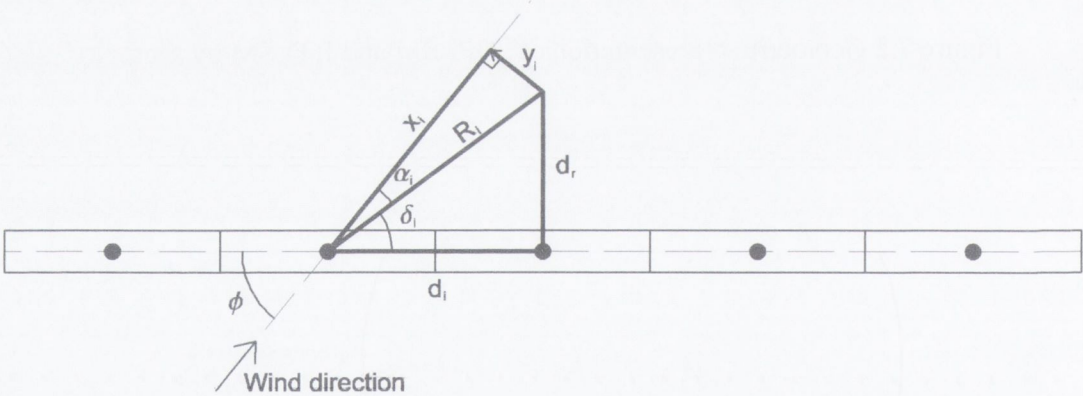


Figure 7.4 Geometric representations of link elements.

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From Figure 7.4, it is seen that the calculation of x_i and y_i can be obtained using the following equations:

$$\delta_i = \tan^{-1} \left(\frac{d_r}{d_i} \right) \quad (7.6)$$

$$R_i = \sqrt{d_i^2 + d_r^2} \quad (7.7)$$

$$\alpha_i = |180 - \phi - \delta_i| \quad (7.8)$$

$$y_i = |R_i \sin \alpha_i| \quad (7.9)$$

$$x_i = |R_i \cos \alpha_i| \quad (7.10)$$

The variables in equations (7.6) - (7.10) are defined in Figure 7.4. The values of R_i and δ_i remain constant for each of the links considered. It is clearly evident that the ' α_i ' value is dependent on the value of ' ϕ ' which leads to changing x_i and y_i values. The y_i values are directly substituted in equation 7.2. The calculated values of x_i are used in the calculation of the dispersion coefficients (σ_y and σ_z) which depend on downwind distance and the appropriate stability class for the particular hour considered. These are calculated using Briggs equations as described in Chapter 3.

7.3.2 Dataset considered

The validation of the GFLSM model has been described in Chapter 3. These results remain applicable for the Hybrid model under crosswind and oblique wind conditions. The further validation of the Hybrid model concentrated on the assessment of model accuracy during parallel winds, and during the hours which concentrations at the receptor should have been affected by emissions from the M4.

- Only certain hours were considered in the assessment. The hours considered were from 0700-2100 hours. The remaining nighttime hours were neglected. The basis for this assumption was that the traffic flow during nighttime was relatively less, and the emphasis was more on the period during which the traffic flow was highest and hence the period considered from 0700-2100 hours.
- Only those hours when the measured background concentrations, C_{bkg} , were less than the monitored concentrations at the receptor location, C_{mon} , were considered.
- Even after the above assumption, some background concentrations though less than the receptor concentration were almost equal to them (background data $\cong$ monitored data). Only those hours where $C_{bkg} < 0.8C_{mon}$ were considered.
- Only hours with parallel winds, $(-15 \leq \phi \leq 15)$ were considered.
- Only hours with wind speeds greater than 1m/s were considered as during calm conditions wind directions are not well defined.

About 6% of the data set (509 hours) remained after all the above conditions were applied. Figure 7.5 presents a wind rose of the wind direction frequencies occurring at the motorway monitoring site and at the Casement Aerodrome over the entire study period.

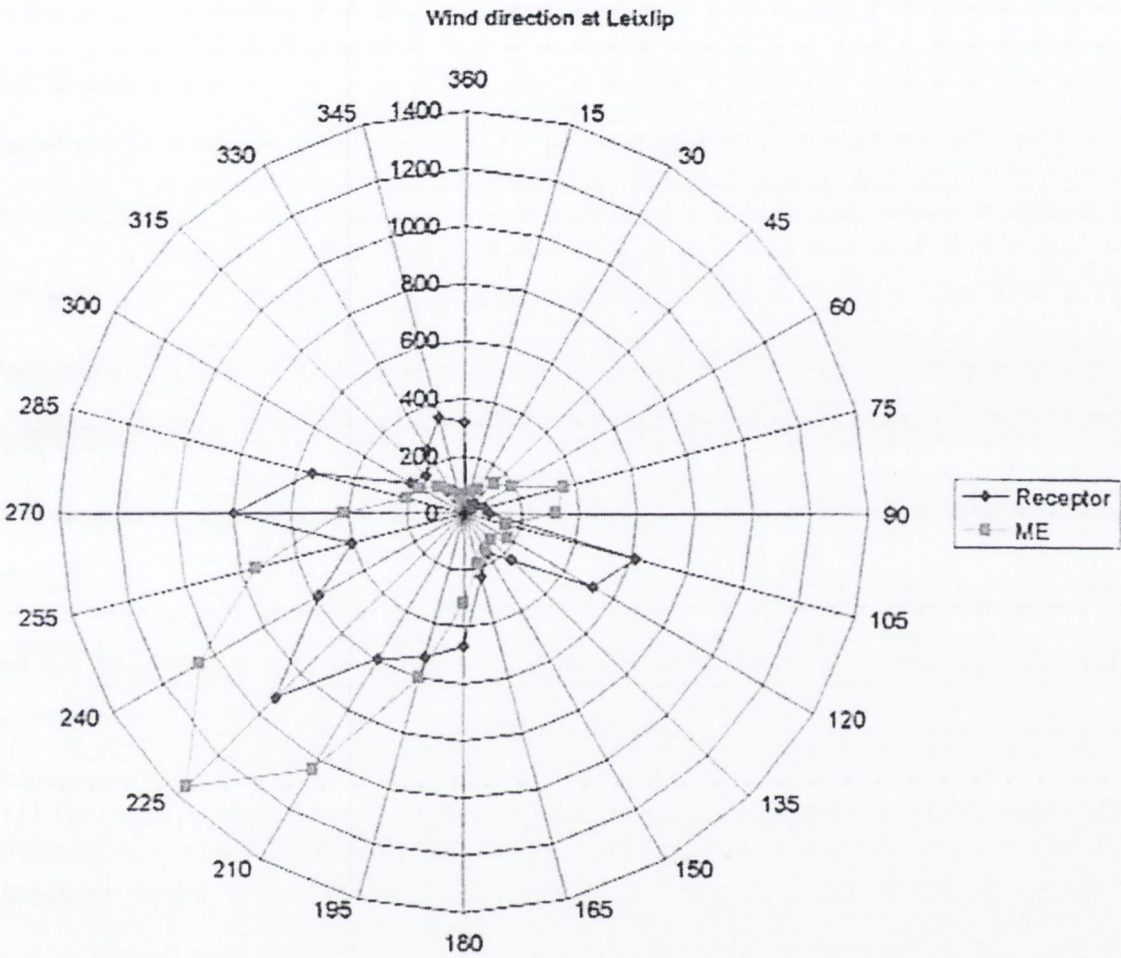


Figure 7.5 Wind direction frequencies at the motorway site (Receptor) and at Casement Aerodrome (ME) (Budd, 2004)

7.3.3 Evaluation of the vehicular emissions.

The evaluation of vehicular emissions using the COPERT III methodology for this particular study site has already been described in Section 3.5.3.

7.3.4 Statistical Parameters.

The statistical parameters considered for model evaluation are those already used throughout this thesis. The details of these statistical parameters and their meaning and interpretation have been described in Section 2.5.

7.4 Results

The performances of the GFLSM and the IITLS models are first compared using the entire year of monitored data collected at the study site. The performance of the Hybrid and GFLSM models are then compared using the restricted dataset described above.

7.4.1 GFLSM and IITLSM comparison.

The final modelled NO_x concentration obtained from the application of any model can be represented as:

$$(\text{NO}_x)_{\text{FP}} = (\text{NO}_x)_{\text{P}} + (\text{NO}_x)_{\text{BKG}} \quad (7.11)$$

Where $(\text{NO}_x)_{\text{FP}}$ is the final predicted concentration, $(\text{NO}_x)_{\text{P}}$ is the model predicted concentration and $(\text{NO}_x)_{\text{BKG}}$ is the background concentration.

It can be observed from equation (7.11) that the final predicted values are dependent on the assumed background concentrations.

Hourly NO_x concentrations were measured at this site throughout the second half of the study period (13/3/2002-15/9/2001). For this period, the comparison of monitored concentrations with the predictions made using the GFLSM and the IITLSM was carried out using individual hourly background concentrations (Case 3, as described in Chapter 3), i.e. for each hour

$$(\text{NO}_x)_{\text{FP}} = (\text{NO}_x)_{\text{P}} + (\text{NO}_x)_{\text{MB}} \quad (7.12)$$

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Where $(NO_x)_{MB}$ is the measured background concentration. For the first half of the study period (15/9/2001-12/3/2002), the background concentrations used are taken from the observed average diurnal variation of NO_x concentration at the background site. The predicted NO_x concentration is obtained from

$$(NO_x)_{FP} = (NO_x)_P + (NO_x)_{DP} \quad (7.13)$$

Where $(NO_x)_{DP}$ is the mean NO_x concentration at the background site, for the hour of the day concerned, taken from calculated diurnal profile shown in Figure 3.13. Hence, throughout the whole year, the final predicted data was obtained by adding the background concentrations to the GFLSM or IITLSM modelled concentrations. For parallel wind conditions, the GFLSM model concentration is zero, hence the total concentration is simply the background concentration (Figure 7.3). The final IITLSM model calculations incorporated the background concentration and the particular relevant crosswind, parallel or oblique concentration dependant on the particular wind direction for that particular hour.

The statistical evaluations of the predicted $(NO_x)_{FP}$ values calculated by employing the IITLSM and GFLSM equations (7.11) -(7.13) are shown in Tables 7.1-7.3. The diurnal profile variations of the monitored and modelled data using the GFLSM and IITLSM models over for the entire study period are shown in Figure 7.6.

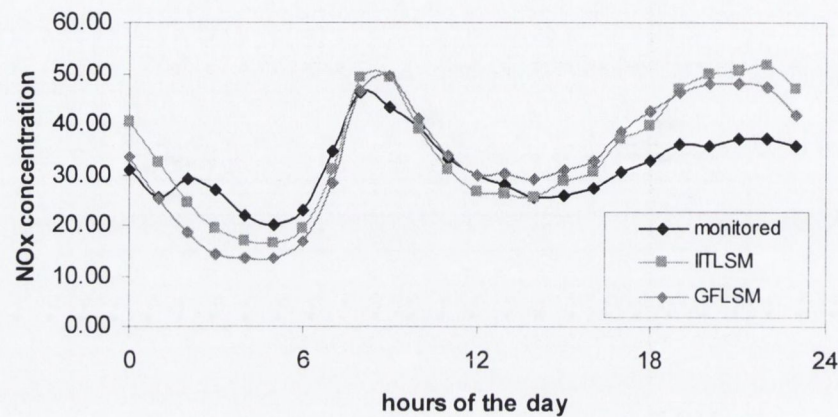


Figure 7.6 Diurnal profile variation for monitored and modelled data (entire year).

Parameters	monitored	IITLS	GFLSM
IA	1.00	0.69	0.73
NMSE	0.00	1.24	1.03
R	1.00	0.43	0.45
FB	0.00	0.08	0.05

Table7.1 Summary of statistical results (entire year)

Parameters	monitored	IITLS	GFLSM
IA	1.00	0.55	0.56
NMSE	0.00	1.40	1.15
R	1.00	0.35	0.38
FB	0.00	-0.02	-0.05

Table7.2 Summary of statistical results (first 6 months)

Parameters	monitored	IITLS	GFLSM
IA	1.00	0.75	0.76
NMSE	0.00	0.89	0.85
R	1.00	0.64	0.65
FB	0.00	0.20	0.19

Table7.3 Summary of statistical results (last 6 months)

From the statistical analysis performed and the results obtained it is observed that there is a very marginal difference between the accuracy of the predicted data obtained using GFLSM and IITLSM models, with the performance of the GFLSM model being slightly better. It is observed from Figure 7.1 that both the models are able to predict the peak concentrations in the earlier part of the day, whereas in the later part of the day the models slightly tend to overpredict the measured concentration.

The statistical analysis on the first six months of monitored and modelled data shows only limited differences between the models, the key difference being in the NMSE values. In this context it was clearly observed that the GFLSM model performed marginally better than the IITLSM when all wind directions are considered. Nevertheless, the inability of the GFLSM to calculate concentrations during parallel winds implies significant scope for improved performance using the Hybrid model.

7.4.2 Hybrid and GFLSM comparison.

The hybrid model was tested against the monitored data and the GFLSM ‘stand alone model’ to determine its effectiveness in predicting concentrations during parallel wind conditions by considering the residual 6% dataset during which actual highway emission impacts were observed. Figures 7.7-7.9 show the diurnal profile variations in the monitored data, GFLSM results and hybrid model results over the entire year, first six months and last six months, respectively.

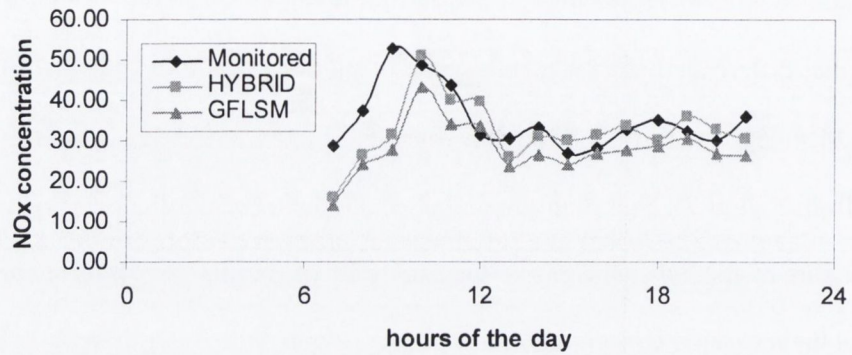


Figure 7.7 Diurnal profile variation for monitored and modelled data (entire year)

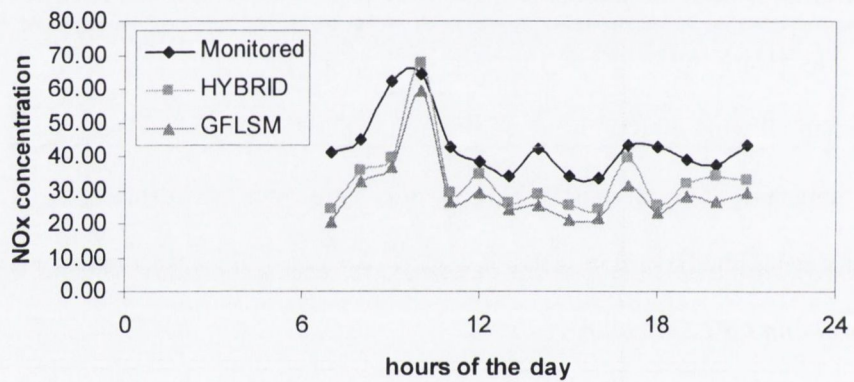


Figure 7.8 Diurnal profile variations for monitored and modelled data (sep01-mar02)

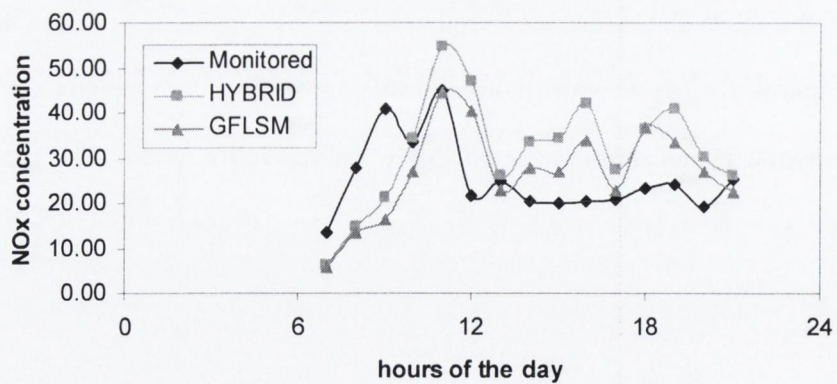


Figure 7.9 Diurnal profile variations for monitored and modelled data (apr02-sep02)

From the diurnal profiles, it is seen that the Hybrid and the GFLSM curves follow each other closely. The Hybrid concentrations are always slightly greater than the GFLSM due the contribution of C_{llwind} (equation 7.4). It was observed that for the first six months both models had a tendency to underpredict the monitored concentrations whereas during the second half of study period, both models had a tendency to overpredict the monitored concentration, with the concentrations predicted by the hybrid model being slightly higher than the GFLSM stand alone model. The diurnal profile obtained for the entire analysis showed that the GFLSM slightly underestimates monitored concentration due to the $C_{llwind} = 0$ assumption, but the hybrid model gives a closer match to the monitored profile.

Statistical analysis of the results shows that the performance of the Hybrid model is much better than the GFLSM model when compared over the entire period of one year and first set of six months data as shown in Tables 7.4 and 7.5. Note that performance of GFLSM under parallel wind conditions is less accurate then when all wind directions and speeds are considered (Table 7.1). There is a marginal decrease in the effectiveness of the Hybrid model during the second six months analysis as shown in Table 7.6. This is associated with the tendency of both models to overpredict measured concentrations in this period. Overall, however, the Hybrid model gives much better and improved results for both short term and long term averages than the GFLSM.

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Parameters	monitored	Hybrid	GFLSM
Mean	33.43	33.57	28.40
IA	1.00	0.57	0.52
NMSE	0.00	0.90	0.92
R	1.00	0.28	0.25
FB	0.00	0.00	-0.16
F2	100	80	80

Table7.4 Summary of statistical results (entire year)

Parameters	monitored	Hybrid	GFLSM
Mean	40.55	34.35	29.45
IA	1.00	0.61	0.57
NMSE	0.00	0.62	0.70
R	1.00	0.36	0.31
FB	0.00	-0.17	-0.32
F2	100	86	86

Table7.5 Summary of statistical results (first 6 months)

Parameters	monitored	Hybrid	GFLSM
Mean	25.16	32.66	27.18
IA	1.00	0.39	0.41
NMSE	0.00	1.42	1.34
R	1.00	0.22	0.21
FB	0.00	0.26	0.08
F2	100	78	78

Table7.6 Summary of statistical results (last 6 months)

7.5 Study Conclusions

This chapter we have presented a comparison of two Gaussian based atmospheric dispersion models, GFLSM and IITLS against monitored data collected from an ambient NO_x measurement campaign conducted on Leixlip M4 motorway using a composite emission factor and hourly background concentrations. Graphical and statistical analyses reveal a high level of agreement between the measured and predicted datasets using both models, with the GFLSM model slightly outperforming the IITLS model. A Hybrid model was developed from these two models by incorporating the parallel concentration term from the IITLS model

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within the GFLSM, and the developed hybrid model was evaluated against the test site data for parallel wind conditions. Statistical and graphical analysis revealed that the Hybrid model was more effective in dealing with parallel wind conditions than the GFLSM model when used alone.

8.1 Summary

The research described in this thesis has addressed the use of dispersion modelling in the amendment of the air quality impacts of road traffic emissions. The aims of the research were to evaluate the use of different models and the input data that should be employed to obtain optimum results.

Air pollution assessment studies incorporating measured and modelled concentrations of traffic pollutants were performed at four selected sites comprising two highway (motorway) sites, one rural town and one street canyon site. Hourly online measurements of CO, NO_x, and NO₂ were considered at the M4 motorway site and street canyon sites, whereas speciated hydrocarbons were considered at the M50 motorway site. Hourly meteorological and traffic data were obtained at all sites, to determine their associated influence on pollutant concentrations.

For the successful completion of any modelling exercises, it is important to know the chemical properties of the pollutants and the appropriate dispersion modelling techniques and the basic background regarding their formulations and applicability depending upon site conditions. Chapter 2 of the thesis presents a comprehensive report on this aspect.

For a proper modelling study, often a screening model is employed to determine the necessity of an elaborate modelling exercise. In this context the DMRB model was assessed at the M4 motorway site.

CALINE4 is the widely used dispersion model used for modelling concentrations from roadways and is regularly used in Ireland. Chapter 3 introduces the GFLSM model which is based on a similar formulation as CALINE4 but is wholly analytical in nature. Detailed

comparisons of monitored and modelled CO and NO_x concentrations were carried out for both models at two motorway sites.

At the M4 site detailed monitoring campaign had obtained a lot of required data (traffic and meteorological and background) for modelling assessment. The hourly background concentrations in this case were available for the last six months of the study and average of these was used as background for the first six months. Graphical and statistical analysis revealed that the GFLSM gave slightly better results for CO. A new proposal regarding the definition of background concentrations by stability class was proposed and shown to give good model efficiency. Generally, in the highway modelling, a CEF is often used, however a new concept of Hourly Emission Factors (HEF) was also considered. It is seen from both the studies that a proper selection of CEFs can give an equally good modelling result compared to those obtained with HEFs. The use of HEF at both the study site has shown that if a proper CEF value is used, there is no need for use of HEF. Sensitivity analysis of the models was carried for CO and NO_x concentrations.

The second site selected for the highway study was adjacent to the M50 motorway. In comparison to the M4 site where detailed data was available for an extended period of twelve months, the M50 motorway focused on capturing the spatial variation of pollutant concentrations downwind of the road. The monitoring was carried out for several hydrocarbons and the receptors were placed at 25m, 120m and 240m from the road which nullified the need for background concentration. As a result of the modelling exercise carried out it was observed that both models (CALINE4 and GFLSM) were able to model the range of background corrected concentrations of hydrocarbons reasonably well particularly at the receptor location closest to the motorway albeit that the individual hourly prediction often

differed substantially from measured values. The performance of modelled values decreased with receptor distance, but the performance of GFLSM was similar to CALINE4 modelling. The models performed extremely well in predicting long term averages but failed in predicting short term modelling performance.

The GFLSM model was also applied at a site in Monasterevin, to predict the change in air quality due to the opening of the M7 bypass of the town. The dataset available here was the least consistent of all cases but probably represents real life modelling better. Monitored and modelled air quality data both showed a change in air quality due to the opening of the bypass; however the change was not accurately depicted in the modelling results. The modelling results though seem to follow the trends evident in the before and after cases and predicted the improved air quality in the after case. The non availability of proper background data impeded modelling accuracy at this site. On an overall basis the GFLSM model seems to perform well when compared with monitored data and with modelled data obtained using CALINE4 and the use of HEF and background concentrations as per stability class can lead to improved modelling results.

The urban street canyon modelling study was conducted at Pearse Street in Dublin City center from May 2006 to December 2006. STREET and OSPM models were tested and evaluated at the Pearse Street canyon. Graphical and statistical comparisons showed that the performance of both models was reasonably good. The OSPM results were found to have better correlation with the monitored data than the STREET values for CO. Despite this, the STREET model remained reasonably accurate, in spite of its simplicity which allows it to be more readily incorporated into transport network models of urban areas. The best possible combination of modelled data arises with the combination of OSPM using HEF. It was similarly observed that

OSPM results had a slightly better correlation with monitored data than the STREET values for NO_x . Further to this, the use of background conditions based on different assumptions (as described in details in Chapter 5 and assessed in Chapter 3 for motorway conditions) was studied for NO_x and led to almost identical conclusions as at the motorway site.

The major importance of modelling NO_x concentrations at street canyons is to determine NO_2 concentrations, as these are more closely associated with adverse human health. These are generally obtained using Stedman's method or the Wilson and Laxen (DEFRA) method. These equations were modified for local Pearse street conditions and a new 'power method' of determining NO_2 concentrations from modelled NO_x concentrations was also proposed. The feasibility of predicting NO_2 concentrations for highways using the developed and standard methods were also assessed for the M4 motorway site in Chapter 6.

From the assessment studies, it was observed that the performance of gaussian models during low wind speeds and parallel wind directions is poor. In this context, a hybrid model was formulated that incorporated aspects of two gaussian based dispersion models to achieve improved predictions for parallel wind directions, as described in Chapter 7.

8.2 Main Findings

M4 motorway study

The main findings from the modelling study carried out at M4 can be summarized as:

The application of the DMRB model shows that it has a tendency for overprediction. With the newer version, though the overprediction is comparatively much less than the older version, the modelling results agree more with the monitoring results at the motorway than at the

roundabout site. The modification of the 5 link roundabout junction to 3 link junction on the basis of average traffic flows is a reliable concept and gives more improved modelling performance for roundabouts. The speed versus emission characteristics show that the emission factors are speed dependant and that the 3 link method of modelling gives lower value of emissions than the 5 link approach.

The detailed modelling exercise involving the use of GFLSM and CALINE4 for predicting CO concentrations showed that both models are suited for prediction capabilities. The CALINE4 modelling results obtained show a better agreement than Budd (2004), this is particularly due to use of an improved CEF. The performance of both the models is similar as indicated by the statistical and graphical analysis. The statistical distribution patterns observed also show a similar trend (Weibull distribution, based on KS statistic). The concept of hourly emission factors based on percentage HGV is also proposed and studied and no significant change was observed.

The GFLSM modelling of NO_x concentrations was assessed using a series of cases for background concentrations. Hour – by – hour concentrations of background values should be used if available (Case 3). However, the classification of background concentration as per stability class (Case 4) is nearly as good.

M50 motorway study

The GFLSM and CALINE4 models were assessed for predicting ‘background corrected’ hydrocarbon concentrations, wherein the receptors were located at 25m, 120m and 240m on either side of the motorway. It was observed from the modelling results that the GFLSM and

CALINE4 models performed similarly. The GFLSM gave a better performance on some measures and CALINE4 others. The performance of both models was better at 25m than 120m or 240m. However, spatial variability of concentrations was found to be well predicted by both models. The use of background corrected concentration measures leads to poorer model evaluation parameters than when background concentrations are included.

Monasterevin bypass study

The GFLSM model was employed to predict the change in air quality due to the opening of a town bypass. The monitored concentrations showed a definite improvement in the air quality with the opening of the bypass. The GFLSM model performed best in predicting the air quality data after the opening of the bypass, but with less accuracy for the 'before case' and for predicting the change in air quality. One of the major reasons for this was the validity of the available background concentration data. The average of the concentrations at 0400 was assumed to be the background concentrations for both pollutants and for both the scenarios (before and after). A significant change was observed in this context for the background concentrations based on this assumption. The use of a background corrected approach seemed to show slightly a better diurnal profile. Another significant drawback for this modelling study was the inadequate dataset, which led to inferior modelling results.

Street Canyon Modelling Study

Two street canyon models, STREET and OSPM were studied in the context of predicting street canyon concentrations. Both models effectively predicted the variations in air quality observed at Pearse Street. Both models seem to be successful in predicting long term concentrations. The OSPM model gave better prediction accuracy than STREET for both CO

and NO_x . The background concentration evaluation study showed that the use of stability class may offer a very good alternative when hourly values are not available.

NO_2 Street Canyon Modelling Study

NO_2 concentrations were predicted from modelled NO_x concentrations using two standard techniques. Both of these techniques were modified for the local conditions. It was also seen that a power law gave the best fit for the local NO_x to NO_2 concentrations ratio.

Hybrid modelling Study

The performance of gaussian models decreases with low wind speed and wind directions. A hybrid model was proposed to increase the efficiency of the GFLSM model for parallel wind conditions by incorporating the parallel concentration term from the IITLS model. The IITLS model was compared to the GFLSM model and it was observed that even though both the model performances were similar, the GFLSM was marginally better than the IITLS model.

It was observed that the prediction capabilities of the GFLSM model were significantly enhanced when the 'parallel concentration term' was included in it in comparison to the GFLSM stand alone model

8.3 Scope for further study

The following section outlines possible avenues for further research regarding highway modelling and street canyon junctions:

- For the M4 study site, formulate HEFs using speed versus emission characteristics as compared to the emission versus percentage HGV used in this study.
- Perform similar modelling exercises using GFLSM or CALINE4 for junctions including roundabouts to determine the ability of the GFLSM model to handle increased complexity.
- Rigorous testing of the proposed hybrid model should be carried out at other motorway sites under parallel wind conditions.
- A vertical assessment of street canyon effects should be carried out at Pearse Street. This would include taking measurements at selected heights on either side of the street and assessing the spatial distribution of pollutants with respect to height, allowing for a vertical profile of the selected pollutants.
- The OSPM modelling in this study has been performed using the laid down mathematical formulae. Comparison of the results so obtained using the software should be made against the modelled results using the equations. It is also necessary to change/modify the standard OSPM input parameter settings to accommodate local Irish conditions.
- Repeat the entire modelling procedure as outlined in Chapter 5 and 6 for another street canyon similar to Pearse Street one, and assess the modelling performance to see whether it is similar to Pearse street canyon modelling.
- Investigate the usefulness of Regional air quality models in providing background concentrations for local air quality assessments and compare to the recommendations of this thesis.

References:

- Alloway, B.J., Ayres, D.C., 1997. 'Chemical principles of Environmental Pollution', *Blackie Academic and Professional*.
- Atkinson, R., 1995. 'Gas phase Tropospheric Chemistry of Organic Compounds'. *Atmospheric Environment* 24(1), 1-14.
- Barletta, B., Meinardi, S., Simpson, I.J., Khwaja, H.A., Blake, D.R., Roland, S., 2002. 'Mixing ratios of volatile organic compounds (VOC's) in the atmosphere of Karachi, Pakistan'. *Atmospheric Environment* 36(21), 3429-3443.
- Benarie, M.M., 1980. 'Urban Air Pollution Modelling'. *MacMillan Press Ltd., London, United Kingdom*.
- Benson, P., 1992. 'A review of the development and application of the CALINE3 and 4 models'. *Atmospheric Environment* 26B (3), 379-390.
- Berkowicz, R., Palmgren, F., Hertel, O., Vignati, E., 1996, 'Using measurements of air pollution in streets for evaluation of urban air quality – meteorological analysis and model calculations'. *The Science of the Total Environment*, 189/190: 321-326.
- Berkowicz, R., Hertel, O., Larsen, S.E., Sørensen, N.N., Nielsen, M., 1997, 'Modelling traffic pollution in streets'. *Ministry of Environment and Energy, National Research Institute, Denmark*.
- Berkowicz, R., 2000, 'OSPM – A parameterised street pollution model'. *Environmental Monitoring and Assessment* 65, 323-331.
- Bogo, H., Gomez, D.R., Reich, S.L., Negri, R.M., San Roman, E., 2001: 'Traffic pollution in a downtown site in Buenos Aires'. *Atmospheric Environment* 35, 1717-1727.
- Bond, G.G., McLaren, E.A., Baldwin, C.L., Cook, R.J., 1986. 'An update of mortality among chemical workers exposed to benzene'. *Br. J. ind. Med* 43, 685-691.
- Broderick, B.M., Budd, U., Misstear, B.D., Ceburnis, D., Jennings, S.G., 2005. 'Validation of CALINE4 modelling for Carbon Monoxide concentrations under free-flowing and congested traffic conditions in Ireland'. *International Journal of Environmental Pollution* 24 (1/2/3/4), 104-113.
- Brimblecombe, P., 1986. 'Air Composition and Chemistry'. *Cambridge Environmental Chemistry Series 6*.
- Buckland, A.T., 1998. 'Validation of a street canyon model in two cities.' *Environmental Monitoring and Assessment* 52, 255-267.
- Buckland A.T. & Middleton, D.R., 1999, 'Nomograms for calculating pollution within street canyons'. *Atmospheric Environment* 33, 1017-1036.

Budd Una., 2004. 'Comparison of Screening and Short Term Modelling with Monitoring at Motorway and Roundabout Sites in Ireland'. *PhD Thesis* submitted in the Department of Civil, Structural and Environmental Engineering, Trinity College Dublin.

Cadle, S.H., Chock, D.P., Monson, P.R., Heuss, J.M., 1977. 'General motors sulphate dispersion experiment: experimental procedures and results'. *Journal of Air Pollution Control Assessment* 27, 33-38.

Carslaw, D., Beevers, S., 1999. 'NO_x and NO₂ predictions at roadside and background locations in London'. *South East Institute of Public health*.

Carslaw, D.C., 2006. 'Risks of exceeding the hourly EU Limit Value for nitrogen dioxide resulting from road transport emissions of primary nitrogen dioxide'. *Proceedings from the 2nd conference on environment and transport, including the 15th conference on transport and air pollution, Reims, France, 12-14 June 2006, no. 107, volume 1, 183-190.*

Central Statistics Office (CSO), 2004. *Vehicles Licensed for the first time, 2003* CSO, Government Stationary Office, Dublin.

Chock, D.P., 1978. 'A simple line source model for dispersion near roadways'. *Atmospheric Environment* 12, 823-829.

Colville, R.N., Hutchinson E.J., Mindell, J.S., Warren, R.F., 2001. 'The transport sector as a source of air pollution'. *Atmospheric Environment* 35, 1537-1565.

Clarke, A.G., Ko, Y.Y., 1996. 'The relative significance of vehicular emissions and other emissions of volatile organic compounds in the urban area of Leeds, UK.' *The Science of the total Environment* 189/190, 401-407.

Council of European Communities (CEC), 1999. Council Directive 1999/30/EC of the European Parliament and of the Council of 22 April 1999 relating to limit values for sulphur dioxide, nitrogen dioxide and oxide of nitrogen, particulate matter and lead in ambient air.

Council of European Communities (CEC), 2000. Council Directive 2000/69/EC of the European Parliament and of the Council of 16 November 2000 relating to limit values for benzene and carbon monoxide in ambient air. Official Journal of the European Communities, 13 December, L 313 (12).

Csanady, G.T., 1972. 'Crosswind shear effects on atmospheric diffusion'. *Atmospheric Environment* 6, 221-232.

Dabberdt, W.F., Ludwig F.L., Katie King., Johnson, W.B., 1973. 'Validation and applications of an urban diffusion model for vehicular pollutants.' *Atmospheric Environment* 7, 603-618.

Dabberdt, W.F., Hoydysh, W., Schorling, M., Yang, F., Holynskyj, O., 1995. 'Dispersion modelling at urban intersections.' *The Science of the Total Environment* 169, 93-102.

Delaney, K., 2006. 'Monitoring and modelling the Air Quality Impacts of Road Traffic Sources.' *MSc Thesis submitted to the Department of Civil, Structural and Environmental Engineering at Trinity College Dublin.*

DePaul, F.T., Sheih, C.M., 1986, 'Measurements of wind velocities in a street canyon'. *Atmospheric Environment* 20, 455-459.

DMRB 2003. Design Manual for Roads and Bridges, Volume 11, Environmental Assessment, Section 3, Part 1- Air Quality. Department of Transport, HMSO, London. February 2003 edition

Eerens, H.C., Sliggers, C.J., van den Hout, K.D., 1993. 'The CAR model: the Dutch method to determine city street air quality.' *Atmospheric Environment* 27B (4), 389-399.

Dewulf, J., van Langenhove, H., Wittman, G., 2002. 'Analysis of volatile organic compounds using gas chromatography'. *Trends in analytical Chemistry* 21(9-10), 637-646.
Ekstrom, M., Sjodin, A., Andreasson, K., 2004. 'Evaluation of CopertIII emission model with on road optical remote sensing measurements.' *Atmospheric Environment* 38, 6631-6641.

Environmental Protection Agency (EPA), 2000. 'Ireland's Environment –Millennium Report'. EPA, Dublin.

Environmental Protection Agency (EPA), 2004. 'Ireland's Environment –the state of the environment'. EPA, Dublin.

Federal Highway Administration (FHA), 2000. 'Microscale and regional modelling and emission models'. United States Department of Traffic- FHA, Washington D.C., USA

Ganguly., R., Budd U., Broderick., B., Misstear., B., 2006. 'Applicability of a screening model at motorway and roundabout sites in Ireland', *Proceedings of 9th World Congress on Environmental Health held on 18-23 June at Trinity College Dublin (TCD), Dublin, Ireland.*

Ganguly., R., Broderick., B., 2006. 'Application of General Finite Line Source Model to Predict Carbon Monoxide concentration adjacent to a motorway in Ireland'. *Proceedings of 2nd International Congress on Computational Mechanics and Simulation held on 8-10 December at Indian Institute of Technology Guwahati, India, 1810- 1816.*

Ganguly., R., Broderick., B., 2006. 'Application of a General Finite Line Source Model for Predicting Hydrocarbon concentration on M50 motorway in Ireland'. *Proceedings of ACME/ISSEC meeting held on 19-20 April at Queens University, Belfast, UK. 111-114.*

Ganguly., R., Broderick., B., 2007. 'Application of a General Finite Line Source Model for predicting Benzene concentration on M50 motorway in Ireland'. *Proceedings of International Conference on Civil Engineering in the New Millennium: Opportunities and*

Challenges (CENeM-2007) held on 11-14 January at Department of Civil Engineering, Bengal Engineering and Science University, Kolkata, India.

Ganguly, R., Broderick, B., 2008. 'Performance Evaluation and Sensitivity Analysis of General Finite Line Source Model for CO concentrations for Motorways in Ireland. A Note.' *Transportation Research Part D*, DOI: 10.1016/j.trd.2008.01.006

Genikhovich, E.L., Ziv, A.D., Iakovleva, E.A., Palmgren, F., Berkowicz, R., 2005. 'Joint analysis of air pollutions in street canyons in St. Petersburg and Copenhagen'. *Atmospheric Environment* 39 (15), 2747-2757.

Gokhale, S., Khare, M., 2004. 'A review of deterministic, stochastic and hybrid vehicular exhaust emission models'. *International Journal of Transport Management* 2, 59-74.

Gokhale, S., Khare, M., 2007. 'Statistical behaviour of carbon monoxide from vehicular exhausts in urban environments'. *Environmental Modelling & Software* 27, 526-535.

Gokhale, S.B., Patil, R.S., 2004. 'Modelling the size separated particulate matter (SSPM₁₀) from vehicular exhausts at traffic intersections in Mumbai'. *Environmental Modelling and Assessment* 98, 23-40.

Goyal, P., Ramakrishna, T.V.B.P.S., 1999. 'A line source model for Delhi'. *Transportation Research Part D* 4 (4), 241-249.

Han, X., Naeher, L.P., 2006. 'A review of traffic related air pollution exposure assessment studies in the developing world'. *Environment International* 32 (1), 106-120.

Harkonen, J., Lahtinen, K., Valkonen, E., Kukkonen, J. 1997. 'An operational model for vehicular pollution from a road network.' *International Journal of Environment and Pollution* 8 (3-6), 436-437

Heeb, N.V., Forss, A.M., Saxer, C.J., Wilhelm, P., 2003. 'Methane, benzene and alkyl benzene cold start emission data of gasoline-driven passenger cars representing the vehicle technology of the last two decades'. *Atmospheric Environment* 37, 5185-5195.

Held, T., Chang, D.P.Y., Niemeier, D.A., 2003. UCD 2001: 'An improved model to simulate pollutant dispersion from roadways'. *Atmospheric Environment* 37 (38), 5325-5336.

Hlavinka, M.W., Korpics, J.J., Bullin, J.A., 1987. 'TEXIN2: a versatile model for predicting CO concentrations near intersections.' *Journal of the Air Pollution Control Association* 37(7), 819-822.

Hosker, R.P., 1985, 'Flow around isolated structures and building clusters: A review'. *ASHRAE Transactions* 91, 1671-1692.

Hussain, M., Lee, B.E., 1980. 'An investigation of wind forces on three-dimensional roughness elements in a simulated atmospheric boundary layer flow: Part II Flow over large arrays of identical roughness elements and the effect of frontal and side aspect ratio variations'. *Report BS 56, Dept. Building Science, University of Sheffield.*

Ionel, I., Sturm, P., Lelea, D., Ungureanu, C., 1999. 'Simulations of the traffic contribution in a Romanian city by means of the CALINE modelling.' *8th Symposium on transport and air pollution, Graz, Austria*.

Ireson, R.G., 1999. 'Intersection Air Quality Modelling'. Project 25-06, National Cooperative Highway Research Programme, Washington D.C., USA.

Jacob, D.J., 1999. 'Introduction to Atmospheric Chemistry'. *Princeton University Press*.

Irwin, J.S., Rosu, M.R., 1988. 'Comments on a draft practise for statistical evaluation of atmospheric dispersion models.' *Proceedings of the 10th Joint Conference on Application of Air Pollution Meteorology with A&WMA, USA*, 6-10.

Jakeman, A.J., Simpson, R.W., Taylor, J.A., 1988. 'Modelling distributions of air pollutant concentrations-III: hybrid modelling deterministic-statistical distributions'. *Atmospheric Environment* 22(1), 163-174.

Jakeman, A.J., Taylor, J.A., 1989. 'Identification, estimation, and simulation of frequency distributions of pollutant concentrations for air quality management'. In: *Cherminisoff (Ed.), Air Pollution Control. Encyclopaedia of Environmental Control Technology*, vol II, 135-138.

Johnson, W.B., Ludwig, F.L., Dabberdt, W.F., Allen, R.J., 1973. 'An urban diffusion simulation model for carbon monoxide.' *Journal of the Air Pollution Control Association* 23, 490-498.

Kiely, G., 1997. 'Environmental Engineering'. *McGraw Hill International (UK) Limited*.

Kono, H., Ito, S., 1990. 'A comparison of concentration estimates by the OMG volume-source dispersion model with three line source dispersion models'. *Atmospheric Environment* 24B, 253-260.

Kouridis, Ntziachristos and Samaras, 2000. COPERT III. 'Computer programme to calculate emissions from road transport'. User's Manual (Version 2.1), EEA, Technical Report No. 50, Copenhagen, 46pp.

Kukkonen, J., Valkonen, E., Walden, J., Koskentalo, T., Aarnio, P., Karppinen, A., Berkowicz, R., Kartastenpaa, R., 2001a. 'A measurement campaign in a street canyon in Helsinki and comparison of results with predictions of OSPM model.' *Atmospheric Environment* 35 (2), 231-243.

Khare, M., Sharma, P., 1999. 'Performance evaluation of general finite line source model for Delhi traffic conditions'. *Transportation Research Part D* 4 (1), 65-70.

Kukkonen, J., Harkonen, J., Karppinen, A., Lusa, K., 2001b. 'Evaluation of CAR-FMI model against measurements near major road.' *Atmospheric Environment* 35 (5), 949-960.

Kukkonen, J., Valkonen, E., Walden, J., Koskentalo, T., Aarnio, P., Karppinen, A., Berkowicz, R., Kartastenpaa, R., 2001. 'A measurement campaign in a street canyon in

Helsinki and comparison of results with predictions of the OSPM model'. *Atmospheric Environment* 35, 231-243.

Lu, H.C., 2002. 'The statistical characters of PM₁₀ concentration in Taiwan area'. *Atmospheric Environment* 36, 491-502.

Luhar, A., Patil, S., 1989. 'A general finite line source model for vehicular pollution prediction'. *Atmospheric Environment* 23, 555-562.

Maffeis, G., 1999. 'Prediction of carbon monoxide acute air pollution episodes: Model formulation and first application in Lombardy'. *Atmospheric Environment* 33, 3859-3872.

Manning, A. J., Nicholson, K.J., Middleton, D.R., Rafferty, S.C., 2000. 'Field study of wind and traffic to test a street canyon pollution model.' *Environmental Monitoring and Assessment* 60, 283-313.

Marmur, A., Mamane, Y., 2003. 'Comparison and evaluation of several mobile-source and line-source models in Israel'. *Transportation Research Part D* 8 (4), 249-265.

Martuzevicius, D., Grinshpun, S.A., Reponen, T., Górný, R.L., Shukla, R., Lockey, J., Hu, S., McDonald, R., Biswas, P., Kliucininkas, L., LeMasters, G., 2004. 'Spatial and temporal variations of PM_{2.5} composition throughout an urban area with high freeway density - the Greater Cincinnati study'. *Atmospheric Environment* 38, 1091-1105

Matzaros, A., 1990. 'Results from a model of road traffic air pollution, featuring junction effects and vehicle operation modes.' *Traffic Engineering and Control* 31 (1), 24-30.

McCrae, I.S., Green, J.M., Hickman, A.J., Hitchcock, G., Parker, T., Ayland, N., 2000. 'Traffic management during high pollution episodes: a review'. TRL Report, UKDETR.

McHugh, C.A., Carruthers, D.J., Edmunds, H.A., 1997. 'ADMS-Urban: an air quality management system for traffic, domestic and industrial pollution.' *International Journal of Environment and Pollution* 8, 666-674.

Mayer, H., 1999. 'Air pollution in cities'. *Atmospheric Environment* 33 (24), 4029-4037.

Mensink, C., Maes, G., 1997. 'Comparative sensitivity study for operational short range atmospheric dispersion models.' *International Journal of Environment and Pollution* 8(3-6), 356-366.

Mensink, C., Colles, A., Janssen, L., Cornelis, J., 2003. 'Integrated air quality modelling for the assessment of air quality in streets against the council directives.' *Atmospheric Environment* 37 (37), 5177-5184.

Meszaros, E., 1981. 'Atmospheric Chemistry – Fundamental Aspects'. *Elsevier Scientific Publishing Company*.

Ministry of Environment (ME) Wellington, New Zealand, 2004. 'Good practice Guide for Atmospheric Dispersion Modelling.' Technical Report prepared by NIWA, AURORA Pacific Limited and Earth Tech Incorporated for the Ministry of Environment, Wellington, New Zealand. www.mfe.govt.nz

Nadarajah, S., Gupta, A.K., 2006. 'Some bivariate gamma distributions'. *Applied Mathematics Letters* 19, 767-774.

Nagendra, S.M.S., Khare, M., 2002. 'Line Source Emission Modelling'. *Atmospheric Environment* 36 (13), 2083-2098.

Nagendra, S., Prakash, M., Monilal, R., Khare, M., 2004. 'Performance evaluation of gaussian based line source models at urban roadways in the Bangalore city'. *Journal of Environmental Engineering and Management* 3(3), 465-475.

Nakamura, Y., Oke, T.R., 1989, 'Wind, Temperature and Stability conditions in an E-W orientated canyon'. *Atmospheric Environment* 22, 2691-2700.

Nelli, J.P., Messina, A.D., Bullin, J.A., 1983. 'Analysis and modelling of air quality at street intersections.' *Journal of the Air Pollution Control Association* 33(8), 760-764.

Noll, K.E., Miller, T.L., Clagget, M., 1978. 'A comparison of three highway line source dispersion models'. *Atmospheric Environment* 12, 1323-1329.

NRA. www.nra.ie

Ntziachristos, L., Samaras, Z., 2000. COPERT III. Computer programme to calculate emissions from road transport. Methodology and emission factors (Version 2.1). EEA, Technical Report No. 49, Copenhagen, 86pp.

Okamoto, S., Ohnishi, H., Yamada, T., Itohiya, T., 1999. 'A database for highway air quality modelling.' *8th Symposium on transport and air pollution, Graz, Austria*. 541-548

O'Donoghue, R.T., 2004. 'Monitoring of Traffic Related Hydrocarbon Concentrations.' *PhD Thesis* submitted to the Department of Civil, Structural and Environmental Engineering at Trinity College Dublin.

Oke, T.R., 1988. 'Street design and urban canopy layer climate'. *Energy Building* 11, 103-113.

Olesen, H.R., 1997a. Presented at the 22 NATO/CCMS International Technical Meeting on Air Pollution Modelling and its Application, France, *cited by* Timmis et al, 2000.

Ott, W. R., 1995. Environmental Statistics and Data Analysis. *Lewis Publishers*.

Petersen, W.B., 1980. 'Users guide for HIWAY-2, highway air pollution model'. 3-17, EPA-600/8-80-018.

Pasquill, F., 1974. Atmospheric Diffusion, second edition. *Ellis Horwood Ltd., Chichester, UK 228pp*.

Peavy, H.S., Rowe, D.R., Tchobanoglous, G., 1985. 'Environmental Engineering' *McGraw Hill Book Company*.

Qin, Y. and Kot, S.C., 1993: 'Dispersion of vehicular emission in street canyons, Guangzhou City, South China'. *Atmospheric Environment* 27B, 283-291

Rao, S.T., Visalli, J.R., 1981. 'On the comparative assessment of the performance of air quality models.' *Journal of the Air pollution Control Association* 31(8), 851-860.

Rao, S.T., Sistla, G., Eskeridge, R.E., Petersen, W.B., 1986. 'Turbulent diffusion behind vehicles: evaluation of roadway models.' *Atmospheric Environment* 20(6), 1095-1103.

Reybolj, D., Sturm, P.J., 1999. 'A GIS based component oriented integrated system for estimation, visualisation and analysis of road traffic air pollution.' 8th *Symposium of Transport and air pollution, Graz, Austria*.

Reynolds, A.W., Broderick, B.M., 2000. 'Development of an emissions inventory model for mobile sources'. *Transportation Research, Part D*, 5, 77-101.

Sharma, P., Khare, M., 2001. 'Modelling of vehicular exhausts- a review'. *Transportation Research Part D*: 6, 179-198.

Shenouda, D.A.S., 1994. 'Modelling air pollution near arterial roads and highways.' *PhD thesis submitted to Department of Civil and Mining Engineering, University of Wollongong, Australia*.

Shenouda, D.A., Schmidt, L.C., 1997. 'Predicting traffic generated carbon monoxide concentrations in Sydney'. *Journal of transportation engineering* 123 (5), 327-336.

Simpson, R.W., Butt, J., Jakeman, A.J., 1984. 'An averaging time model of SO₂ frequency distributions from a single point source'. *Atmospheric Environment* 18 (6), 1115-1123.

Steadman, J.R., and Dore, C.J., (1998). 'An empirical model for quantifying current and future benzene and 1, 3 butadiene concentrations at the roadside'. AEA Report

AEAT.4301 (2). AEA Technology plc.

Stedman, J.R., Goodwin J.W.L., Katie King., Murrells, T.P., Bush, T.J., 2001. 'An empirical model for predicting urban roadside nitrogen dioxide concentrations in the UK.' *Atmospheric Environment* 35, 1451-1463.

Stern, A.C., 1984. 'Fundamentals of air pollution, Vol (1-5)' *Academic Press N.Y.*

Sturm, P.J., Almbauer, R., Sudy, Ch., Pucher, K., 1997. 'Application of computational methods for determination of traffic emissions.' *Journal of the Air and Waste management Association* 47, 1204-1210.

Surman, P.G., Simpson, R.W., Stokoe, J., 1982. 'Application of Larsen's model to Brisbane, Australia'. *Atmospheric Environment* 16 (11), 2609-2614.

Taylor, M.A.P., Anderson, M., 1982. 'Modelling pollution and energy use in urban road networks.' *Proceedings of the ARRB*, 11(6).

Timmis, R., Wilkinson, S., Carruthers, D.J., McHugh, C.A., 2000. 'Recent studies to validate and compare atmospheric dispersion models for regulatory purposes in UK'. *International Journal of Environment and Pollution* 14(1-6), 431-442.

United Kingdom Department of the Environment, Transport and the Regions (UKDETR), 2000. 'Review and Assessment: Selection and use of dispersion models.' www.environment.detr.gov.uk/airq/laqm/tg300/pdf/index.htm

United States Environmental Protection Agency (USEPA), 1999. 'Appendix W to Part 51 Guideline on Air Quality Models.' www.epa.gov/scram001

USEPA 2000. PAMSGRAM. Vol. 18, June 2000. AMTIC PAMS, Office of Air Quality Planning and Standards (www.epa.gov/ttn/amtic/pamsgram.html).

Vardoulakis, S., Gonzalez-Flesca, N., Fisher, B.E.A., 2002a. 'Assessment of traffic-related air pollution in two street canyons in Paris: implications for exposure studies'. *Atmospheric Environment* 36, 1025-1039.

Vardoulakis, S., Fisher B.E.A., Gonzalez-Flesca, N. and Pericleous, K., 2002b. 'Model Sensitivity and uncertainty analysis using roadside air quality measurements.' *Atmospheric Environment* 36, 2121-2134.

Vardoulakis, S., Gonzalez-Flesca, N., Fisher, B.E.A., Pericleous, K., 2005. 'Spatial variability of air pollution in the vicinity of a permanent monitoring station in central Paris'. *Atmospheric Environment* 39, 2725-2736.

Watson, J.G., Chow, J.C., 2001. Ambient air sampling. In: Baron, P.A., Willeke, K. (Eds.), *Aerosol Measurement: Principles, Techniques and Applications*. Wiley-Interscience, New York, pp. 821 (Chapter 27).

WHO/UNEP., 1992. 'Urban air pollution in mega cities of the World.' *World Health Organisation/United Nations Environment Programme*, Blackwell, Oxford.

WHO., 1995. 'Update and revision of the Air Quality Guidelines for Europe'. WHO, Geneva, Switzerland

Wealdon District Council 2000. 'Stage II Air Quality Review and Assessment.'

Available from:
www.wealden.gov.uk/Environment_and_Transport/Air_Quality/air_quality_2.PDF

Wight, G.D., 2000. Fundamentals of Air Sampling. *CRC Press, Inc., Boca Raton, FL*, p. 111.

Wilmott, C.J., 1981. 'On the validation of models'. *Physical Geography* 2, 184-194.

Wilson, P., Laxen, D., 2002. 'A new approach to deriving NO₂ from NO_x for Air Quality Assessments of Roads'

Available from <http://www.uwe.ac.uk/aqm/review/noxno2report.pdf>

Yamartino, R.J., Wiegand, G, 1986, 'Development of simple models for the flow, turbulence and pollutant concentrations within an urban street canyon'. *Atmospheric Environment* 20, 2137-2156.

Zannetti, P., 1990. Air pollution modelling: theories, computational methods and available software. *Computational Mechanics Publications*, Southampton.

Zimmerman, J.R., Thompson, R.S., 1975. 'Users Guide for HIWAY, a highway air pollution model.' EPA-650/4-74-008.

<http://envfor.nic.in/divisions/iass/cia/Annex5.htm>

<http://www.cordis.europa.eu/transport/home.html>