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DEVELOPMENT AND APPLICATION OF AN INTEGRATED AIR QUALITY MODELLING SYSTEM FOR TRAFFIC RELATED POLLUTION IN URBAN AREAS

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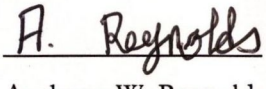
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"Cíallaíonn an t-innealtóireacht úsáid ealaíonta na heolaíochta"

(Engineering is the artful use of Science)

SUMMARY

An Air Quality Modelling System (AQMS) has been developed for metropolitan areas in Europe and applied in Dublin. The primary objective of this AQMS is to incorporate the latest knowledge on traffic and air quality at a high level of spatial and temporal resolution, restricted only by data availability. The AQMS consists of three main modules, namely a traffic module, an emissions rate module and a pollutant dispersion module. These are all integrated with a Geographic Information System (GIS). The accuracy of the AQMS model is established by validating the individual components.

A case study research strategy was followed which generalises the specific case of Dublin. The traffic module employed is SATURN (Simulation and Assignment of Traffic in Urban Road Networks) and SATCHMO (SATURN Travel CHoice MOdel SATURN); the emissions factors employed were derived from the European Union MEET (Methodologies to Estimate Emissions from Transport) project; and the dispersion model is an enhanced version of CALINE4 (CALifornia LINE source model version 4) entitled CALINE4R. The emissions rate module is designed to operate at a level of detail compatible with both the traffic and dispersion modules. It estimates hot-stabilised, start-up and evaporative emissions for ten different pollutants, and two modes of vehicle operation (cruise and creep).

The AQMS is validated at three study sites in Europe, initially in Dublin, and subsequently at Melton Mowbray, UK and Hannover, Germany. One of the major advantages of the AQMS is that, where available, it can employ traffic data from urban traffic control systems and this has been successfully demonstrated in Dublin using traffic data from SCATS (Sydney Co-ordinated Adaptive Traffic System) and in Melton Mowbray using traffic data from SCOOT (Split Cycle Optimisation and Offset Technique).

A bottom-up emissions and fuel consumption inventory is compiled for the greater Dublin area for a base year (1991), and their relative changes in a present year (1996) and two future years (2006 and 2016) are calculated. In addition, a comparison of an emission and fuel consumption inventory compiled using a top-down approach and a combined bottom-up approach for 1996 is performed. The fuel consumption inventory is validated against

retail fuel sales in Dublin. Abatement strategies to reduce total emissions involving the use of transport policies and alternative fuels are evaluated.

A novel method to predict the location of potential hotspots in urban areas and the formation of an air emissions index is developed. The air quality in the vicinity of three heavily trafficked sites in Dublin is estimated. The first is located at the junction with the highest traffic volume, while the second is located at the junction with the greatest congestion. The third hotspot is situated at the location with the greatest combined potential for emissions and subsequent concentrations, this being identified on the basis of the emissions for each link.

The AQMS has the facility to incorporate alternative traffic or pollutant dispersion modules. In addition, new or improved emission factors can be incorporated into the AQMS as they become available. This flexibility is achieved through the modular design, which separates the individual components. As a predictive tool, the AQMS is well balanced in terms of the accuracy of state-of-the-art traffic, emissions and pollutant dispersion models.

It is envisaged that the AQMS will be maintained and managed by the DTO at their offices in Dublin.

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ABBREVIATIONS

A/C	air conditioning
AA:	Automobile Association
AAKT:	annual average kilometres travelled
AC:	alternating current
ADMS-urban:	atmospheric dispersion modelling system - urban
AEI:	air emissions index
AIRPOL4:	air pollution model version 4
ALAPCO:	Association of Local Air Pollution Control Officers
APCA:	Air Pollution Control Association
API:	air pollutant index
AQAT-3:	air quality analysis tools version 3
AQE:	air quality impact
AQI:	air quality index
AQMS:	air quality modelling system
AQS:	air quality standard
AQTAN:	air quality technical analysis notes
AUTOMOD:	automobile model
BÁC:	Bus Átha Cliath
BMC:	background measured concentration
BMW:	Bavarian Motor Works
C_4H_6:	1,3-butadiene
C_6H_6:	benzene
CALINE2:	California line source model version 2
CALINE4:	California line source model version 3
CALINE4:	California line source model version 4
CALINE4R:	California line source model version 4 revised
CAL-MoVEM:	California motor vehicle emission model
CALTRANS:	California Department of Traffic
CAR-FMI:	contaminants in the air from a road - Finnish Meteorological Institute
CCTV:	closed circuit television
CD:	computational dynamics
CDOH:	Colorado Department of Highways

CE-CERT:	College of Engineering - Centre for Environmental Research and Technology
CEF:	composite emission factor
CFCF:	composite fuel consumption factor
CFR:	code of federal regulations
CH_4:	methane
CMEM:	composite modal emissions model
CMP:	cold mileage percentage
CNG:	compressed natural gas
CO:	carbon monoxide
CO_2:	carbon dioxide
CODEMA:	City of Dublin Environmental Management Association
CONCAWE:	The oil companies study group for conservation of clean air and water in Europe
COPERT:	computer program to calculate emissions from road transport
CORINAIR:	core inventory air emissions
COST:	European Co-operation in the field of scientific research;
CPB3:	canyon plume box model version 3
CPF:	catalyst pass function
CRC:	Co-ordinating Research Council
CSO:	Central Statistics Office
CTEM:	combined traffic and emissions rate model
DC:	direct current
DGV:	digitalisierte Graz vanfahren
DMRB:	design manual for roads and bridges
DOE:	Department of the Environment
do-min:	do – minimum traffic scenario in Dublin
do-str:	do – strategy traffic scenario in Dublin
DOT:	Department of Transport
DRIVE:	dedicated road infrastructure for vehicle safety in Europe
DS:	degree of saturation
DTO:	Dublin Transport Office
DTU:	Technical University of Denmark
EC:	European Community
EEA:	European Environment Agency
EEC:	electronic emission control

EECT:	engine/emissions control technology
EF:	emission factor
EFD:	emission factor database
EGF:	element growth factor
EGR:	exhaust gas recirculation
EIA:	environmental impact assessments
EIIP:	emission inventory improvement programme
EL:	element length
EMEP:	European monitoring and evaluation programme
EMFAC:	emission factor model
EMFAC7E:	emission factor model version 7E
EPA:	Environmental Protection Agency
EPAINT:	EPA Intersection model
ESB:	Electricity Supply Board
ESRI:	Environmental System Research Institute
ETC-AE:	European Topic Centre - air emissions
ETC-AQ:	European Topic Centre - air quality
ETEM:	enhanced traffic and emissions model
ETMRN:	European training and mobility research network
EU:	European Union
EUDC:	European urban driving cycle
FB:	fractional bias
FC:	fuel consumption
FCF:	fuel consumption factor
FDOE:	Federal Department of Energy
FDOT:	Federal Department of Traffic
FHWA:	Federal Highway Administration
FHWAINT:	FHWA Intersection model
FID:	flame ionisation detector
FLINT:	Florida intersection model
FLS:	finite line source
FOREMOVE:	forecast of emissions from motor vehicles
FORTRAN:	formula translation
FTP:	Federal test procedure
GC:	gas chromatography
GDA:	greater Dublin area

MicroFacCO:	microscale automobile emission factor model for CO
MIMO:	microscale model
MISKAM:	Mikro Skaliges Klima- und Ausbreitungs model
MOBILE3:	mobile source emission factor model version 3
MOBILE4:	mobile source emission factor model version 4
MOBILE5a:	mobile source emission factor model version 5a
MOBILE6:	mobile source emission factor model version 6
MODEM:	modelling of emissions in urban areas
MODIM:	modelling of imissions
MVEIM:	motor vehicle emissions inventory model
MVERA:	motor vehicle emissions rate algorithms
MVFC:	motor vehicle fuel consumption
N_2O:	nitrous oxide
NATO-CCMS:	North Atlantic Treaty Organisation - committee on the challenges of modern society
NCHRP:	National Cooperative Highway Research Program
NDIR:	nondispersive infrared
NM-HC:	non methane hydrocarbons
NMSE:	normal mean square error
NM-VOC:	non methane - volatile organic compounds
NO:	nitrogen monoxide
NO_2:	nitrogen dioxide
NOTLINE:	Nottingham line source model
NO_x:	nitrogen oxides
NRA:	National Roads Authority
NSCA:	National Society for Clean Air and environmental protection
NWS:	National Weather Service
NYCDEP:	New York City Department of Environmental Protection
NYS-DOT:	New York State - Department of Traffic
O-D:	origin-destination
OECD:	Organisation for Economic Corporation and Development
OSPM:	operational street pollution model
P-2:	percentage of 2
PC:	personal computer
PCM:	powertrain control module
pcu:	passenger car unit

PM:	particulate matter
PM_{10}:	particulate matter less tha 10 microns in diameter
$PM_{2.5}$:	particulate matter less tha 10 microns in diameter
PMFAC:	particulate matter emission factor model
POLLEN:	modele d'inventaire des emissions de pollutants du traffic routier aux niveaux national
PROKAS_B:	Programm zur Berechnung von KFZ-Bedingten Abgaskonzentrationen an Strassen version B
PROKAS_V:	Programm zur Berechnung von KFZ-Bedingten Abgaskonzentrationen an Strassen version V
QBC:	quality bus corridor
QUARG:	Quality of urban air review group
RDMS:	relational database management system
REF:	relative emission factor
RME:	rapeseed methyl ester
ROADFAC:	road factor emission model
RON:	research octane number
RPM:	road pollution monitor
RTWNSW:	Road Traffic Authority New South Wales
RVP:	reid vapour pressure
SATCHMO:	SATURN Travel Choice Model
SATURN:	simulation and assignment of traffic in urban road networks
SAVIAH:	small area variations in air quality and health
SCATS:	Sydney co-ordinated adaptive traffic system
SCF:	speed correction factors
SCOOT:	split cycle optimisation and offset technique
SF:	scale factor
SI:	scale index
SME:	sunflower methyl ester
SO_2:	sulphur dioxide
SP:	specific power
SQL:	structured query language
SR-60:	State Route - 60 in California
SR-90:	State Route - 90 in California
STAPA:	State and Territorial Air Pollution Control Officers Association
TCD:	Trinity College Dublin

TEOM:	tapered element oscillating microbalance
TEXIN3:	Texas intersection model version 3
TRAPOS:	optimisation of modelling methods for traffic pollution in streets
TRB:	Traffic Research Board
TREMOD:	transport and emission-estimation model
TRI:	Transport Research Institute
TRL:	Transport Research Laboratory
TSP:	total suspended particles
TUG:	Technical University - Graz
TÜV:	Technischer Uberwachungs Verein
TW:	two wheeler
TWC:	three way catalyst
UCD:	University College Dublin
UK-DETR:	United Kingdom - Department of the Environment, Transport and the Regions
UK-DOT:	United Kingdom - Department of Transport
UK-NAQS:	United Kingdom - national air quality standard
UN-ECE:	United Nations – economic cooperation for Europe
US-EPA:	United States - Environmental Protection Agency
UV:	ultraviolet
VBA:	visual basic for applications
VDAS:	vehicle data acquisition system
VERL:	Vehicle Emissions Research Laboratory
VHT:	vehicle hours travelled
VIM:	vehicle impact model
VKT:	vehicle kilometres travelled

1. INTRODUCTION

1.1 BACKGROUND

The atmosphere of the world's cities is increasingly affected by air pollution. Hence, deteriorating air quality is fast becoming one of the most pressing and unrelenting environmental problems of our times. Poor air quality in large metropolitan areas is not a new concern; however the nature and type of air pollution has changed over the years. Swift [1729] in a letter to the 'Dublin Weekly Journal' made a reference to the effects of air pollution on the many thousand poor inhabitants of Dublin nearly two hundred years ago. Swift stated that "The constant thick clouds of smoke that hang over Dublin, is so nauscoue, the air so corrupted, that the smell of the smoke is perceptible some miles off, in so much that few, or none, ever escape without some disorder". Swift further noted that the smoke has intoxicated their brains that they are void of all senses. He concluded that, "the chief cause of the bad air about Dublin proceeds from the great quantity of smoke in the coal used here".

In the past, pollutants were emitted primarily from domestic sectors and later from industrial and power generation sectors. The pollutants of concern were smoke, SO_2 and TSP. However, fuel control regulations have been effective in dramatically reducing domestic emissions, while fuel switching, and other measures (e.g. IPC licensing and more efficient boilers) have been effective in reducing industrial emissions. Now, emissions from road traffic are the principal source of air pollutants in all large conurbations throughout the world. The pollutants of concern from mobile sources include NO_2, PM_{10}, $PM_{2.5}$, CO, VOC, C_6H_6 and C_4H_6. A report on Ireland's Environment [EPA, 2000] 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". Traffic also emits greenhouse gases such as CO_2 and CH_4. Ireland's international commitment is to limit greenhouse gas emissions (i.e. carbon dioxide) in the period 2008 - 2012 to thirteen per cent above 1990 levels [EPA, 2000].

Pollutant emissions can have substantial impacts on the local environment, including increased degradation of buildings and health effects. In addition, this impact is usually due to the aggregated effects of several air pollutants. The environmental evaluation of

these impacts (i.e. an air quality analysis) can be achieved using either of two approaches. The more comprehensive would consist of large-scale atmospheric monitoring, carried out at a wide range of sites and maintained for a long duration at each. This approach would involve significant expense, both initial and recurrent. In addition, it is difficult to make future projections or evaluate abatement strategies from historic pollutant concentrations alone as future conditions may change. The second option is to develop either a physical or mathematical model of the problem and conduct a more limited programme of monitoring specifically targeted at providing sufficient results to allow the model to be accurately calibrated and verified. However, as pollutant transport and chemical processes defy accurate emulation by means of physical models, the use of a mathematical air quality model seems most appropriate.

Air quality analysis for mobile sources is complex and normally performed by a combination of computer models [FHWA, 2000]. There are primarily three types of model required to perform an air quality analysis. The first type of analysis represents the process of estimating traffic activity and fleet composition. This process is usually performed with the aid of a traffic model. The second type of analysis estimates emissions produced by traffic fleets. This is normally performed with the aid of an emission rate model, which estimates vehicular emissions in grams per unit time or distance (or both). When emission rates are combined with motor vehicle activity data, the result is a spatial and temporal estimation of emissions. This is commonly known as an emission inventory. The third type of analysis is the estimation of ambient pollutant concentrations in the atmosphere. This analysis is performed using a pollutant dispersion model. The pollutant dispersion model may incorporate photochemistry and deposition modules.

The emissions rate component in the above analysis crucially links the traffic and pollutant dispersion components, and errors therein can have substantial consequences on the final output of an air quality model. While many traffic and dispersion models are relatively well developed and at a mature stage, it is widely acknowledged by the scientific community that emission rate models lag some way behind. Part of the reason for this is that traffic models are straightforward to validate: traffic variables (e.g. flow, queues, and average speed) can be observed without the use of sophisticated equipment, and numerous data sets exist for the validation of pollutant dispersion models. In comparison, emission rate models are extremely expensive to validate. Common methods include remote sensing, on-board instrumentation and tunnel measurements. All methods involve the use of

expensive equipment. Therefore, other methods have to be developed to validate emission rate models.

In addition, there are many fundamental questions regarding current methods for estimating local pollutant concentrations in urban areas. For example, what spatial (e.g. macro-scale and micro-scale) and temporal (e.g. hourly and annual) level of detail is required? What traffic parameters are important? As there are many different types of traffic, emission rate and pollutant dispersion models - what type and complexity of model should be employed?

The lack of compatibility between traffic, emission rate, and pollutant dispersion models is another difficulty inherent in current air quality analysis [Ireson, 1999]. These three types of models have evolved separately over time, with the result that the outputs of one model may not be compatible with the inputs of the next. Indeed many of the models were not developed to provide the type of analysis required of them today. For example, traffic models were originally developed to help size and locate highway and transit facilities in a region. Similarly emission rate models were originally developed to estimate area-wide emissions for input into emissions inventories and not to provide predictions of emission rates of vehicles travelling on individual roadways. Many dispersion models were originally designed for continuous point source emissions over long periods of time (e.g. annual averages). Consequently, these models have to be adapted or redeveloped for urban air quality analysis.

Policy makers need a fully integrated system of models to be able to address local urban air quality problems accurately and efficiently. Only when the traffic, emissions, and dispersion components of an air quality model are linked together properly with a similar level of precision and accuracy, can strategies to mitigate urban air pollution be evaluated effectively.

1.2 OBJECTIVE OF RESEARCH

The primary objective of this project was to develop and implement a scientifically sound and practical methodology to estimate a motor vehicle emission inventory and the resultant local pollutant concentrations in urban areas.

This broad objective includes the following issues:

- Review the literature on the current state-of-the-art in air quality assessment;
- Determine appropriate estimating procedures or models to estimate traffic related air pollution in urban areas;
- Evaluate the current state-of-the-practice in urban air quality modelling;
- Assess the suitability of existing highway and intersection air quality model components (i.e. traffic, emissions rate, and pollutant dispersion);
- Develop an improved integrated model and computer software program for urban air quality assessment;
- Validate this model and its individual components against observed data measurements;
- Formulate a method to compare different pollutant emissions; and
- Develop and apply a methodology to assess potential pollutant hotspots in an urban area.

In addition, it was required to compile emissions and fuel consumption inventories for the entire greater Dublin area.

1.3 RESEARCH PROJECT DOMAIN

Due to the inherent complexity of urban air quality analysis and economic constraints on the project, it was decided to limit this research to the adoption of the most suitable existing traffic and pollutant dispersion models. The traffic model employed in this study was developed by the ITS/WS Atkins and was implemented by the DTO. It is managed and maintained at their offices and the results from it were made available for this study. In addition, an emissions rate model was developed from emissions data measured under a European Union project. The pollutant dispersion model employed was developed by CALTRANS. Deficiencies in the individual components made it necessary to modify and enhance them to make them more compatible with each other.

This integration of individual well-accepted models ensures that the new AQMS will be acceptable for regulatory purposes, including demonstrations of attainment with air quality standards, and EIA analyses. Any new model has to be extensively tested and validated over long periods of time in order to gain acceptability in the scientific community. The cost of developing a new model can be enormous, for example the NCHRP awarded the

Centre for Environmental Research and Technology in California over US$2 million for the development of a state-of-the-art comprehensive modal emissions model [Barth and Norbeck, 1994].

A core concept of this project was to concentrate on developing the three modelling components together. This is fundamental, as the modelling required in each field can be very complex and time consuming. Consequently, there is a danger of becoming too involved in one area, and bringing it beyond what is applicable to the others. Often, researchers in this field have developed either traffic or dispersion models in great detail and consequently paid little attention to the other.

1.4 NOVEL ASPECTS OF RESEARCH

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

1. This project brings together state-of-the-practice and state-of-the-art in air quality modelling (see Chapter 2). Frequently, many research models have proven very difficult, if not impossible, to implement on large urban scales.
2. A MVEIM has been formulated that can use traffic data from both a traffic model and an urban traffic control system (see Chapter 3).
3. Prior to this project there existed no suitable models for estimating emissions rates from Irish vehicles in urban areas (see Chapter 4).
4. MEET emissions data were adapted for use at a local scale (i.e. high spatial resolution) in an urban area (see Chapter 4).
5. The pollutant dispersion model, CALINE4, has been restructured and reprogrammed. The enhanced version, known as CALINE4R, should be thought of as an updated and expanded version of CALINE4 (see Chapter 6).
6. The AQMS is transferrable as it has been applied and validated in three different European urban areas (see Chapter 7).
7. The AQMS can incorporate real-time traffic data from two different urban traffic control systems i.e. SCATS and SCOOT (see Chapter 7).
8. An extensive and comprehensive traffic-related emissions and fuel consumption inventory has been compiled for the entire greater Dublin area (see Chapter 8).
9. As the fuel consumption and emissions factors were derived from the same sources, the emission inventory was indirectly validated at a macroscopic level by

comparing predicted fuel consumption against retail fuel sales data in Dublin (see Chapter 8).

10. As the environmental impacts of emissions are often as a result of a combination of pollutants, indices (AEI and API) were formulated to compare different pollutants for air quality analysis purposes (see Chapter 9).
11. A new method was developed to determine potential air pollution hotspots. While, traditionally, junctions with either the highest traffic volume or the greatest traffic queues were chosen, the new method makes use of a combination of link-by-link emission estimates and an AEI (see Chapter 9).

1.5 LAYOUT OF THESIS

This thesis is divided into ten Chapters and three Appendices:

Chapter one has introduced the problem considered and outlines the objectives of this research project. The project domain is specified. In addition, the novel aspects of the project are identified.

Chapter two reviews the literature related to emission inventories and air quality modelling. This literature review leads to the specification of an 'ideal' but 'realistic' AQMS. The Chapter concludes with the selection of a pollutant dispersion model, an emission rate model and a traffic model for use in this project.

Chapter three describes the development of a motor vehicle emission inventory model. The model consists of four core modules; a traffic module, an EECT module, a MVERA module, and a MVFC module. The model also includes a database of relevant emission factors.

Chapter four reports on the methodology employed during the formulation of the emission factors for the emissions rate model. An approach is developed to estimate queuing emission factors from speed-dependent emission functions. Emissions from conventional fuels are compared qualitatively, as are emissions from the primary alternative fuels.

Chapter five describes the translation of the MVEIM to a functional software program. The MVEIM is developed in Microsoft® Access™ and Microsoft® SQL Server™ along with Microsoft® Excel™, while ArcView® is used for visualisation of the results. The results of a

sensitivity analysis on the MVEIM are presented along with the salient features of the MVEIM.

Chapter six presents the history of the development of the air pollution dispersion model employed. The main components of the model are described along with the associated algorithms employed. However, a literature review revealed a number of deficiencies in the current version of the model. In response, a modified version of the model is developed. These modifications are described in detail.

Chapter seven presents the application of the combined emission inventory and air pollutant dispersion model at different sites in three different European cities. The first is in Dublin, the second in Melton Mowbray and the third is in Hannover. The model was successfully validated at each site by comparing predicted levels of roadside pollution with measured data.

Chapter eight describes the compilation of an emission and fuel consumption inventory for a base year (1991), the present (1996) and two future years (2006 and 2016). Separate emission and fuel consumption inventories are compiled for the Dublin transport strategy (generally known as the do-strategy option) and a do-minimum strategy in both future years. The fuel consumption inventory for 1996 is validated against retail fuel sales data. Finally, the potential impact of alternative fuels is quantitatively evaluated.

Chapter nine presents an overview of ambient air quality in Dublin. Potential 'hotspots' in the city are investigated by applying the model at a selected number of sites. Traditionally, it is believed that these sites occur at junctions with either the highest traffic volume or the greatest congestion. A new approach is developed to identify potential hotspots in urban areas and to compare different pollutants.

Chapter ten summarises the work carried out during the course of this project and the main conclusions drawn from the research. The main scientific contributions of this research to the field of 'air quality modelling' are articulated. In addition, some recommendations for future work are given.

Appendix A contains a list of the scientific communications (journals, conferences and presentations) produced from this research.

The list of organisations and agencies that provided data and reports for this project are listed in *Appendix B*.

Appendix C contains a legend for the process flowcharts and entity diagrams presented in Chapter five.

2. BACKGROUND AND LITERATURE REVIEW

2.1 INTRODUCTION

This background Chapter reviews the key literature related to modelling the air quality impacts of traffic emissions. The compilation of motor vehicle emission inventories is described in detail. A state-of-art review is performed on current available motor vehicle emission inventory models that are potentially applicable in Ireland. The models are classified into three different categories, namely macro-scale, meso-scale and micro-scale. An advanced emissions rate model developed in the USA is described. A general introduction to air quality modelling is given. Following that, the modelling of roadside concentrations is described in detail. Next, the use of geographic information systems in relation to emission inventories and air quality modelling is articulated. One of the objectives of this research was to specify an 'ideal' but 'realistic' AQMS. The specification draws on both state-of-the-art and state-of-the-practice. Based on this specification, a pollutant dispersion model, an emission rate model, and a traffic model are chosen for use in this project.

The Chapter begins with a review of the attributes of an emission inventory including types of emission inventories, uses of emission inventories, preparation of emission inventories and estimation of emission inventory uncertainty is identified.

2.2 DEFINITION OF AN EMISSIONS INVENTORY

An emissions inventory is a database of emission source activities, activity statistics, emission factors, emission measurements and the emission estimates derived from these data [Stapleton, 1996]. Seika [1996] stated that, "the aim of an emission inventory is to provide information on all emission sources within a given area and the amount of pollutants coming from them". The UK-DETR defines an atmospheric emissions inventory as "an organised collection of data relating to the characteristics of processes or activities which release pollutants to the atmosphere across a study area" [UK-DETR, 1998a]. An emission inventory can also be considered as an aggregation of data, each having four separate characteristics [Pulles and Builtjes, 1998]:

- The (chemical and/or physical) identity of the 'pollutant' being emitted;
- The (economic and/or societal) 'activity' that causes the emissions;
- The (geographic/spatial) 'location' of the emission; and
- The 'time' dependence of the emission.

The European Topic Centre on Air Quality defines an atmospheric emissions inventory as "a collection of data presenting an emission of a pollutant (to air) and related parameters" including the following [Van Aalst et al., 1998]:

- Chemical identity - characterises the chemical properties of the pollutant;
- Activity or technology - characterises the cause of the emission and relates it to (anthropogenic or biogenic) activity;
- Location - describes the location on the map;
- Time dependence - describes the temporal resolution of the inventory.

The time resolution of the emissions in principle follows the time resolution of the activity rate.

Simply put, an emissions inventory is a compilation of all sources of air pollution within a given area in a given time frame.

In general, emission inventory data may be grouped according to typology [Cirillo et al., 1996]:

- Point sources - An emission from a single point e.g. a power plant chimney;
- Line sources - An emission along a defined line e.g. road transport, railways, inland navigation, shipping or aviation;
- Area sources - Low intensity emissions from sources (such as building heating systems) which are assumed to be distributed evenly on the basis of administrative areas, e.g. countries, electoral wards, and districts; and
- Grid sources - Background emissions from a multitude of sources, which are combined into regular grids, e.g. the OECD 50 x 50 km or EMEP 150 x 150 km grids covering Ireland.

The grid source type may be viewed as an extension of the area source type. An emissions inventory model for motor vehicles normally consists of line sources and area sources. Emissions from traffic on major roads are modelled as line sources, while evaporative and cold-start emissions may be modelled as area or line sources. Traffic from minor roads can be modelled as area sources also. In the context of emission inventory complexity, Holman [1999] stated that "estimating road transport emissions is the most complex, as emissions come from such a large number of different sources, each with different emission characteristics".

Creelman [1997] differentiates between actual and potential emission inventories. Actual rates of emissions reflect the true mass of pollutants emitted and are usually based on source measurement data (e.g. stack gas monitoring). Potential emissions are estimates of the maximum mass of pollutants emitted in a given time period and are based on projections (e.g. chemical balance equations). Potential maximum emissions are normally used in the prediction of worst-case air quality. As an example, the total emissions of sulphur dioxide from 1kg of fuel can be obtained by combusting the fuel and measuring the emissions (i.e. actual emissions) or by using a chemical mass balance equation and computing the theoretical amount (i.e. potential emissions). This latter method assumes that all sulphur in the fuel is transformed into sulphur dioxide, which may not be the case.

2.2.1 Types of Emissions Inventories

An emissions inventory can be categorised into two primary groups, namely 'bottom-up' and 'top-down' [Costa and Baldasano, 1996], [Gilson et al., 1997], [Janssen et al., 1998], [Ko, 1995], [Kram et al., 2000], [Lindley et al., 1999], [Samaras et al., 1995], [Seika, 1996], [SEIPH, 1995] and [Van Amstel et al., 1999]. One definition of these two types of inventories is given as [Gilson et al., 1997]:

- Bottom-up approach: tends to model emissions at street level, and from it allowing urban-scale inventories by an integration process; and
- Top-down approach: follows the opposite trends, which consist of adopting the algorithm initially developed for countrywide studies to micro-scales.

The bottom-up approach [SEIPH, 1995] seeks first of all to quantify activity in a geographically disaggregated form, and then to apply emission factors. Hence, emissions for each part of the activity are quantified separately and can be aggregated depending

upon need. An example is the collation of road traffic data and fleet composition for all roads over a specified time period in a study area, and the subsequent application of factors for each category of vehicle and mode of operation on each road. Although this approach results in very accurate geographical distributions, it is unsuitable for large study areas because of the great effort involved in compilation [Costa and Baldasano, 1996].

The top-down approach [SEIPH, 1995] provides emission estimates by taking a mean statistic over a large geographical area, for example, the total production of carbon monoxide. A number of surrogate statistics (e.g. traffic density) are then employed to estimate temporal and spatial variations. For example, a total emission for an urban area will require the total vehicle kilometres travelled, which is typically supplied from the NRA or other appropriate data source. The activity statistic is then multiplied by a corresponding emission factor relating to an average vehicle. The advantage of this approach is that it yields an accurate global inventory [Costa and Baldasano, 1996]. Seika [1996] notes that this approach is best used when data is limited.

Samaras et al. [1995] compiled top-down and bottom-up emission inventories for the city of Thessaloniki in Greece. Estimates of activity data and emission factors were carried out independently and were then equated and reconciled to produce estimates with the fewest possible uncertainties. Samaras et al. [1995] identified a number of parameters for comparison, for example, total mileage, emission factors, fuel consumption, and vehicle composition. The exercise displayed that in principle, it was possible to bring in line top-down and bottom-up assessments.

The purpose of an emission inventory, the area covered (geographical extent) and the specific resolution being collected (sources relating to an area, line or specifically to a point) should determine whether a top-down or bottom-up approach should be used [SEIPH, 1995]. Loibl et al. [1993] suggested that the methodology for compiling an urban emissions inventory should be a combination of both approaches. Seika [1996] noted that inventories are usually a mixture of both approaches, with the share of top-down calculated sources increasing with the size of the study domain.

2.2.2 Uses of an Emissions Inventory

There are a number of reasons to compile an emissions inventory. For example, as an aid to the interpretation of ambient air quality measurements, as an input to air quality models,

as an input to policy-making with respect to abatement strategies, to assist in evaluating the effect of existing and proposed policies and, for general public information. Field [1995] noted that an emissions inventory coupled with a pollutant dispersion model are arguably the most important tools available in determining policies to meet air quality targets.

The UK-DETR [1998a] identified five specific reasons to compile a general emissions inventory, which are similar to those distinguished by Ball and Radcliffe [1979]. These apply equally to emission inventories developed for road traffic.

The first reason is to provide an overview of the intensity of emission sources in a study domain and to establish the absolute or relative contribution of different sources. In this case the different sources are the various categories of vehicles. Using GIS, maps can be generated depicting the intensity of emissions across a study domain. Specific 'hot-spots' can be identified and marked for further study, or as an indicator of those areas which may be 'at risk' of exceeding air quality limits.

Secondly, they can help guide the siting of air quality monitoring stations. For example, an emissions inventory with a high temporal and spatial scale will indicate when and where the highest concentration pollution fields at a local level are most likely to be found. Alternatively, it will indicate which territories are the most representative for a regional area air quality monitoring network.

Thirdly, an emissions inventory can help in estimating the cost and extent of any required emission controls. In the case of a MVEIM, these controls could include transport policies, traffic management schemes, and infrastructure changes.

However, an emissions inventory in itself will not provide sufficient information to assess whether a particular domain or receptor will fail to attain air quality objectives, either now or in the future. Therefore, a fourth use for an emissions inventory is as an input to an air quality model to estimate pollutant concentration fields. Such models translate the time and spatial patterns of air emission discharges into time and spatial patterns of the resulting states of the natural environment, described by ambient concentrations according to a variety of weather conditions.

Finally, the emissions inventory along with a pollutant dispersion model can be used to assess trends in air quality. By varying the inputs to the inventory in a way that emulates

future scenarios (such as due to a change in fuel, or emission limits), it is possible to quantify and qualify their impact on air quality.

Buckingham et al. [1997] list the following motivations for the compilation of an emissions inventory:

- Input to discussions with various international bodies;
- Input to decision-making with respect to abatement strategies;
- Assist in assessing the effectiveness of existing policies;
- A guide to the interpretation of air quality measurement data;
- Input to air quality models; and
- General public information.

Creelman [1997] stated that, "emissions are a common denominator in the public's mind for judging environmental impacts, since what is emitted can often be seen while ambient pollution concentrations are more difficult to grasp".

2.2.3 Preparation of an Emissions Inventory

Guidelines exist for the preparation of emission inventories. These guidelines set out techniques and procedures required to estimate emissions from different source groups including motor vehicles. However they tend to be at a nationwide level, rather than for a specific urban area. The currently available guidelines include:

- The CORINAIR methodology [Bouscaren, 1992];
- The 'Preparation and Use of Atmospheric Emission Inventories' by the UK-DETR [UK-DETR, 1998a];
- The 'Procedures for Emission Inventory Preparation' by the EPA [US-EPA, 1992f];
- The 'Review Study on European Urban Emission Inventories' by the ETC-AE [Cirillo et al., 1996];
- The 'Guidelines for National Greenhouse Gas Inventories' by the IPCC [Houghton et al., 1996]; and
- The 'Atmospheric Emission Inventory Guidebook' by the EEA [McInnes, 1996].

The ETC-AE 'Review Study on European Urban Emission Inventories' [Cirillo et al., 1996] does contain some information on the compilation of an emission inventory for urban areas. It suggests a proposed 'information sheet' for urban inventories and proceeds to give an example of this method as applied to Rome, Italy in 1993. The methodology is very generic in nature and the spatial resolution was only 1 x 1 km grid. The resolution is sufficient for background concentrations estimation, but is of no use in predicting localised hot-spots or pollution episodes.

2.2.4 Estimation of Emissions Inventory Uncertainty

Emission inventories are not usually thought of as models, but in fact they are. A model is a representation of reality. In an emission inventory, the model may be as simple as the product of an emission factor and a corresponding activity or, a complex, computer-based model may be used to estimate the emission factor, the activity, or both. Emission inventories are by their nature inexact [Field, 1995]. The method of compilation, quality of the emission factors employed in calculations, source statistics and physical data affect emission inventory uncertainty [Taylor, 1995]. Uncertainties in models can be categorised into three types namely 'Natural', 'Model', and 'Input Data' uncertainties [Isukapalli, 1999].

Natural uncertainty is due to unavoidable unpredictability (randomness). For example, a diurnal temperature cycle can affect certain pollutant emission rates (e.g. volatile organic compounds) and therefore contributes to natural uncertainty. In addition, there is inherent variability in the processes that cause emissions, such as parameters vary with time, over space, or across individuals in a population. For example driver behaviour (gentle or aggressive) affects emissions.

Models are necessarily simplified representations of phenomena being studied. The primary types of model uncertainty are [Isukapalli, 1999]:

- Model Structure: uncertainty arises when there are alternative sets of technical or scientific assumptions;
- Model Detail: uncertainty arises due to simplifications in conceptual and mathematical formulation for purposes of tractability;
- Extrapolation: models that are calibrated and validated for one portion of input space, but they may be completely unsuitable for making estimations in other regions of the parameter space;

- Model Resolution: selection of spatial and temporal resolution and/or averaging frequently involves uncertainty in model application; and
- Model Boundaries: a model may have limited boundaries in terms of time, space, and number of chemical species.

Uncertainties in input data come from a large variety of sources. For example, measurement errors, which can involve (a) random errors in analytic devices (e.g. the imprecision instruments to measure emissions), (b) systematic biases that occur due to imprecise calibration, or (c) inaccuracies in the assumptions used to infer the actual quantity of interest from the observed readings of a surrogate or proxy variable. Other substantial sources of error include the use of input data that is out-of-date (e.g. employing emission factors for a non-catalyst car to represent a modern car) or estimated/measured data from a small sample (e.g. assuming emission factors derived from cars is representative of all vehicles). Indeed, Singer [1998] states that the "current travel-based inventory models use emission factors measured from potentially biased vehicle samples". Further uncertainty in model application arises from uncertainties associated with measurement data employed in model calibration.

Uncertainty associated with model formulation and application can also be classified as 'reducible' and 'irreducible' [Isukapalli, 1999]. Natural uncertainty is inherent or irreducible, while input data and model uncertainty contain both reducible and irreducible components.

The US-EPA, STAPA and ALAPCO published guidelines for evaluating emission inventory uncertainty as part of the emission inventory improvement program [EEIP, 1996]. Various approaches for estimating uncertainty in the context of an emission inventory are presented by EEIP [1996]. The primary findings of this study by EEIP are summarized in Table 2.1. They are categorised as being qualitative, semi-quantitative, or quantitative. While it was outside the scope of this project to estimate emission inventory uncertainty, it is important to recognise that it does exist. For example, Huson [1985] notes that the uncertainty inherent in the output from mathematical models frequently can cause controversy.

Roe and Reisman [1997] note that these broad categories (i.e. qualitative, semi-quantitative, or quantitative) should not be considered hard and fast. For example, the Monte Carlo simulation method, which is included as a direct simulation method may be semi-

quantitative, if the emission parameter distributions are estimated using expert opinion rather than measured data. In addition, the propagation of errors method could be considered quantitative, if the emission parameter statistics are developed from actual data.

Table 2.1: Summary of common methods employed to estimate emission inventory uncertainty [source: derived from EEIP, 1996]

Method	Reference	Description
Qualitative Methods		
Qualitative Discussion	Steiner et al., 1994	Sources of uncertainty are catalogued and discussed; direction of bias and relative degree of imprecision are given, if known.
Subjective Data Quality Ratings	Saeger, 1994 US-EPA, 1995c;	Subjective rankings based on professional judgment and expert opinion are assigned to each emission factor or associated parameter
Semi-quantitative methods		
Data Attribute Rating System	Beck et al., 1994; US-EPA, 1995c;	Numerical values representing relative uncertainty are assigned to each emission factor or variable through objective methods.
Expert Estimation Method	Horie & Shorpe, 1989; Horie, 1988; Linstene & Turoff, 1975; SCAQMD, 1982;	Emission distribution parameters (e.g. mean, standard deviation, and distribution type) are estimated by experts. Simple graphical and analytical techniques can then be used to estimate confidence limits from the distributional data.
Propagation of errors method	Balentine et al., 1994; Benkovitz & Oden, 1989; Benkovitz, 1985; Environment Canada, 1994; Managat et al., 1984;	Emission parameter averages and standard deviations are obtained from measurements or estimated using expert judgement. The error (f) in the final result (F) is derived from the error in each measurement or number used to get that result. The error in a result, F±f, for F = f(x,y,...) is found from: $f = (dF/dx)\, e_x + (dF/dy)\, e_y + ...$ where dF/dx is the partial derivative of F with respect to x, e_x is the uncertainty in x, etc.
Quantitative Methods		
Direct Simulation Method	Efron & Tibshirani, 1991; Freeman et al., 1986; Gatz & Smith, 1995a; 1995b; Iman & Helton, 1988a, 1998b; Oden & Benkovitz,1990;	Monte Carlo simulation and other numerical methods are used to estimate directly the central value and confidence intervals of individual emission estimates.
Direct or Indirect Measurement (validation method)	Claiborn et al., 1995; Fujita et al., 1992; Mitchell et al., 1995; Peer et al., 1992; Pierson et al., 1990; Spellicy et al., 1992;	Direct (stack sampling) or indirect (tracer studies) field measurements of emissions are used to compute emissions and uncertainty directly. The measurements also provide data for validating emission rate models
Receptor Modeling method (source apportionment method)	Chow et al., 1992; Lowenthal et al., 1992; Scheff et al., 1995; Watson et al., 1984;	Can be used to provide a measure of the relative contribution of each source type but not absolute emission estimates. Works best for non-reactive pollutants for which a unique fingerprint exists for all source categories
Inverse Air Quality Modeling Method	Chang et al., 1993; 1995; Hartley & Prinn, 1993; Mulholland & Seinfeld, 1995;	Air quality simulation models are used in an inverse, iterative approach to estimate the emissions required to produce observed concentrations.

2.3 MOBILE SOURCE EMISSIONS INVENTORY

The most common modelling approach employed to compile a mobile source emission inventory is based on two processing steps [Bailey, 1995], [Joumard, 1998], [Meyer, 1997], [Holman, 1999], [André, 1995], [Creelman, 1997], [Sawyer et al., 2000]:

1. Determining a set of emission factors which specifies the rate at which emissions are generated (exhaust and evaporative emissions); and
2. Determining an estimate of vehicle activity as a function of vehicle class, time of day, location, speed, density, etc.

The emissions inventory is computed from the product of the results of these two steps. From this process, a temporally and spatially resolved emission inventory can be obtained. In reality, however, the compilation of a motor vehicle emissions inventory is a much more complex process.

2.3.1 VEHICLE ACTIVITY ESTIMATION

Vehicle activity data is usually obtained from either traffic surveys or traffic models. Data from traffic surveys are more desirable, as they provide information on actual traffic patterns on actual roadways. However, such surveys have the major limitation that they only supply data pertaining to particular inspection times and locations, rather than a complete study area and they are often out of date. In comparison, a traffic model represents a software simulation of the physical road network and traffic environment contained therein [Warner, 1985]. The current generation of these models can be very detailed and simulate entire urban domains [Algers et al., 1997]. However, it is recognised that even the most complex traffic models still do not contain all the information needed for the compilation of a complete inventory of emissions of pollutants to the atmosphere. It is clear that traffic and travel surveys will continue to be one of the most significant methods of obtaining critical information needed for traffic planning and decision making in the new millennium [Griffiths et al., 2000]. In addition they are the primary source of input data for many traffic models.

The major disadvantage of the above methods is that they use passive traffic data (derived from either traffic models or traffic surveys). The UK-DETR [1998a] discuss in detail the major disadvantages of employing data from either traffic models or sample counts/surveys in emissions inventory calculations. Chapin [1993] suggests that traffic

volumes, both overall and on local arterials, may be underestimated by as much as 10 to 20%. This in turn, may result in underestimating emissions by as much as 50% [Eisele et al., 1996]. Any error in traffic flow rate will cause by itself a proportional error in emissions calculation, but if vehicle speeds are derived from such a flow rate, the error in emissions could increase dramatically due to the speed effect on pollutants [Negrenti, 1998]. Therefore, correct traffic flow is crucial for confidence in any emission prediction model. In addition, mobile source emissions inventories are often out of date by the time they are compiled. One approach to overcoming these disadvantages is to exploit the data readily available in many urban traffic control systems. Data from traffic control systems can be obtained in real-time but are again limited to the location of counters. However, real-time methods cannot be used to evaluate the impacts of proposed transport policies, traffic management schemes or abatement strategies such as the use of alternative fuels, but they can provide a base case for evaluation. Therefore an integrated traffic and emissions rate model is required for future simulations.

2.3.2 Factors Influencing Vehicular Emissions

The types of vehicle activities, that produce emissions, and the corresponding emissions produced are given in Table 2.2 [Guensler, 1993]. These elevated emissions result from engine conditions that give rise to incomplete combustion, and from catalyst temperatures that are too low for efficient control of exhaust gas emissions [Pozniak, 1980], [Heywood, 1988], [Jacobs et al., 1990], [Stone et al., 1990], [Joy, 1992], [Guensler, 1993].

Table 2.2: Emission producing vehicle activities and emissions produced [source: Guensler, 1993]

Emission Producing Vehicle Activity	Type of Emission Produced
Vehicle Kilometers Traveled	Running Exhaust Emissions Running Evaporative Emissions
Cold Engine Starts	Elevated Running Exhaust Emissions
Warm or Engine Starts	Elevated Running Exhaust Emissions
Engine Hot Soaks	Evaporative Emissions
Engine Idling	Running Exhaust Emissions Running Evaporative Emissions
Exposure to Diurnal Temperature Sweep	Evaporative Emissions
Vehicle Refueling	Evaporative Emissions
Modal Behavior that causes enrichment / enleanment (e.g. high power demand, heavy engine loads or engine motoring)	Elevated Running Exhaust Emissions

A literature review revealed many factors that affect the rate of emissions and fuel consumption [Arekani et al., 1992], [Bailey et al., 1990], [Barth et al., 1996], [Darnton, 1997], [Faiz et al., 1996], [Ferreira, 1983], [Guensler, 1993], [Heseltine and Nelson, 1995],

[Hughes, 1992], [OMTC, 1982], [Rogers, 1984], [Seshardi and Harrisson, 1993], [Singh, 1997], [Stead, 1999]. These factors can be broadly divided into four types: (a) vehicle parameters, (b) vehicle operating environment, (c) vehicle operating conditions and (d) fuel parameters. The primary components in each of these categories are given in Table 2.3.

Table 2.3: Factors that influence vehicle fuel consumption and emissions

Vehicle Parameters	Vehicle Operating Environment	Vehicle Operating Conditions	Fuel Parameters
Vehicle mass; Engine size; Engine type; Vehicle power; Fuel system; Catalyst type; Transmission type; Tyre type & size; Tyre pressure; Wheel alignment; Vehicle shape; Oil viscosity; Vehicle age; Inspection & Maintenance; Emission controls.	Roadway gradient; Ambient temperature; Altitude; Humidity; Diurnal temperature sweep; Pavement type (e.g. cement or tarmac); Surface conditions (e.g. wet or dry).	Driving behavior (e.g. gentle or aggressive); Throttle position; Manifold pressure; Cold/hot start mode; Average speed; Acceleration & speed variation; Modal activities; Trip length; Trips per day; Load (e.g. A/C, payload or towing); Engine temperature; Air/fuel ratio.	Fuel type; Oxygen content; Fuel volatility; Sulphur content; Benzene content; Olefin & Aromatic content; Lead & metals content.

It is acknowledged by the scientific community that all these factors contribute to vehicle emissions, and from a research model perspective, it is important to be able to include all these factors. However, it must be remembered that although there are a substantial number of influencing factors, not all have significant effects on fuel consumption or emission rates. Current emission rate models appear to account for some but not all of the factors listed in Table 2.3. From an applications perspective, it is not practical to include all factors. Washington [1998] stated that the "modelling efforts need to focus primarily on quantifying first order effects". Therefore, a number of surrogate parameters should be utilised, with the final selection depending on the data that is relatively easy to obtain or estimate for a regional fleet of vehicles. An example of a surrogate parameter is the use of an average operating speed to represent acceleration, deceleration, and cruise. Emission rate models based on modal emission rate measurements indicate that, even in small-scale applications, average speed is the most influential factor with speed variation being less important [Hansen et al., 1995], [Joumard et al., 1995a], [Sturm et al., 1996].

2.3.3 Mechanics of Exhaust Emissions

The power to move a vehicle comes from combustion of fuel in its engine. Vehicle fuels are generally mixtures of hydrocarbons (i.e. compounds that contain hydrogen and carbon atoms) and are denoted by the generic formula $C_{\alpha}H_{\beta}$. Combustion can be viewed as the

burning or rapid oxidation of a fuel. The combustion of $C_\alpha H_\beta$ is complete if all the carbon in the fuel is converted to carbon dioxide, all the hydrogen is converted to water, and nitrogen in the air remains unaffected. The minimum amount of air required to accomplish this task is known as theoretical air (denoted as $\lambda=1$) and can be calculated from the stoichiometry of the chemical equation. When the air stream exceeds the theoretical amount required ($\lambda>1$), unused oxygen appears in the combustion products. When the amount of air is less than the theoretical amount ($\lambda<1$), the combustion is incomplete. The chemical reaction for complete combustion of a hydrocarbon fuel and air (assuming air consists of nitrogen and oxygen only) is:

$$C_\alpha H_\beta + \lambda\left[\alpha+\frac{\beta}{4}\right](O_2+3.76N_2) \rightarrow \alpha CO_2 + 3.76\lambda\left[\alpha+\frac{\beta}{4}\right]N_2 + (\lambda-1)\left[\alpha+\frac{\beta}{4}\right]O_2 + \frac{\beta}{4}H_2O \qquad 2.1$$

In reality, the combustion process is not ideal and automotive engines emit several types of pollutants. In incomplete combustion, the products contain carbon monoxide, carbon, particulate matter and unburned hydrocarbons as well as carbon dioxide, oxides of nitrogen and water vapour. The quantity $\lambda\left[\alpha+\beta/4\right]$ represents the air-to-fuel ratio in the above chemical reaction. Low values of $\lambda\left[\alpha+\beta/4\right]$ produce rich fuel mixtures (enrichment) while high values of $\lambda\left[\alpha+\beta/4\right]$ produce lean fuel mixtures (enleanment) and misfire may occur. Vehicle high power demand activity (e.g. hard accelerations, heavy loads, and steep roadway gradients) creates periods of enrichment. In contrast, high vehicle speeds coupled with low acceleration rates create enleanment periods. Enleanment also occurs with sharp deceleration or rapid load reduction events, and sometimes during long deceleration.

Under enrichment conditions, significantly elevated quantities of carbon monoxide and hydrocarbons due to incomplete combustion are produced. It is worth noting that enrichment occurs by design, as vehicle manufacturers use enrichment to provide for high power demand episodes.

Under enleanment conditions, carbon monoxide production decreases due to more complete combustion, while hydrocarbon emissions increase slightly. Recent research [An et al., 1998] has shown that rapid load reduction events can cause extremely high short-

duration emissions of hydrocarbons, while long deceleration events are mainly associated with longer-lasting hydrocarbon puffs.

The most important factor affecting the formation of nitrogen monoxide is the flame temperature, which is theoretically at a maximum at stoichiometric conditions and will decrease during both enrichment and enleanment. The rate of formation of nitrogen monoxide is exponentially proportional to flame temperature. In addition, nitrogen monoxide formation decreases linearly with increasing residence time of the fluid in the combustor. However, increasing residence time also has the desirable effect of reducing carbon monoxide and hydrocarbon emissions.

2.3.4 START-UP VEHICLE EMISSIONS

The primary sources of emissions from motor vehicles are the exhaust gases and hydrocarbons/VOCs produced by evaporation of the fuel [Hickman et al., 1998]. When an engine is started below its normal operating temperature, it uses fuel inefficiently. Consequently, the quantities of pollutants emitted are greater than when it is running under hot stabilised conditions. In addition, vehicles with a catalyst require a certain period of time before the catalyst can operate efficiently [Farrauto and Heck, 1999]. Hence, a vehicle starting with a cold engine has considerably higher emissions than one with an engine at normal operating temperature.

When the engine is cold, the commanded (by a choke in old vehicles, and an automatic system in modern vehicles) air-fuel mixture is rich in fuel compared to the ideal stiochiometric conditions, and there is not enough oxygen in the air-fuel mixture to completely combust the fuel. This increased fuel is commanded to reduce the tendency of the engine to stall when it is cold and to compensate for poor mixing and fuel conditions in the intake manifold. The incomplete combustion of the fuel results in elevated emissions of carbon monoxide and hydrocarbons, which are too high to be completely handled by the catalytic converter. As the engine warms up, combustion efficiency increases and emission levels decrease.

The catalytic converter will not start working properly until it reaches a 'light-off' temperature of approximately 300°C. Catalyst temperature rise is a function of initial catalyst temperature, exhaust gas temperature, exhaust gas volume flow rate, and emission

concentrations. Guang Zhu [1999] found that it generally takes 6 km for the catalyst to be fully active in summer conditions, and longer in winter.

In modern vehicles, onboard computer systems, control the air-fuel ratio, and hence the elevated emissions are a direct function of the computer control system, which varies from vehicle to vehicle. The vehicles operate in either open-loop or closed-loop mode. In closed-loop operation, the emission control system monitors the oxygen concentration in the exhaust gas. Incomplete combustion is indicated by low oxygen concentration and consequently the on-board computer adjusts the air-to-fuel ratio and other combustion parameters to correct for this scenario. During the first few minutes of operation or when the engine power demand deviates rapidly, a vehicle operates in open-loop control. Under open-loop control, incomplete combustion can occur and consequently elevated emissions are produced.

Thus when many vehicles in a fleet take frequent short trips, the start emissions can account for a significant fraction of the total emissions. The magnitude of these elevated emissions is a function of commanded air-fuel ratios, catalyst temperature, and engine temperature.

2.3.5 High Emitters

A small percentage of vehicles emit a disproportionate percentage of pollutant emissions, especially for carbon monoxide and hydrocarbons [Wolf et al., 1998]. These so-called 'high emitters' or 'super emitters' exhibit higher emissions rates under all operating conditions than 'normal emitters'. The emissions of normal- and high-emitting vehicles can differ by one or more orders of magnitude. For example, high gaseous emitter vehicles have been found to display approximately 5-10 times the particulate emission rates of normal emitters [Durbin et al., 1999]. Studies using 'remote-sensing' have shown that less than 10% of the road vehicles can be responsible for up to 50% of emissions [Bishop and Stedman, 1996]. Faiz et al. [1996] using remote sensing studies also argues that 10% of vehicles are responsible for 50% of the emissions. Another study found that the passenger cars with the highest 10% of carbon monoxide emissions generated approximately 58% of the total carbon monoxide emitted from all cars, while the 10% highest hydrocarbon-emitting cars generated 65% of the total hydrocarbons emitted from cars [Stephens, 1994]. In Michigan, the highest emitting 5% of passenger cars were seen to generate 45% of all carbon monoxide from cars, and the highest emitting 5% of passenger cars in California generated

38% of all carbon monoxide emitted from cars [Stephens et al., 1997]. Experiments at Los Alamos National Laboratory in the USA found that as little as 10% of the traffic fleet could produce over 50% of total emissions [Williams et al., 1997]. These findings have been confirmed by another laboratory-based study [An et al., 1995]. In the UK, Revitt et al. [1999] found that 31% of vehicles produced 76% of the total hydrocarbon emissions. A study in Australia found that up to 80% of emissions are caused by only 20% of vehicles [Reid, 1997]. Pierson et al. [1999] found that 10% of vehicles produced nearly 50% of total hydrocarbon emissions. Revitt [1985] noted that researchers at the University of Middlesex found that 12% of vehicles contributed up to 50% of the total fleet emissions in the UK.

A remote-sensing study in Colorado [Zhang et al., 1993] found that the fraction of high emission polluters increases with vehicle age. For example, studies [Sjodin and Lenner, 1995] indicate that a yearly deterioration rate for catalyst cars of 30% for carbon monoxide and 20% for hydrocarbons. New vehicle emissions tests in Ireland are targeting this problem. Even though these carbon monoxide emission tests comprise a two-speed idle test, studies [Walsh et al., 1996] have shown that high-emitter vehicles in an idle test are also high-emitters on-road. Wolf et al. [1998] stated that vehicles with poor start emissions characteristics should not be categorised with vehicles that have poor hot-stabilized emission characteristics.

2.3.6 Determination of Source Strength

As there exist many base emission factors, and considering the fact that none were measured from Irish motor vehicles (with the exception of a very limited amount of data on alternative fuels), an evaluation of the available factors was required. Data from over one hundred published reports were collated. However, it became obvious that some data was not useful.

For example, emission factors measured a decade ago are, in general, much higher than those from recent tests [Chiquetto, 1995a]. Today's vehicles produce less total emissions than they did twenty-five years ago [Green and DeCicco, 2000], [UK-DETR, 1997]. The primary reasons for this are tighter emission standards and technological improvements (e.g. increase in efficiency and better emission control equipment such as three-way catalytic converters, carbon canisters and particulate traps) of new vehicles. The three-way catalytic converter reduces emissions of nitrogen oxides, hydrocarbons and carbon

monoxide. The carbon canister uses activated carbon to capture evaporative emissions, while the particulate trap captures particulates.

Figure 2.1 displays the vehicle emission control history for carbon monoxide emitted by passenger cars, assuming that the first legislation in 1970 (i.e. 70/220/EC) [Murley, 1999] is equal to one hundred percent. As can be seen from Figure 2.1 each emission control limit was enforced for a number of years prior to a stricter limit being introduced. Similar trends exist for other pollutants such as particulate matter and nitrogen oxides. However, legislation was not introduced for other pollutants until later. For example, emission legislation for nitrogen dioxide and particulate matter was first introduced in 1977 (i.e. 77/102/EC) [Murley, 1999]

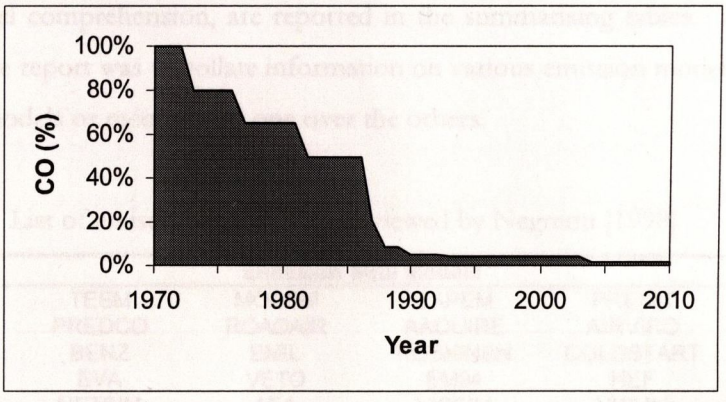


Figure 2.1: Carbon monoxide exhaust emission control history for cars

Other data was of poor quality. For example, background concentrations were not measured during the tests. Guensler [1993] has documented a number of problems in emission factor data collection efforts:

1. Only one or a very limited number of vehicles was tested.
2. The driving cycles employed were not representative of actual road activity;
3. The response time of measuring equipment was not fast enough;
4. Background ambient air concentrations were not measured;
5. Exhaust gas flow-rates exceeded constant volume sampling pump capacity; and
6. Driving cycle speed traces were retained instead of actual speed traces.

In addition, there is generally a lack of quality assurance supplied with the data and consequently it is difficult to estimate the accuracy of the data.

Information on the state-of-the-art of vehicle emission modeling software was collated as part of the COST-319 action – MEET [Negrenti, 1998]. A number of the emission models reviewed by Negrenti [1998] have been made readily available and are easy to use because they are combined with a user-friendly GUI. In contrast, experts can only operate other models such as TREMOD. Finally, some models are not available to the general public. Data on thirty-nine emission models currently used in Europe was collated [Negrenti, 1998]. The models were compared under a range of headings including spatial and temporal scale, traffic input, pollutants, fleet description, vehicle kinematics, and experimental data sources. Table 2.4 presents the reviewed emission models. However, Negrenti concluded that the most relevant items to be looked at for the purpose of a model classification are the spatial and temporal scales and the traffic fleet composition. These pieces of information, together with many others considered relevant for an adequate model comprehension, are reported in the summarising tables. As the primary objective of the report was to collate information on various emission models, Negrenti did not rank the models or recommend one over the others.

Table 2.4: List of emission rate models reviewed by Negrenti [1998]

Emission Rate Models			
TEEM	MODEM	TAPEM	PREMIT
PREDCO	ROADAIR	AAQUIRE	AIRVIRO
BENZ	EMIL	KOSKINEN	COLDSTART
EVA	VETO	EM94	HEF
NETSIM	AEA	VISSIM	VISUM
NEMIS	EMISMOB	LIISA	CAREMIS
TEE	ASHDOWN	DGV	KEMIS
SCRAP	TEE-TURBAN	VERSIT	ROADFAC
VEMI	MADI-EM	EMOD	COPERT
TEDMAN	TREMOD	CITAIR	--

Shearn et al. [1997] performed a literature review on twenty-two existing vehicle emission models (see Table 2.5) to ascertain which models might be suitable for integration with SCOOT [Hunt et al., 1981]. SCOOT is an urban traffic control system developed in the UK.

The models were compared under such headings as average speed, speed/acceleration changes, other vehicle kinematics, other input parameters, pollutants estimated, and country of origin. Shearn et al. [1997] stated that the most relevant items to be looked at (for the purpose of integrating with SCOOT) are the input data required. Shearn et al. concluded that none of the models reviewed were suitable for use with SCOOT because of the mismatch between the type of traffic data produced by SCOOT and that required by the emissions rate models.

Table 2.5: List of emission rate models reviewed by Shearn et al. [1997]

Emission Rate Models			
AAQUIRE	EVA	NEMIS	VERSIT
AIRVIRO	HEB	PREMIT	VETO
ASHDOWN	KOSKINEN	ROADFAC	WSL (AEA)
BENZ	LINZ MODEL	TAPEM	COPERT
DGV	MADI-EM	TEE	--
EM94	MODEM	TRAF-NETSIM	--

Namdeo [1998] performed a review of vehicle emission rate models that could be used in the UK. The models reviewed include, MOBILE6; EMFAC; DMRB; LRC emissions database; TRL emission factors; CORINAIR; MEET; and ROADFAC. The US modelling software (MOBILE6 and EMFAC) cannot be applied in Ireland, as the vehicles are very different to those in the USA. The other models are only semi-independent of each other as they share emission data.

Cloke et al. [1997] reviewed several emission rate models that have been employed, or could be useful, for predicting vehicle emissions in the UK. The models are categorised into three types namely, emission factor models, average speed models and modal models. The models reviewed include, DMRB, COPERT, MODEM, HBEFA, and DGV. The study noted that many of the models (e.g. DMRB and MODEM) are limited to the estimation of emissions from hot stabilised engines and the models that account for start-up and evaporative emissions do so in a very simple manner using empirical relationships.

2.3.7 Major Sources of Error

The compilation of an emission inventory is often associated with a high degree of error. This is especially true with a multitude of individual emission sources and continuously varying vehicle and engine-operating modes [Samaras and Zachariadis, 1998]. In principle, errors in emission inventory models may be divided into two categories, random and systematic. Random errors are caused by:

- Inaccuracy in the measurement devices and techniques employed e.g. not properly calibrated, and/or not sensitive enough;
- Inherent variability in the emission behaviour of different vehicle models e.g. models predict different emissions levels for the same class of vehicle;

- Lack of sufficient number of representative measurements e.g. assuming one vehicle represents an entire fleet; and
- Erroneous data with regard to vehicle usage e.g. errors in vehicle kilometres travelled.

Systematic errors may be further divided into two types, errors concerning emission factors and errors concerning traffic data and vehicle composition. Errors in emission factors include employing driving cycles that are considerably different from real driving conditions, and a lack of sufficient measurements.

Guensler [1993] listed five main sources of error in emission inventory models. These are:

1. Ignoring a number of important vehicle emission-producing activities e.g. start-up and evaporative emissions;
2. Drawing inappropriate statistical inferences based upon collected data e.g. assuming passenger cars represent an entire fleet;
3. Under-representing the contribution to average emission rates of high-emitting vehicles;
4. Failing to collect data from a representative sample fleet e.g. only measuring emissions from a small number of vehicles; and
5. Linking already uncertain emission rate estimates with uncertain vehicle activity estimates.

Lindley and Longhurst [1998] emphasise that there is a potential for error at every stage of the emission inventory estimation process, from the initial input data representing the polluting activity, through to the additional assumptions about those activities and finally with the use of emission factors to represent the activity as an emission

2.3.8 Comparative Studies of Emission Rate Models

Sturm et al. [1996; 1997] distinguishes between three different approaches to compiling emission inventories based on input data and area of application. These consist of (a) emission computation methods based on real driving behaviour (modal modelling), (b) methods based on road stretch analysis, and (c) mileage-related emission balances. The first method is used to compile emission inventories on a micro-scale level (e.g. a specific junction or road), and is used to calculate emission factors [Hassel et al., 1995]. The

second method is used to compile inventories on a regional level (e.g. an urban area), and is normally based on average driving speed. This method may give rise to inaccuracies because it does not account for accelerations and decelerations. The third method is used to compile inventories on a national or global level. This method is normally based on vehicle kilometres travelled per annum, and the emission factors employed are not speed dependent, i.e. the same velocity is assumed for different types of roads in a study area (for example COPERT classifies roads as urban, rural or motorway). Sturm et al. [1996; 1997] found that the total emissions inventory compiled by each method varied substantially.

The amount of detail required by a method depends on the application. As emission inventories are only as accurate as the original data employed to compile them, it is not possible to compile an inventory with a degree of accuracy higher than that of the original input data. Accordingly, the quality of the input data with respect to both the applicability of emission factors used, and the level of detail employed to describe the traffic network, has a significant impact on emission estimates. For example, estimated emissions of nitrogen oxides and hydrocarbons were reduced by 35% and 28% respectively when up-to-date emission factors were employed [Sturm et al., 1996].

Zachariadis [1995] compared the results of two macroscale models, namely COPERT [Eggleston et al. 1993] and KEMIS [Hausberger et al., 1994] and one micro-scale model, namely the DGV [Sturm et al., 1994], used for the estimation of road traffic emissions. COPERT is a calculation methodology employing mean speed-dependent emission factors. KEMIS employs passenger car emission factors developed by TUV Rheinland and heavy-duty vehicle and motorcycle emission factors developed at the TU-Graz. The DGV model employs average instantaneous emission maps from twelve vehicles to calculate average emissions for all passenger cars. The result of using the three different models for emission calculations was illustrated with an example for the city of Thessaloniki in Greece [Zachariadis and Samaras, 1996; 1997]. The main conclusion to be drawn from the study is that average speed-dependent emission factors are of adequate precision when compiling aggregated area source type inventories. The importance of high emission incidents such as hard accelerations may have a negligible effect if they are included in an emissions inventory of mean hourly emissions in a large area. This is due to the fact that accelaeration and deceleration are taken into account implicitly in speed-dependent emission factors. However, the study showed that the effect of gradient, altitude and cold-start on vehicle emissions is important. If the effects of specific roadway topography on a finer detail (e.g. street junctions) have to be analysed, then accelerations, decelerations and

queuing need to be taken into account. The study is critical of all three models (i.e. COPERT, KEMIS and DGV) because they do not take sufficient account of cold-start emissions.

Winther [1998] examined motor vehicle emission factors from three emission rate models, namely COPERT II [Ahlvik et al., 1997], HBEFA [INFRAS, 1995], and the DTU model [Winther, 1997]. Emissions factors for carbon monoxide, volatile organic compounds and nitrogen oxides were assessed. The study concentrated on petrol UN-ECE 15.04 and catalyst cars with engine capacities ranging from 1.4 to 2 litres. For passenger cars equipped with a catalyst, the emission factors in COPERT II suggest a reduction in the efficiency of catalytic converters at high vehicle speeds. However, this is not authenticated by the DTU measurements. The HBEFA emission factors show a reduction in the efficiency of the catalytic converter for oxides of nitrogen only. The vehicle emission factors deviate among the three emission prediction models. For example, the DTU model estimates carbon monoxide emissions, which are 50 to 75% higher than those other models. In contrast, the DTU volatile organic compounds and oxides of nitrogen estimated emissions are about 40 and 50% lower, respectively, than the emissions obtained with the other models.

Samaras and Zachariadis [1994] compared the methodologies employed in COPERT [Eggleston et al. 1993] and MOBILE5a [US-EPA, 1993]. MOBILE5a is the US-EPA's regulatory emission rate model for all states except California. Like COPERT, it is a macro-scale model. However, unlike COPERT, which can be validated using fuel sales data, MOBILE5a does not estimate fuel consumption. Emission data in MOBILE5a is obtained from US Federal Test Procedures, while emission data in COPERT is collated from various laboratories throughout Europe. MOBILE5a assumes three operating modes, namely cold-start, hot-stabilised and hot-start. In comparison, COPERT considers only two operating modes, namely hot- and cold-start. Evaporative emission factors from MOBILE5a are refined. For example, COPERT categorises cars as either controlled (i.e. equipped with a carbon canister) or uncontrolled, while MOBILE5a categorises cars into numerous different types depending on the age of the vehicle (i.e. model year). Samaras and Zachariadis [1994] emphasise that MOBILE5a should only be applied in countries where the vehicle fleet is somewhat similar to that in the USA.

Metz and Samaras [1994] compared two forecasting models for road traffic emissions, namely FOREMOVE [Samaras and Zierock, 1994] and BMW. The FOREMOVE model

incorporates the COPERT emission rate model. The focus of the comparison was to estimate future emissions of carbon monoxide, hydrocarbons, oxides of nitrogen and particulate matter from German cars. The primary inputs for both models were similar (e.g. increased traffic and more cars with catalysts). Both models predicted significant decreases for all pollutants. However, the estimated reductions were significantly different. An analysis of the inputs revealed that the discrepancy was principally due to the emission factors employed and the mileage distribution for older cars.

Joumard et al. [1994] compared two forecasting models, namely FOREMOVE [Samaras and Zierock, 1994] and POLLEN [Joumard, 1993]. POLLEN was developed to estimate fuel consumption and pollutants emitted by all transport modes from 1970 to 2010 in France. An analysis of the algorithms employed in each model showed that both adopt essentially similar basic computation methods for estimating emissions, but arrive at significantly different results due to differences in the emission factors used, and in the basic statistical data employed. Differences in the underlying assumptions in the development of future scenarios were also relevant.

Samaras and Zachariadis [1998] applied COPERT [Eggleston et al. 1993] and CONCAWE [CONCAWE, 1990] to twelve countries employing as input the fuel supplied by these countries to CORINAIR. They found that COPERT estimates of evaporative emissions from conventional cars are generally higher, particularly in countries with high annual vehicle mileage and high fuel volatility, than CONCAWE estimates. In the case of controlled cars (i.e. cars equipped with a carbon canister), COPERT appears to overrate the impact of the evaporative control system. For example, it assumes that cars equipped with a carbon canister produces one-fifth of the emissions of an uncontrolled vehicle. The efficiency of the carbon canister as estimated by both COPERT and CONCAWE is 96% and 83% respectively.

Zachariadis and Samaras [1996, 1997] compared four models used to calculate urban emission inventories across Europe, namely, HBEFA [INFRAS, 1995], MODEM [Jost et al. 1992], DGV [Sturm et al., 1994] and COPERT [Eggleston et al. 1993]. HBEFA, MODEM and DGV are micro-scale models while COPERT is a macro-scale model. The HBEFA [INFRAS, 1995] is a result of a combined Swiss and German project, which started in the mid 1980s and concluded in 1995. MODEM was carried out as part of the EC DRIVE programme in the early 1990's and contains hot emission factors for cars only [Joumard et al., 1995b]. The focus of the study was on the methods employed by each

model for the estimation of emissions. Even though most emission models in Europe have been developed independently of each other, they contain many common points. However, important differences also exist between the models, the most notable being:

- CO and HC emissions of catalyst cars, for which DGV estimates considerably higher emissions at lower speeds;
- NO_x emissions of catalyst and diesel cars, for which MODEM estimates were 2 to 3 times higher at lower speeds; and
- HC emissions of diesel cars, for which COPERT forecasts substantially higher low-speed emissions.

At medium and high vehicle speeds, all four models predict relatively similar results for all pollutants with the exception of NO_x. COPERT, for example, predicts up to 50% higher NO_x emissions than HBEFA. The study concluded that the range of emission estimates for the three instantaneous models (HBEFA, MODEM and DGV) are quite small; more importantly, this range is no greater than the error band for vehicle emission measurements. The models are validated against each other and not against field data. The study reported that while emission factors are not a linear function of speed, they display an approximately linear behaviour within the speed range typical for each type of road. The study found that non-linearity at mean speeds less than 20 km/hr is not important because it is highly unlikely that the average speed in a region would be so low. As the study was considering the compilation of emission inventories for typical areas of 500x500 m^2 and as such emissions in individual streets were not of great interest.

Creelman [1997] compared a number of on-road motor vehicle emission factor methods under the headings cost effectiveness, practicality, uncertainty, and upgrade potential. The methods reviewed included MOBILE for MCMA [Radian, 1993], MOBILE5a [US-EPA, 1993], and COPERT II [Aklvik et al., 1997]. Creelman [1997] noted that COPERT II has been subjected to the same type of validation studies as MOBILE. The practicality of COPERT II was rated 'acceptable', the cost effectiveness was rated 'good', but the uncertainty and upgrade potential was rated 'poor'. COPERT II was upgraded to COPERT III [Ntziachristos and Samaras, 2000].

2.4 TRAFFIC AND EMISSIONS RATE MODELS

A mobile source emissions inventory model normally consists of a traffic model and an emissions rate model.

Negrenti [1998] reviewed thirty-nine existing emission rate models. Of these, only eleven were combined with a traffic or traffic model. The main features of these CTEMs are given in Table 2.6 along with associated limitations. For example, many were developed for specialised applications or areas and, as such, are not applicable to Ireland. The emissions rate components of some CTEMs are out-of-date and have not been upgraded. Bostock [1994] stated that the "availability of comprehensive, accurate and up-to-date emissions input data is a fundamental requirement for accurate predictions from an emissions model". Most CTEMs predict conventional motor vehicle pollutants such as carbon monoxide, nitrogen dioxide, carbon dioxide, hydrocarbons, sulphur dioxide, and particulate matter, while only one predicts methane and benzene. None of them appear to have the facility to predict $PM_{2.5}$ or 1,3-butadiene. Only MADI-EM has a limited database of emission factors for alternative fuels, and only EVA includes different types of emissions (e.g. start-up, evaporative and hot-stabilised). However, EVA classifies vehicles into only four categories and it estimates only three pollutants. In summary, currently available CTEMs have limited capabilities.

Table 2.6: Combined traffic and emissions models reviewed by Negrenti [1998]

Emissions Model	Traffic Model	N° of Pollutants	Spatial Scale	Temporal Scale
PREMIT	TRANSYT	4	micro	sec./mins.
AIRVIRO	STRAUSS	3	macro	any
EVA	Traffic Assignment	3	micro	any
TRAF-NETSIM	NETSIM	3	micro	mins./hrs.
VISSIM	VISSIM	5	micro	sec./hrs
VISSUM	DYNEMO	5	macro	hrs./days
NEMIS	NEMIS	3	micro	?
EMISMOB3	TRIPS	10	macro	hrs./yrs.
MADI-EM	DUCK	5	micro	secs./days
TEDMAN	TEDMAN	9	micro	hrs/yrs.
CITAIR	PMV	14	micro	any

2.4.1 CLASSIFICATION OF CTEMS

Historically traffic and emission models have been developed independently for distinct purposes [Savonis, 2000]. Traffic models were developed to estimate the effect of infrastructure and management improvements on traffic flows and congestion levels. Over time, the modelling process has been refined to include greater detail. Emission models

have evolved and improved over time also. The two fields are subject to extensive study but are performed in separate ways and links between the traffic and emission models are still weak [Gilson et al., 1997], and consequently, they are not always compatible. One of the major difficulties in integrating traffic and emission models is the relative level of accuracy of the two. For example, the accuracy of very precise vehicle activity or traffic composition data is partly lost if the emissions data is relatively poor. Table 2.7 demonstrates the spectrum of possible approaches. The right-hand-side of Table 2.7 lends itself to improved accuracy and precision, but is very labour intensive. On the other hand, the left-hand-side of Table 2.7 is not very accurate. Data intensity, cost, computing resources and explanatory power increase from left to right [Rogers et al., 1997]. In theory, the right-hand-side of Table 2.7 should be more accurate.

Table 2.7: Possible approaches of combining vehicle activity and emissions factors [source: adapted from Guensler, 1998]

VEHICLE ACTIVITY				
Total Trips/Day	Vehicle Class Kilometres Travelled at Mean Speeds	Technology Group Modal Simulation	Specific Vehicle Activity Simulation	Specific Vehicle-Engine Activity Simulation
← *Aggregate*				*Disaggregate* →
Average Fleet (g/trip)	Vehicle Class Average Speed (g/km)	Technology Groups Vehicle Mode (g/km and g/s)	Individual Vehicles Vehicle Mode (g/s)	Individual Vehicles Vehicle Engine Mode (g/KW-s)
EMISSION FACTORS				

Zachariadis and Samaras [1997] note that this is not necessarily the case because the refined models require a large experimental database, which is not always available, and consequently the results can be more uncertain. In addition, the overall uncertainty often cannot be reduced by the use of sophisticated and complex methods because it is a product of the variability in real world emissions.

Emission estimates must also be temporally and spatially resolved in a domain. In fact, the level of spatial and temporal aggregation of traffic emission models needed by dispersion models may help define the minimum level of model aggregation required [Bachman, 1999]. Spatial resolution essentially distinguishes macro-models from micro-models. Table 2.8 differentiates CTEMs into three categories (macro-, meso- and micro-scale).

The microscopic approach is based on car following principles and is typically computationally intensive. The macroscopic approach is based on the average movement of a group of vehicles, which improves their computational performance but reduces the

detail of representation. The mesoscopic approach lies between the other two approaches and balances computational performance and accuracy of representation.

Table 2.8: Classification of combined traffic and emissions rate models

Category	Micro-scale	Meso-scale	Macro-scale
Application area	local scale	local to regional scale	regional scale
Spatial classification	major & minor roads	major & minor roads	major roads only
Temporal classification	sec.-by-sec.	minutes-to-hourly	hourly-to-daily
Input data	actual driving behaviour	segments of links	similar links combined
Road specific data	gradient	gradient	none
Vehicle activity	vehicle-engine simulation	cruise & queue	average speed
Vehicle classification	specific vehicle-engine	technology category	fleet average
Emissions modelling method	emission maps based on engine data	emissions modal matrix	total emissions over a cycle
Emissions units	g/kW-s.	g/km & g/s	g/km

2.4.2 Comparison of CTEM Approaches

The following sections describe the macro-, micro- and meso-scale approaches to combined traffic and emissions rate models.

2.4.2.1 Macro-scale approach

Many transport related emissions inventories are estimated using a macro-scale calculation method, as compatible traffic models are available for most main urban areas and are relatively comprehensive. However, this approach possesses a number of deficiencies. For example, vehicle classification is generally limited to three or four types, and the traffic models take no account of engine/emissions control technologies. It should be noted that traffic models do not need this level of detail for traffic purposes but as traffic-emission models they do. In addition, travel activity data is limited and the predictions of vehicle activity (vehicle kilometres travelled and average speed) lack the spatial resolution and precision required to properly assess control measures [Stopher, 1993]. Since average speed models were designed for free flow conditions, they are not applicable to congested urban areas [Reynolds and Bell, 1992]. In addition, "speed-based models explain, at best, one third to one half of the variation in trip emissions" [LeBlanc, 1998].

Reiter [1997] states that the "correct representation of emissions in urban traffic requires a detailed representation of flow in proximity to junctions". Emissions are substantially higher near intersections than at mid-link because vehicles usually spend a sizeable quantity of time queuing near the stop-line than they do at mid-link [Bell et al., 1996b]. Lee [1983] also found that "vehicle emissions and fuel consumption at or near street intersections are

usually higher than at other street segments because the intersection frequently causes vehicles to slow, stand, and accelerate". Leung [1997] found that ambient concentrations of benzene were over twelve times greater in heavy congestion (18.6 ppb) as compared to free flowing traffic (1.5 ppb). Claggett et al. [1981] measured carbon monoxide concentrations at an urban junction over a period of six weeks. Sensors were placed midway along the approach link and at the stop-line (i.e. beginning of vehicle queue). A separate measurement campaign was performed at a local freeway. The results are summarised in Table 2.9. The measured concentrations were nearly twice as high at the head of the queue zone as compared to the mid-block or freeway levels. This occurred even though traffic volumes 3.2 times higher were observed at the freeway site, and the average wind speed was much lower at the freeway site. These observations emphasise the need to model different vehicle modes of operation on each link and not assume that a mean speed dependent emission factor will suffice. Guensler [1993] states that the best speed correction factor models explain about fifty-percent of the variation in emissions. Therefore other contributing parameters should also be explored, such as vehicle modal activity (e.g. idle, acceleration and deceleration) and the influence of high-emitters.

Table 2.9: Summary of measurements from Claggett et al. [1981]

Parameter	Mid-link	Queue zone	Freeway
Average traffic volume (vph)	2239	2239	7255
Average vehicle speed (mph)	39	0-28	43
Average wind speed (mph)	7.5	7.5	4.0
CO maximum concentration (ppm)	24	43.7	24.8
CO average concentration (ppm)	3.3	12.8	6.7

There are also deficiencies in the methods used to derive SCF and the importance of certain vehicle modes of operation may be underestimated. In general, these modes of operation are more polluting than steady cruising velocities and emissions from interrupted traffic flow (due to congestion, junctions, and roundabouts) are higher than those from uninterrupted flow. Joumard et al. [1995b] noted that there could be substantially different emission results for driving cycles with approximately the same average speed. McCrae [1991] found that the use of a single speed and thus a single emission rate could introduce a significant degree of error in the estimation of pollutant concentrations. LeBlanc et al. [1995] indicated that a model based on vehicle speed alone does not provide sufficient carbon monoxide emission rate predictive capabilities for a fleet. Bell [2000] stated that, "macroscopic models are not suitable for exploring ways to manage traffic to alleviate air pollution problems caused by traffic in urban areas".

Kelly and Groblicki [1993] found that a single power acceleration can produce more carbon dioxide than is emitted in the balance of a single short trip (< 8 km). Mild acceleration perturbations at high speeds can lead to substantially elevated emissions compared with the steady-state values [Barth et al., 1999]. A qualitative assessment of the affect of vehicular modal operation on emission production is given in Table 2.10 for three pollutants (CO, HC and NO).

Table 2.10: Qualitative effect of vehicular modal operation on emission production [source: Seshardi and Harrison, 1993]

Vehicle mode	Mode type	CO	HC	NO
Cruise	*Low speed*	Low	Low	Low
	High speed	Very low	Very low	Moderate
Acceleration	*Soft*	Low	Low	High
	Hard	Moderate	High	Moderate
Deceleration	*Average*	Very high	High	Very low
Idle	---	High	High	Very low

2.4.2.2 Micro-scale approach

In comparison with the macro-scale approach, a micro-scale inventory calculation method should provide comprehensive results that can be used with a greater degree of confidence at the local scale than those offered by a macroscopic calculation method. In reality, however, emission inventories calculated by such methods suffer from major deficiencies on both the traffic and the emissions prediction sides. Algers et al. [1997] reviewed fifty-eight existing micro-simulation traffic models from all around the world and identified four principal limitations:

- Imperfect simulation of human behaviour;
- Difficulty in modelling a network close to reality;
- Hardware limitations; and
- Poor simulation results and analysis.

It is worth noting that users as well as model designers cited these limitations. According to Algers et al. [1997], limitations associated with 'imperfect simulation of human behaviour' and 'difficulty in modelling a network close to reality' are cited most often. Clearly, it is very challenging if not impossible to obtain the dual aim of 'real human behaviour' and network modelling. Hardware limitations are not cited very often because of the speed of today's modern computers. Only a small number of model designers cite

poor simulation output and analysis as a major limitation. This seems to be a drawback rather than a limitation. However, if one wishes to link the results to another model (e.g. emission rate model), this can cause major problems. With respect to the environment, 52% of the reviewed models estimate emissions, 48% estimate fuel consumption, while only 16% estimate roadside pollution levels.

Algers et al. [1997] also found that it is not yet practical or feasible to model second-by-second movement of each specific vehicle, and its interaction with other vehicles, pedestrians and cyclists, on all roads within a large urban area. Marsden [1997a] who stated that, "vehicle behaviour is not being modelled exactly as found on the street" supports this view. Bullock and Urbanik [2000] claim that many users view micro-simulation models sceptically. Bachman et al. [1998] stated that, "it is unlikely that widespread data availability allows modelling on a vehicle per vehicle basis, nor is it likely that modelling at that level is practical or useful for regional scale modelling". A comparison of three micro-simulation models (DRACULA, NEMIS and AIMSUN2) applied in Leeds found that "none of the models could represent all the features found in the test network" [Fox, 1999]. Marsden [1997a] also claims that the microscopic approaches require parameters with a greater accuracy than current traffic models can provide. Any benefits gained in employing microscopic emissions calculations are lost by misrepresentations of actual vehicular behaviour on roadways. Samaras and Zachariadis [1994] concluded that, "the uncertainty of emission estimates increases sharply when the spatial and temporal scale becomes finer".

Microscopic type inventories, by their very nature, are labour and data intensive and require high performance computing technologies. Regan [1996] notes that, "the need for such expensive data makes the use of instantaneous emissions models limited in day-to-day engineering practice". Bachman [1999] also claims that modelling individual vehicle engine dynamics for a large metropolitan area is not realistic or practical due to extensive input data requirements. In addition, current research at Georgia Institute of Technology [Bachman et al., 1996] indicates that relationships between various operating modes and emissions for any given vehicle are very complex. Cloke et al. [1997] found that many advanced emission rate models (i.e. modal models) have been developed to estimate hot stabilised emissions for passenger cars in a limited range of driving conditions. Therefore, any potential increase in accuracy that these advanced models afford is negated by the omission of start-up and evaporative emissions. Cloke et al. [1997] also notes that the use of these advanced emission rate models beyond the range of data on which they are based (e.g. employing passenger cars emission estimates to represent an entire fleet) rapidly

increases their uncertainty and inaccuracy. Joumard et al. [1999a] states that instantaneous emission models for passenger cars available in Europe did not prove to be reliable for their specific application field, and provided a false image of accuracy that can lead to completely erroneous conclusions. In addition, Bell [2000] stated that "although the emission factors data is poor for macro- and meso-scopic modelling it does not really exist for microscopic modelling". Sturm et al. [1996] emphasises, with respect to micro-scale simulations, that it is not always necessary to employ the most detailed model. The most important selection criterion is to choose the appropriate model for a specific purpose.

2.4.2.3 Meso-scale approach

From the above discussion, it can be observed that macro-scale models are not considered accurate enough, while micro-scale models are restricted by data (both traffic activity and emissions) availability. While it is acknowledged that each individual vehicle will have its own emission rate, it is clearly inappropriate to dis-aggregate emission estimations to this degree of detail. Regan [1996] found that "the current trend in emissions modelling seems to be towards the middle ground of developing models that capture the spatial details of pollutant emissions without the need to simulate space-time trajectories of individual vehicles". Heseltine and Nelson [1995] suggest using a 'category analysis' method whereby it is assumed that emissions are constant over a relatively homogenous sub-category of vehicles and period of activity. In this method, a primary task is to identify these homogenous vehicle sub-categories and travel activities. Simultaneously, appropriate emission factors for each sub-category have to be established. Previous meso-scale models have employed one value for average speed and one fixed value in acceleration mode (e.g. 0.75 m/s^2 in Chiquetto [1995b] and 2.8 m/s^2 in Matzoros [1988]).

The US-EPA and the FHWA held a workshop for the purpose of identifying and discussing current emission modelling research efforts in the USA [Siwek, 1997]. The workshop concluded that the level of model complexity required must first be defined before the direction of further research is decided. What is required is a level of complexity between the precise microscopic approach on one hand and the inaccurate macroscopic approach on the other. Bachman [1999] states that the level of complexity required should lie between the largest vehicle emissions research efforts at CE-CERT [Barth and Norbeck, 1993, 1994] and the current US designated method (MOBILE5a) [US-EPA, 1993]. CE-CERT has developed a modal emissions model based on vehicle-engine power while MOBILE5a employs an average speed approach.

2.5 COMPREHENSIVE MODAL EMISSIONS MODEL

As already stated, the most advanced emissions model in the world was developed by CE-CERT in the USA. This section provides a brief description of the model. Further details may be found elsewhere [Barth and Norbeck, 1993; 1994], [Barth et al., 1997; 1999], [An et al., 1997]. The author spent four months at CE-CERT during the summer of 1998 working on this project, and much of this experience is represented in the motor vehicle emission inventory model described in Chapter three.

The research focussed on developing the model for a Ford Taurus. The overall objective is to develop and verify a CMEM that accurately reflects impacts of speed, engine load, and start conditions on emissions under a comprehensive variety of driving characteristics and vehicle technologies.

2.5.1 STRUCTURE OF CMEM MODEL

Figure 2.2 illustrates the structure of the CMEM. The complete CMEM comprises six modules, as indicated by the six rectangular boxes. These modules model engine power demand, engine speed, fuel/air ratio, fuel-rate, engine-out emissions, and catalyst-pass function. The model requires two groups of input parameters as indicated by the round boxes as shown in Figure 2.2.

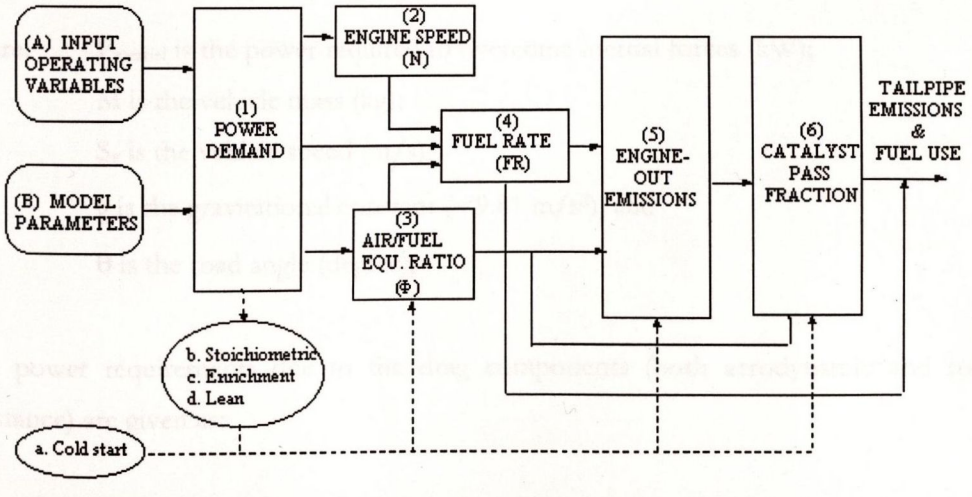


Figure 2.2: Outline structure of CMEM [source: Barth et al., 1999]

The output from the model is fuel consumption and tailpipe emissions. The model encompasses four modes of operation, namely cold-start, stoichiometric operation, enrichment and enleanment. Evaporative emissions are not taken into account.

In the CMEM, the emission process is divided into different components or modules that correspond to physical phenomena associated with vehicle operation and emissions production. Each component is then modelled as an analytical representation consisting of the various parameters that are characteristic of the process.

2.5.1.1 Power demand module

The CMEM tracks an individual vehicle's power demand and engine equipment status. Power demand is predicted using static vehicle parameters (vehicle mass, cross-sectional area, rolling resistance coefficient, and aerodynamic drag coefficient), dynamic vehicle parameters (speed, and acceleration), and environmental parameters (wind resistance, road grade, air density, temperature, and altitude).

The power demand at the wheels is a combination of the power required to overcome the inertial and drag forces. The inertial power requirements are given as:

$$P_{inertial} = \frac{M}{1000} \cdot S_v \cdot (a + g \cdot \sin\theta) \qquad 2.2$$

where: $P_{inertial}$ is the power required to overcome inertial forces (kW);
M is the vehicle mass (kg);
S_v is the vehicle speed (m/s);
g is the gravitational constant (≈ 9.81 m/s^2); and
θ is the road angle (degree);

The power requirements due to the drag components (both aerodynamic and rolling resistance) are given as:

$$P_{drag} = \frac{S_v}{1000} \cdot \left(M \cdot g \cdot C_r + \frac{\rho}{2} \cdot S_v^2 \cdot A_F \cdot C_a \right) \qquad 2.3$$

where: P_{drag} is the power required to overcome drag forces (kW);

C_r is the rolling resistance coefficient;

ρ is the mass density of air (g/m^3);

A_F is the vehicle cross-sectional frontal area (m^2); and

C_a is the aerodynamic drag coefficient.

The total tractive power requirements placed on the vehicle at the wheels is given as:

$$P_{tractive} = P_{drag} + P_{inertial} \qquad \textbf{2.4}$$

where $P_{tractive}$ is the tractive power requirement at the wheels. The following relationship is employed to translate this tractive power requirement to demanded engine power requirement:

$$P_{engine} = \varepsilon \cdot P_{tractive} + P_{acc} \qquad \textbf{2.5}$$

where: P_{engine} is the demanded engine power requirement (kW);

ε is the combined efficiency of the transmission and final drive (%); and

P_{acc} is the engine power demand associated with the operation of accessories such as power steering, air conditioning, brakes and electrical loads (kW).

2.5.1.2 Engine speed module

Engine speed is expressed in terms of vehicle speed:

$$N(t) = S_R \cdot \frac{R(L)}{R(L_g)} \cdot S_v(t) \qquad \textbf{2.6}$$

where: $N(t)$ is the engine speed at time t (rev./sec.);

S_R is the ratio of the engine rotational speed in a specific gear to the vehicle linear speed (rev./metre);

$R(L)$ is the gear ratio in L^{th} gear, $L = 1, \ldots L_g$;

$R(L_g)$ is the gear ratio in top gear; and

$S_v(t)$ is the vehicle speed at time t (m/s).

The term $\frac{R(L)}{R(L_g)}$ is to account for vehicles travelling in different gears.

2.5.1.3 Air-fuel equivalence ratio module

One of the most important components of the CMEM is approximating the emission control mechanisms of the vehicle. In older vehicles, emission control is accomplished through a combination of mechanical, pneumatic or hydraulic mechanisms. The engine control regulates the fuel and air intake as well as spark-timing and EGR to achieve the desired performance in power output, fuel economy and emissions. Modern vehicles are equipped with complex emission control systems that closely regulate fuel injectors.

The emission control function is modelled using the equivalence ratio, defined as:

$$\phi = \frac{(A/F)_o}{(A/F)} \qquad 2.7$$

where: ϕ is the fuel-air equivalence ratio;

$(A/F)_o$ is the air/fuel ratio at stoichiometry; and

(A/F) is the commanded air/fuel ratio.

The fuel-air equivalence domain is divided into three regions; rich, stoichiometric (approximately $0.98 < \phi < 1.02$) and lean.

2.5.1.4 Fuel rate module

The fuel rate can be modelled using the following equation:

$$FR = \phi\left(J_f \cdot N_{speed} \cdot V_{engine} + \frac{P_{engine}}{\eta_i}\right)\frac{1}{HV_{fuel}} \qquad 2.8$$

where: FR is the fuel use rate (g/s);

ϕ is the fuel-air equivalence ratio.

J_f is the engine friction factor (kJ/rev.-litre);

where $\eta_{catalyst}$ is the efficiency of the catalytic converter (%). The catalyst efficiency is determined from an empirical relationship.

2.5.2 TEST VEHICLE

The test vehicle was a 1991 Ford Taurus with approximately 60,000 miles, equipped with a 3.0L V-6 engine, fuel injection, a 4-speed automatic overdrive transmission, air conditioning, speed cruise control and an EEC system. During all experiments the vehicle was operated using a commercial source of regular unleaded California reformulated gasoline. The vehicle was fitted with on-board instrumentation to measure pollutants in real world conditions.

2.5.2.1 On-board emissions instrumentation

Carbon monoxide, carbon dioxide and hydrocarbons are measured with a NDIR automotive emission analyzer. The NDIR analyzer consists of an infrared source, three-infrared filters (one each for CO, CO_2 and HC), a sample cell, and three-infrared detectors. The light source produces a wide range of light frequencies covering the infrared band and extends in both directions into the visible and ultraviolet spectrums. The filters are optical band-pass filters used to select a specific band of infrared light centred on an exact wavelength. The wavelength of the filter coincides with the specific gas to be measured and consequently multiple gas measurement requires multiple filters. At the ends of the sample cell, windows allow the infrared light to pass through the gas sample being measured. Finally, the detector, which is sensitive to infrared light wavelengths, converts the beam of light into an output voltage. Each NDIR analyser uses a single-beam measurement technology to provide fully corrected CO, CO_2, and HC emission concentrations. The NDIR uses a two-point span calibration (high and low) in addition to a zero gas (air) calibration.

Nitrogen monoxide is measured using a replaceable fuel cell technology sensor and appropriate hardware and software. The nitrogen monoxide sensor consists of three electrodes (sensing, counter and reference) separated from each other by an electrolyte. Sample gas enters through a gaseous capillary diffusion barrier, which limits the flow of gas to the sensing electrode. The sensor electrodes are supplied with a bias voltage at all times. The sensor is sensitive to temperature gas flow-rate and pressure changes and its response time curve is highly non-linear. It also exhibits a performance phenomenon known as

post-calibration drift after prolonged periods of continuously measuring nitrogen monoxide. For this reason experiments were limited in duration and the sensor was validated with a calibration gas before and after each experiment. The sensor can use a 1- or 2-point calibration span in addition to a zero gas (air).

Constant heated gas streams are taken from the exhaust (both pre- and post catalyst), through heated filled sample lines, into both analyzers. All the sample lines and the NDIR are heated above 80 °C to avoid water condensation. A silica filter then dries the gas sample before it enters the nitrogen monoxide sensor. In other words, the NDIR measures a 'wet' gas stream while the nitrogen monoxide sensor measures a 'dry' gas stream.

The power supply of 12V DC and 110V AC required by the instrumentation is supplied by an independent 12V system with a DC to AC (modified sine wave) inverter. Energy usage (battery voltage and current draw) is monitored at all times during testing. Previous studies have shown that measurement variations are linked to low voltage and therefore providing a consistent stable power supply is crucial.

2.5.2.2 Vehicle parameters instrumentation

Various operating parameters from the vehicle PCM are collected by the VDAS. The PCM provides two basic kinds of parameters: digital (or discrete) and analog. The discrete parameters are those that can only be in one of two states such as on or off, open or closed, high or low, yes or no. Switches and solenoids provide the discrete parameters. Analog parameters are quantities displayed as a measured value in the appropriate units e.g. voltage, pressure, temperature, time, and speed. The vehicle parameters collected include: engine rpm, oxygen sensor voltage, throttle position, throttle position mode, engine coolant temperature, intake air temperature, intake idle air percent, fuel injector pulse width, pressure feedback EGR voltage, EGR vacuum regulator percent, short term fuel percent, spark advance, battery voltage, reference voltage, vehicle speed, transmission gear selection, brake booster switch, open loop operation flag, emissions canister purge flag, Lo fan flag, Hi fan flag, A/C flag and power steering pressure flag.

The VDAS consists of a MT2500 Scanner connected to a PC with one serial port for input. Proprietary software allows the display and recording of vehicle data in text or graphic formats.

2.5.2.3 Global positioning system

Vehicle velocity and grade information can be estimated from the position data collected with the GPS receiver. The vehicle is equipped with an Ashtech Z-12 GPS receiver and antenna, which collects position data from orbiting satellites. An accuracy of 1-2 cm can be achieved using double-differential GPS phase differencing, in which differencing is first performed between the mobile and stationary units to eliminate satellite-related errors, and then between satellites to eliminate receiver clock errors. The processed data is then evaluated for deviations in elevation (to determine the grade of specific road segments) and position over time (to determine the velocity and subsequently the acceleration of the vehicle).

2.5.3 CMEM INPUTS

The CMEM requires two groups of input data, namely input operating variables and vehicle model parameters.

The specifications for the Ford Taurus are given in Table 2.11.

Table 2.11: Specification of 1991 Ford Taurus

Static Input Parameter	Symbol	Value
Maximum Horsepower	P_{max}	140 hp
Weight	M	2020 kg
Rolling resistance coefficient	C_r	0.015
Aerodynamic drag coefficient	C_d	0.42
Frontal area	A_f	3.1 m^2

These values are combined with the constants given in Table 2.12.

Table 2.12: Constants employed in calculations

Constant	Symbol	Value
Gravitational constant	G	9.81 m/s^2
Air density	ρ	0.00236 g/m^3
Road grade	θ	0°

The following dynamic input parameters are assumed.

Table 2.13: Dynamic parameters assumed for the CMEM

Dynamic Input Parameter	Symbol	Value
Lower heating value of gasoline	HV_{fuel}	44 kJ/g
Transmission efficiency	ε	92.5%
Engine indicated efficiency	η_I	40%
Stoichiometric air/fuel ratio	$(A/F)_o$	14.6
Engine friction factor	J_f	0.25 kJ/(rev*litre)

2.5.4 TESTING

Testing was performed in CE-CERT's VERL. Field measurements were also carried out on the Moreno Valley Freeway (I-215/SR-60), as well as at Penske Speedway in Fontana, and at El Mirage dry lakebed in the Mojave Desert.

2.5.4.1 Dynamometer testing

Dynamometer testing of the vehicle was performed in order to validate the on-board instrumentation, in CE-CERT's VERL. The dynamometer tests included the FTP cycle and two cycles developed previously by CE-CERT personnel. These cycles known as NCHRP_e and NCHRP_h represent freeway and arterial driving conditions respectively. Table 2.14 presents the operating envelopes for the three driving cycles. For comparison purposes, the operating envelope for the Ford Taurus is also given. The minimum specific power is negative as the vehicle is slowing down.

During these tests, emissions data was collected from both the on-board instrumentation and the VERL instrumentation. The accuracy of the VERL instrumentation exceeds the on-board instrumentation. Empirical formulas were developed by the author to compensate for these discrepancies.

Table 2.14: Comparison of operating envelopes of three driving cycles with a Ford Taurus

Travel Activity	FTP	NCHRP_e	NCHRP_h	Ford Taurus
Max speed (mph)	55	74.9	60.6	94
Max. acceleration (mph/s)	3.3	6.1	5.7	9
Max. deceleration (mph/s)	-3.3	-7.6	-7.4	-9

2.5.4.2 Speedway and desert testing

Modal experiments were performed at Penske Speedway and El Mirage dry lakebed. Nine modes of vehicle operation were employed in the modal experiments: constant velocity, hard, medium and soft accelerations and decelerations, idle and cruise. The speedway has a very slight positive grade while the lakebed is flat. All electrical devices and the air conditioning were turned off for the duration of the tests. The same researcher drove in all tests at the speedway and at the dry lakebed.

2.5.4.3 Freeway testing

Field tests were also performed on the shared section of I-215 and SR-60, which extends from SR-90 to where SR-60 and I-215 split and is known locally as the Moreno Valley freeway. This section of freeway is a major north/south thoroughfare between the city of Moreno Valley and the rest of the South Coast Basin in California. For the most part, it has three general-purpose lanes going in both directions. It has a considerable grade (approximately 2.9%), ascending more than 760 feet over 5-miles from west to east.

In this field test, the route was driven in both directions repeatedly during a 24-hour period to determine the effect of time of departure and the direction of travel on time of travel. The trips comprised of a pair of 8 northbound and 8 southbound trips from SR-90 to the I-215/SR-60 split. The trips commenced at 0430, 0730, 1030, 1330, 1630, 1700 and 2230 hours respectively. A test carried out at 2030 hours had equipment failure unrelated to the measuring instrumentation.

All trips were driven by one of two researchers who were instructed to drive in a 'conservative' manner. In all but one of the freeway tests, the driver remained in the middle lane where possible and did not pass any other vehicle during the entire trip. This driving is not as 'aggressive' as the normal behaviour for the average driver who changes lanes frequently in an attempt to reduce trip times. During the trips, both speed and acceleration of the vehicle in front of the test vehicle limited speed and acceleration of the test vehicle. The test at 0430 hours was driven in the inside lane of the freeway so that a constant speed could be achieved for the trip. Data collection for these tests commenced at the beginning of the on-ramp and finished at the end of the off-ramp. Only pre-catalyst emissions, GPS and VDAS data were collected on these tests. The longest journey time travelling north and south was 576 and 611 seconds respectability, while the shortest time of travel going north and south was 336 and 350 seconds respectively.

2.5.5 SAMPLE RESULTS

All the emissions data collected during the tests were collated into a database. Figure 2.3 to Figure 2.6 illustrates the variation of carbon dioxide, carbon monoxide, hydrocarbons, and nitrogen monoxide emissions with specific power, for the 1991 Ford Taurus. The pollutants all display a similar trend. For example, the emissions are relatively constant during both positive and negative high power demand periods. At low power demand periods, there is considerable variation in the emissions, due to the transition from stiochiometric to enrichment operating conditions. This transition impacts on some pollutants less (e.g. carbon monoxide in Figure 2.3) than others (e.g. nitrogen monoxide in Figure 2.5). In addition, there is nearly an order of magnitude difference between normal and enriched modes of operation.

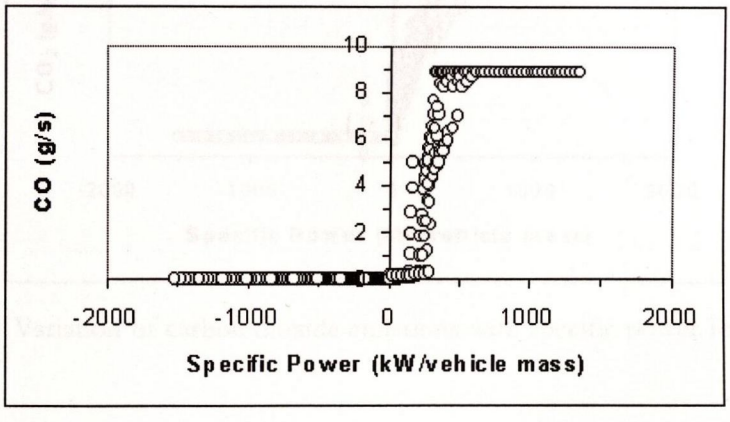


Figure 2.3: Variation of carbon monoxide emissions with specific power for a 1991 Ford Tauras

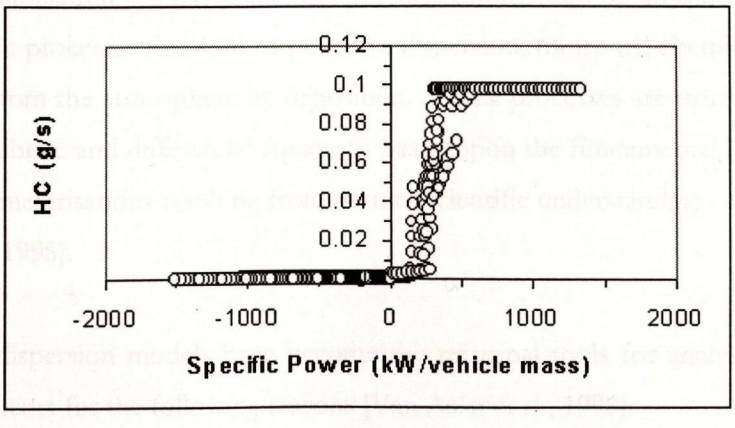


Figure 2.4: Variation of hydrocarbon emissions with specific power for a 1991 Ford Tauras

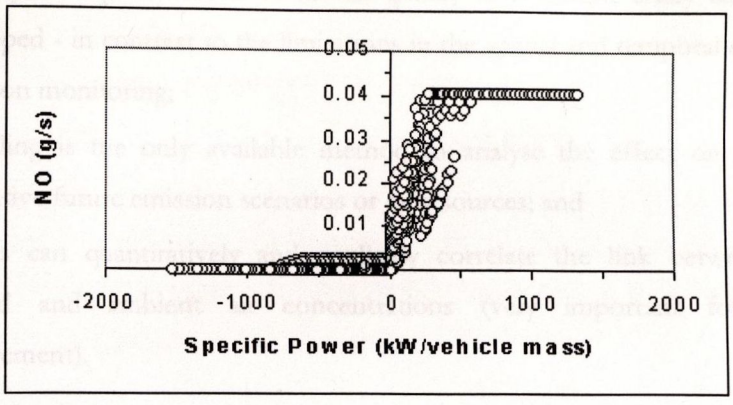


Figure 2.5: Variation of nitrogen monoxide emissions with specific power for a 1991 Ford Tauras

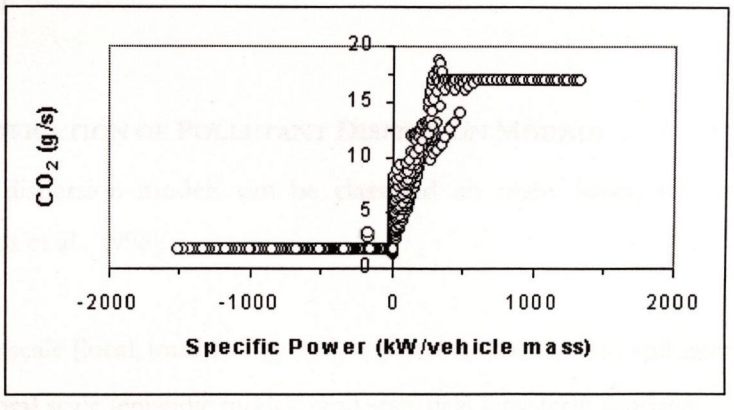


Figure 2.6: Variation of carbon dioxide emissions with specific power for a 1991 Ford Tauras

2.6 POLLUTANT DISPERSION MODELLING

Air pollution simulation is a technique that provides information on air quality. It is based on atmospheric processes that lead to pollutant dispersion, transport, chemical conversion and removal from the atmosphere by deposition. These processes are usually represented by a set of algebraic and differential equations based upon the fundamental laws of science as well as parameterisations resulting from current scientific understanding of the processes [Hwang et al., 1998].

Atmospheric dispersion models have become the principal tools for analysis in most air quality assessments for the following reasons [Van Aalst et al., 1998]:

- A complete representation of the air quality in a specific study domain may be developed - in contrast to the limitations in the spatial and temporal distribution of pollution monitoring;
- Modelling is the only available method to analyse the effect on air quality of alternative future emission scenarios or new sources; and
- Models can quantitatively and explicitly correlate the link between pollutants emitted and ambient air concentrations (very important for air quality management).

The term 'air quality dispersion model' covers a wide range of applications, from simple models including graphs, tables or formulae, to sophisticated computer programs [UK-DETR, 1998b].

2.6.1 Classification of Pollutant Dispersion Models

Air pollutant dispersion models can be classified on many bases, for example on the [Moussiopoulos et al., 1996]:

- Spatial scale (local, local-to-regional, regional-to-continental, and global);
- Temporal scale (episodic models, and statistical long-term models);
- Treatment of the transport equations (Lagrangian and Eulerian models);
- Treatment of various processes (chemistry, wet and dry deposition); and
- Complexity of the approach.

Clark [1983] classifies pollutant dispersion models into three primary types, namely physical, stochastic, and deterministic. A physical model is a reproduction of actual topographical and meteorological conditions at a laboratory scale size, while a statistical model uses empirically derived relationships between monitored ambient pollutant concentrations and other parameters (e.g. wind speed and traffic volume). In comparison, Turner [1979] defined a deterministic model as "a mathematical expression of the effects of the atmosphere upon air pollutants". Zanetti [1993] classifies deterministic pollutant dispersion models as Gaussian, Eulerian, and Lagrangian.

2.6.2 Review of Available Pollutant Dispersion Models

A large variety of models for air pollution dispersion have been developed for different applications. As part of the COST-615 action, Schatzmann et al. [1997] compared fifty-nine air quality models under the headings type, purpose, characteristics, domain, and primary assumptions employed. COST-615 was one of four parts of the COST programme 'Science and Research for Better Air in European Cities'. The objective of the programme was to launch a major concerted effort in the field of environmental protection with special emphasis on European conurbations.

The European Topic Centre on Air Quality developed a model documentation system with the aim of providing guidance to any model user in the selection of the most appropriate model for his application [Moussiopoulos et al., 1995], [deLeeuw et al., 1996], [Tønnesen et al., 1997]. An overview of ninety-four models employed (but not necessarily developed) in Europe is presented in the model documentation system. The models are compared under the following headings: Institution, Application, Type of model, Domain, Simulation period, Horizontal resolution, Vertical resolution, Transport scheme, Dry deposition, Wet deposition, Chemistry, Emissions, Meteorology, Boundary conditions, and Reference.

Kupiszewska [1997] performed an audit of existing sectoral models for transport, air pollution, land use and population modelling. Thirteen air pollution models currently employed in the UK were reviewed. The UK-DETR [1998b] provides a list of dispersion models (eighteen in total) as a guide to potential users in the UK. Other reviews in this area include [Olesen and Mikkelsen, 1992], [Kretzschmar et al., 1994], [Gryning and Schiermeier, 1996], [Madany, 1997], [Gryning and Millan, 1994], [Van Dop and Kallos, 1992], [Rasse, 1998], [Szepesi, 1989]. None of the reviews recommended any specific model. Instead they collated data concerning specific models for potential users. In comparison, the Guideline on Air Quality Models (Appendix W to part 51) [US-EPA, 1998] was established to promote consistency in the use of models within the air management process. It identifies preferred air dispersion models for regulatory applications in the USA [US-EPA, 1998].

2.6.3 Modelling of Roadside Pollutant Concentrations

The prediction of pollutant concentrations near roads and highways frequently involves the use of mathematical dispersion models [Noll et al., 1978]. While various types of models have been developed, "most frequently, due to their simplicity and direct applicability for

estimates on a local scale, various versions of the Gaussian line-source model have been used for dispersion evaluations from a road" [Härkönen et al., 1996].

The Gaussian model employs a three-dimensional cartesian co-ordinate system, namely down-wind, cross-wind and vertical. The model assumes that pollutants are transported downwind of a source, giving rise to a plume. The concentration profile of this plume is described as bell-shaped in the lateral and vertical directions, with the highest concentrations at the centre-line of the plume.

McCrae [1991] stated that, "Gaussian theory has been widely adopted to emulate pollutant concentrations as a function of distance between a receptor and the centre point of a road under study". Bielli et al. [1998] stated that the "Gaussian plume models are the most widely used because of their simplicity since more complicated alternatives perform no better in common applications". The US-EPA in its guidance on air dispersion modelling of toxic substances in urban areas [US-EPA, 1999] states that "the Gaussian plume model is a widely used technique for estimating the impacts of non-reactive pollutants because of its good performance against field measurements, and because it is computationally efficient relative to other types of models, such as grid and puff models". Chiquetto [1993] noted that most existing models for estimating air pollution from traffic follow the Gaussian dispersion theory. Cloke et al. [1997] noted that the most common mathematical approach, in terms of predicting local impacts of pollutant concentrations is the Gaussian dispersion algorithm. In addition, most Gaussian models represent emissions from a junction or highway as a fictitious line down the centre of the roadway [Datz, 1994]. The ETC-AQ in their review of air quality models [Moussiopoulos et al., 1995] found that micro-scale (< 1km) Gaussian models are currently used for regulatory purposes, policy support, and scientific research in Europe.

Many Gaussian dispersion models have been developed to estimate the roadside concentration of traffic related pollutants. These include ADMS-urban [McHugh et al., 1997a], CAR-FMI [Härkönen et al., 1995], GFLSM [Luhar and Patil, 1989], PROKAS_V [Romberg et al., 1996], MODIM [Hesek, 1998], HNS-ROAD [Fekete, 1983], CALINE4 [Benson, 1992], HIWAY2 [Petersen, 1980], GM-LINE [Chock, 1978], TEXIN3 [Hlavinka, 1995], AIRPOL4 [Carpenter and Clemena, 1975], and FLINT [Wayson, 1998].

CRC [1986] compared eight Gaussian dispersion models used to estimate roadside traffic related air pollution. The models were compared under such headings as Input, Assumptions, Modal Range, Output, and Special Features.

Prior to selection and use of any model, it should be properly validated and independently if possible [Zanetti, 1998]. The UK-DETR guidelines on the 'selection of dispersion models' [UK-DETR, 1998b] suggest that factors such as model accuracy, validation and ease of use need to be taken into account.

2.6.4 GAUSSIAN FORMULATION FOR LINE SOURCE

Nikolaou et al. [1997] present a detailed description of modelling pollutant dispersion near roadways.

The basic advection-diffusion equation governing the dispersion of pollutants can be written as [Seinfeld, 1986]:

$$\frac{\partial \chi}{\partial t} = S + u\frac{\partial \chi}{\partial x} + v\frac{\partial \chi}{\partial y} + w\frac{\partial \chi}{\partial z} + \frac{\partial}{\partial x}\left(K_x \frac{\partial \chi}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial \chi}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial \chi}{\partial z}\right) \qquad 2.11$$

where: χ is the concentration;

t is time;

S is internal effects such as sources or sinks;

x, y, z are directions in the cartesian co-ordinate system;

u, v, w are wind velocity components in the x, y, z directions respectively; and

K_x, K_y, K_z are eddy diffusivities in the x, y, z directions respectively.

This equation is difficult to apply. However, a number of simplifying assumptions can be applied to the equation such as:

- Pollutants are emitted from a continuous source;
- The process is steady state, hence the quantity $\frac{\partial \chi}{\partial t} = 0$;

- Major transport direction due to wind is chosen to lie along the x-axis, hence v and w are equal to zero and consequently $v\frac{\partial \chi}{\partial y}=0$ and $w\frac{\partial \chi}{\partial z}=0$;
- K_i is constant in any direction; and
- Wind speed u is constant at any point in the x, y, z system.

After applying the above assumptions, Equation 2.11 can be reduced to the following form:

$$0=S+u\frac{\partial \chi}{\partial x}+\frac{\partial}{\partial x}\left(K_x\frac{\partial \chi}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial \chi}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial \chi}{\partial z}\right) \qquad \textbf{2.12}$$

The diffusion term in Equation 2.12 (x-drection) can be written as:

$$\frac{\partial}{\partial x}\left(K_x\frac{\partial \chi}{\partial x}\right)=K_x\frac{\partial^2 \chi}{\partial x^2}+\frac{\partial}{\partial z}\left(\frac{\partial K_x}{\partial z}\right) \qquad \textbf{2.13}$$

Since K_x is a constant then $\frac{\partial K_x}{\partial z}=0$. Similarly this can be applied to the y and z diffusion terms in Equation 2.12 as both K_y and K_z are constants also.

Also, for a continuous source, advection in the x-direction is much more important for the transport of the material than turbulent diffusion:

$$u\left(\frac{\partial \chi}{\partial x}\right)>>K_x\left(\frac{\partial^2 \chi}{\partial x^2}\right) \qquad \textbf{2.14}$$

Therefore the diffusion term $K_x\left(\frac{\partial^2 \chi}{\partial x^2}\right)$ is assumed equal to zero since it is small. Consequently, Equation 2.12 reduces to:

$$u\left(\frac{\partial \chi}{\partial x}\right) = S + K_y\left(\frac{\partial^2 \chi}{\partial y^2}\right) + K_z\left(\frac{\partial^2 \chi}{\partial z^2}\right) \qquad \textbf{2.15}$$

As eddy diffusivities K_i (where i = x, y, or z) are not readily available, Gaussian solutions to the diffusion equation have been proposed. Cramer [1959] tested the following functional form of the Gaussian equation using data collected by Calder [1949]:

$$\chi = \frac{Q}{\sqrt{2\pi} \cdot \sigma_y \cdot \sigma_Z \cdot \bar{u}} \left\{ \exp\left[-\frac{1}{2}\left(\frac{y^2}{\sigma_y^2} + \frac{z^2}{\sigma_z^2} \right) \right] \right\} \qquad \textbf{2.16}$$

where: Q is the continuous point source strength (g);

σ_y and σ_z are the standard deviations of the concentration distribution in y- and z-directions;

$\bar{u}$ is the mean wind speed (m/s).

Gaussian models were originally developed for continuous point sources, and have since been adapted for finite line sources. A schematic diagram of horizontal dispersion from a finite line source is shown in Figure 2.7.

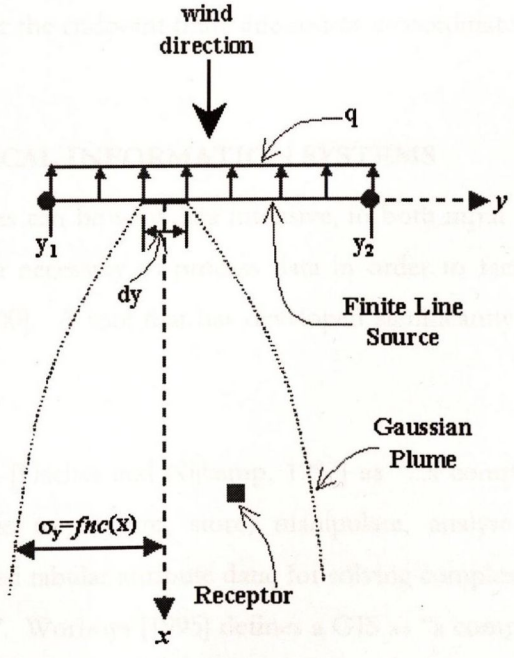


Figure 2.7: Horizontal dispersion downwind from finite line source [source: adapted from Benson, 1989]

The wind is assumed perpendicular to the roadway (i.e. finite line source) and the emissions strength is assumed constant across the line source. The horizontal dispersion coefficient σ_y is shown as a function of distance downwind x. Zanetti [1990] stated that, "even though the plume concentrations are quite irregular, a sufficient long averaging time (e.g. one hour) generates bell-shaped concentration distributions that can be well approximated by the Gaussian distribution in both the horizontal and (to a lesser degree) the vertical".

The downwind ground level concentration computed using a crosswind Gaussian formulation for a line source of finite length has the following functional form [Benson, 1989]:

$$\chi(x,y) = \frac{q}{\pi \cdot \sigma_z \cdot u} \cdot \int_{y_1 - y}^{y_2 - y} \exp\left(\frac{-y^2}{2\sigma_y^2}\right) \qquad 2.17$$

where: $\chi(x, y)$ is the ground level concentration at a particular location downwind x and y;

q is the continuous line source strength (g);

u is the wind speed (m/s);

σ_y and σ_y are the horizontal and vertical Gaussian diffusion parameters; and

y_1 and y_2 are the endpoint finite line source y-coordinates.

2.7 GEOGRAPHICAL INFORMATION SYSTEMS

As emissions inventories can be very data intensive, in both input and output, specialised computer programs are necessary to process data in order to facilitate presentation and visualisation [Willis, 2000]. A tool that has developed significantly in the recent years for this purpose is a GIS.

A GIS may be defined [Fischer and Nijkamp, 1993] as "...a computer-based information system which attempts to capture, store, manipulate, analyse and display spatially referenced and associated tabular attribute data, for solving complex research, planning and management problems". Worboys [1995] defines a GIS as "a computer-based information system that enables capture, modelling, manipulation, retrieval, analysis and presentation of geographically referenced data". Put simply, a GIS facilitates the representation of, and the

storage/manipulation of spatial data in an intuitive manner. Therefore, it is useful in modelling the spatial contexts of activity and emission patterns and the interaction of temporal characteristics with spatial attributes. Another important feature of GIS is its ability to bridge the gap between analysts and policy-makers' need for easy understand of data [Bachman, 1999]. In addition, Walia [1998] stated that the "spatial nature of environmental data warrants the use of tools like GIS for spatial analyses".

Fedra [1999] notes that the analysis of traffic-generated pollutants requires the integration of models with GIS and large volumes of data. Fedra [1999] distinguishes between GIS and environmental modelling (e.g. air quality models, and emission rate models). For example, in GIS, the fundamental concept is one of location, and of spatial distribution and relationship. The primary elements are spatial objects. In contrast, the basic concept in environmental modelling is one of state, expressed in terms of numbers or mass, of interaction and dynamics. The basic elements are species, which may be chemical and environmental media such as air.

A literature review revealed that GIS has been previously employed in the compilation of emission inventories and applied to air quality analysis.

2.7.1 GIS AND EMISSION INVENTORIES

Lindley and Longhurst [1998] state that the powerful processing tools in GIS for spatial and attribute data makes it extremely useful for emission inventory applications. The NATO-CCMS pilot workshop on air pollution transport and diffusion over coastal urban areas emphasised the need for an emissions inventory database to be compatible with a GIS [Melas et al., 1995]. Bachman et al. [1996] noted that the modelling capabilities of a GIS are well suited to the modelling of mobile-source emissions because vehicle activities and the emissions associated with them can be correlated with specific points in time and space. In addition, Bachman et al. [1998] noted that future emission models will need spatially resolved subfleet characteristics to determine mobile emission inventories so that comprehensive and accurate estimates may be made. Bruckman et al. [1991] developed a model, CAL-MoVEM that employed a GIS and an emission rate model (EMFAC7E) to develop emission estimates for input into a photochemical model. An urban emissions inventory was compiled for the Greater London area on a 1 x 1 km^2 grid basis from point, area and line source activities and aggregated to give total pollutant loads by employing a

GIS [Crabbe et al., 1999]. Researchers at Georgia Institute of Technology developed a GIS-based emissions model – MEASURE [Bachman, 1999].

2.7.2 GIS AND AIR QUALITY

Many air dispersion models are now available with a GIS such as ADMS-urban. A number of researchers have linked the CALINE series of models to a GIS. For example, Nasef [1995] developed a GIS to support roadway impact assessment, which incorporated CALINE4. Nasef recommended that the system be linked with a traffic emission model to replace the screening procedures currently employed. Hallmark [1996] linked a GIS with two dispersion models (i.e. CALINE3 and CAL3QHC) to estimate pollutant concentration levels in the vicinity of 'drive-thru' restaurants and banks. Researchers at the University of Huddersfield mapped urban air pollution at the small area scale (10 m^2) using regression analysis in the ARC/INFO GIS package [Smallbone, 1998]. Collins [1998] employed also a number of statistical methods (e.g. Kriging, and Interpolation) and CALINE3 to predict traffic related pollution in Huddersfield within the framework of a GIS. Li et al. [1999] employed HIWAY2 within a GIS to analyse the distribution of the concentration of pollutants along roadways. Wood [1997] identified the magnitude and spatial nature of residual errors between predicted and actual air quality impacts using a GIS. Rebolj and Sturm [1999] integrated an emission rate and dispersion model within a GIS framework. The SAVIAH project [Briggs et al., 2000] developed a GIS-based, regression mapping technique to model spatial patterns of traffic-related air pollution. Shivarama et al. [1998] integrated a GIS and two air quality models (i.e. PEM2 and TRIAD) into a spatial decision support system for air quality management. Kingham [1993] examined links between ambient air pollution and respiratory health in the Lancashire town of Preston within a GIS environment. Researchers at the University of Northampton employed a number of dispersion models, for example CALINE3, ISC3 and ADMS-urban, to estimate exposure to traffic related pollution (i.e. nitrogen dioxide) within a GIS environment [deHoogh, 1999]. Wills [1998] investigated environmental health indicators for epidemiology and policy applications using CALINE3 within ArcView® desktop mapping and GIS software. Jensen [1998] integrated the Danish OSPM and a GIS to investigate population exposure to traffic air pollution. Scott [1998] expanded the analytic capabilities of the traditional GIS to display pollutant concentrations generated by the US-EPA dispersion model ISCST3 in three-dimensional space. Forkenbrock and Schweitzer [1999] investigated the extent to which the air quality consequences of a traffic system change would disproportionately affect minority or low-income populations in the USA. The approach applied a GIS to

blend US Census data with the results from emission and dispersion models of vehicle-generated pollutants to discern whether disproportionate effects would occur.

2.8 AQMS SPECIFICATION

The literature review above demonstrated a number of advantages and disadvantages of existing emission inventory and air quality models. Based on this review, a specification for an 'ideal' but 'realistic' integrated AQMS is formulated. The specification below draws on the assets and inadequacies of the models and methods described in this Chapter.

1. Three components defining traffic activity and composition, emission rates and pollutant dispersion should be used, and all three should be of comparable accuracy. The integrated model should be modular in design so that individual components can be falsified (i.e verified and validated) or replaced.
2. The model should estimate the production of the primary regulated pollutants, toxics and greenhouse gases in space and time.
3. The model should operate at a meso-scopic level (e.g. simulating categories of vehicles and their operating mode). At the very least, the effect of congestion at different locations should be taken into account explicitly.
4. There should be a comprehensive representation of vehicle categories. Since traffic models normally classify vehicles into two or three types, a vehicle type mapping should be performed to incorporate a large number of categories.
5. The model should be capable of employing real (from an urban traffic control system) or passive (from a traffic model) traffic data.
6. The most up-to-date reliable emission rate model should be employed and it should be developed for the country or region of application.
7. The model should quantify separate hot-stabilised, start-up and evaporative emissions. As vehicle emission standards tighten, start-up and evaporative emissions will become more and more prominent.
8. The model should be capable of being updated continuously as new and better emissions data become available.
9. The model should be as generic as possible, so that it can employ data from the large range of existing monitoring systems.
10. A GIS should be employed for data presentation and visualisation. This will allow for the spatial allocation of emissions and pollutant concentrations.

11. The model should be validated using retail fuel sales data and roadside pollutant measurements.
12. The model should be applied and validated at a number of locations to ensure transferability.

Finally, a good AQMS should incorporate the latest traffic, emissions and pollutant dispersion knowledge at a low level of spatial aggregation (restricted only by data availability).

2.8.1 POLLUTANT DISPERSION MODEL

As already stated, Bachman [1999] suggests that the level of spatial aggregation of mobile source emissions needed by air quality models could define the minimum level of model aggregation required. In the light of this, an appropriate dispersion model was first selected for use in this project.

On the basis of the preliminary literature review and evaluation of fundamental requirements (e.g. availability of source code, published literature, user manual, and validation), it was decided to employ CALINE4 for local dispersion (kerbside) modelling for the following reasons:

1. The source-code was made available by the developers, CALTRANS [Kear, 1998]. This allowed modifications to be made to the program.
2. Complete documentation is available, ranging from the scientific and technical description down to the user's manual.
3. Extensive model evaluation and validation has been performed both by the developers and independently.
4. The model is computationally efficient.
5. Although, the model was developed in the USA, it is employed throughout the world for roadside pollution prediction. For example, it has been used in Australia [Shenouda and Schmidt, 1997], Bangladesh [Rahman, 1999], Canada [Loranger et al., 1995], China [Chan, 1995], Colombia [Martínez et al., 1999], India [Luhar and Patil, 1989], Ireland [Sweetman, 2000], Italy [Corti and Carnevale, 2000], Japan [Kajihara, 1999], Korea [Min-Jung, 1999], Lebanon [El-Fadel and Shazbak, 1999], Romania [Ionel et al., 1999], Saudi Arabia [Nasef, 1995], South Africa [Gondwe, 1998], and the UK [Sokhi, 1998a] amongst others.

6. Finally, the model compares favourably with other dispersion models.

CALINE4 is the latest version of the CALINE series of models [Benson, 1992]. The UK-DETR [1998b] in its guidelines on the 'Selection and Use of Dispersion Models' classifies CALINE4 as an "advanced" model. Hung et al. [1991] claims that CALINE4 offers the best potential in urban pollution modelling, and it "is the only Gaussian model that claims to be able to model relatively low wind speeds of 0.5 m/s and deal with three situations: open terrain, bluff and canyon". A bluff is similar to a street canyon except it applies to depressed roadways (i.e. below ground level but not covered). Held et al. [1998] stated that, "CALINE4's accuracy is well balanced with the accuracy of state-of-the-art predictive models for emissions and traffic". Bielli et al. [1998] found that the state-of-the-art includes various kinds of Gaussian models of different complexity and characteristics, among which the most relevant for evaluating dispersion phenomena in urban areas is CALINE4. Hassan et al. [2000] stated that "Gaussian plume models such as CALINE4 have extensively being used in assessing the impacts of existing and proposed sources of air pollution on local and urban air quality". The NCHRP in the USA (project 25-6) awarded a contract to develop an Integrated Air Quality Intersection Computer Model [Yedlin et al., 1998]. The suitability of existing intersection air quality models was assessed and the use of CALINE4 was recommended. Ireson [1998] stated that CALINE4 was "efficient and reliable for most conditions" and "able to treat key worst-case processes". Singh [1997] reported CALINE4 as the best model for application in flat terrain. In a review of dispersion models used for environmental assessment process in the UK, Barrowcliffe [1994] notes that consultancies have, almost universally, chosen to employ CALINE4 for traffic emissions. QUARG noted that there is a growing use of commercially available models from the USA of which the most commonly used is CALINE4 [QUARG, 1993a]. Zandi [1997] states with regard to the CALINE series of models that, "more complex models are unnecessary for most applications because of the uncertainties in estimating future emission factors and traffic volumes". Leung et al. [1996] stated that CALINE4 was the most commonly used model for predictive modelling of air pollution due to traffic. Collins [1998] stated that "CALINE4, and its predecessors, have been widely used across the USA and now also in the UK". Nanni et al. [1996] stated that, "for studies of line sources (i.e. highways), models are available which are adequate for flat terrain and steady-state conditions (i.e. US-EPA recommended CALINE-3)". Khare and Sharma [1999] found that "the most widely used models are Gaussian based viz. CALINE4 and CALINE3". Vanderheyden et al. [1997] states that the "numerical modelling of vehicular emissions using the United States Environmental Protection Agency's CALINE4 and

CAL3QHC dispersion models to predict air quality impacts in the vicinity of roadways is a widely accepted means of evaluating vehicular emissions impacts". Vanderheyden et al. [1997] further stated that, "the numerical models can account for atmospheric dispersion in both open or suburban terrain". An evaluation of CALINE4 in complex terrain [Benson et al., 1986] found that the "model performance for receptors near the roadway in complex terrain is judged adequate for impact assessment purposes". However, Benson et al. [1986] noted that "predictions for more distant receptors are much less reliable" than for closer receptors. Namdeo [1995] concluded that, "CALINE4 is the best model for application in flat terrain, with limited use in complex terrain". The Environmental Unit of Enterprise Ireland, with commercial and local authority clients also employs CALINE4 to estimate traffic related pollution in Dublin [Sweetman, 2000].

The highest level of spatial resolution that CALINE4 can handle is a segment of a roadway (i.e. width and length of one vehicle), while the highest level of temporal resolution that the model can handle is one-hour. An appropriate emissions rate model will have a level of spatial and temporal resolution, which is comparable to that of CALINE4.

2.8.2 EMISSIONS RATE MODEL

Guensler [1993] stated that the "first item to keep in mind, from an emission inventory standpoint, is that estimation of vehicle activity must necessarily be a secondary process". In addition Guensler [1993] believes that emission producing vehicle activity must be identified initially, and then emission rates associated with those activities must be developed. Finally, vehicle activity should be quantified. Too often, emission inventory developers identify traffic activities first, through the development of a traffic model and then select corresponding emission factors. This can lead to significant discrepancies, as some vehicle emission producing activity may be omitted. For example, while it is well known that a small percentage of vehicles (high- and super-emitters) are responsible for the majority of emissions, none of the CTEMs reviewed include high or super emitters.

This review has highlighted a wide range of emission rate models that are available to accept traffic information as an input. The literature review was performed to gather information on these existing models, and to determine their suitability for use in this project.

Following this review, it was decided to employ the MEET emissions data. MEET is a European Commission (Directorate for Transport) sponsored project under the Fourth Framework Programme. The MEET project was undertaken to provide a basic, Europe-wide procedure for evaluating the impact of transport on air pollutant emissions and energy consumption. It brings together the most comprehensive and up-to-date information on vehicle emissions and activity statistics which, together, make it possible to estimate the emissions resulting from almost any transport operation. The primary objective of the project was to provide a set of data and models, allowing different European users, and especially European Union projects, to calculate the pollutant emissions and the fuel or energy consumption of the different transport modes at strategic level, for the past, present and future situations.

The main attractive features of MEET, which render it suitable for the present project, are:

1. The raw data employed is collated from all over Europe;
2. The vehicle test population represents a cross-section of the existing traffic fleet;
3. Emissions produced by a large number of vehicles were measured under various driving conditions e.g. regulatory driving cycles and instrumented vehicles;
4. Many of the driving cycles were real-world driving cycles;
5. It was developed for all of Europe, therefore can be applied in Dublin;
6. The most up-to-date and comprehensive emissions data currently available in Europe – released in July 1999;
7. A large range of pollutants are included (e.g. carbon monoxide, nitrogen oxide, sulphur dioxide and particulate matter), green house gases (e.g. carbon dioxide and methane) and toxics (e.g. benzene and 1,3-butadiene);
8. Emissions are divided into three types i.e. hot stabilised, start-up and evaporative emissions;
9. Roadways are categorised into three types i.e. urban, rural and motorway;
10. The facility to predict future emission estimates is incorporated by taking into account changes in vehicular technology and emission legislation; and
11. MEET is a fuel-based methodology therefore it can be validated against fuel sales data first before compiling an emission inventory.

However, there are a number of deficiencies in the MEET methodology. For example, vehicle modes of operation are not taken into account explicitly. These issues will be addressed in Chapter four.

2.8.3 TRAFFIC MODEL

The traffic module adopted in this study comprises both the SATURN [Van Vliet, 1992] and the SATCHMO [Willumsen et al., 1993] models. The SATURN model was originally developed at the Institute of Transport Studies, University of Leeds. WS Atkins developed SATCHMO for multi-modal simulation. The SATURN & SATCHMO model was originally implemented for the greater Dublin area as part of the Dublin Transport Initiative in the mid-1980s. It has been up-graded a number of times since then. The model has been extensively calibrated and validated by the Dublin Transport Office [McCabe, 1998]. The simulation results from the model were made available for this research study.

2.9 SUMMARY

This background Chapter reviewed the key literature related to air quality modelling. The compilation of motor vehicle emission inventories was described in detail. A state-of-the-art and state-of-the-practice review was performed and presented on current available motor vehicle emission inventory models. A brief introduction to air quality modelling was outlined. The modelling of roadside concentrations was illustrated. The use of geographic information systems in relation to emission inventories and air quality modelling was articulated and found to be a necessary part of air quality analysis. A specification for an 'ideal' but 'realistic' AQMS was drawn up. Based on this specification, a dispersion model, an emission rate model, and a traffic model were selected for use in this project. The design of the proposed integrated AQMS meets the goals and objectives stated in Chapter one. In addition the model avoids the constraints of extensive data development and cost.

The next Chapter describes, in detail, the conceptual design of the MVEIM developed for use in this project.

3. CONCEPTUAL DESIGN OF MVEIM

3.1 INTRODUCTION

This Chapter discusses the formulation of a MVEIM and the underlying theories associated with its design. The primary modules of the MVEIM are illustrated in a flow diagram and are subsequently described in detail. A database of relevant emission and fuel consumption factors - which are derived from the MEET project amongst others, is also described. The inherent assumptions employed in the MVEIM are identified. Finally, the integration of the MVEIM with a GIS for visualisation and analysis purposes is presented.

3.2 MVEIM COMPONENTS

While there is a general agreement that new processes need to be formulated and subsequently models developed to overcome current deficiencies in emission inventory models, there is disagreement over the best method to achieve this [Washington, 1996]. One of the primary objectives of this research project was to develop a method of determining traffic model-based urban emissions inventories, which reflect the need to include different modes of vehicle operation, but on a 'practical' and 'realistic' basis. In addition, the traffic activity and emissions factors should be of comparable accuracy, both in spatial and temporal resolution. The calculation technique employed in the MVEIM is generally known as a meso-scale method. The MVEIM comprises of four primary modules, namely:

- A traffic module;
- An engine/emissions control technology module;
- A motor vehicle emissions rate algorithms module; and
- A motor vehicle fuel consumption module.

In addition, the MVEIM incorporates an emissions and fuel consumption factors database. The relationships between the individual modules and emissions factors database and their respective inputs and outputs are illustrated in Figure 3.1.

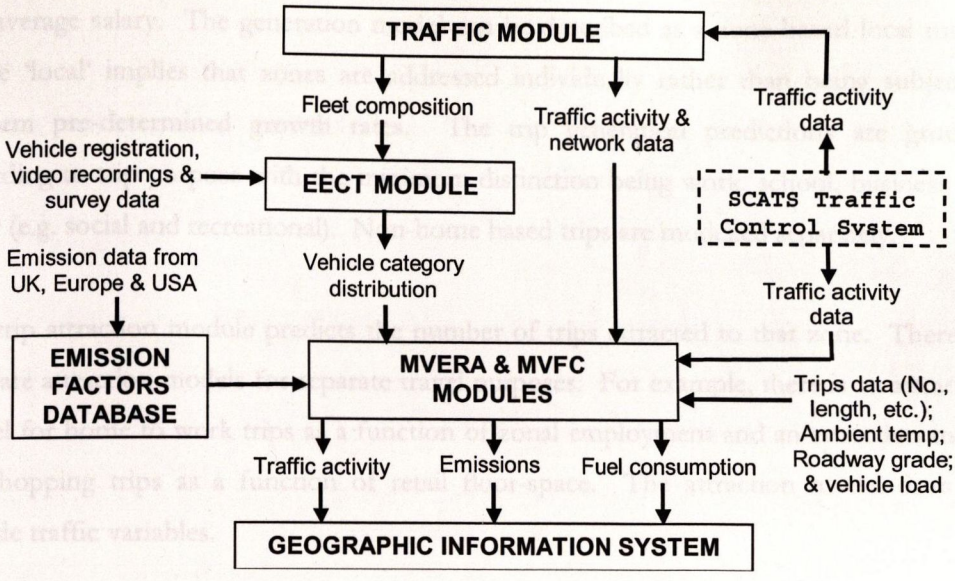


Figure 3.1: Schematic layout of the MVEIM showing the main components

3.2.1 TRAFFIC MODULE

As stated in Chapter two, the traffic module adopted in this study comprises both SATURN [Van Vliet, 1995] and SATCHMO [Hall, 1996] models.

SATURN & SATCHMO provides a detailed representation of the greater Dublin transportation system including junctions (priority, signal and roundabout) for both average weekday morning peak and afternoon inter-peak hours. The period from 8 am to 9 am is assumed to be representative of the peak hour while that from 2 pm to 3 pm is assumed to be representative of the inter-peak hour [SDG, 1994].

For modelling purposes, the city is divided into three hundred and sixty-seven zones, which together cover the greater Dublin area. Each fine zone is based on Ward and District Electoral Divisions as specified by the CSO [1996]. The zones do not overlap.

SATURN & SATCHMO is divided into four primary modules: trip generation and attraction, trip distribution, modal split, and assignment. The units in which these modules operate are trips. A trip can be defined as a one-way movement from an origin to a destination, each of which the traveller has a purpose.

The trip generation module predicts the number of trips generated in a zone as a function of the socio-economic characteristics of that zone. These characteristics include total population (working and school aged), places (employment and school), total households

and average salary. The generation model can be described as a zone-based local model, where 'local' implies that zones are addressed individually rather than being subject to uniform pre-determined growth rates. The trip generation predictions are grouped according to trip purpose with the minimum distinction being work, school, business and other (e.g. social and recreational). Non-home based trips are modelled separately.

The trip attraction module predicts the number of trips attracted to that zone. There are separate attraction models for separate travel purposes. For example, there is an attraction model for home to work trips as a function of zonal employment and an attraction model for shopping trips as a function of retail floor-space. The attraction model does not include traffic variables.

In the trip distribution module, the forecasted number of trips generated by each origin zone attracted to each destination zone is modelled.

The modal split module determines the mode of transport that is used. The functional form employed is the 'availability' or 'non-availability' of a car to distinct categories of individuals or market-segments. The categories with a car-available at the time of their trip have a choice of using the car or public transport (i.e. bus or rail). On the other hand, the categories with no-car-available at the time of the trip are limited to public transport. The choice methodology is arranged in a hierarchical configuration. The actual modal split is determined by employing 'logit' formulation and the application of generalised 'cost' parameters. These cost parameters are calculated from research methods (e.g. stated preference surveys) and the relative costs of private and public transport. Private transport costs includes such variables as vehicle operating cost and parking charges, while public transport costs including fares and time such as vehicle, transfer, walk and waiting.

The assignment module uses two sub-models to assign trips between all zone pairs to links, based on the minimum time (or cost, or combinations of time and cost) path between zones and also on capacity constraints. The first sub-model employs cyclic flow profiles to represent the movement of platoons of motor vehicles over a road network. This sub-model takes account of the interaction of different flows at roundabouts, signal controlled and priority junctions. It requires data concerning the flow on each link in the network to determine queues, capacities and time delays. A separate sub-model employs a 'trip-matrix' to determine these flows. The module also assigns passengers to public transport networks. Mode choice and assignment in congested urban networks are co-dependent.

There are two generic inputs for SATURN & SATCHMO, namely the 'trip-matrix' and the 'network', which may be regarded as 'demand' and 'supply' inputs. Figure 3.2 illustrates this concept.

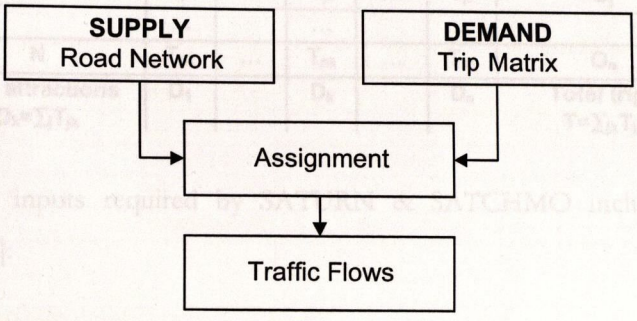


Figure 3.2: Matching demand with supply in SATURN & SATCHMO

The trip-matrix (see Table 3.1) specifies the number of trips from zone to zone and the 'network' specifies the geographical location and topography of the roadways upon which the trips take place. The primary source of raw data for the trips-matrices is a comprehensive set of kerbside surveys and public transport origin/destination interviews (i.e. on-board/at bus-stop/rail-station interviews). Obviously, it is next to impossible to generate trip-matrices to cover all of Dublin from the above methods. Therefore, traffic count surveys and air passenger traffic were used to assist in the derivation of 'most-likely' trip-matrices. The air passenger traffic indicated the number of people travelling to and from the airport. The latter trip-matrices can be used to ensure that the assigned flows match the observed flows within certain pre-defined limits. Individual matrix cells represent the number of trips from one zone to another. Total trips to and from a specific zone for a given period of time are determined from trip matrix column and row totals. Separate matrices are created for two time periods (peak and inter-peak) and four modes of transport (car, HGV, bus and rail).

The physical network comprises all motorways, main roads, secondary roads, and the more commonly used minor streets. The junctions are represented by a series of uniquely numbered four-digit nodes while the segments of roadways are represented by links. The links are defined in terms of the nodes at either end. Traffic enters a link at one node and exits at another node. A 'turn' is represented by a sequence of three node numbers: start, end and next. The network in Dublin is divided into two distinct parts – 'inner' and 'outer'. The inner network has a relatively high number of junctions in comparison to roadways while the outer network mainly contains road data.

Table 3.1: The origin-destination matrix [source: Kupiszewska, 1998]

Zones	1	...	k	...	n	Trip productions $O_j=\sum T_{jk}$
1	T_{11}	...	T_{1j}	...	T_{1n}	O_1
	...		...		...	
j	T_{j1}	...	T_{jk}	...	T_{jn}	O_j
	...		...		...	
N	T_{n1}	...	T_{nk}	...	T_{nn}	O_n
Trip attractions $D_k=\sum_j T_{jk}$	D_1		D_k		D_n	Total trips $T=\sum_{jk} T_{jk}$

In summary, the inputs required by SATURN & SATCHMO include the following [Chiquetto, 1995b]:

- O-D matrix;
- Bus routes and frequencies;
- Road network coding (zones, nodes, links, centroids, gateways);
- Link data (length, capacity, number of lanes, flow directions, free flow traffic speed);
- Turn data (saturation flow, turns allowed, turning capacity);
- Junction types (priority, signalised, roundabout);
- Node co-ordinates;
- Equivalent vehicle lengths;
- Parameters such as minimum gap acceptance between vehicles; and
- Traffic signal data, stage lengths, offsets and cycle times.

Both the trip-matrices and road network are employed in a 'route choice' model which allocates trips to 'routes' throughout the network, as a result of which total volume flows along links may be summed and the corresponding network 'costs' calculated.

SATURN & SATCHMO divides motor vehicles into a three-category classification system (LDV, HGV and bus).

The output parameters passed from the SATURN & SATCHMO traffic module to the MVERA module are shown in Table 3.2 (vehicle type is passed to the EECT module).

Table 3.2: Shared parameters between SATURN & SATCHMO and MVERA modules

Parameter	Classification	Type	Unit
link length	network data	static	km
link type	network data	static	urban, rural or motorway
junction type	network data	static	signal, priority, or round-about
vehicle type	fleet characteristic	dynamic	LDV, HGV or bus
traffic volume	travel activity	dynamic	vehicles/hr
link velocity	travel activity	dynamic	km/hr
queue length	travel activity	dynamic	pcu
link time-delay	travel activity	dynamic	seconds
turn time-delay	travel activity	dynamic	seconds
n° of primary-stops	travel activity	dynamic	---
n° of stop-starts	travel activity	dynamic	---

One pcu is assumed to occupy a length of 5.75 m [Bell, 1978]. Three pcus are equivalent to one bus or one HGV. Time delays (both link and turn) are the average delays experienced by each pcu during the time period modelled. The free flow time is the time that would be spent travelling on a link operating at its free-flow velocity. The total travel time is the sum of both free flow and respective time delay (either link or turn). Primary stops occur when a vehicle arrives at the back of a queue and stop-starts occur when a vehicle moves up in a queue.

3.2.2 EECT Module

In emission inventory modelling, fleet distribution must be described in detail because it affects many parameters employed in emissions rate determination [Bachman et al, 1996]. However, the traffic module employed categorises the entire vehicle population into only three types (LDV, HGV and bus), thus ignoring vehicle age, engine displacement, gross vehicle weight, fuel type, and so forth.

A further breakdown of the fleet distribution on a spatial and temporal basis is determined by the EECT module. The process of converting one dataset to another is known as a vehicle-type mapping. This mapping procedure is illustrated graphically in Figure 3.3. In this illustration, the gross vehicle categories of the traffic module are given across the top of a matrix. The category mapping simply gives the percentage distribution for each category/year bin that corresponds to the appropriate MVERA category. These mappings can be created using knowledge of the traffic module categories that correspond to the different MVERA categories. Technology categories can be defined as groups of vehicles that have been identified as having significant emission rate differences.

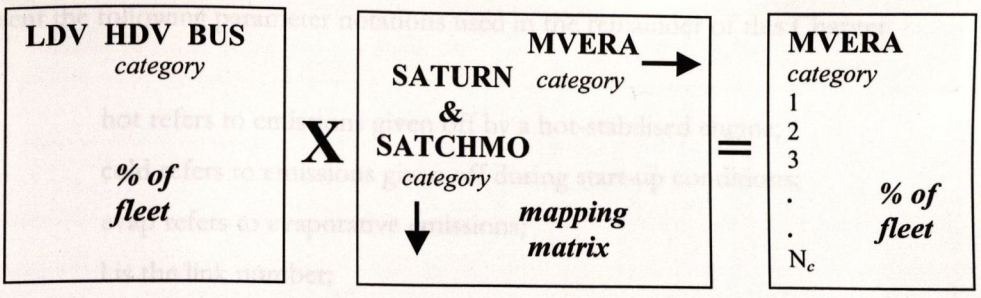


Figure 3.3: SATURN & SATCHMO to MVERA module vehicle category mapping procedure

One of the major advantages of employing this type of procedure is that different vehicle categories from other traffic models can be used with the MVERA module. This means that the MVEIM can be applied in places where a SATURN & SATCHMO traffic module is not available.

Through the mapping procedure, the EECT module estimates the relative percentages, for individual links or zones, of each vehicle category (LDV, HGV and bus), defined on the basis of engine capacity, engine type (spark ignition, compression ignition), fuel delivery system (carbureted, fuel injection), emission control system (open-loop, closed-loop), and catalyst type (no catalyst, oxidation catalyst, three-way catalyst). Subsequently, the age profile of the fleet and the type of fuel burned can be determined for each link.

As already stated, a small percentage of vehicles emit a disproportionate percentage of pollutant emissions. Identifying the percentage of normal- and high-emitting vehicles in an urban area and quantifying their emissions is vital for accurate emission inventory accounting [Wolf et al., 1998]. By spatially and temporally distinguishing these vehicles, abatement strategies, which specifically target high-emitters, can be better evaluated. For example, older vehicles have higher emissions than new vehicles and cars that originate in lower socio-economic zones tend to be old. Buses and public service vehicles on specific routes in Dublin are also known to be old.

3.2.3 MVERA Module

The primary function of this module is to determine the composite or total emission rate for each link in the network per unit time. This is achieved in a two-step process, namely determination of link segments and subsequent emission calculation. Each of these steps is

now described in detail. Before discussing the formulation for this methodology, we present the following parameter notations used in the remainder of this Chapter.

hot refers to emissions given off by a hot-stabilised engine;
cold refers to emissions given off during start-up conditions;
evap refers to evaporative emissions;
l is the link number;
t is the specific time period under consideration (sec.);
p is the pollutant (CO, NO_x, PM_{10}, VOC, etc.);
v is the vehicle category (e.g. cars, trucks, buses, motorcycles, etc.) and sub-category (size of engine or weight);
y is the vehicle manufacture year; and
r is the road type (urban, rural or motorway);
g is the average grade of the roadway (%);
s is the average speed of the vehicle (km/hr)
w is the average weight load on the vehicle i.e. passengers or payload (%);
T is the ambient temperature (°C);
P is the RVP of a fuel (kPa);
f is the fuel type (e.g. petrol, diesel and LPG);
N_v is the number of vehicles in category v;
N_y is the number of vehicles in category v, manufactured in year y; and
N_l is the number of links in a study-domain.

3.2.3.1 Determination of link segments

For modelling purposes, each lane on a roadway is divided into a number of segments reflecting the areas in which vehicles are most likely to be in cruising (i.e. free flow) or queuing (i.e. creep) mode. A free flow link is defined as a segment of roadway having a constant width, traffic volume, travel speed, and vehicle emission factor. A queue segment is defined as a segment of roadway with a constant width and emission source strength, on which vehicles are idling for a specified period of time.

As emission factors are normally given in g/s or g/km, link segments are divided according to both time and distance travelled.

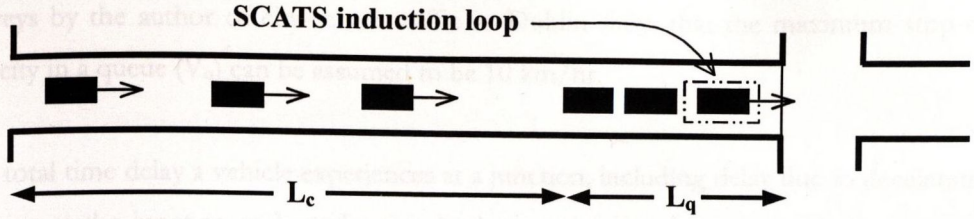


Figure 3.4: Division of a link into segments representing lengths spent cruising and queuing respectively

In mathematical form, the time taken for a vehicle to travel from one end of the roadway to the other is made up of the sum of the following components:

$$t(l,t) = t_c(l,t) + t_q(l,t) \qquad 3.1$$

where: $t(l,t)$ is the total time taken to traverse link l (in s);

$t_c(l,t)$ is the time spent in 'cruise' mode on link l (in s); and

$t_q(l,t)$ is the time spent in 'queue' mode on link l (in s).

The movement of a vehicle queuing at an intersection or roundabout, whereby it progressively approaches the junction through a number of stop-starts is known as creep. A stop-start consists of an increase in velocity followed by a decrease in velocity (as depicted graphically in Figure 3.5). For example, when an intersection traffic light turns 'red', a queue forms on a roadway leading to a junction. A vehicle joining the back of the queue will have to come to a complete stop (i.e. velocity equal to zero) and idle for a period of time. When the light turns 'green', a number of vehicles will traverse the junction. The vehicle at the back of the queue will move up the queue but it may not traverse the junction (i.e. it may have to wait for another 'green' light). This movement up the queue is known as a stop-start. The combined stop-start and idle is generally known as 'creep'.

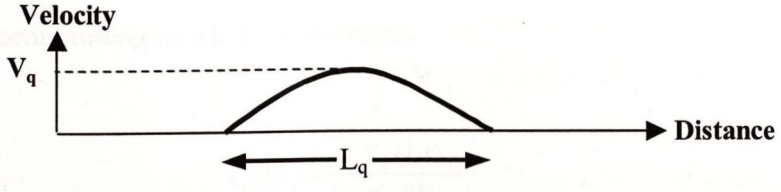


Figure 3.5: Velocity-distance diagram of stop-start manoeuvre in a traffic queue

Surveys by the author of city-centre traffic in Dublin show that the maximum stop-start velocity in a queue (V_q) can be assumed to be 10 km/hr.

The total time delay a vehicle experiences at a junction, including delay due to deceleration, queuing at the junction and accelerating back to cruise speed is commonly known as the 'control delay'.

The traffic module determines the time spent queuing at the end of roadway and the number of vehicles queuing (in pcu), from which the length of the queue segment (in km) is determined as:

$$L_q(l,t) = \frac{N_q(l,t)\left[L_{pcu} + L_{sp}\right]}{1000} \qquad 3.2$$

where: $L_q(l,t)$ is the length of the queue segment on link l (in km);

$N_q(l,t)$ is the number of pcu's queuing at a junction on link l;

L_{pcu} is the length of a pcu (in m); and

L_{sp} is the distance between two vehicles (in m);

The vehicle is assumed to be in cruising mode for the remaining portion of the link. The distance along a link travelled by a vehicle in cruising mode is calculated as:

$$L_c(l,t) = L(l) - L_q(l,t) \qquad 3.3$$

where: $L_c(l,t)$ is the length of the cruise segment on link l (in km);

$L(l)$ is the length of link l (in km);

The time spent cruising on a link l is therefore:

$$t_c(l,t) = \frac{L_c(l,t)}{3600 \cdot V(l,t)} \qquad 3.4$$

where: $t_c(l,t)$ is the time spent cruising on link l (in s); and

V(l,t) is the average vehicle velocity on link l (in km/hr).

The above calculations assume that all vehicles have to come to a complete stop at the end of a link. In other words, every vehicle approaching a junction will have to queue. In reality, a percentage of the vehicles will pass through the junction without queuing, and therefore will not have to slow down. Figure 3.6 graphically represents the two typical trajectories of a vehicle traversing an intersection, with the y-axis parallel to the roadway. For simplicity of explanation, it is assumed that the approach and departure roadways to and from the intersection respectively are both one-way and that vehicles do not make a right or left turn.

Trajectory A (in Figure 3.6) is typical of a vehicle that does not stop or slow down while traversing the intersection. These vehicles are assumed to have a steady-state velocity while travelling both on the roadway and through the intersection. However, the average velocity of the two adjoining roadways may be different. Consequently there is a change in slope of the trajectory at the x-axis to represent this change in velocity.

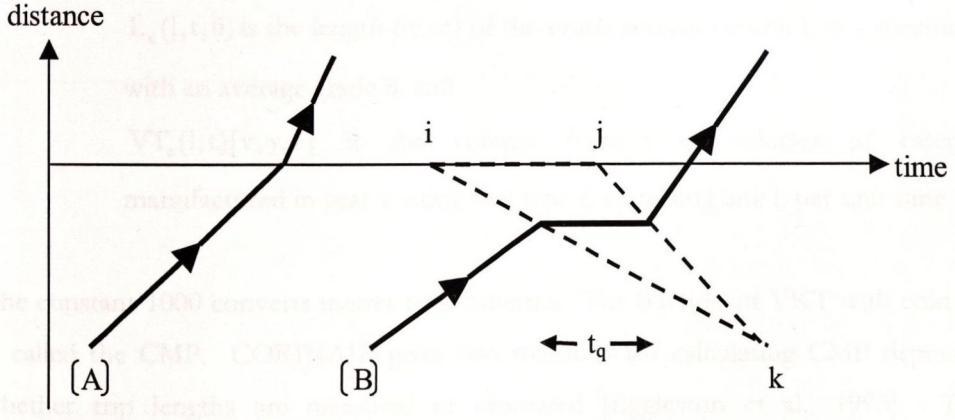


Figure 3.6: Time-distance diagram of vehicle movements and queuing areas at an under capacity signalised intersection

Trajectory B (in Figure 3.6) is typical of a vehicle that stops and queues at the intersection. The vehicle decelerates from its cruising velocity on the approach roadway, before it stops to queue for a period of time t_q and subsequently accelerates away to reach it new cruising velocity on the departure link. The triangular area i-j-k enclosed by the dashed-lines defines the queuing area at the junction. The diagram does not illustrate over-capacity at a junction, since averaged-hourly values are employed, and it is assumed that the junction will clear in any given hour. In addition, an instantaneous stop is assumed for each vehicle (i.e. vehicular acceleration and deceleration are not taken into account).

3.2.3.2 Emissions calculation methodology

The hot exhaust emissions (i.e. CO, CO_2, SO_2, NM-VOC, CH_4, NO_x, PM_{10}, $PM_{2.5}$, C_4H_6, and C_6H_6) from traffic cruising on a link per unit time (in this case an hour) is:

$$E_c^{p,hot}(l,t) = \sum_{i=1}^{N_v}\sum_{j=1}^{N_y}\left[\frac{CEF_c^{p,hot}[v,y,f,w,s,r,\theta]\cdot L_c(l,t,\theta)\cdot VT_c(l,t)[v,y,f]}{1000}\right] \quad \textbf{3.5}$$

where: $E_c^{p,hot}(l,t)$ is the hot emission rate per unit time t (e.g. g/hr), of a particular pollutant p emitted by all traffic cruising on link l;

$CEF_c^{p,hot}[v,y,f,w,s,r,\theta]$ is the average representative hot speed dependent composite emission factor (in g/km) for pollutant p, relevant for vehicle category v, manufactured in year y, using fuel type f, carrying an average weight load w, travelling at an average speed s, on roadway r, with an average road grade θ;

$L_c(l,t,\theta)$ is the length (in m) of the cruise section on link l, in a specific time t, with an average grade θ; and

$VT_c(l,t)[v,y,f]$ is the volume fraction of vehicles of category v, manufactured in year y, using fuel type f, traversing link l, per unit time t.

The constant 1000 converts metres to kilometres. The fraction of VKT with cold engines is called the CMP. CORINAIR gives two methods for calculating CMP depending on whether trip lengths are measured or estimated [Eggleston et al., 1993]. The two definitions are given as:

$$CMP = 0.698 - 0.051L_{trip,m} - (0.01051 - 0.000770L_{trip,m})T_{amb} \quad \textbf{3.6}$$

and

$$CMP = 0.6474 - 0.02545L_{trip,e} - (0.00974 - 0.000385L_{trip,e})T_{amb} \quad \textbf{3.7}$$

where: $L_{trip,m}$ is average measured trip length (km);

$L_{trip,e}$ is average estimated trip length (km); and

T_{amb} is ambient temperature (^{0}C).

These empirical relationships are derived from data collected from surveys (throughout Europe) performed during the development of COPERT [Eggleston et al., 1993]. The sensitivity of CMP to temperature and trip length is shown in Figure 3.7. This methodology assumes that the maximum CMP on any given link is 70% and that a vehicle has reached hot stabilised running conditions before 25 km. It is highly unlikely that more than 70% of the vehicles on any given roadway would be operating under start-up conditions. In addition, other studies found that a vehicle takes an average of 6 km before it is fully warmed up [Farrauto and Heck, 1999]. It may be concluded that Eggleston et al. assumptions appear reasonable.

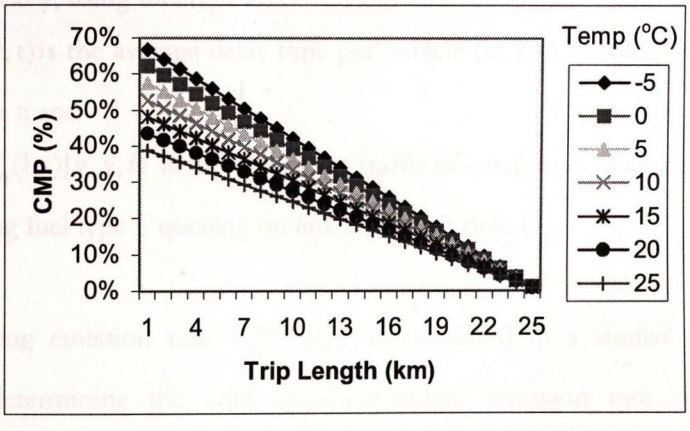


Figure 3.7: Sensitivity of cold-mileage-percentage to trip length and temperature

The cold emissions from road traffic cruising on link l per unit time is:

$$E_c^{p,cold}(l,t) = E_c^{p,hot}(l,t,\theta) \cdot REF_c^p[v,y,f] \qquad 3.8$$

where: $E_c^{p,cold}(l,t)$ is the cold emissions per unit time t (e.g. g/hr), of a particular pollutant p emitted by all traffic cruising on link l; and

$REF_c^p(v,y,f)$ is the relative emission ratio for pollutant p, relevant for the vehicle category v, manufactured in year y, using fuel type f.

As already stated, at signalised junctions, roundabouts, etc. and during periods of heavy traffic, vehicles are delayed due to primary and secondary queues or 'stops'. Primary 'stops' occur at traffic signals while secondary 'stops' occur due to congestion away from signalised junctions. In these states, travel-distance independent emissions are produced. The hot emissions from road traffic queuing on link l per unit time is:

$$E_q^{p,hot}(l,t) = \sum_{j=1}^{N_v} \sum_{k=1}^{N_y} \left[CEF_q^{p,hot}[v,y,f] \cdot t_q(l,t) \cdot VT_q(l,t)[v,y,f] \right] \qquad \textbf{3.9}$$

where: $E_q^{p,hot}(l,t)$ is the hot emission rate per unit time (e.g. g/hr) of a particular pollutant p emitted by all traffic queuing on link l;

$CEF_q^{p,hot}[v,y,f]$ is the average representative hot queuing composite emission factor (in g/sec) for pollutant p, relevant for vehicle category v, manufactured in year y, using fuel type f,

$t_q(l,t)$ is the average delay time per vehicle (in sec) queuing on link l, per unit time t; and

$VT_q(l,t)[v,y,f]$ is the volume of traffic of category v, manufactured in year y, using fuel type f, queuing on link l, per unit time t.

The cold queuing emission rate $E_q^{p,cold}(l,t)$ is calculated in a similar manner to that employed in determining the cold speed-dependent emission rate with an average representative queuing emission factor $E_q^{p,cold}[v,y,f]$ for a cold engine being used. As already stated, some vehicles will pass through a junction without having to queue and consequently $VT_c(l,t)[v,y,f]$ does not necessarily equal $VT_q(l,t)[v,y,f]$.

The evaporative emissions from road traffic traversing link l per unit time t is:

$$E^{p,evap}(l,t) = CEF^{p,evap}[v,y,f,T,P] \cdot VKT(l,t)[v,y,f] \qquad \textbf{3.10}$$

where: $E^{p,evap}(l,t)$ is the evaporative emission rate per unit time (e.g. g/hr) of a particular pollutant p, emitted by vehicles traversing link l;

$CEF^{p,evap}[v,y,f,T,P]$ is the average representative evaporative composite emission factor (in g/km) for the pollutant p, relevant for vehicle category v, manufactured in year y, using fuel type f, at an average temperature T, and having fuel RVP P; and

$VKT(l,t)[v,y,f]$ is the vehicle-kilometres-travelled on link l, per unit time t, by vehicles of category v, manufactured in year y, using fuel type f.

Road traffic also gives rise to particulate matter (PM_{10} and $PM_{2.5}$) from brake-wear, tyre-wear and re-entrained roadway dust. The main source of information on these particulates is AP-42 [US-EPA, 1996] and the validity of applying this data to an emission inventory for Dublin is open to question. It is likely however that any errors arising will be smaller than those incurred if these sources were ignored completely. It should be noted that engine exhaust emissions for particulate mater are included in Equation 3.5.

The total emission of a particular pollutant for all traffic on each link is calculated by summing the individual emission components:

$$E^{p}(l,t) = \left[E_c^{p,hot}(l,t) + E_q^{p,hot}(l,t)\right] \cdot (1 - CMP) + \left[E_c^{p,cold}(l,t) + E_q^{p,cold}(l,t)\right] \cdot CMP + \left(E^{p,evap}(l,t)\right) \quad \textbf{3.11}$$

The estimate of the emission inventory for pollutant p, due to traffic on all links per unit time t is:

$$E^{p}(t) = \sum_{l=1}^{N_l} E^{p}(l,t) \quad \textbf{3.12}$$

As already stated, the traffic module contains traffic activity and fleet composition data per road segment for the morning peak and afternoon inter-peak hours on a typical weekday. The yearly estimate of emissions is therefore:

$$E^{P}(yr)=\sum_{w=1}^{52}\left[\left(\sum_{wd=1}^{5}\sum_{h=1}^{24}k_1E^{P}(l,peak)+k_2E^{P}(l,interpeak)\right)+\left(\sum_{we=1}^{2}\sum_{h=1}^{24}k_3E^{P}(l,interpeak)\right)\right] \quad 3.13$$

where: yr is yearly or annual;

k_1 and k_2 are constants to relate peak and inter-peak weekday (wd) data to hourly data; and

k_3 is a constant to relate inter-peak weekend (we) data to hourly data.

3.2.4 EMISSION FACTORS DATABASE

Since no emission factors are available specifically for Ireland (except for alternative fuels), the emissions factors employed in this study are derived from the MEET project. In addition, these emission factors were supplemented with data from three alternative sources:

1. Emission factors developed for the UK (e.g. LRC, DMRB and TRL);
2. Emission factors produced under EU initiatives (e.g. CORINAIR, MODEM and EEA's Atmospheric Emissions Inventory Guidebook) and other independent European studies (e.g. HBEFA); and
3. The US-EPA's manual (AP-42) on the 'Compilation of Air Pollution Emission Factors' and other US studies (only PM_{10} and $PM_{2.5}$ emission factors for brake, tyre and pavement wear are applicable to Ireland).

The methodology implemented in the MVERA module has been designed in such a way as to make use of virtually all the available types of vehicle emission data, which are applicable to Ireland. Since this methodology is generic, future improved emission factors can be readily incorporated into the database.

3.2.5 MVFC MODULE

This MVFC module calculates fuel consumption for the various modes of transport in a similar manner to that employed in the MVERA module for estimating emissions. For example, the cruise-related fuel consumption is:

$$FC_c^{hot}(l,t) = \sum_{i=1}^{N_v} \sum_{j=1}^{N_y} \left[\frac{CFCF_c^{hot}[v,y,f,w,s,r,\theta] \cdot L_c(l,t,\theta) \cdot VT_c(l,t)[v,y,f]}{1000} \right] \quad \textbf{3.14}$$

where: $FC_c^{hot}(l,t)$ is the fuel consumption per unit time (e.g. g/hr), by all traffic cruising on link l;

$CFCF_c^{hot}[v,y,f,w,s,r,\theta]$ is the average representative hot composite fuel consumption factor (in g/km) relevant for vehicle category v, manufactured in year y, using fuel type f, carrying an average weight load w, travelling at an average speed s, on roadway r, with an average road grade θ;

The constant 1000 converts metres to kilometres. The cold emissions from road traffic cruising on link l per unit time is:

$$FC_c^{cold}(l,t) = FC_c^{hot}(l,t) \cdot REF_c[v,y,f] \quad \textbf{3.15}$$

where: $FC_c^{cold}(l,t)$ is the fuel consumption per unit time (e.g. g/hr), by all traffic cruising on link l; and

$REF_c(v,y,f)$ is the relative fuel consumption ratio relevant for the vehicle category v, manufactured in year y, using fuel type f.

The hot fuel consumption from road traffic queuing on link l per unit time is:

$$FC_q^{hot}(l,t) = \sum_{j=1}^{N_v} \sum_{k=1}^{N_y} \left[CFCF_q^{hot}[v,y,f] \cdot t_q(l,t) \cdot VT_q(l,t)[v,y,f] \right] \quad \textbf{3.16}$$

where: $FC_q^{hot}(l,t)$ is the is the fuel consumption rate per unit time (e.g. g/hr) by all traffic queuing on link l; and

$CFCF_q^{hot}[v,y,f]$ is the average representative hot composite fuel consumption factor (in g/sec) relevant for vehicle category v, manufactured in year y, using fuel type f.

The cold queuing fuel consumption rate $FC_q^{cold}(l,t)$ is calculated in a similar manner to that employed in determining the cold speed-dependent fuel consumption rate with an average representative queuing fuel consumption factor $FC_q^{cold}[v,y,f]$ for a cold engine being used.

The total fuel consumption by all traffic on each link is calculated by summing the individual emission components:

$$FC(l,t) = \left[FC_c^{hot}(l,t) + FC_q^{hot}(l,t)\right] \cdot (1 - CMP) + \left[FC_c^{cold}(l,t) + FC_q^{cold}(l,t)\right] \cdot CMP \qquad 3.17$$

The estimate of the total fuel consumption by all traffic on all links per unit time t is:

$$FC(t) = \sum_{l=1}^{N_l} FC(l,t) \qquad 3.18$$

The yearly or annual estimate of fuel consumption is:

$$FC^P(yr) = \sum_{w=1}^{52} \left[\left(\sum_{wd=1}^{5} \sum_{h=1}^{24} k_1 FC^P(l,peak) + k_2 FC^P(l,interpeak) \right) + \left(\sum_{we=1}^{2} \sum_{h=1}^{24} k_3 FC^P(l,interpeak) \right) \right] \qquad 3.19$$

The fuel consumption factors are stored in a database analogous to the emission factor database. Similar to the emission factors database, the fuel consumption factors are primarily derived from the MEET project and supplemented by other sources.

3.3 INHERENT ASSUMPTIONS OF THE MVEIM

Like any other model, the MVEIM has inherent assumptions and constraints. The primary assumptions are:

- The EECT module is heavily dependent on available statistical data.

- Traffic composition is homogenous and constant through a specified domain, e.g. a link.
- Vehicle speed is calculated as space-mean-speed and consequently is constant along any link.
- All delayed vehicles come to an instantaneous stop and instantaneously reach allocated cruise speed.
- The vehicle activity data adequately represents the traffic characteristics on all links.
- The emission factors stored in the EFD adequately represent the vehicle population in the study domain.

While these simplifying assumptions fall short of reality, they are reasonable in light of the overall precision required of the AQMS being developed. In addition, thay are compensated for in other modules of the MVEIM. For example, a vehicle joining a queue will not come to an instantaneous stop (i.e. it will decelerate). However, the effects of deceleration and acceleration are taken into account implicitly in the emissions factors employed in the MVEIM.

3.4 INTEGRATION WITH A GIS

As already stated, a GIS is utilised to facilitate presentation and visualisation of the fuel consumption and emissions inventories. The critical decision is how to integrate the MVEIM with a GIS. Two primary approaches exist, namely full integration or coupling [Karimi and Houston, 1996].

In the full integration method, a GIS programming language is employed to create and implement the MVEIM. Consequently, the MVEIM becomes one of the analytical functions of the GIS. The primary advantage of this method is a common data structure and data model for representing real world features. Also data handling and visualisation can be executed within one software system. However, there are processing limitations in the full integration methodology, as a GIS lacks the ability to perform sophisticated mathematical operations or computationally-intensive modelling efficiently [Densham and Goodchild, 1990].

In the coupling method, a GIS is employed to help prepare model-input data, and display model results. The model exists as a stand-alone program. The primary benefit of this approach is that each system complements the other. For example, the MVEIM provides

data to the GIS for spatial analysis and the GIS can be employed to prepare input files and allow model results to be displayed in a map form. The major drawback with this integration method is that repetitious processes such as converting model output to GIS, can be laborious and may have to be performed over and over again by the user, after each model run. However, this conversion process can be automated by using writing code in FORTRAN, C/C++, Microsoft® VBA or any other programming language.

It was decided to employ the coupling method and use the GIS to display the MVEIM results. The DTO had previously coupled a GIS to the traffic module SATURN & SATCHMO [McCabe, 1998]. Therefore, the approach followed was to extend the capabilities of the GIS to incorporate the MVEIM results.

3.5 SUMMARY

A conceptual MVEIM was described in detail in this Chapter. The model consists of four modules, namely a traffic module, an EECT module, a MVERA module, and a MVFC module. The model also includes a database of relevant emission and fuel consumption factors derived from MEET data and supplemented by others. The inherent assumptions employed in the conceptual model were listed. The conceptual model is to be integrated with a GIS for visualisation and analysis purposes.

The development and formulation of the emission factors employed within the MVEIM are described in detail in the next Chapter. In addition, a comparison is drawn between the emission levels from conventional and alternative fuels.

4. DEVELOPMENT OF EMISSION FACTORS

4.1 INTRODUCTION

An international project, MEET is the primary source of emissions data employed in this study [Joumard, 1999]. The development of a set of appropriate emission factors is a complex issue. An emission factor may be viewed as a ratio of an emission and a corresponding activity. The primary sources (i.e. laboratories and countries of origin) of the raw emission data used in the MEET methodology are given. Emission factors can be categorised into three types, namely hot stabilised, cold-start extra and evaporative. The formulation of a comprehensive set of speed-dependent emission functions factors are described. MEET emissions data was primarily developed for regional emissions inventories. One of the objectives of this study is to adapt the MEET emissions data for use at a local scale (i.e. high spatial resolution) in an urban area. Consequently, creep-dependent emission factors are developed so as to incorporate vehicle delay. Another objective is to investigate the potential that alternative fuels have to reduce emissions from traffic. However, prior to selecting any alternative fuel, a thorough comparison between emissions of petrol and diesel vehicles, and from conventional fuels and alternative fuels is necessary. Finally, the related areas in which more research is needed are identified.

4.2 SOURCES OF EMISSIONS DATA EMPLOYED

This Chapter describes the development of the emission factors for the MVEIM. Much of the information provided is taken from the relevant MEET Deliverables [Hassel, 1995], [Hassel and Weber, 1997a], [Hickman, 1997], [Hickman et al., 1998], [Joumard and Sérié, 1997], [Joumard, 1999], [Kourtidis et al., 1999], [Rijkeboer, 1997], [Samaras and Ntziachristos, 1998], [Samaras et al., 1997, 1998a], [Sérié and Joumard, 1997], [Sturm et al., 1998] and other sources that describe the MEET project.

Emissions data for the MEET project was collated from the following European Laboratories and Institutes:

- Aspen Utvecklings AB, Lund Sweden;
- EMPA, Dübendorf, Switzerland;

- INFRAS AG, Bern, Switzerland;
- INRETS, Bron cedex, France;
- Institute for Transport Sciences (KTI), Budapest, Hungry;
- Laboratory of Applied Thermodynamics, Aristotle University, Thessalonki, Greece;
- MTC, Bilprovning, Sweden;
- National Environmental Research Institute (NERI), Roskilde, Denmark;
- Norwegian Institute of Air Research; Lilleström, Norway;
- PSA Peugeot-Citroën, Colombes, France;
- Swedish Environmental Research Institute, Göteborg, Sweden;
- Technical University, Graz, Austria;
- TNO, Delft, the Netherlands;
- Transport Research Institute, Zilina, Slovakia;
- Transport Research Laboratory, Crowthorne, United Kingdom; and
- TÜV Rheinland, Abschlussbericht, Germany.

4.3 BASIC PRINCIPLES

As described in Chapter three, vehicle emissions for any pollutant can be regarded as being composed of three components:

$$E^{p} = E^{p,hot} + E^{p,cold} + E^{p,evap} \qquad 4.1$$

where: E^{p} is the total emission for a particular pollutant p (in kg);

$E^{p,hot}$ is the pollutant emission produced when an engine is in a hot stabilised mode (in kg);

$E^{p,cold}$ is the pollutant emission produced after an engine is started or before catalyst light-off (in kg); and

$E^{p,evap}$ is the pollutant emission by evaporation of the fuel (in kg).

Each of the three contributions (hot, start and evaporative) to the total emission depends on an associated emission factor and one or more parameters relating to the operation of the vehicle, so that in general:

$$E_{ta}^{p} = EF_{ta}^{p} \cdot ta \qquad 4.2$$

where: E_{ta}^{p} is one of the contributions to total emissions;

EF_{ta}^{p} is an activity related emission factor; and

ta is the traffic activity relevant to this type of emission.

The parameters EF_{ta}^{p} and ta are themselves functions of other variables. The development of each of these emission functions EF_{ta}^{p} is described next.

4.4 HOT EMISSIONS FACTORS

The MVEIM requires emissions information on vehicles under two different modes of operation (cruise and queue). The most widely available emissions data for estimating the quantity of pollutants emitted from motor vehicles is based on the average speed of the vehicle. Due to the limitations of the available emission measurements, it is not practical to formulate a complete set of emission functions for all vehicle categories. In the MVEIM, the mean speed is taken into account in all cases, but the other dependencies (i.e. gradient, load, mileage and temperature) are applicable only for those vehicle classes where the necessary data is available, and for which the data demonstrated a significant effect. For example, the data did not show any effect of accumulated mileage on motorcycle emissions (i.e. the emissions were approximately equal for motorcycles with high and low accumulated mileage). Consequently, it is assumed that this effect is negligible. It is worth noting that other parameters are known to affect emissions, for example, air conditioning and altitude. Although the principles of their effects are known, there is insufficient emissions data to estimate quantitative values.

4.4.1 CRUISE EMISSIONS FACTORS FOR LIGHT-DUTY-VEHICLES

The activity related emission factor for hot emissions is expressed primarily as a function of vehicle speed [Samaras and Ntziachristos, 1998]. The average speed emission functions are based on aggregated emission data for various driving cycles, whereby the driving cycles are represented by their average speeds alone. This data is collated according to vehicle technology, capacity class and model year and a speed dependent emission function is derived.

A total of 9,039 emission tests on 2,522 vehicles conducted over a range of driving cycles were collected. Only emissions data corresponding to driving cycles not employed in vehicle type approval tests were used in order to avoid possible emission underestimation due to the low driving dynamics of regulatory driving cycles. Therefore, the emission functions developed are considered to originate from cycles representing real-world driving conditions. Various laboratories formulate these cycles to describe actual driving situations in their own countries. Consequently, emission measurements were obtained from over 41 different real-world driving cycles covering mean speeds between 5.2 km/hr and 130 km/hr. The kinematic quality of driving cycles is a major factor in measured emission representativity [Joumard et al., 1999b]. Table 4.1 lists the driving cycles employed and their primary characteristics (i.e. duration, distance, mean speed, maximum speed and maximum specific power). The specific power of a vehicle can be approximated as twice the product of the speed (S_v) and acceleration (a):

$$SP = 2S_v \cdot a \qquad \textbf{4.3}$$

The units of S_v are km/hr, a is km/hr-s, and SP is $(km/hr)^2/s$ or kW/kg. The total vehicle specific power is the engine power-out less the sum of the power required to overcome rolling, drag and gradient resistances. Mathematically the specific power is:

$$SP = 2S_v\left[76.2\frac{g \cdot HP}{m_v \cdot S_v} - f_{rr} \cdot g - \frac{\rho}{2}\frac{g \cdot C_D \cdot A_v \cdot S_v^2}{m_v} - g \cdot \sin(\theta)\right] \qquad \textbf{4.4}$$

where: g is gravitational constant ($\approx 9.81\ m/s^2$);

HP is the engine horsepower (bhp);

S_v is the vehicle speed (m/s);

m_v is the weight of the vehicle (kg);

f_{rr} is the rolling resistance coefficient;

ρ is the air density (kg/m^3);

C_D is the aerodynamic drag coefficient;

A_v is the frontal area of the vehicle (m); and

θ is the roadway grade (degree).

The constant 76.2 converts from horsepower to m-kg/sec. The resistance terms are all negative since they act against the vehicle.

Table 4.1: Driving cycles included in the MEET project

Driving cycle	Duration (sec)	Distance (km)	Mean speed (km/hr)	Max. speed (km/hr)	Max. Sp. Power (kW/kg)
AutoR-1	734	15.13	74	113.9	269.6
BAB-1000	1000	--	118	160	--
BAB-436	420	--	107	130	--
BAB-736	750	--	110	150	--
Congested-Traffic	1040	1.92	6.64	44.9	236.0
Highway	765	16.502	78	96.4	193.4
MODEM-1	635	3.45	19.5	60	224.2
MODEM-10	430	1.87	15.6	44.4	238.5
MODEM-11	962	11.35	42.5	88.2	242.4
MODEM-12	423	2.44	20.8	49.9	184.0
MODEM-13	526	2.62	17.9	55.7	248.8
MODEM-14	383	3.41	32.1	67	250.1
MODEM-2	168	0.88	18.8	60	263.1
MODEM-3	282	1.08	13.8	39.1	133.5
MODEM-4	132	0.41	11	31	92.5
MODEM-5	1027	6.33	22.2	73.5	404.4
MODEM-6	91	0.13	5.2	26.1	90.3
MODEM-7	100	0.84	30.2	82.4	456.2
MODEM-8	250	1.11	15.9	53.5	185.3
MODEM-9	95	0.2	7.6	27.5	58.3
MODEM-Motorway	452	12.68	101	128.7	461.4
MODEM-Road	712	8.49	42.9	109.2	277.2
MODEM-Urban Free Flow	355	2.25	22.8	62.3	151.6
MODEM-Urban-Slow	428	1.71	14.3	42.3	126.0
Route-2	809	9.27	42	77.6	285.1
T-100	400	11.1	100	107.3	107.6
T-115	400	12.8	115	122.4	101.1
T-130	400	14.4	130	137.7	110.2
T-85	400	8.9	85	93	99.8
TRL-1	580	4.46	27.71	48	--
TRL-2	551	11.66	76.17	96	--
TRL-3	566	12.02	76.43	96	--
TRL-4	573	6.21	39.02	64	--
TRL-5	542	13.74	93	112	--
TRL-6	501	13.05	93.03	112	--
TRL-Motorway	641	17.5	102.64	118.6	285.5
TRL-Rural	1090	16.5	55.71	95	281.2
TRL-Urban	1222	6.14	18.58	47.7	198.8
UFLUI-2	1054	5.62	19.5	45.2	221.6
ULENT-2	814	1.67	7.5	22.5	93.3

Since the specific power multiplied by the vehicle mass is the kinetic power, the specific-power measures kinetic energy used during a driving episode. In the case of MODEM-Urban-Slow, the maximum specific power is 126.0 kW/kg. In MODEM-Motorway, the

maximum specific-power is much greater, reaching 461.4 kW/kg. During high power episodes, the kinetic power required to overcome vehicle inertia typically dominates the total power requirements. Consequently, during high power operation, a constant specific power approximately represents constant total power. The specific power levels of 400 kW/kg represent high power driving.

The dynamics of the driving cycles, which are particularly significant during urban driving, are taken into account implicitly. Best-fit emission functions were formulated by plotting the emissions measured during various driving cycles against the mean speed of the cycle. Based on the distribution of the emissions, binomial regression analysis was employed to produce correlation coefficients. In most cases, large discrepancies between emission measurements and the best-fit curves are observed and the correlation coefficients are low. This raises serious doubts about the reliability of the emission functions.

The large discrepancies in MEET data suggest inconsistencies between the values measured in the different laboratories and tests. It was thought that these variations in measurements were possibly caused by factors other than those adopted for vehicle categorisation. Consequently, a further analysis of the measured data was carried out to determine whether substantial distinctions existed between vehicles conforming to different standards. Specifically, the effects of the laboratory where the measurements took place, total mileage driven and engine size were analysed to determine whether these parameters could be responsible for the disparity in measured emissions data. This investigation was predominantly based on regulatory driving cycles, and it was assumed that the parameters listed above had an equal affect on emissions over both real-world and regulatory driving cycles. Unfortunately, the study did not bear conclusive results since enormous gaps existed in the measured emissions data between the various vehicle categories. In addition, the emission measurements were not taken specifically for the purpose of such an investigation.

4.4.2 Cruise Emissions Factors for Heavy-duty-vehicles

Much less emission measurement data is available from heavy-duty-vehicles, and consequently, it is not possible to develop emission functions to the same level of detail as for light-duty-vehicles [Hickman, 1997]. Heavy-duty-vehicles are more diverse than light-duty-vehicles with gross-vehicle-weight ranging from 3.5 to 40 tonnes. Also, their operation ranges from very disrupted trips (such as an urban bus journey or refuse

collection round) to high-speed transport of passengers and goods on motorways. In contrast to light-duty-vehicles, nearly all heavy-duty-vehicles have diesel engines. In addition, the first emission control legislation for heavy-duty-vehicles came into force in 1993 as opposed to 1970 for light-duty-vehicles. Therefore, there is less diversity with respect to age categories. Regulatory emission tests for heavy-duty-vehicles are based on engine performance and not on the complete vehicle as with light-duty-vehicles. The European type approval test involves the measurement of emissions under 13 steady-state scenarios. These scenarios are defined in terms of the speed of the engine and its load.

Emissions data was collated from a number of European laboratories in the MEET project. The measurements were performed for heavy-duty-vehicles with no payload, travelling on a road with zero gradient. For urban buses and coaches, the emissions were measured with a 50% payload. Regression analysis was performed on the measurement data and a third-order polynomial was formulated with respect to vehicle speed. The polynomial has the following functional form:

$$\varepsilon = a_o + a_1 \cdot s + a_2 \cdot s^2 + a_3 \cdot s^3 + \frac{a_4}{s} + \frac{a_5}{s^2} + \frac{a_6}{s^3} \qquad 4.5$$

where: ε is the rate of emission rate (in g/km) for an unloaded heavy goods vehicle, or a bus or coach, on a roadway with an average gradient of zero;

a_o is a constant;

$a_1 - a_6$ are the speed coefficients; and

s is the average speed of the vehicle (km/hr).

Unfortunately, goodness-of-fit and confidence intervals were not supplied with the emissions data.

4.4.3 Cruise Emissions Factors for Two-wheelers

Emissions from two-wheelers have received less attention than light-duty-vehicles [Rijkeboer, 1997]. However, two-stroke engines can emit substantial quantities of hydrocarbons.

A large difficulty with two-wheelers is the variety of vehicles available in terms of mass, engine power, and engine working principle. In addition, there are on-road, off-road and hybrid machines. There is also different legislation with which the vehicles have to comply. For example, there is an UN-ECE Regulation (UN-ECE R47) for mopeds and an UN-ECE R40 for motorcycles.

Emissions measurement data is scarce. It is assumed that the operation of mopeds is not influenced by traffic and consequently they are nearly always operated at maximum capability. Therefore, speed-independent emission factors were formulated for mopeds. Speed dependent emission factors were developed for various classes of motorcycles. It should be remembered that due to the small sample of data, the degree of uncertainty is substantial. For example, only data from 24 motorcycles was available for the MEET project.

4.4.4 EMISSIONS CORRECTION FACTORS

As already stated, hot emission factors are formulated initially as a function of the mean vehicle speed. Depending on the vehicle type and available data, modification factors (which may themselves be functions of other parameters) are employed to allow for road gradient, vehicle load, vehicle mileage, ambient temperature and air conditioning. The resulting formula has the form:

$$EF^{p,hot} = fnc\{s\} \cdot ECF_{\theta}^{p,hot} \cdot ECF_{w}^{p,hot} \cdot ECF_{am}^{p,hot} \cdot ECF_{T}^{p,hot} \cdot ECF_{a/c}^{p,hot} \qquad \textbf{4.6}$$

where: $EF^{p,hot}$ is the corrected hot emission factor for pollutant p (in g/km);

$fnc\{s\}$ is the speed dependent emission for standard conditions (in g/km);

$ECF_{\theta}^{p,hot}$ is the hot emission correction factor for gradient, θ;

$ECF_{w}^{p,hot}$ is the emission correction factor for weight-load, w;

$ECF_{am}^{p,hot}$ is the hot emission correction factor for vehicle accumulated mileage, am;

$ECF_{T}^{p,hot}$ is the hot emission correction factors for temperature, T; and

$ECF_{a/c}^{p,hot}$ is the emission correction factors for air conditioning, a/c.

The gradient of a road has the effect of increasing or decreasing the resistance of a vehicle to traction, and consequently the power required to overcome the resistance due to the road grade. Emissions are directly related to power - as the power increases so do the emissions. Emissions were measured for six road categories (motorway, dual carriageway, extra urban roads, main urban roads, long urban streets, and short urban streets), and each road category is divided into four types of traffic flow conditions (free flow, slight congestion, moderate congestion, and heavy congestion). Each of these is split in turn into five classes of gradient (i.e. -6%, -3%, 0%, 3%, and 6%) with two different load factors (10% and 90%) per gradient class. A regression analysis was performed on the measured data and a sixth-order polynomial with respect to average vehicle speed is formulated to correct for grade. Unfortunately goodness-of-fit and confidence intervals were not supplied with the emission factors. The polynomial has the following functional form:

$$ECF_{\theta}^{p,hot} = b_6 \cdot s^6 + b_5 \cdot s^5 + b_4 \cdot s^4 + b_3 \cdot s^3 + b_2 \cdot s^2 + b_1 \cdot s + b_o \qquad 4.7$$

where: $ECF_{\theta}^{p,hot}$ is the hot emission correction factor travelling at speed s, on road gradient θ;

b_o is a constant;

$b_1 - b_6$ are the speed coefficients; and

s is the average speed of the vehicle (in km/hr).

Similarly, regression analysis was also performed to derive equations for the effect of load on emissions. Data for intermediate load status (i.e. between 10% and 90%) is not available. However, it may be assumed that the emission rate varies linearly between the low and high load values. A third-order polynomial with respect to average vehicle speed and gradient in percent is formulated to correct for load. The polynomial has the following functional form:

$$ECF_{w}^{p,hot} = c_o + c_1 \cdot \theta + c_2 \cdot \theta^2 + c_3 \cdot \theta^3 + d_1 \cdot s + d_2 \cdot s^2 + d_3 \cdot s^3 + \frac{d_o}{s} \qquad 4.8$$

where: $ECF_{w}^{p,hot}$ is the vehicle load correction hot emission factor travelling at speed s, on road gradient θ;

c_o is a constant;

$c_1 - c_3$ are the gradient coefficients;

$d_o - d_3$ are the speed coefficients; and

s is the average speed of the vehicle (in km/hr).

The impact of mileage on vehicle emission performance is due to two primary reasons [Ntziachristos and Samaras, 1999]. Firstly, the normal wear of the engine, as well as deposition build-up on the cylinder wall and head, and ageing of the catalyst are responsible for an increase in emissions from older vehicles. Secondly, the probability of severely damaged engine parts or malfunctioning or increases with age. Regular maintenance and implementation of inspection and maintenance schemes (similar to those in the USA) could reduce the impact of such vehicles. In the MEET project, an effort was made to distinguish between three different mileage regions (i.e. < 10,000 km, 10,000 to 100,000 km and > 100,000 km). In the run-in region (<10,000 km), an emission deterioration of approximately 60% is evident for carbon monoxide, nitrogen dioxide and hydrocarbons. However, the total emissions are very low in this region and consequently, the increase is negligible. The same effect is found in the second region (10,000 to 100,000 km) except the emission level is much higher and consequently the increase is substantial. Emissions seem to stabilise after an accumulated mileage point in the region of 100,000 km. Emissions are estimated to be up to three times higher than the original values for vehicles having more than 120,000 km. The effect of mileage on carbon dioxide emissions is negligible. Degradation lines have been defined by regression analysis and subsequently normalised according to the mean mileage of the sample. A first-order polynomial with respect to average vehicle speed, accumulated mileage and the product of speed and mileage is formulated to correct for the effect of mileage, which has the following functional form:

$$ECF_{am}^{p,hot} = h_o + h_1 \cdot s + h_2 \cdot am + h_3 \cdot am \cdot s \qquad \textbf{4.9}$$

where: $ECF_{am}^{p,hot}$ is the mileage correction factor travelling at speed s, for accumulated mileage am;

h_o is a constant;

h_1 is the speed coefficient;

h_2 is the accumulated mileage coefficient;

h_3 is the product coefficient of speed and accumulated mileage; and

s is the average speed of the vehicle (in km/hr).

Low ambient temperatures also affect hot emissions, which are indirectly proportional to ambient temperature. A linear correlation established that average carbon monoxide emissions increase up to 108% between -20 °C and 22.5 °C. Therefore, linear equations independent of speed are formulated for carbon monoxide, nitrogen dioxide and hydrocarbons, which have the following functional form:

$$ECF_T^{p,hot} = k_o + k_1 \cdot T \qquad 4.10$$

where: $ECF_T^{p,hot}$ is the hot emission temperature correction factor;

k_o is a constant; and

k_1 is the temperature coefficient.

The higher load imposed on the engine by an air conditioning compressor will affect emission levels. For example, the power consumption of an air condition unit in a car can be as high as 7.5 kW. Measurement data was collated and compared for 12 petrol and 12 diesel vehicles with and without the air-conditioning in operation. When the air-conditioning was operating, carbon dioxide emissions increased by 20% for all vehicles. Other emissions from petrol vehicles also increased (but not in a consistent way). Diesel vehicles showed an increase in the range of 20 to 30% for carbon monoxide, nitrogen dioxide and carbon dioxide when compared to measurements taken with the air conditioning turned off. Hydrocarbons exhibit a large variation but no obvious differentiation at an average level. Although air-conditioning operation has an effect on emissions, correction factors are subject to the limitations imposed by the huge scatter in the measurement data.

4.5 START-UP EMISSIONS FACTORS

The start-up (also known as cold-start) extra emission can be defined as the total emission after engine start exceeding the hot engine emission for the same distance travelled. The MEET cold-start emission calculation is primarily based on a reference emission value, the distance travelled since start-up, the average vehicle speed and the ambient temperature. The reference emission value is the cumulative emission of a cold-start trip with average speed of 20 km/hr, at an ambient temperature of 20 °C, and a period until the engine is

warmed-up or catalyst reaches light-off. This distance is generally known as the cold-distance. Excess emissions are produced during the whole of the cold distance.

A methodology for cold (start-related) emissions has been developed empirically, using emissions measurements collated from a number of European laboratories. The prerequisite for adopting particular emissions data in the MEET project was that measurements had been observed for each vehicle with both a hot and cold engine, but otherwise identical test conditions. The difference between both sets of measurements (i.e. hot and cold) can be taken to represent the excess emissions resulting from the cold operation. Modification factors (which may themselves be functions of other parameters) are employed to correct for speed, ambient temperature, and distance travelled.

4.5.1 START-UP EMISSIONS FACTORS FOR LIGHT-DUTY-VEHICLES

The emissions measurements from various laboratories and individual tests from any given laboratory display a wide variation [Joumard and Sérié, 1997]. The total number of measurements collated was 2,568, where a single emission measurement is defined as one collected from a vehicle tested over the same driving cycle for both a cold and hot start, irrespective of the pollutant being observed. This total of 2,568 is made up of 1,784 petrol cars with a catalytic converter, 460 petrol cars without a catalytic converter, 315 diesel cars without a catalytic converter, and 9 diesel cars with a catalytic converter. The majority of tests were performed within the temperature range of 3.0 to 19.6 °C. Emissions measurements at other ambient temperatures (i.e. -9 to 26 °C) were employed to determine the affect of ambient temperature on cold start emissions.

For each vehicle category and each pollutant, a base excess emission value was determined at standard conditions, namely a start temperature of 20 °C and an average trip speed of 20 km/hr. Then, correction functions were developed for actual start temperature T, average speed s, and also for the distance travelled d. The general formula for start-related excess emissions (in g) is:

$$\text{excess emission (g)} = \omega \cdot \left[\text{fnc}_1\{s\} + \text{fnc}_2\{T\} - 1\right] \cdot \text{fnc}_3\{\delta\} \qquad \textbf{4.11}$$

where ω is the reference excess emission at 20 °C and 20 km/hr (in g);

s is the average speed during the cold period (in km/hr);

T is either the ambient temperature for a cold-start or the engine start temperature for vehicle starts at an intermediate temperature (in °C);

δ is the ratio of actual trip distance to cold distance; and

fnc_1, fnc_2 and fnc_2 are regression functions of speed, temperature and distance travelled respectively.

4.5.2 START-UP EMISSIONS FACTORS FOR HEAVY-DUTY-VEHICLES

Very little extra emission measurements are available for heavy-duty-vehicles. However, an approximation of their excess emissions has been obtained from an analysis of emission measurements from tests carried out on ten heavy-duty-engines [Kurtul and Graham, 1992]. These tests were carried out on an engine dynamometer, under the US heavy-duty transient test cycle. The duration of test is 1,200 seconds. The tests were first performed on a cold engine (roughly 20 °C start-temperature) and then repeated for a hot engine. The temperature of the coolant was measured during the cold tests, and it was found to reach the hot start value after 600 to 800 seconds. The difference between the hot and cold test emissions measurements is the cold excess emission, as the tests covered all of the cold start period. Due to the fact that the emissions data only comprised measurements from one operating cycle and, in addition, were only carried out at one ambient temperature, it was not feasible to ascertain whether the excess emission obtained is very representative.

Cold start emission factors for buses can be assumed to be the same as those of heavy-goods-vehicles, since most buses have diesel engines and conform to similar legislation.

4.5.3 START-UP EMISSION FACTORS FOR TWO-WHEELERS

The MEET project does not include any start-up emission factors for two-wheelers [Rijkeboer, 1997]. In addition, a literature search did not reveal any sources of start-up emissions factors for motorcycles or mopeds.

4.6 EVAPORATIVE EMISSIONS FACTORS

Evaporative emissions are primarily associated with petrol engined vehicles as petrol is a lot more volatile than diesel. In addition, the speciation of evaporative emissions changes with increasing ambient temperature in favour of the most volatile hydrocarbon species, thus changing the speciation of traffic emissions during the course of the day [Kourtidis et al., 1999]. In general there are four types of evaporative loss:

1. Refuelling losses occur when the vehicle is being refuelled. The contents of saturated vapours are displaced by the liquid fuel, and are normally vented to the atmosphere. Refuelling losses are usually attributed to the fuel handling chain and not to the vehicle emissions.
2. Diurnal breathing losses occur as a result of the diurnal temperature cycle causing vapour expansion inside the fuel tank as the ambient temperature rises during the daylight hours. Without an emission control system, some of this increased volume of fuel vapour is vented to the atmosphere. At night, when the temperature drops, vapour contracts and fresh air is drawn into the petrol tank through the vent. This lowers the concentration of hydrocarbons in the vapour space above the liquid petrol and consequently a concentration gradient forms between the two (i.e. vapour space and petrol). This concentration gradient gives rise to additional evaporation of petrol until a new equilibrium is reached between the two (at which time the evaporation stops). The corresponding units are g/day.
3. Hot soak losses occur when a vehicle is switched off after operation. Heat from the engine and exhaust system increases the temperature of the fuel in the system that is no longer flowing. Carburettor float bowls are particularly significant source of hot soak emissions. The corresponding units are g/procedure.
4. Running losses are the result of vapour generated in fuel tanks during vehicle operation. Running losses are most significant during periods of high ambient temperatures. The combined effect of high ambient temperature and exhaust system heat can generate a significant amount of vapour in the fuel tank. They are also caused by periodic purging of the evaporative emission control canister [Kishan et al., 1993] or from the carburettor on older cars. There are two types, namely, hot and warm. It is thought that the emission rate may vary linearly with altitude [Collins and Scott, 1993] and exponentially with RVP [Salles et al., 1996]. The corresponding units are g/km.

Refuelling and hot soak losses are normally treated as stationary sources. Refuelling losses occur at fuel stations and hot soak losses occur primarily at car parks and off-street parking. Diurnal breathing losses are calculated on a daily basis and thus it is difficult to apportion them on a link-by-link basis. Only running losses can be calculated on a link-by-link basis.

From a very limited dataset of emissions measurements, an evaporative emission function was developed in terms of RVP and average monthly ambient temperature [Samaras et al., 1997]. The RVP is a measure of fuel volatility in kPa. Similarly, the hot soak losses emission factor formulated is a function of fuel volatility and average monthly ambient temperature. The diurnal breathing losses emission factor derived is a function of minimum ambient temperature during the day and the average temperature rise during the day.

4.7 CREEP EMISSIONS FACTORS

As described in Chapter three, the movement of a vehicle queuing at an intersection or roundabout, whereby it progressively approaches the junction through a number of stop-starts is known as creep. Queuing is made up of both idling and creeping. Idling is an inefficient engine-operating mode and produces substantially higher rates of pollution than driving at optimum speeds [Hallmark and O'Neill, 1996]. The average speed of the vehicle while creeping and idling is assumed to be less than 10 km/hr. MEET does not supply emission factors for either idling or creeping, so they must be estimated from the speed-dependent emission factors. Hence, the emission factors for each vehicle type at 10 km/hr are determined using the speed-dependent emission factors described already by Equation 4.6. These mean cruise emission factors at 10 km/hr are multiplied by 2.78 m/sec (10 km/hr) to obtain the queuing emission factors in mg/sec.

4.8 EMISSIONS FROM ALTERNATIVE FUELS

An area that promises enormous potential for the reduction of emissions from engines (and in particular diesel engines) is alternative fuels, such as natural gas and bio-diesel. However, emission factors for such alternative fuels are very scarce. In addition, they are usually only measured for new and well-tuned engines. Due to the limited quantity of emissions data, it is prudent to compare emissions of conventional fuels (such as diesel and petrol) to those of alternative fuels and thus derive correction factors.

4.8.1 COMPARISON OF EMISSIONS FROM DIESEL AND PETROL

Prior to comparing various types of alternative fuels, it is a useful exercise to compare emissions from the two conventional fuels (i.e. petrol and diesel). Since petrol is not used very frequently in goods vehicles or buses, the comparison will concentrate on cars. Table 4.2 shows a relative qualitative comparison of pollutants from petrol and diesel cars. For

some pollutants, petrol engines are cleaner than diesel engines and therefore produce lower emissions (e.g. PM_{10}), whereas for others the opposite applies (e.g. HC). In general however, diesel cars are cleaner that petrol cars without catalysts [NSCA, 1998]. Diesel engine emissions of CO, HC and NO_x are generally lower than those from an un-controlled (without a TWC) petrol engine [Poulton, 1994]. However, the use of a TWC lowers the petrol engine emissions to that of a diesel engine. A detailed comparison of emissions from diesel and petrol engined vehicles is given elsewhere [QUARG, 1993b], [Holman, 1999].

Table 4.2: Comparison of emissions of pollutants from diesel and petrol cars [source: adapted from NSCA, 1998]

Pollutant	Diesel	Petrol
NO_x	Initially higher than petrol with catalyst	Reduced by catalyst in new cars but equivalent to diesel in the long term
HC	Lower than petrol, further reduced by oxidation catalyst	Higher than diesel - emitted from exhaust and fuel tank evaporation. Emissions increase when traffic is congested and the engine is cold
C_6H_6	No evaporative emissions, and low emissions in exhaust	Dependent on the C_6H_6 and HC content of the petrol, but about three times higher than diesel
C_4H_6	Higher from diesel cars, but reduced by oxidation catalyst	Lower from petrol cars
CO	Lower than petrol - reduced by oxidation catalyst	Reduced by catalyst. Increases when traffic is congested and the engine is cold
PM	The best diesel cars have emissions twice those of a petrol vehicle	Emissions are half those of the best diesel cars
CO_2	Diesel is a denser fuel so more CO_2 is given off per litre burnt. However the greater efficiency of the diesel engine means that overall they emit less CO_2	Comparisons of greenhouse gas emissions (including CH_4 and NO) from diesel and petrol with catalyst have found that emissions from petrol cars are 20% higher
SO_2	Emitted from diesel exhausts	Maximum of 0.2%

Petrol and diesel both comprise of hydrocarbons. Petrol contains lighter hydrocarbons in the range of C_4 to C_{12}, while diesel contains heavier hydrocarbons in the range C_{12} to C_{19}. The quality of petrol is defined by the RON and varies between 93 and 97. The quality of diesel is defined by the Cetane number and its value varies between 45 and 55.

4.8.2 Improved Conventional Fuels

The European Union has revised the environmental standards on petrol and diesel fuels [Murley, 1999]. In December 1998, the European Commission published a new directive 98/70/EC (amends Directive 93/12/EC) with far-reaching consequences regarding the environmental requirements for petrol and diesel fuel. Currently, two standards, EN 228 and EN 590, which were adopted in 1993, give a comparable composition of petrol and diesel through out Europe. In the new Directive, more stringent requirements are specified. The Directive will be implemented in two stages: the first stage being introduced

in 2000 and the second in 2005. Table 4.3 shows the specifications for petrol and Table 4.4 those for diesel.

Table 4.3: Environmental specifications for petrol

Parameter	Unit	2000		2005
		Min.	Max.	Max.
Research octane number	--	95	--	--
Motor octane number	--	85	--	--
Reid vapor pressure (summer)	kPa	--	60	--
Distillation - evaporated at 100 °C	% v/v	46	--	--
- evaporated at 150 °C	% v/v	75	--	--
Hydrocarbon analysis – olefins	% v/v	--	18	--
- aromatics	% v/v	--	42	35
- benzene	% v/v	--	1	--
Oxygen content	% m/m	--	2.7	--
Oxygenates – methanol	% v/v	--	3	--
- ethanol	% v/v	--	5	--
- iso-propyl alcohol	% v/v	--	10	--
- tertiary-butyl alcohol	% v/v	--	7	--
- iso-butyl alcohol	% v/v	--	10	--
- ethers with 5 or more carbons	% v/v	--	15	--
Other oxygenates	% v/v	--	10	--
Sulphur content	mg/kg	--	150	50
Lead content	g/l	--	0.005	--

Table 4.4: Environmental specifications for diesel

Parameter	Unit	2000		2005
		Min.	Max.	Max.
Cetane number	--	51	--	--
Density (at 15 °C)	kg/m^3	--	845	--
Distillation (95% point)	°C	--	360	--
Polycyclic aromatic hydrocarbons	% m/m	--	11	--
Sulphur content	mg/kg	--	350	50

4.8.3 Comparison of Emissions from Alternative Fuels

Any alternative fuel that displaces diesel or petrol will have to perform well relative to numerous criteria, such as contribution to emissions of criteria pollutants (e.g. CO and NO_x), toxics (butadiene and benzene) and greenhouse gases (CO_2 and methane) [Maples et al, 2000]. There are many types of alternatives fuels being considered. These include LPG, CNG, methanol, ethanol, bio-diesel, etc.

LPG is a mixture of light-hydrocarbons, which are gaseous at standard temperature and pressure and which liquefy readily at moderate pressures or reduced temperatures. The main components of LPG are propane (C_3H_8), propylene (C_3H_6) and butane (C_4H_{10}).

The principal component of natural gas is methane (CH_4), generally comprising 87 to 90% by volume of the hydrocarbons depending on the source of the gas. It also contains ethane (C_2H_6), propane (C_3H_8), butane (C_4H_{10}), and pentane (C_5H_{12}).

A number of reports compare, in general, pollutant emissions from vehicles using alternative fuels to those using conventional fuels [Deluchi, 1991], [Gover et al., 1996a; 1996b], [Haseley, 1996], [Lewis and Gover, 1995], [Lewis, 1997], [Poulton, 1994], [Rijkebour and Hendriksen, 1993], [Samaras et al., 1998b], [TRL, 1994], [FDOE, 1995].

Poulton [1994] collated data on alternative fuels from around the world, concluding that "much of the exhaust emissions data relating to the use of alternative fuels are from limited testing of initial prototype alternative-fuelled vehicles, with mostly bi-fuel conversions (not optimised engines) resulting generally in a large and sometimes highly variable (higher or lower) range of emissions values". Therefore the values are better expressed qualitatively rather than quantitatively. Table 4.5 [Poulton, 1994] gives a qualitative comparison of the vehicle exhaust pollutant effect of using alternative fuels, with reference to a petrol vehicle with a TWC. While the results in Table 4.5 cannot be employed in modelling the actual impact of using alternative fuels in motor vehicles, they do indicate which alternative fuels are best (with respect to reducing emissions). It serves no useful purpose investigating further alternative fuels that will increase emissions.

Table 4.5: Qualitative pollutant emissions performance of alternative fuels in comparison to petrol [source: adapted from Poulton, 1994]

Fuel	CO	NO_x	Total HC	NM-HC	CO_2
Petrol	Baseline	Baseline	Baseline	Baseline	Baseline
Diesel	Lower	Higher	Equal/Lower	Lower	Lower
Methanol	Equal	Variable	Lower	Lower	Lower
Ethanol	Equal	Variable	Lower	Lower	Lower
CNG	Lower	Variable	Equal/Higher	Lower	Lower
LPG	Lower	Variable	Lower	Lower	Lower
Hydrogen	Lower	Equal/Lower	Lower	Lower	Lower

Overall, all the alternative fuels given in Table 4.5 indicate a reduction in NM-HC and CO_2. In addition, THC is shows a reduction with the exception CNG (higher CH_4 emissions). The effect of CO and NO_x emissions from alternative fuels is more varied. For example, CO emissions are either equal to or lower than petrol, while NO_x emissions can be lower, the same or higher than petrol.

Gover et al. [1996a; 1996b] compared the relative benefits of using LPG, CNG, electricity, alcohols and bio-diesels (RME and SME) over petrol and diesel. However, the study concentrated on LCA. LCA considers the environmental burdens (i.e. emissions) that are emitted from all stages related to a process or product from 'cradle-to-grave'. In other words, LCA accounts for the fact that emissions occur during production, traffic, use and final disposal. Gover et al. [1996b] did provide scale factors for various alternative fuels as compared to petrol and diesel engines. The fuel consumption scale factors are in terms of MJ of energy. The petrol engines were primarily cars and LGVs, while the diesel engines were buses and HGVs. From Table 4.6, it can be seen that LPG produces lower emissions than petrol for all pollutants except NO_x. However, fuel consumption (in terms of MJ consumed) remains the same.

Table 4.6: Average alternative fuel scale factors for various pollutants [source: Gover et al., 1996b]

Alternative Fuel	Conventional Fuel	CO_2	CO	HC	NO_x	PM	FC
LPG	*Petrol*	0.88	0.47	0.46	1.1	--	0.98
LPG	*Diesel*	--	2.0	2.1	0.2	0.24	1.1
CNG	*Petrol*	0.82	0.23	1.34	0.69	--	1
CNG	*Diesel*	--	1.0	1.5	0.15	0.15	1.2
Bio-diesel	*Diesel*	1.02	0.78	0.8	1.18	0.76	1.05
Ethanol	*Petrol*	1	0.4	1	0.35	--	0.85
Ethanol	*Diesel*	0.83	1.07	1.46	0.9	0.19	1
Methanol	*Petrol*	0.95	0.69	0.78	0.83	--	0.85
Methanol	*Diesel*	0.81	0.81	0.6	0.43	0.19	1

Lewis and Gover [1995] collated and summarised the LCA benefits of using LPG, CNG and methanol over diesel and petrol. In addition, the study produced averaged vehicle use emissions factors for the aforementioned fuels. These are given in Table 4.7. The study collated data from a number of sources [Gover et al., 1996a; 1996b], [Rijkebour and Hendriksen, 1993], [Deluchi, 1991], [Agentum et al., 1993], [Johansson et al., 1992], [Hammarström, 1988] and [Auto-Oil, 1995]. The results from each study were presented in tabular form and averaged. Lewis and Gover [1995] concluded that although there are substantial variations between the various fuel types in terms of the stage at which the emissions occur, the range of life-cycle emissions is very small, and overall emissions are similar for all fuels. By changing fuels, it may be possible to transfer the emissions from vehicle usage to production. As this project is primarily focussed on local on-road air quality, emissions during production of the fuel are not considered.

Table 4.7: Average indicative emission factors from a range of fuels, measured in g/vkm [source: Lewis and Gover, 1995]

Pollutant	Petrol	Diesel	LPG	CNG	Methanol
CO_2	186.2	149.6	148.6	148.7	141.4
CO	3.37	0.43	1.48	0.82	3.22
NO_x	0.22	0.69	0.19	0.19	0.24
Total HC	0.3	0.08	0.11	0.44	0.12
SO_2	0.02	0.08	0	0	0.003
PM	0.005	0.1	0.004	0.004	0

One of the best sources of information on the use of alternative fuels is the US Alternative Fuel Vehicle Demonstration and Performance Tracking Program [FDOE, 1995]. While emissions factors for vehicles in the USA are not applicable in Europe, the different emissions levels give an indication of the relative increase or decrease that can be expected with the use of these fuels.

An extensive literature review [Samaras et al., 1998b] comparing the effects of four alternative fuels (i.e. CNG, alcohols, dimethyl ether and bio-diesel) on emissions was carried out as part of the COST-319 action. As with conventional fuelled vehicles, the emission factors vary from vehicle to vehicle and consequently the relative reduction or increase in emissions will vary also. In addition, emission factors for these fuels have been mainly produced in relation to vehicles of current technologies [Samaras et al., 1998b]. Due to the limited quantity of experimental data, it is not practical to differentiate between the effects of different types of emissions (i.e. hot stabilised, start-up and evaporative). Table 4.8 gives a summary of the effects on emissions of using various alternative fuels over conventional fuels for specific vehicle classes. The range of scale factors is indicated as ratio of the emissions with the alternative fuel over the emissions with the conventional fuel. It should be noted that the scale factors given in Table 4.8 have a substantial level of uncertainty and therefore should be considered only as an estimate of the potential effects of alternative fuels on emissions [Samaras et al, 1998b]. In Table 4.8, LDVs includes cars and LGVs while HDVs includes HGVs and buses. It can be seen from the table that certain pollutants decrease while other pollutants increase. For example, emissions of CO and NO_x decrease with use of CNG (instead of petrol) in LDVs, while the HC emissions increase.

Table 4.8: Effects of alternative fuels on emissions in various vehicle classes [source: Samaras et al., 1998b]

Alternative Fuel	Conventional Fuel	Vehicle	CO	HC	NO_x	PM
CNG	*Petrol*	*TWC LDV*	0.4-0.5	1.5-2.0	0.4-0.6	---
CNG	*Diesel*	*HDV*	0.1-1.0	0.2-6.0	0.1-1.0	0.05-0.2
Methanol	*Petrol*	*TWC LDV*	0.7-0.9	0.7-0.8	0.8-1.0	---
Ethanol	*Petrol*	*TWC LDV*	0.4-1.4	1.0-1.3	0.4-1.0	---
Methanol	*Diesel*	*HDV*	0.8-3.0	0.6-3.0	0.2-0.4	0.2-0.6
Ethanol	*Diesel*	*HDV*	1.1-1.3	0.7-1.5	0.87-0.9	0.2-0.6
DME	*Diesel*	*HDV*	---	---	0.2-0.5	0.05-0.3
Bio-diesel	*Diesel*	*HDV*	0.75-0.8	0.2-0.8	1.1-1.2	0.6-1.2

4.9 FURTHER RESEARCH REQUIREMENTS

The quantity of emissions data currently available is insufficient in many areas prohibiting accurate assessments. Therefore, further detailed research and measurement is required. For example, the emissions database needs to be continuously updated to account for new vehicles and alternative technologies. There is a limited quantity of data for heavy-duty-vehicles and motorcycles (especially VOCs for motorcycles). Emissions factors should be formulated to account for different vehicle modes of option (e.g. acceleration and deceleration). The influences of auxiliaries (e.g. air conditioning) also need to be quantified. In addition, there should be increased focus on quantifying emissions during operating modes that produce high emissions, such as enrichment and enleanment. Further analysis of the large discrepancies in emissions measurements between laboratories is necessary. Additional measurements of emissions for non-regulated pollutants (e.g. $PM_{2.5}$) need to be carried out. Improved procedures for the measurement and modelling of evaporative emissions need to be developed. Investigation of hot-start effect on emissions (i.e. start-up before the engine cools down) should be carried out. The effects of driving conditions on emissions, in order to assess the impact of small changes in driving behaviour on emissions in urban areas should be investigated. The potential reduction of emissions due to using alternative fuels and improved fuel quantity need to be examined more thoroughly. The MEET project did not include any emissions data from Ireland. Hence, there is a major requirement for emission testing from Irish vehicles.

4.10 SUMMARY

This formulation of emission factors for the MVEIM was given in detail in this Chapter. The emissions were divided into three groups, namely hot-stabilised, cold start-up and evaporative. Emission factors for two types of vehicle operation (i.e. speed-dependent and

queue) were described. An area that shows an important potential for emission reductions from vehicles is through the use of alternative fuels. A summary of the advantages and disadvantages of the primary alternative fuels with respect to emissions was outlined. Finally, due to the substantial gaps in knowledge in this area, further research that needs to be performed was summarised.

The translation of the MVEIM into a functional software program is described in the next Chapter. In addition, the results of the MVEIM sensitivity analysis are given.

5. MVEIM SOFTWARE DEVELOPMENT

5.1 INTRODUCTION

Chapter three described the formulation and conceptual design of the MVEIM, while the development of suitable emission factors was discussed in Chapter four. A primary objective of this research was the implementation of the MVEIM as functional software program. The structure of each module and sub-module in the MVEIM is described in detail. The salient features of the MVEIM are listed. Finally, the results of a sensitivity analysis are presented. The MVEIM, as implemented can account for:

- Emissions of 6 pollutants (CO, NO_x, SO_2, PM_{10}, $PM_{2.5}$, NM-VOC), 2 greenhouse gases (CO_2 and CH_4) and 2 toxins (C_4H_6 and C_6H_6);
- Three different types of emissions (hot-stabilised, cold and evaporative);
- Five different types of fuels (petrol, diesel, LPG, CNG, bio-diesel);
- Ninety-four specific vehicle technology groups;
- The influence of vehicle load and vehicle accumulated mileage;
- Vehicle modal activity (explicit modelling of cruise/queue effects and implicit modelling of acceleration/deceleration effects);
- Three types of roadways (urban, rural and motorway);
- The impact of ambient temperature; and
- The effect of roadway grade.

The MVEIM, as implemented does account for:

- The explicit impact of acceleration and deceleration;
- High and super emitters;
- Off-road motor vehicles;
- The effect of air conditioning; and
- The impact of vehicle inspection and maintenance.

5.2 SOFTWARE DESIGN

As described in Chapter three, the MVEIM consists of four primary modules, namely a traffic module, an EECT module, a MVERA module and a MVFC module. The module also includes a number of sub-modules, which will be described later. This modular structure allows individual elements of the software package to be run independently or in a batch process. As stated in the Chapter three, it was decided to employ the coupling method and use the GIS to display the MVEIM results rather than develop the MVEIM within a GIS software package.

A large EFD was created (originally in Microsoft® Access™ and later in Microsoft® SQL Server™ 7.0) using data from a wide range of studies on conventional and alternative motor fuels used in cars, LDVs, HDVs, buses and motorcycles. One of the major disadvantages of using Microsoft® Access™ is that a 'SQL query' can only search twenty-four data-tables in total. Consequently, the base emission factors database was migrated to Microsoft® SQL Server™. The algorithms in the MVEIM are implemented using a combination of VBA / SQL queries in Microsoft® Access™ / Microsoft® SQL Server™ and macros in Microsoft® Excel™. Microsoft® Excel™ is employed for statistical analysis and presentation of the results.

The ArcView® GIS software package was employed in this study. The package along with Arc/Info® is a product of ESRI of Redland, California. It differs from Arc/Info® in that Arc/Info® is designed to develop GIS data while ArcView® is designed to interact with GIS data, which has already been created. All activities within ArcView® are organised with a Project, which may consist of a number of Views, Tables, Charts, Layouts and Scripts (Scripts are programs in the Avenue™ language). Although the MVEIM is a very valuable tool on its own, integrating it with a GIS results in an even more powerful tool.

Managing and running the MVEIM requires technical skills in:

- Surveying, traffic network modelling and associated software (SATURN & SATCHMO);
- Spreadsheets (i.e. Microsoft® Excel™);
- Databases (i.e. Microsoft® Access™ and Microsoft® SQL Server™); and
- GIS software (ArcView®).

In addition, proficiency in Microsoft® Windows NT™, SQL and Arc/Info® Avenue™ language is required.

Considerable data compilation and processing is mandatory prior to using the MVEIM. For example, information on vehicular trip length, fuel RVP, AAKT, ambient temperature, and fleet composition, to name but a few, is required. Potential sources for each of these data requirements are discussed in the description of the relevant modules.

A flexible design was adopted for the MVEIM so that it could be used in a range of different applications. The model can run in two modes: batch and user-oriented. In batch node, the model accepts traffic data from SATURN & SATCHMO and the user can pre-select various options depending on the final emission inventory required. These options and their corresponding input bins are presented in Table 5.1. It is worth noting that all input bins are not available for each option. For example, the do-minimum and do-strategy traffic scenarios only exist for 2006 and 2016. Some of the options are co-dependent also. For example, the vehicle speed input bin is available only if a specific vehicle activity is selected (i.e. cruise). In addition, miscellaneous bins exist for ambient temperature (-10 °C to 30 °C) and fuel RVP (0 kPa to 150 kPa).

Table 5.1: Options and corresponding input bins available within the MVEIM

Level	Option	Input bin
Temporal Environment	Year	1991, 1996, 2006 & 2016
	Scenario	base, do-min & do-str
	Hour	am & pm
Spatial Environment	Zone	county or zone number
	Link	link number
	Roadway type	urban, rural & motorway
	Roadway grade	-6%, -3%, 0%, +3% & +6%
Fleet Composition	Vehicle category	LDV, HGV & bus
Traffic Activity	Modal activity	cruise & queue
	Vehicle load	10%, 50% & 90%
	Vehicle speed	10 to 130 km/hr
	Accumulated mileage	0 to 250,000 km
Pollutant	Type	CO, NM-VOC, PM_{10}, CO_2, C_4H_6, C_6H_6, $PM_{2.5}$, SO_2, CH_4 & NO_x
Emission	Type	hot, cold & evaporative

If certain data files are not populated, then the MVEIM ignores them. For example, if no information exists on vehicle load, then the model assumes a default value of 50%. Similarly, if roadway grade is missing, the default value is 0%. Alternatively, the user can

over-write certain default parameters. For example, the current default vehicle categories in the MVEIM are LDV, HGV and bus, but if required, the user can define a new vehicle category (e.g. car). The default parameters arise from SATURN & SATCHMO.

5.3 MVEIM MODULES

The modules in the MVEIM, although separate, are connected together through dependent and co-dependent files and programs. For clarity of presentation, each module is presented separately, and indeed many modules do function independently of each other. In most cases, however, their design and use is affected by inputs/outputs of other modules in the MVEIM.

5.3.1 EECT MODULE

The objective of the EECT module is to estimate the vehicle technology group distribution within each of the vehicle categories as defined by SATURN & SATCHMO (i.e. LDV, HGV and bus). However, as the MVEIM was designed to use traffic data from other sources (e.g. SCATS urban traffic control systems), other vehicle categories may be defined by the user.

The structure of the EECT module can incorporate an unlimited number of vehicle types considered to possess different emission characteristics, assuming that the corresponding emission factors are available. For each vehicle category, the EECT module distinguishes different sub-categories and technology groups defined on the basis of successive EU/ECE emission legislation, technology concept (improved conventional, open loop, closed loop), engine capacity or gross vehicle weight, and fuel type. Sub-categories are employed to more realistically represent differences in motor vehicle characteristics within these primary categories. However, the sub-categories employed are those that can be supported by data on emissions factors and travel activity. The classification is done principally for compatibility with the available emissions factors dataset. Table 5.2 shows the complete vehicle classification system. Only vehicle technology groups (94 in total) that have control legislation governing emissions are shown. The MVEIM also contains emission factors for CNG and bio-diesel amongst others.

Table 5.2: Vehicle classification system employed in the EECT module

Class	Fuel	Weight	Engine Size	Model year	Technology group
Car	Petrol	< 2.5 t	<1.4 l	until 1971	Pre-regulation
			1.4-2.0 l	1972 – 1977	70/220 & 74/290/EC
			>2.0	1978 – 1980	77/102/EC
				1981 – 1984	78/665/EC
				1985 – 1992	83/351/EC
				1986 – 1991	Open loop catalyst
				1991 – 1996	91/441/EC (EURO I)
				1996 – 2001	94/12/EC (EURO II)
				2001 – 2005	EURO III
				2005 –	EURO IV
	Diesel	< 2.5t	< 2.0 l	until 1986	Uncontrolled
			> 2.0 l	1986 – 1996	88/436 & 91/441/EC (EURO I)
				1996 – 2001	94/12/EC (EURO II)
				2001 – 2005	EURO III
				2005 –	EURO IV
	LPG	< 2.5t	All	until 1986	Conventional
				1986 – 1996	88/436 & 91/441/EC (EURO I)
				1996 – 2001	94/12/EC (EURO II)
				2001 – 2005	EURO III
				2005 –	EURO IV
LGV	Petrol Diesel	<3.5 t	All	until 1995	Uncontrolled
				1995 – 1998	93/59/EC (EURO I)
				1998 –	96/69/EC (EURO II)
				2001 – 2005	EURO III
				2005 –	EURO IV
HGV	Diesel	3.5 – 7.5 t	All	until 1993	ECE R49 & 88/77/EC
		7.5 - 16 t		1993 – 1997	91/542/EC stage I (EURO I)
		16 - 32 t		1997 – 2001	91/542/EC stage II (EURO II)
		32 - 40 t		2001 – 2005	EURO III
		> 40 t		2005 –	EURO IV
Bus	Diesel	All	All	until 1993	ECE R49 & 88/77/EC
				1993 – 1997	91/542/EC stage I
				1997 – 2001	91/542/EC stage II
				2001 – 2005	EURO III
				2005 –	EURO IV
TW	Petrol	All	< 50 cc (moped only)	until 1996	ECE R 47
				1997-1998	COM(93)449 Stage 1
				After 1999	COM(93)449 Stage 2
			> 50 cc 4 stroke	until 1996	ECE R 40.01
				After 1997	COM(93)449
			> 250 cc 4 stroke	until 1996	ECE R 40.01
				After 1997	COM(93)449
			> 50 cc 2 stroke	until 1996	ECE R 40.01
				After 1997	COM(93)449

From 1970 to 1985, EC member states followed the UN-ECE Regulation 15 (R 15) amendments on emissions of pollutants from vehicles less than 3.5 tonnes. The UN-ECE R15 notation and the corresponding EC directives are given in Table 5.3.

Table 5.3: Comparison between EC legislation and UN-ECE vehicle categories

UN ECE R15	EC Directive
Pre ECE vehicles	Pre-regulation
ECE 15 01	70/220/EC
ECE 15 01	74/290/EC
ECE 15 02	77/102/EC
ECE 15 03	78/665/EC
ECE 15 04	83/351/EC

The governing legislation in Table 5.3 overlaps, because more than one type of vehicle may have been sold in Ireland at a particular time. For example, vehicles (i.e. petrol cars) that conformed to 83/351/EC and 'open loop' catalyst were both available during the years 1986 to 1991.

The EECT module computes a weighted average of the vehicle technology groups within a vehicle category based on the number of vehicles reregistered in that technology group. In addition, each vehicle technology group is weighted by its corresponding AAKT.

A sample calculation of the weighted average for the vehicle category - bus is presented for Dublin in 1998 in Table 5.4. As can be seen from the right hand column of Table 5.2, a bus comprises of five technology groups:

- ECE R49 & 88/77/EC;
- 91/542/EC stage I;
- 91/542/EC stage II;
- EURO III; and
- EURO IV.

The first column in Table 5.4 gives these technology groups within the vehicle category - bus. The second column gives the number registered in each technology group in Dublin in 1998. This data was obtained from vehicle licensing records. The third column in Table 5.4 gives the AAKT for each technology group. The fourth category gives the VKT for each vehicle technology group. The VKT is the product of the second and third columns

in Table 5.4. Finally, the weighted average (fifth column) is computed for each technology group. The vehicle category - bus comprises 48.1% of ECE R49 & 88/77/EC, 22.9% of 91/542/EC stage I, and 29.0% of 91/542/EC stage II.

Table 5.4: Sample computation of weighted average for vehicle category - bus

Technology groups within vehicle category bus in 1998	N° registered in 1998	AAKT	VKT ('000)	Weighted Average
ECE R49 & 88/77/EC	1,187	40,000	47,480	48.1%
91/542/EC stage I	470	48,136	22,624	22.9%
91/542/EC stage II	596	48,136	28,689	29.0%
EURO III	0	0	0	0%
EURO IV	0	0	0	0%
TOTAL	*2,253*		*98,793*	*100.0%*

Figure 5.1 presents the entities involved in the EECT module while Figure 5.2 presents the flow of algorithm. The legend for the process flow charts and entity diagrams is given in Appendix C.

As illustrated in Figure 5.2, the EECT module uses three input files. The spatial (i.e. zone) and temporal (i.e. time period) resolution along with the vehicle category is pre-selected by the user. The data input files required by the EECT module are:

- `Tech_group_desc` (Vehicle Technology group description) file;
- `Fleet_composition` file; and
- `AAKT` (Annual Average Kilometres Travelled) file.

The input data files are imported into the MVEIM database as tables. A table consists of rows (records) and columns (fields). The records correspond to an item in the database, while the fields characterise the various types of data that are associated with each record. Data in different 'tables' are connected to each other through 'keys'. A key is a field that is used to identify a record and a primary key uniquely identifies each record. Often the key is part of the data that is stored or derived for that data. There are two types of key fields: primary and foreign. A primary key uniquely identifies each record in a table, while a foreign key corresponds to the value of a primary key in a related table. This links two tables together. In the `Tech_group_desc` table, the primary key is 'Tech_group_ID'. This primary key is linked in a one-to-many relationship with the 'Tech_group_ID' fields in both the `AAKT` and `Fleet_composition` files. The fields (e.g. vehicle class, fuel, weight, engine size and emission legislation) in the *`Tech_group_descript`* file are

attributes of each specific technology group. For example, a 1998 1.2 litre petrol car can be categorized into the technology group {cars, petrol, <2.5 tonne, <1.4 litre, 94/12/EC} and the primary key for this vehicle type is '1_1_9'. It should be noted that keys (both primary and foreign) are internal to the MVEIM and have no meaning outside of it. These are normally set as arbitrary values.

The data for the `Fleet_composition` and `AAKT` files is obtained from vehicle registration information and statistical data. In addition, data employed in this module can be derived from traffic surveys, video detection systems and SCATS induction loop data.

Several sources of existing official data are also useful. For example, the Central Statistics Office, Dublin Transport Office, Dublin Corporation, Bus Átha Cliath, National Roads Authority, Department of Environment and Local Government, Automobile Association, Department of Transport, and the Department of Energy.

For each application, the user must populate the `Fleet_composition` and `AAKT` files to the level of detail required for that application.

The EECT produces the `Veh_Tech_distrib_per_Veh_Cat` data file, which is exported to the MVERA module.

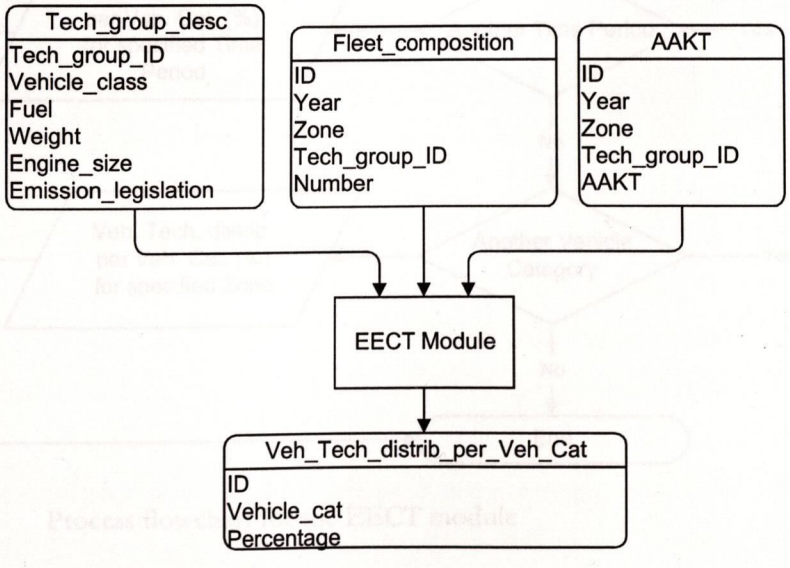


Figure 5.1: EECT module entities

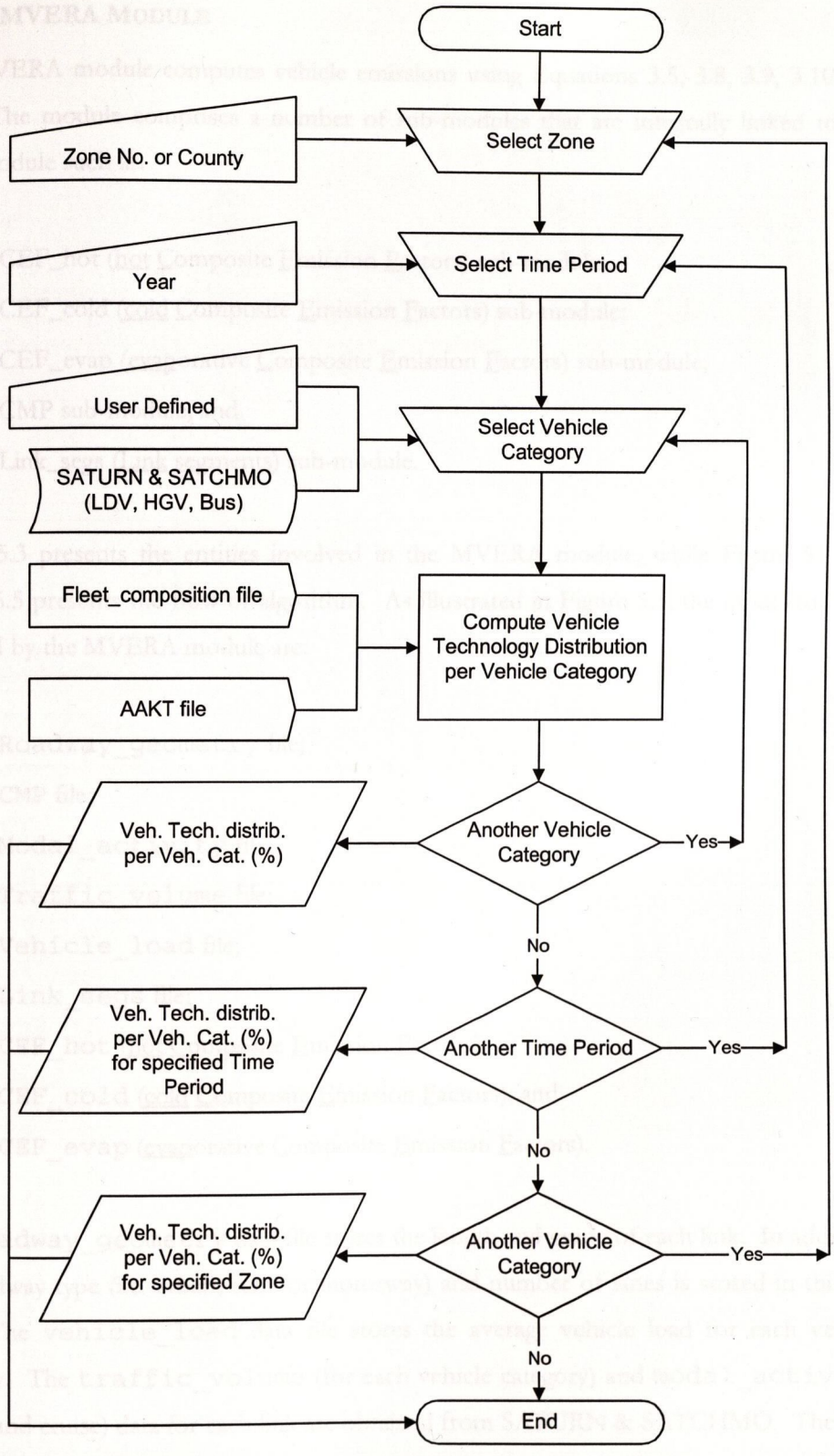


Figure 5.2: Process flowchart for the EECT module

5.3.2 MVERA MODULE

The MVERA module computes vehicle emissions using Equations 3.5, 3.8, 3.9, 3.10 and 3.11. The module comprises a number of sub-modules that are integrally linked to the main module such as:

- CEF_hot (hot Composite Emission Factors) sub-module;
- CEF_cold (cold Composite Emission Factors) sub-module;
- CEF_evap (evaporative Composite Emission Factors) sub-module;
- CMP sub-module; and
- Link_segs (Link segments) sub-module.

Figure 5.3 presents the entities involved in the MVERA module, while Figure 5.4 and Figure 5.5 presents the flow of algorithm. As illustrated in Figure 5.3, the input data files required by the MVERA module are:

- `Roadway_geometry` file;
- `CMP` file;
- `Modal_activity` file;
- `Traffic_volume` file;
- `Vehicle_load` file;
- `Link_segs` file;
- `CEF_hot` (hot Composite Emission Factors);
- `CEF_cold` (cold Composite Emission Factors); and
- `CEF_evap` (evaporative Composite Emission Factors).

The `roadway_geometry` data file stores the length and grade of each link. In addition, the roadway type (i.e. urban, rural or motorway) and number of lanes is stored in this file also. The `vehicle_load` data file stores the average vehicle load for each vehicle category. The `traffic_volume` (for each vehicle category) and `modal_activity` (queue and cruise) data for each link are obtained from SATURN & SATCHMO. The hot, cold and evaporative composite emissions factors are computed by the CEF_hot, CEF_cold, CEF_evap sub-modules respectively (described in the following sections). The output from the MVERA module is exported to ArcView® for visualisation or to

Microsoft® Excel for analysis. In addition, the output is exported to CALINE4R for estimation of ambient roadside pollutant concentrations.

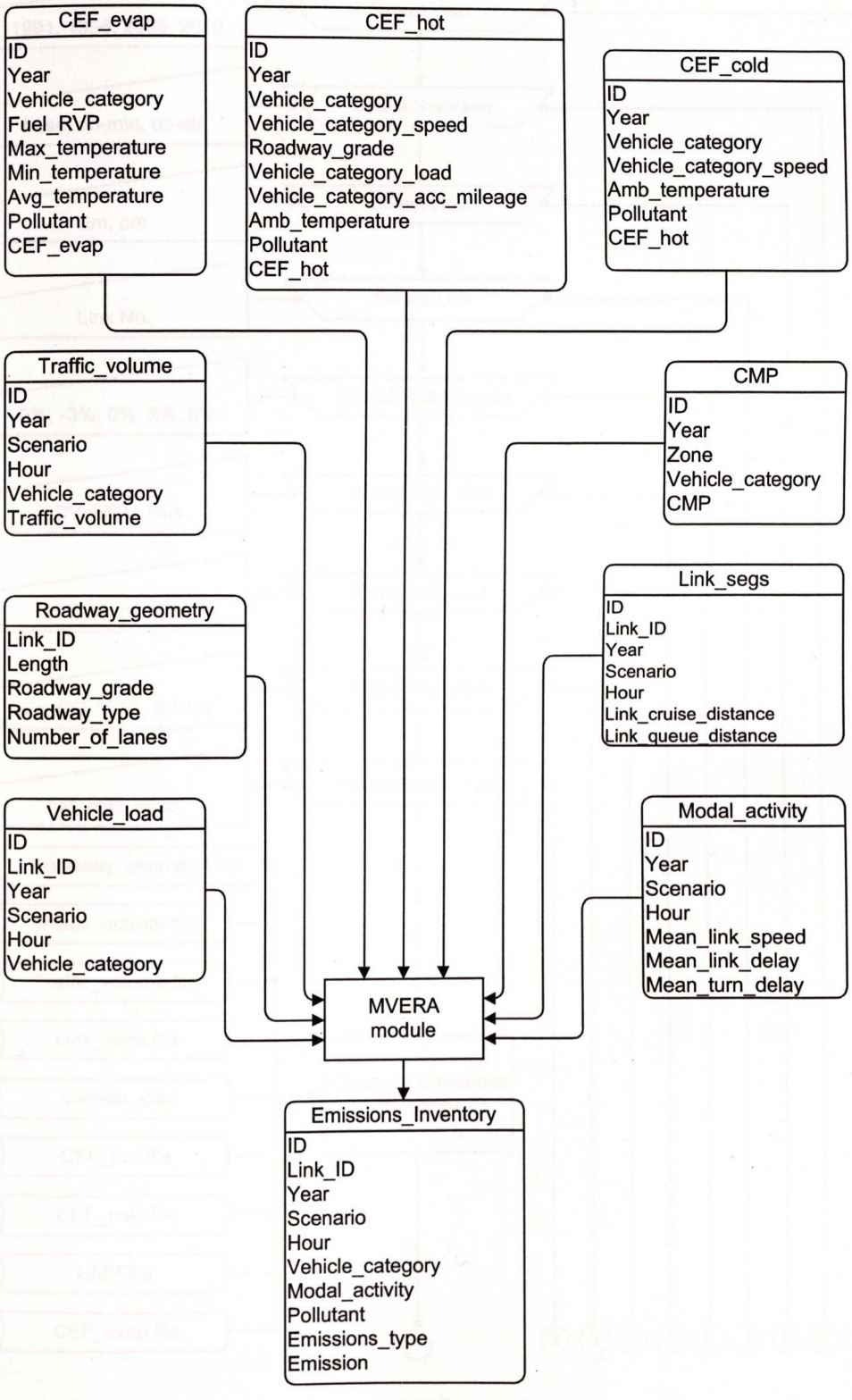


Figure 5.3: MVERA module entities

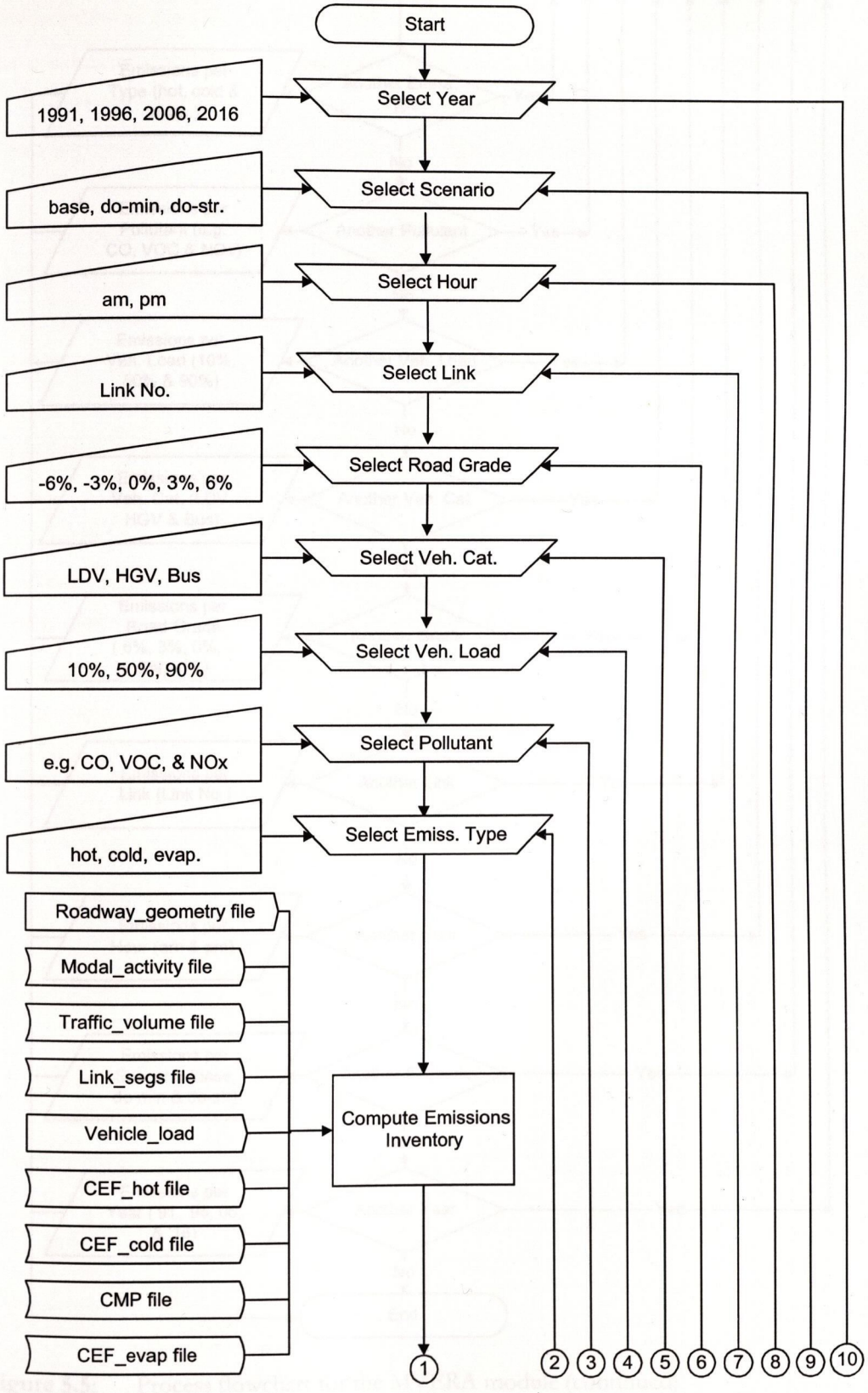


Figure 5.4: Process flowchart for the MVERA module

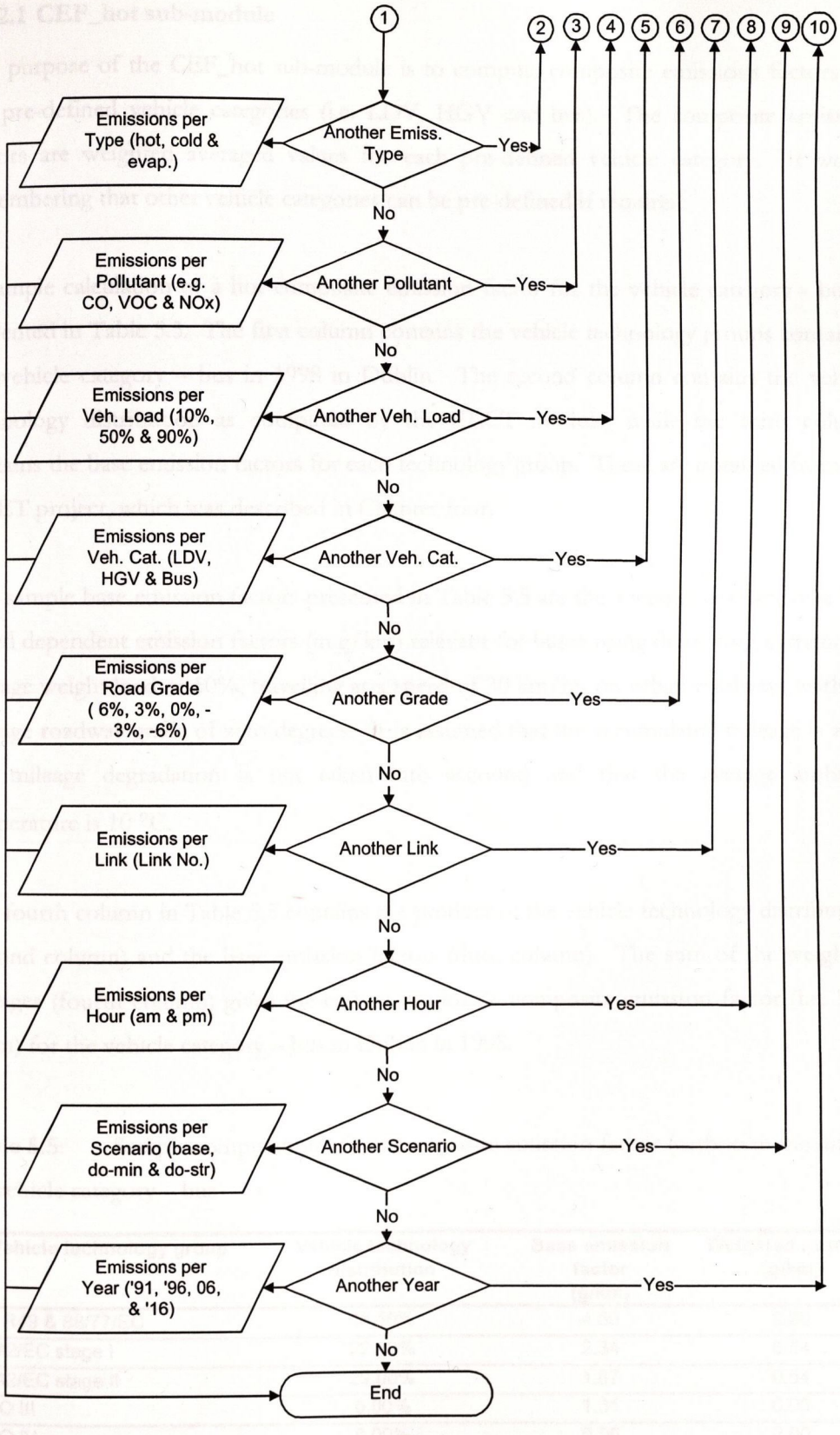


Figure 5.5: Process flowchart for the MVERA module (continued)

5.3.2.1 CEF_hot sub-module

The purpose of the CEF_hot sub-module is to compute composite emissions factors for the pre-defined vehicle categories (i.e. LDV, HGV and bus). The composite emission factors are weighted averaged values for each pre-defined vehicle category. It worth remembering that other vehicle categories can be pre-defined if required.

A sample calculation of a hot composite emission factor for the vehicle category - bus is presented in Table 5.5. The first column contains the vehicle technology groups contained the vehicle category – bus in 1998 in Dublin. The second column contains the vehicle technology distribution as computed by the EECT module, while the third column contains the base emission factors for each technology group. These are obtained from the MEET project, which was described in Chapter four.

The sample base emission factors presented in Table 5.5 are the average representative hot speed dependent emission factors (in g/km) relevant for buses using diesel fuel, carrying an average weight load of 50%, travelling at a speed of 30 km/hr, on urban roadways, with an average roadway grade of zero degrees. It is assumed that the accumulated mileage is zero (i.e. mileage degradation is not taken into account) and that the average ambient temperature is 10 °C.

The fourth column in Table 5.5 contains the product of the vehicle technology distribution (second column) and the base emission factors (third column). The sum of the weighted averages (fourth column) gives the carbon monoxide composite emission factor (i.e. 3.34 g/km) for the vehicle category – bus in Dublin in 1998.

Table 5.5: Sample computation of hot composite emission factor (carbon monoxide) for vehicle category – bus

Vehicle technology group	Vehicle technology distribution	Base emission factor (g/km)	Weighted average (g/km)
ECE R49 & 88/77/EC	48.10%	4.69	2.26
91/542/EC stage I	22.90%	2.34	0.54
91/542/EC stage II	29.00%	1.87	0.54
EURO III	0.00%	1.31	0.00
EURO IV	0.00%	0.96	0.00
Composite emission factor	---	---	*3.34*

Composite emission factors for other pollutants and other vehicle categories are computed in a similar manner.

Figure 5.6 presents the entities involved in the CEF_hot sub-module while Figure 5.7 presents the flow of the algorithm. As illustrated in Figure 5.6 the input data files required by the CEF_hot sub-module are:

- `BEF_hot` (hot Base Emission Factors) file; and
- `Veh_Tech_distrib_per_Veh_Cat` file.

The information in the `BEF_hot` data file is obtained from the MEET project, which was described in Chapter four.

The output data file (`CEF_hot`) is exported to the MVERA module.

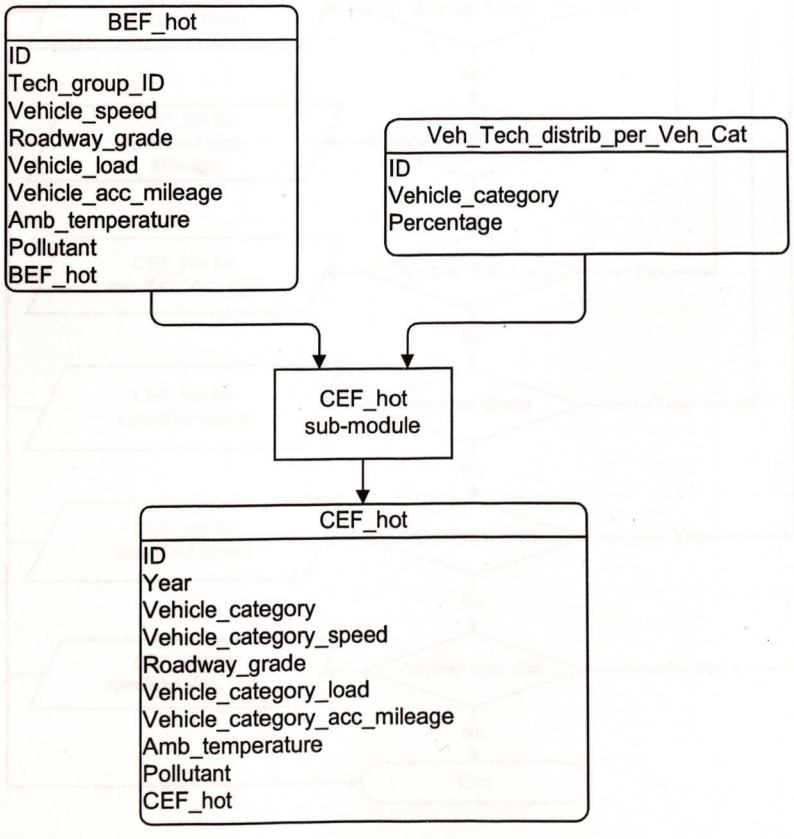


Figure 5.6: CEF_hot sub-module entities

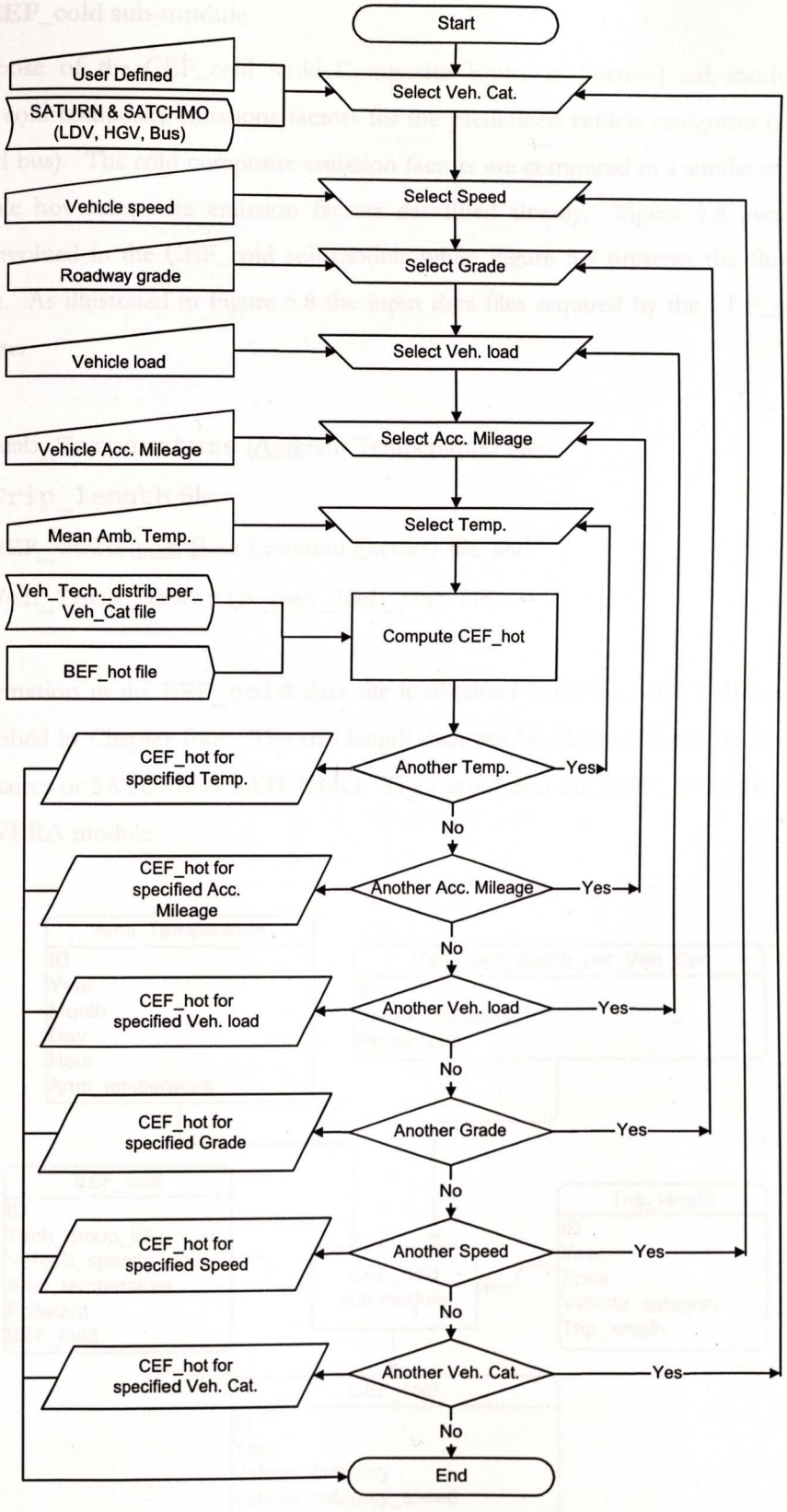


Figure 5.7: Process flowchart for the CEF_hot sub-module

5.3.2.2 CEF_cold sub-module

The purpose of the CEF_cold (cold Composite Emission Factors) sub-module is to compute cold composite emissions factors for the predefined vehicle categories (i.e. LDV, HGV and bus). The cold composite emission factors are computed in a similar manner to the sample hot composite emission factors described already. Figure 5.8 presents the entities involved in the CEF_cold sub-module while Figure 5.9 presents the flow of the algorithm. As illustrated in Figure 5.8 the input data files required by the CEF_cold sub-module are:

- `Amb_Temperature` (Ambient Temperature) file;
- `Trip_length` file;
- `BEF_cold` (cold Base Emission Factors) file; and
- `Veh_Tech_distrib_per_Veh_Cat` file.

The information in the `BEF_cold` data file is obtained from the MEET project, which was described in Chapter four. The trip length data can be obtained from traffic surveys, questionnaires or SATURN & SATCHMO. The output data file (`CEF_cold`) is exported to the MVERA module.

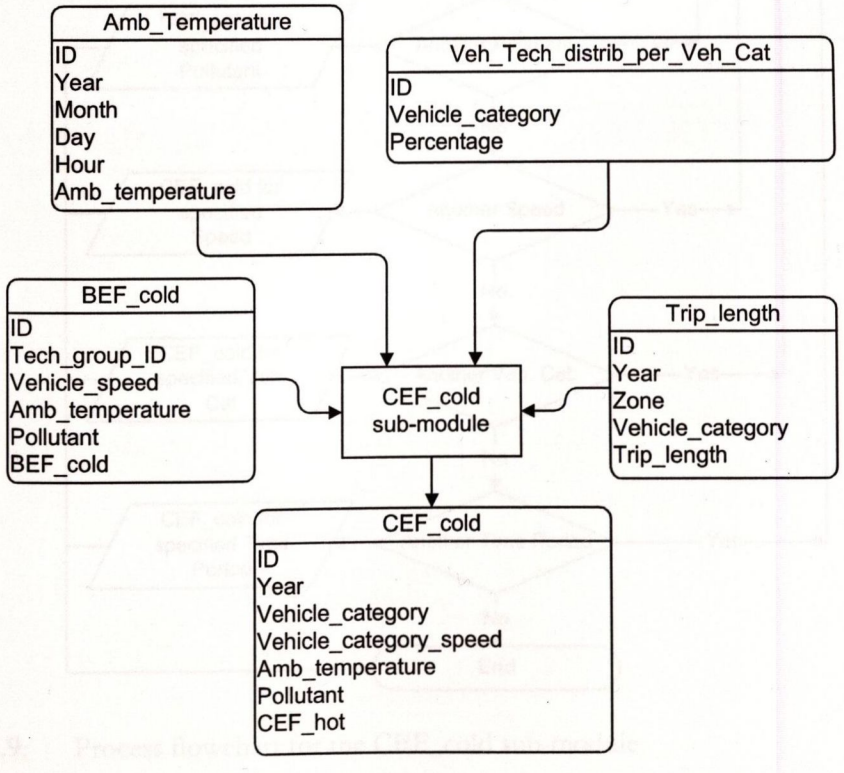


Figure 5.8: CEF_cold sub-module entities

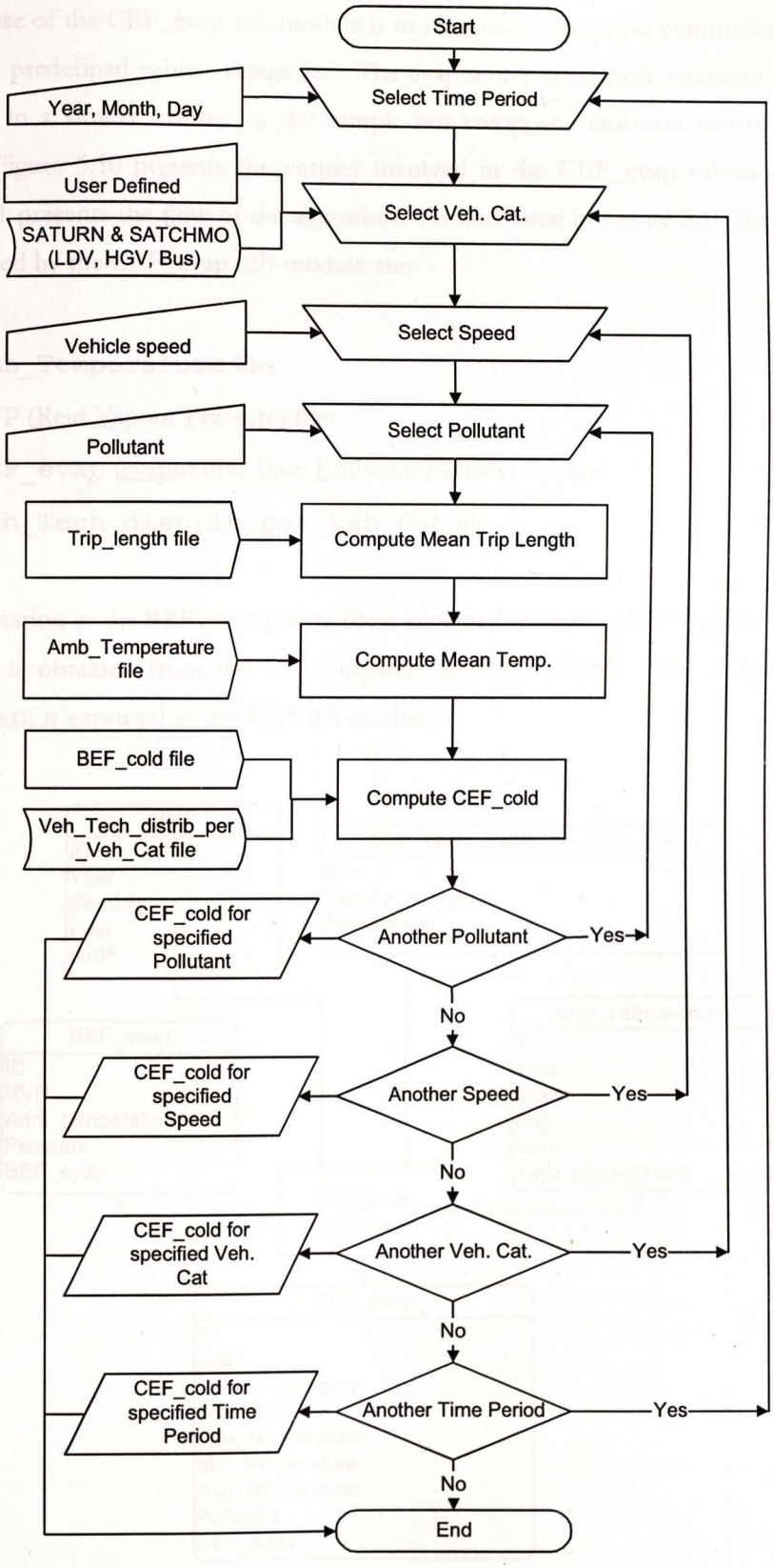


Figure 5.9: Process flowchart for the CEF_cold sub-module

5.3.2.3 CEF_evap sub-module

The purpose of the CEF_evap sub-module is to compute evaporative composite emissions factors for predefined vehicle categories. The evaporative composite emission factors are computed in a similar manner to the sample hot composite emission factors described already. Figure 5.10 presents the entities involved in the CEF_evap sub-module while Figure 5.11 presents the flow of the algorithm. As illustrated in Figure 5.10 the input data files required by the CEF_evap sub-module are:

- `Amb_Temperature` file;
- `RVP` (Reid Vapour Pressure) file;
- `BEF_evap` (evaporative Base Emission Factors) file; and
- `Veh_Tech_distrib_per_Veh_Cat` file.

The information in the `BEF_evap` data file is obtained from the MEET project, while the RVP data is obtained from the Oil companies or CONCAWE. The output data file (`CEF_evap`) is exported to the MVERA module.

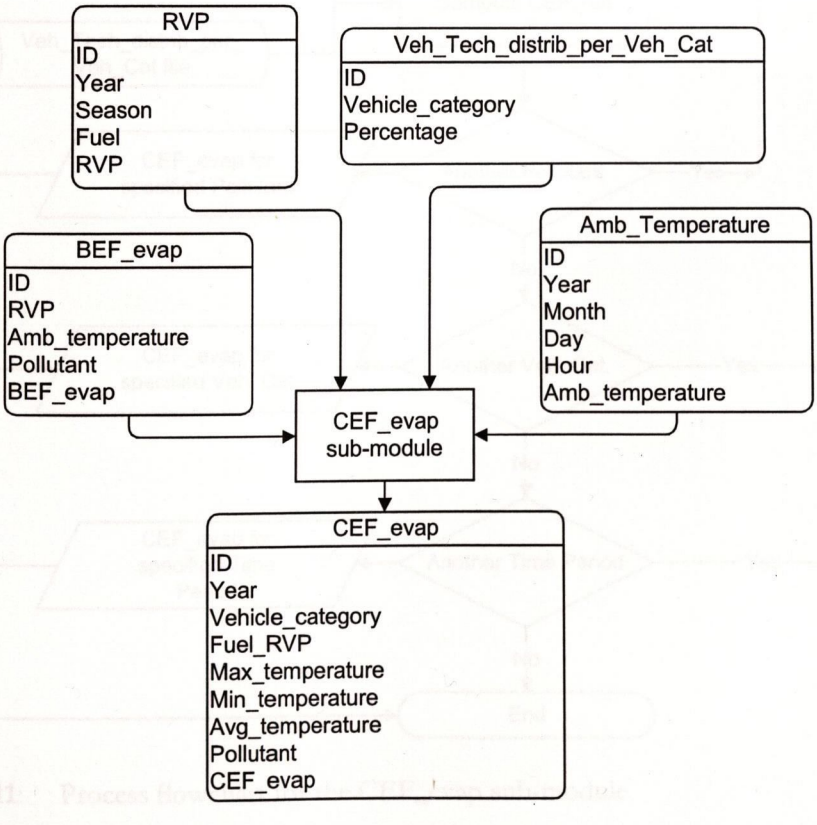


Figure 5.10: CEF_evap sub-module entities

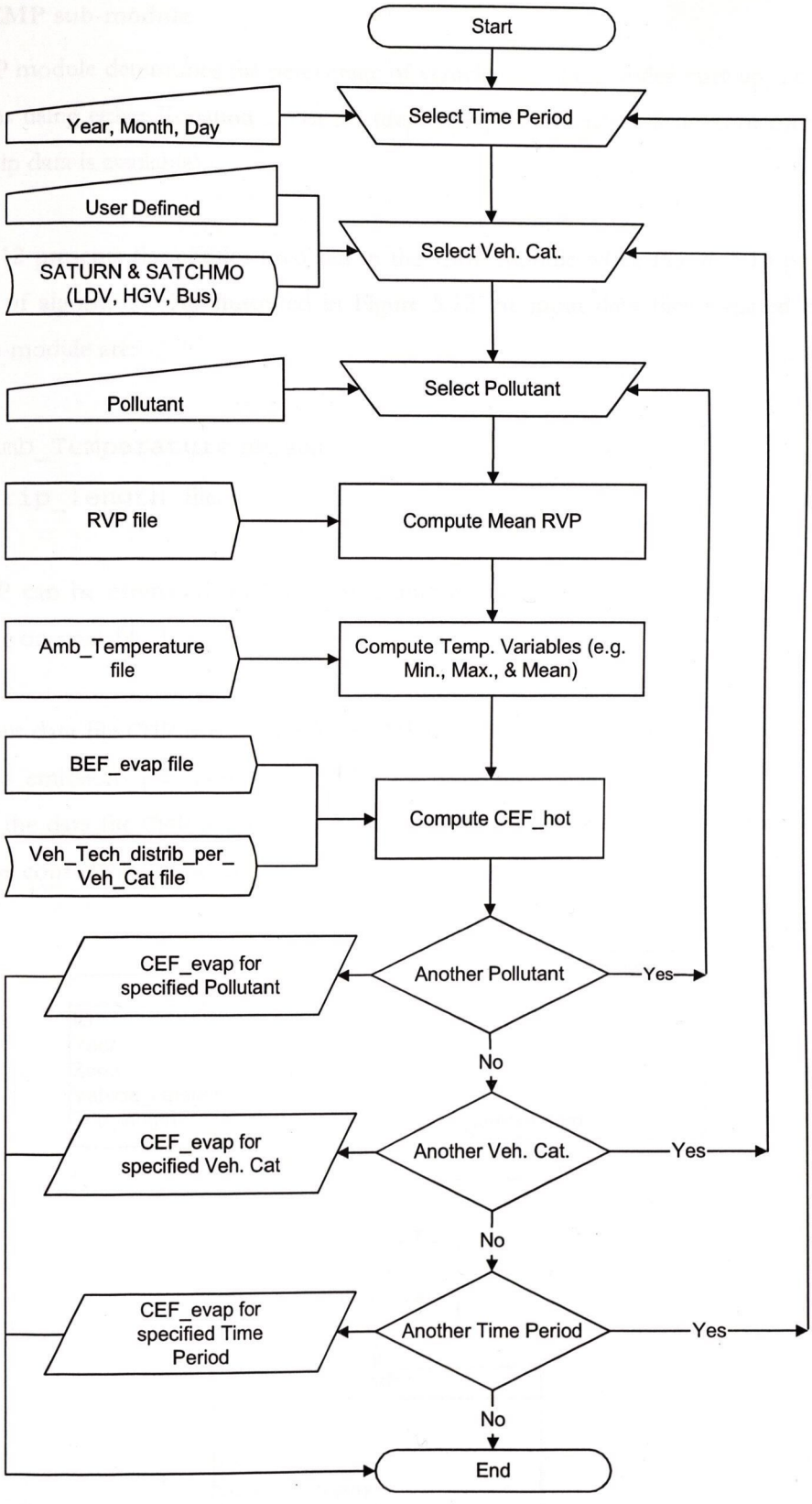


Figure 5.11: Process flowchart for the CEF_evap sub-module

5.3.2.4 CMP sub-module

The CMP module determines the percentage of vehicles travelling under start-up (i.e. cold) conditions using either Equation 3.6 or 3.7 (depending on whether measured or estimated vehicle trip data is available).

Figure 5.12 presents the entities involved in the CMP module while Figure 5.13 presents the flow of algorithm. As illustrated in Figure 5.12 the input data files required by the CMP sub-module are:

- `Amb_Temperature` file; and
- `Trip_length` file.

The CMP can be estimated for each zone, time period and composite vehicle category depending on available data.

The output data file `CMP` is exported to the MVERA module. It is employed to compute the excess emissions produced due to vehicles travelling under start-up conditions. In addition, the data file `CMP` is exported to the MVFC module where it is used to compute excess fuel consumption due to vehicles travelling with cold engines.

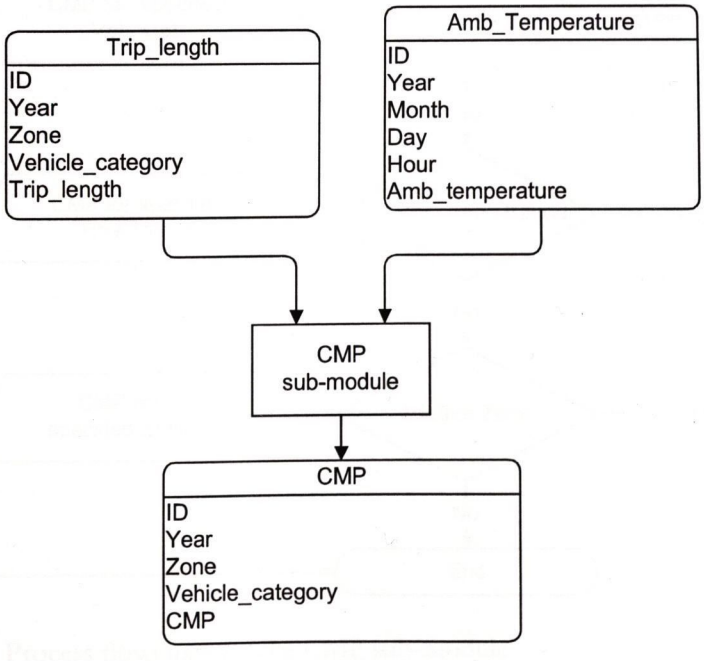


Figure 5.12: CMP sub-module entities

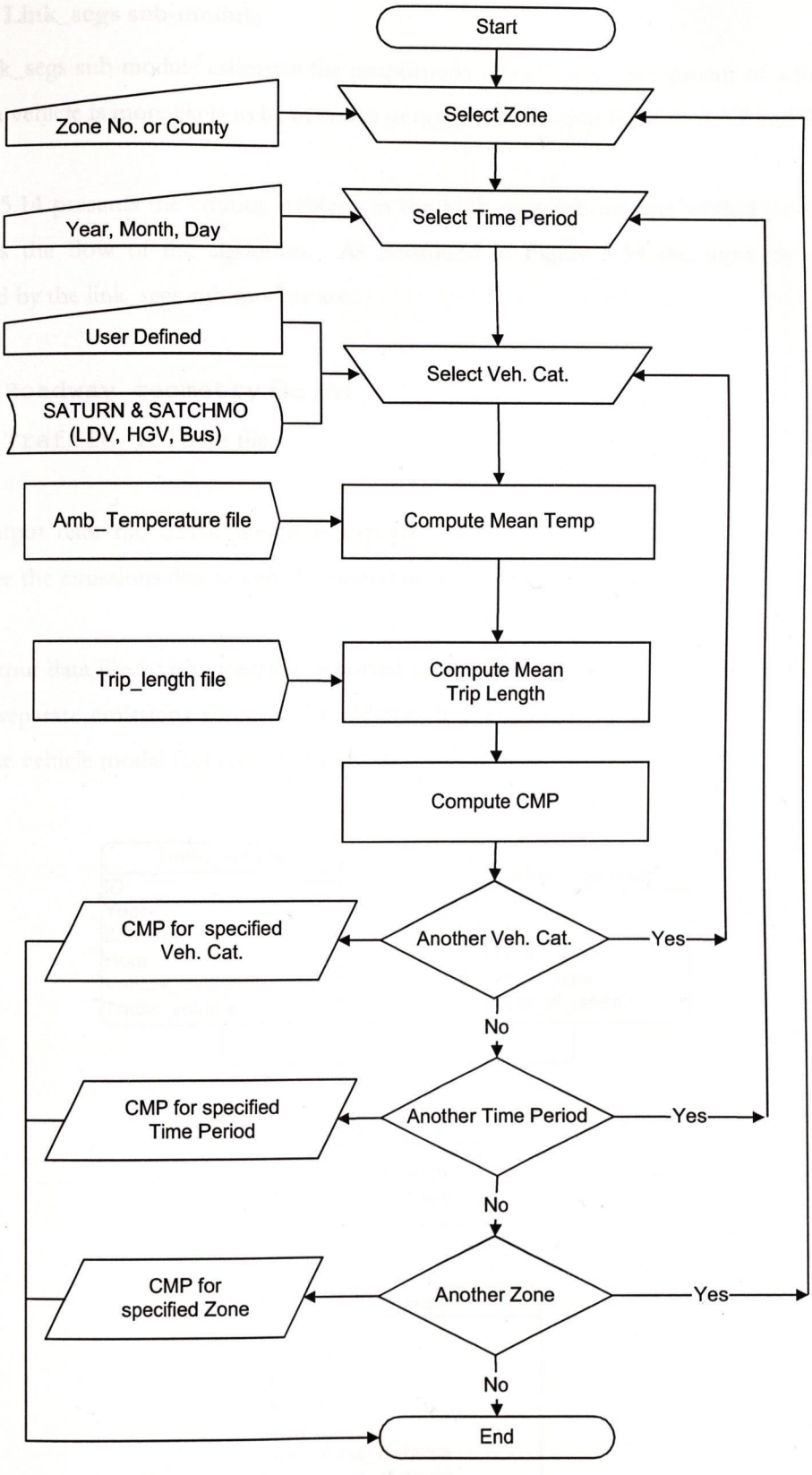


Figure 5.13: Process flowchart for the CMP sub-module

5.3.2.5 Link_segs sub-module

The link_segs sub-module estimates the proportions of each link (or segment of a link) in which a vehicle is more likely to be in cruise or queue mode using Equations 3.2 and 3.3.

Figure 5.14 presents the entities involved in the Link_segs sub-module while Figure 5.15 presents the flow of the algorithm. As illustrated in Figure 5.14 the input data files required by the link_segs sub-module are:

- `Roadway_geometry` file; and
- `Traffic_volume` file.

The output data file `Link_segs` is exported to the MVERA module. It is used to compute the emissions due to vehicles operating in cruise or creep mode.

The output data file `Link_segs` is exported to the dispersion model CALINE4R also, to define separate emissions sources. In addition, it is employed by the MVFC module (to compute vehicle modal fuel consumption).

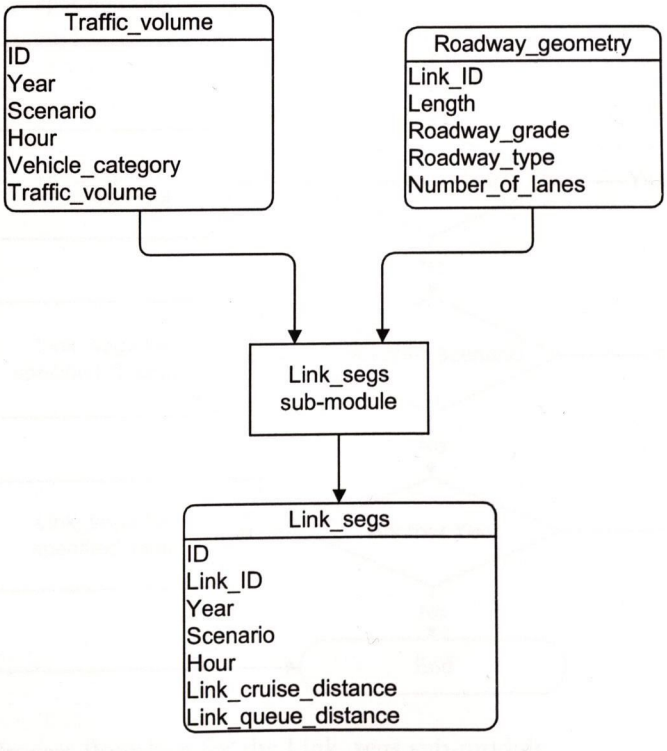


Figure 5.14: Link_segs sub-module entities

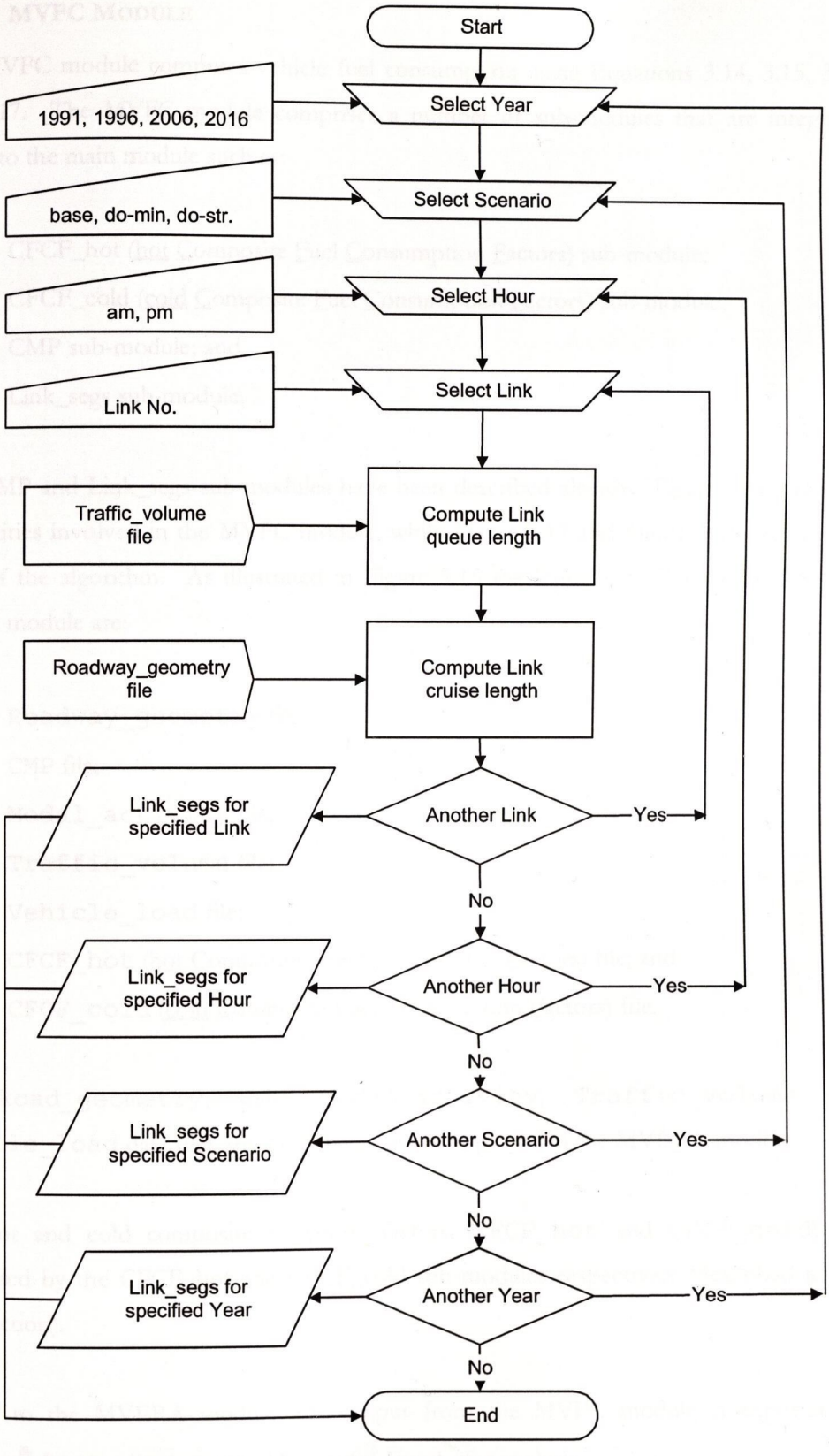


Figure 5.15: Process flowchart for the Link_segs sub-module

5.3.3 MVFC MODULE

The MVFC module computes vehicle fuel consumption using Equations 3.14, 3.15, 3.16 and 3.17. The MVFC module comprises a number of sub-modules that are integrally linked to the main module such as:

- CFCF_hot (hot Composite Fuel Consumption Factors) sub-module;
- CFCF_cold (cold Composite Fuel Consumption Factors) sub-module;
- CMP sub-module; and
- Link_segs sub-module.

The CMP and Link_segs sub-modules have been described already. Figure 5.16 presents the entities involved in the MVFC module, while Figure 5.17 and Figure 5.18 present the flow of the algorithm. As illustrated in Figure 5.16 the input data files required by the MVFC module are:

- `Roadway_geometry` file;
- `CMP` file;
- `Modal_activity` file;
- `Traffic_volume` file;
- `Vehicle_load` file;
- `CFCF_hot` (hot Composite Fuel Consumption Factors) file; and
- `CFCF_cold` (cold Composite Fuel Consumption Factors) file.

The `Road_geometry`, `CMP`, `Modal_activity`, `Traffic_volume` and `Vehicle_load` data files are the same as those employed in the MVERA module.

The hot and cold composite emissions factors (`CFCF_hot` and `CFCF_cold`) are computed by the CFCF_hot and CFCF_cold sub-modules respectively (described in the next section).

Similar to the MVERA module, the output from the MVFC module is exported to ArcView® for visualisation or to Microsoft® Excel™ for analysis.

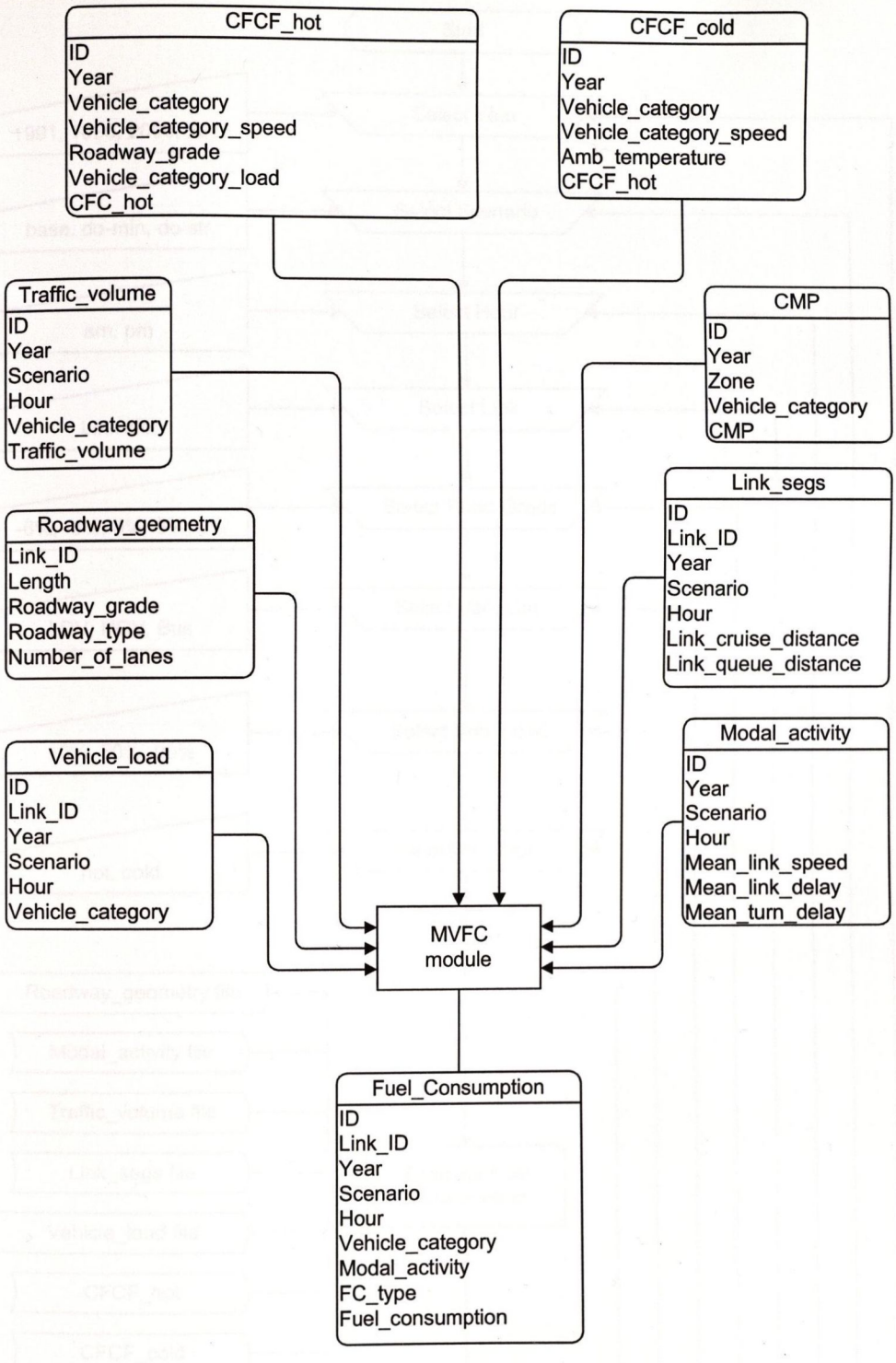


Figure 5.16: MVFC module entities

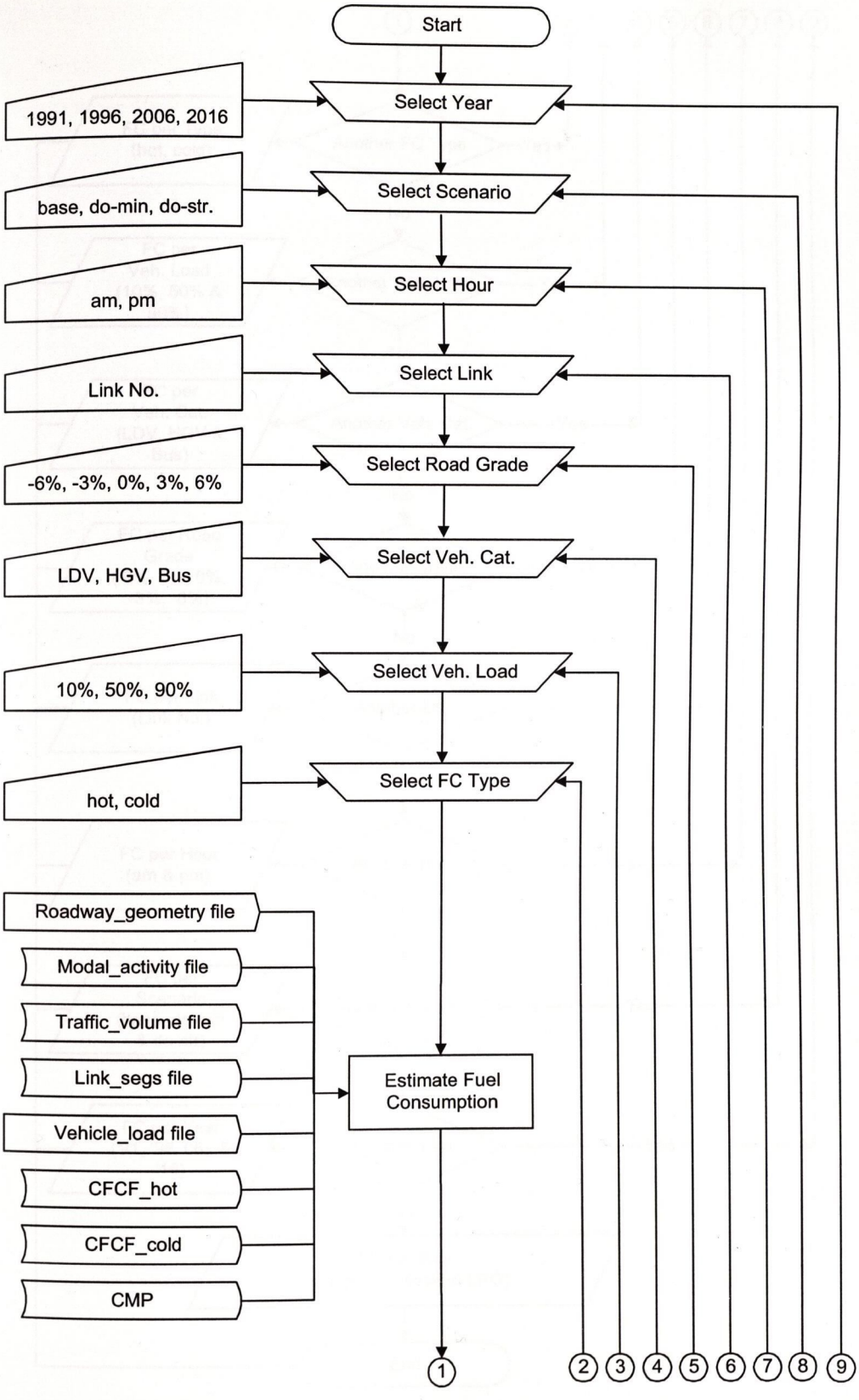


Figure 5.17: Process flowchart for the MVFC module

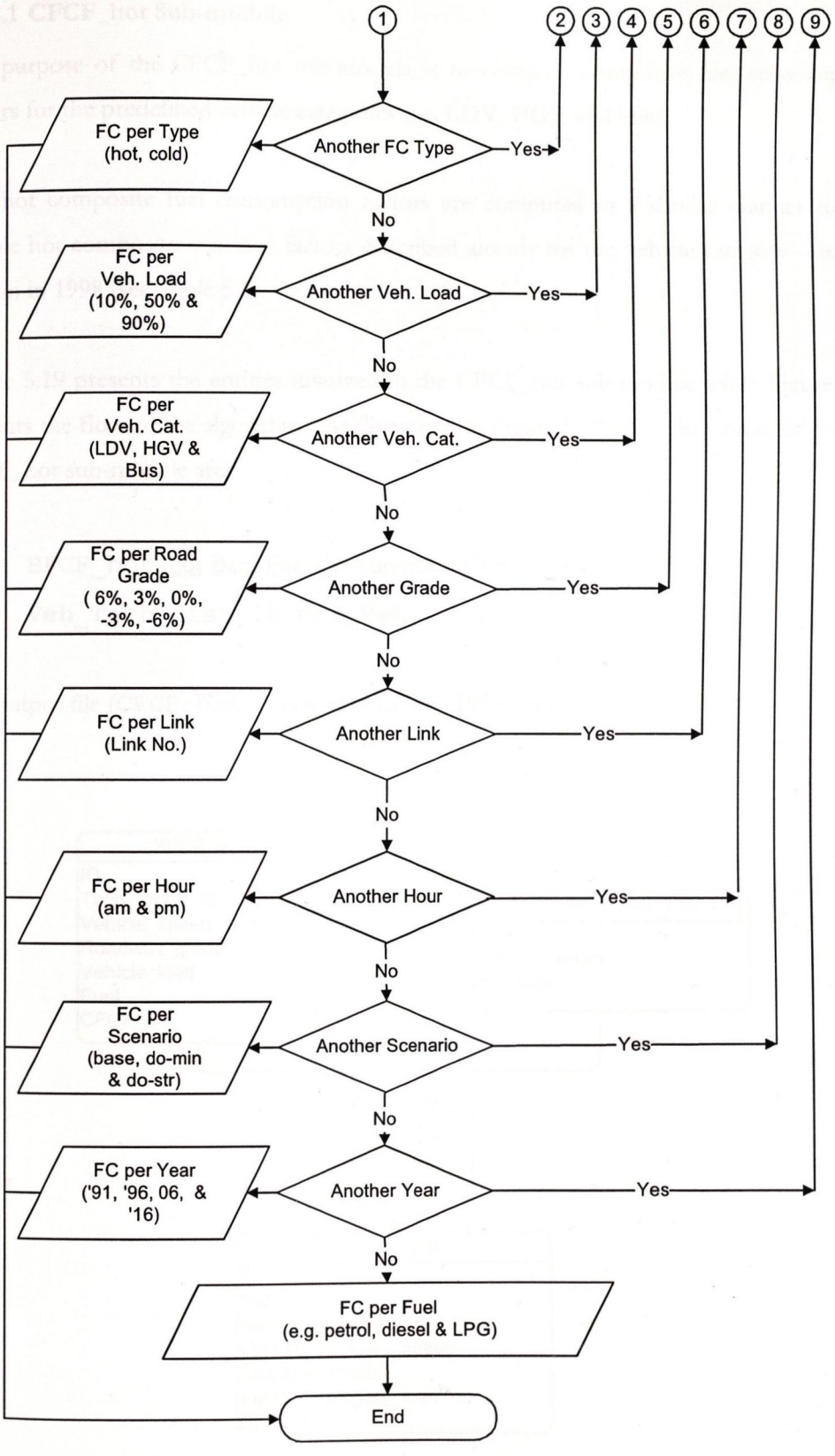


Figure 5.18: Process flowchart for the MVFC module (continued)

5.3.3.1 CFCF_hot Sub-module

The purpose of the CFCF_hot sub-module is to compute composite fuel consumption factors for the predefined vehicle categories (i.e. LDV, HGV and bus).

The hot composite fuel consumption factors are computed in a similar manner to the sample hot composite emission factors described already for the vehicle category – bus in Dublin in 1998 (see Table 5.5).

Figure 5.19 presents the entities involved in the CFCF_hot sub-module while Figure 5.20 presents the flow of the algorithm. As illustrated in Figure 5.19 the inputs required for the CFCF_hot sub-module are:

- `BFCF_hot` (hot Base Fuel Consumption Factors); and
- `Veh_Tech_distrib_per_Veh_Cat` file.

The output file (`CFCF_hot`) is exported to the MVFC module.

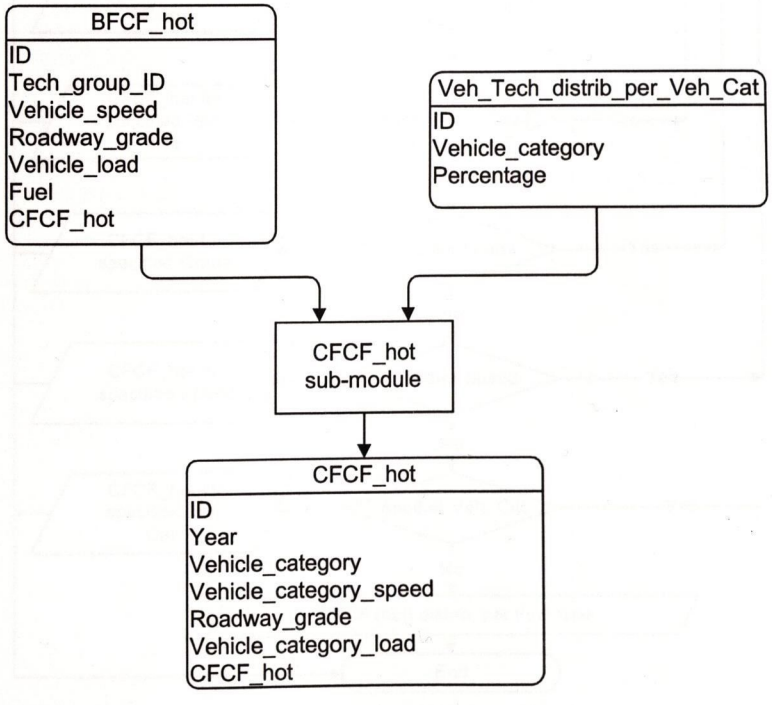


Figure 5.19: CFCF_hot sub-module entities

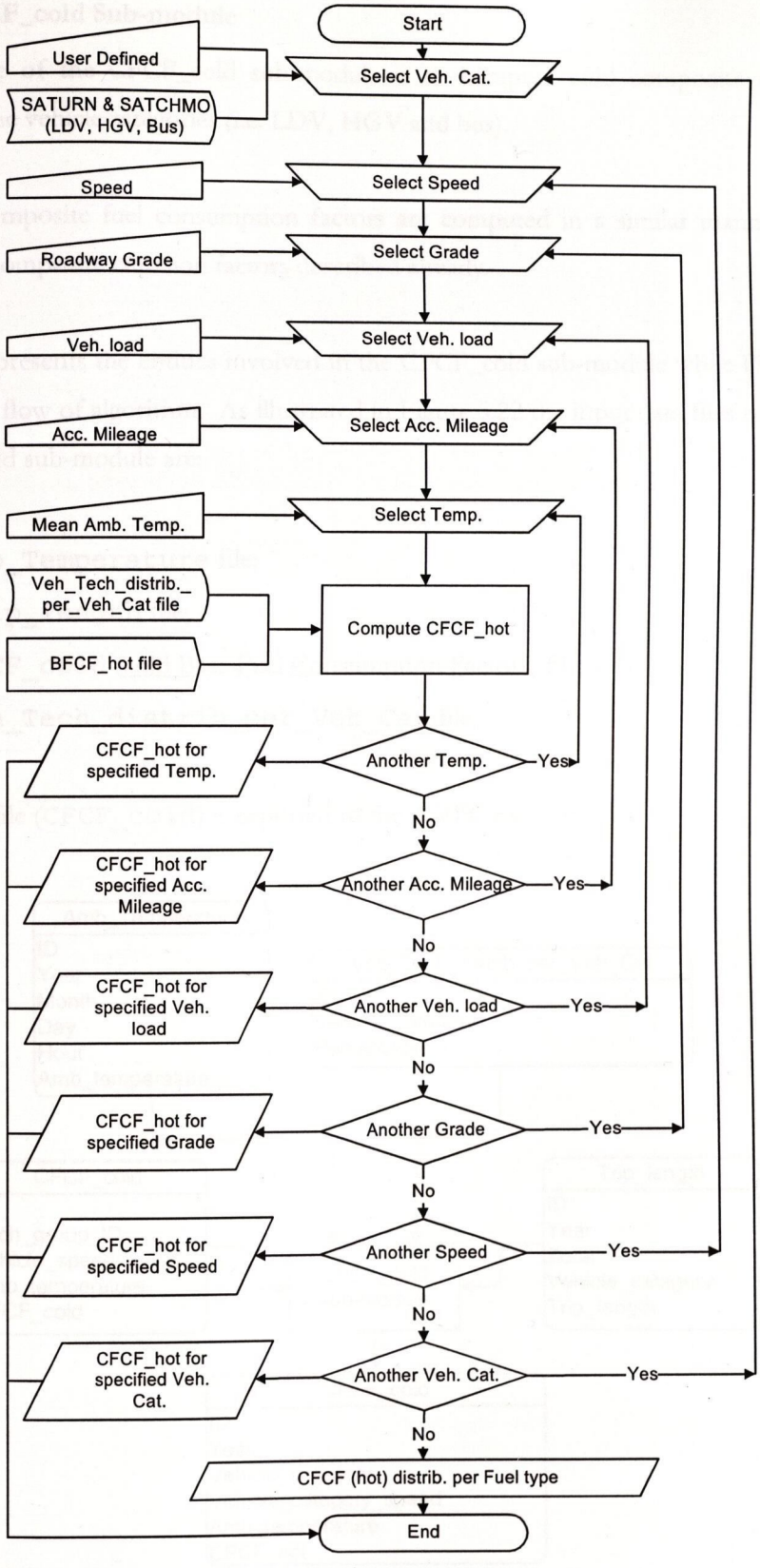


Figure 5.20: Process flowchart for the CFCF_hot sub-module

5.3.3.2 CFCF_cold Sub-module

The purpose of the CFCF_cold sub-module is to compute cold composite emissions factors for the vehicle categories (i.e. LDV, HGV and bus).

The cold composite fuel consumption factors are computed in a similar manner to the sample hot composite emission factors described already.

Figure 5.21 presents the entities involved in the CFCF_cold sub-module while Figure 5.22 presents the flow of algorithm. As illustrated in Figure 5.22 the input data files required by the CEF_cold sub-module are:

- `Amb_Temperature` file;
- `Trip_length` file;
- `BFCF_cold` (cold Base Fuel Consumption Factors) file; and
- `Veh_Tech_distrib_per_Veh_Cat` file.

The output file (`CFCF_cold`) is exported to the MVFC module.

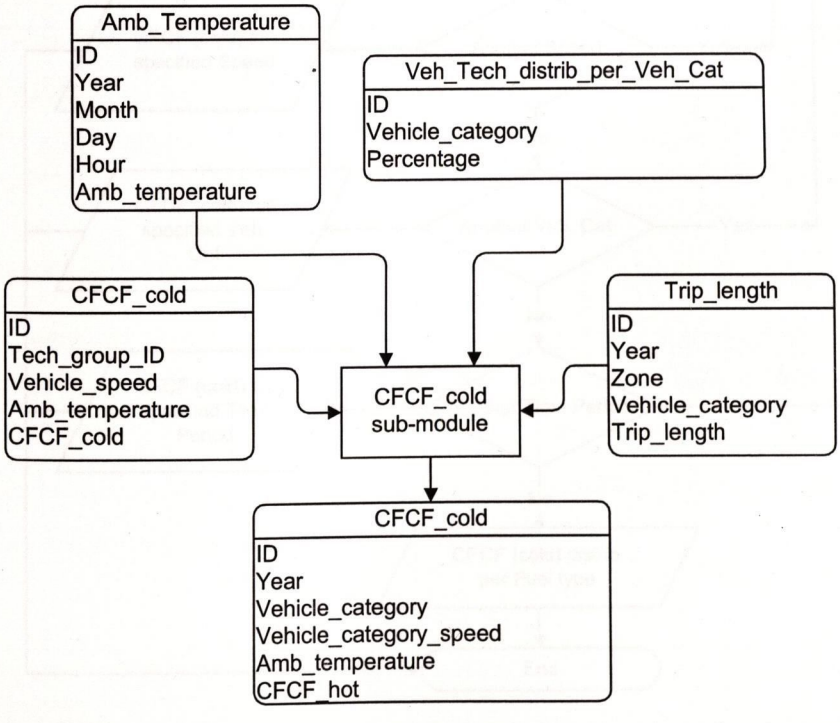


Figure 5.21: CFCF_cold sub-module entities

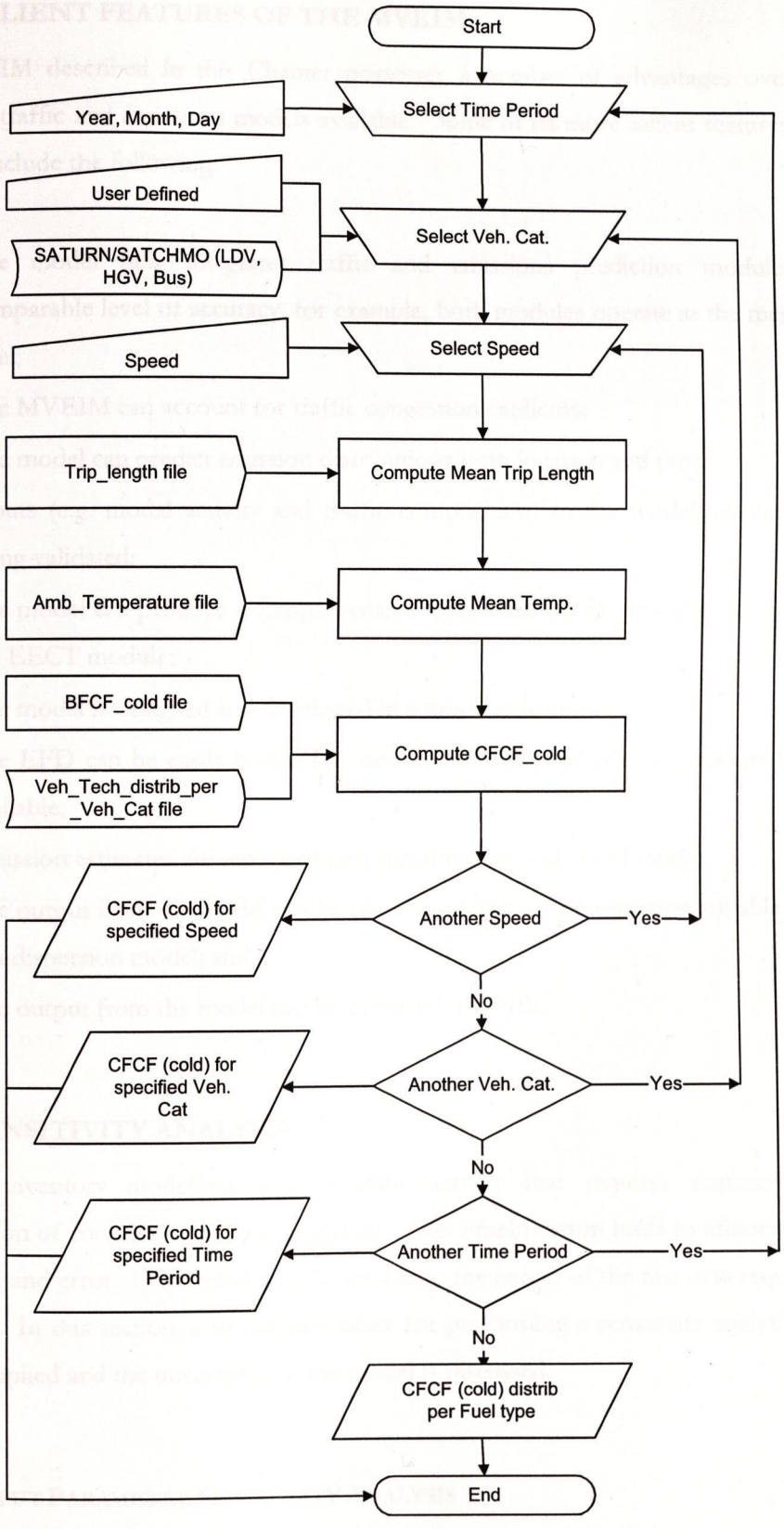


Figure 5.22: Process flowchart for the CFCF_cold sub-module

5.4 SALIENT FEATURES OF THE MVEIM

The MVEIM described in this Chapter possesses a number of advantages over other combined traffic and emissions models available. Some of its more salient features of the MVEIM include the following:

- The model fully integrates traffic and emissions prediction modules at a comparable level of accuracy, for example, both modules operate at the meso-scale level;
- The MVEIM can account for traffic congestion explicitly;
- The model can predict emission distributions both in space and time;
- Inputs (e.g. modal activity and traffic composition) to the model are capable of being validated;
- The model can produce a comprehensive representation of the traffic fleet through the EECT module;
- The model is designed and developed in a modular format;
- The EFD can be easily updated as newer and improved emission factors become available;
- Emission estimates are separated into specific types and travel mode;
- The output from the model can be transferred into a representation suitable for use in a dispersion model; and
- The output from the model can be exported to a GIS.

5.5 SENSITIVITY ANALYSIS

Emission inventory modelling is a scientific activity that requires abstraction and simplification of complex real world processes. This simplification leads to inherent model uncertainty and error. Uncertainty also arises due to the nature of the raw data required for the model. In this section, a simple procedure for performing a sensitivity analysis of the model is applied and the uncertainty in the model is discussed.

5.5.1 INPUT PARAMETER SENSITIVITY ANALYSIS

Sensitivity analysis is a means of evaluating the comparable significance of the MVEIM's output to its variable input parameters. One of the most common techniques used in sensitivity analysis is the 'non-interactive' procedure. Calculations are performed initially by employing the best-estimated values (nominal parameter values) of the input

parameters. All input parameters are then fixed at these nominal values, except one, which is varied in a sequential and independent manner about its nominal value. It is important that the range of values used in this analysis is feasible and realistic. The calculations are then repeated for all input parameters, and the resultant set of output values displays how the MVEIM behaves with respect to each. This procedure demonstrates the relative importance of changes in each input variable in terms of the resultant output values.

This methodology is generic, straightforward and relatively easy to perform. The results are amiable to graphical and tabular representation as they are numerical and do not involve complex formulae. Most importantly, the methodology is independent of the model structure and is therefore generally applicable to all models. The main disadvantage of the methodology is that input parameters are varied individually and therefore interactions between them are not resolved. Also, the methodology is fundamentally empirical in nature and therefore does not draw on what is already known of the MVEIM structure.

A sensitivity analysis was performed with all of the primary model input parameters. By varying ten input parameters that depend heavily on statistical data, a non-interactive sensitivity analysis for the MVEIM was performed. These parameters are given in Table 5.6. The composition and age profile of the fleet was kept constant throughout the sensitivity analysis.

Table 5.6: Standard input parameters and their nominal value for the MVEIM sensitivity analysis

Input Parameter	Nominal value	Variation
Vehicle load (%)	50%	55%
Roadway grade (%)	0%	3%
Accumulated mileage (km)	10,000	11,000
Cruise length (m)	500	550
Fuel RVP (kPa)	100	110
Vehicle speed (km/hr)	30	33
Ambient Temperature (°C)	10	11
Queue length (m)	500	550
Trip length (km)	14	15.4
Traffic volume (vehicles)	5,000	5,500

Each input parameter was increased individually by 10% with the exception of roadway grade, which was varied from 0% to 3%.

5.5.2 SENSITIVITY ANALYSIS RESULTS

The variation of the computed output is presented in Figure 5.23 to Figure 5.32. Some of the results are surprising, but are a consequence of the emission factors used rather than the MVEIM (for example, the effect of roadway grade is not available for all pollutants). Some of the input parameters display a reduction effect, whereby changes in output are smaller than the corresponding changes in the input parameter value. For example, a 10% increase in speed reduces all emissions and fuel consumption. In addition, a 10% increase in trip length results in a reduction in all emissions due to the decreasing influence of start-up (cold) vehicle operation. The model is most sensitive to queue length, followed by traffic volume and cruise length. The model is least sensitive to accumulated mileage, because very little data was collated on this effect. Fuel RVP only affects NM-VOC, 1,3-butadiene and benzene.

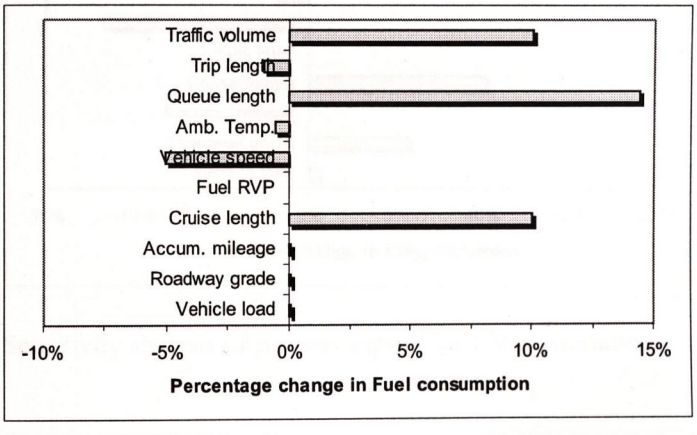


Figure 5.23: Sensitivity analysis of primary inputs for fuel consumption estimation

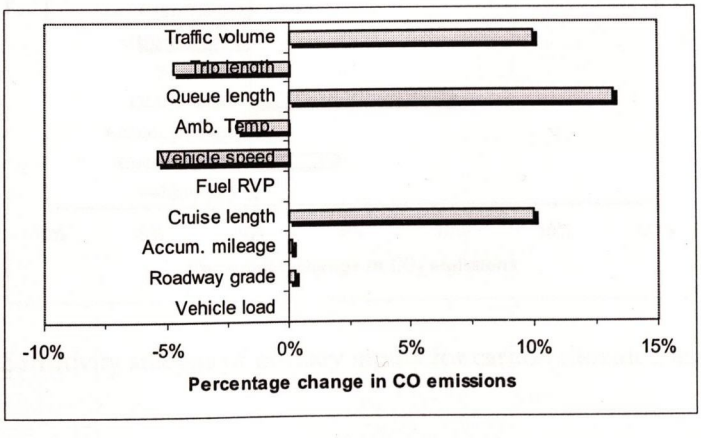


Figure 5.24: Sensitivity analysis of primary inputs for carbon monoxide estimation

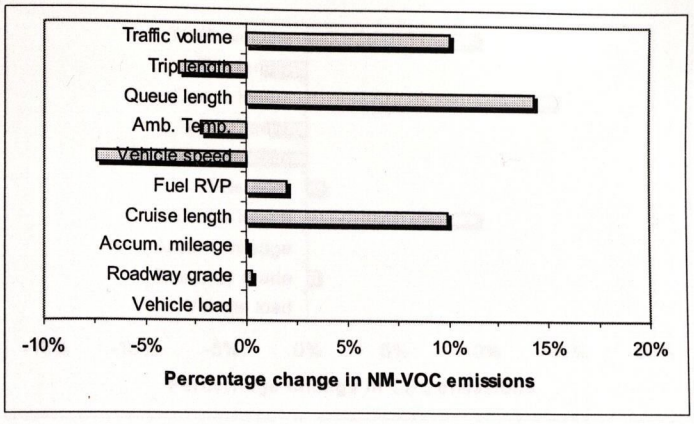


Figure 5.25: Sensitivity analysis of primary inputs for NM-VOC estimation

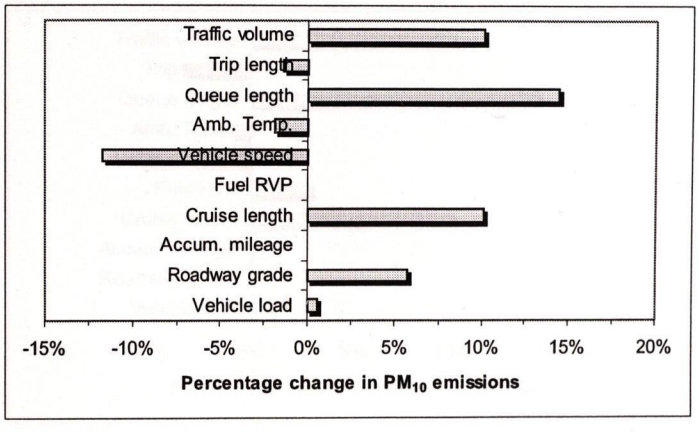


Figure 5.26: Sensitivity analysis of primary inputs for PM_{10} estimation

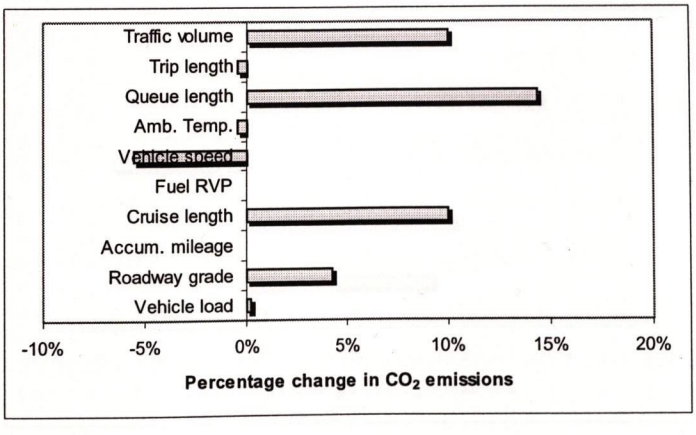


Figure 5.27: Sensitivity analysis of primary inputs for carbon dioxide estimation

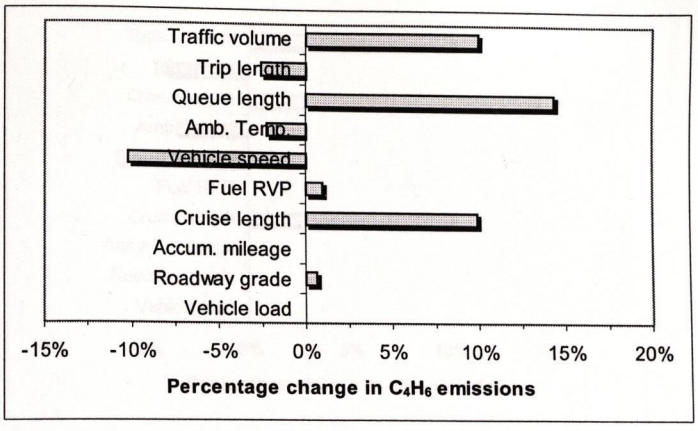


Figure 5.28: Sensitivity analysis of primary inputs for 1,3-butadiene estimation

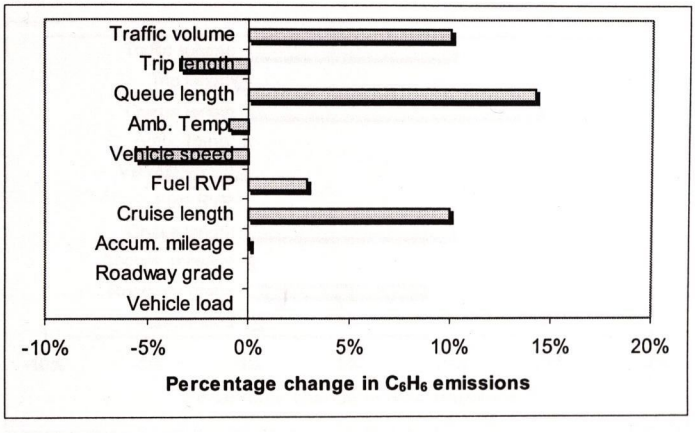


Figure 5.29: Sensitivity analysis of primary inputs for benzene estimation

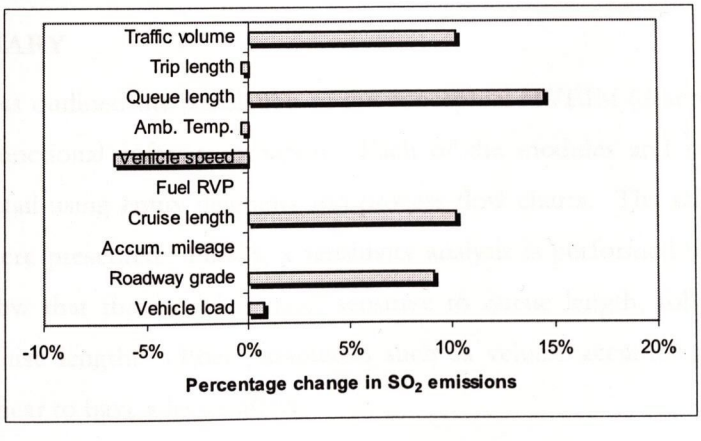


Figure 5.30: Sensitivity analysis of primary inputs for sulphur dioxide estimation

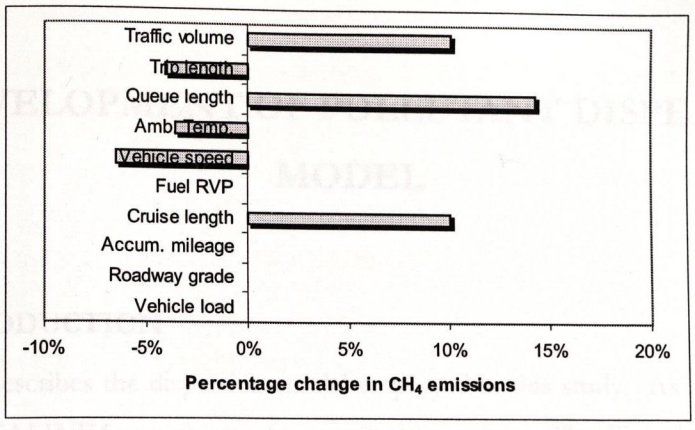


Figure 5.31: Sensitivity analysis of primary inputs for methane estimation

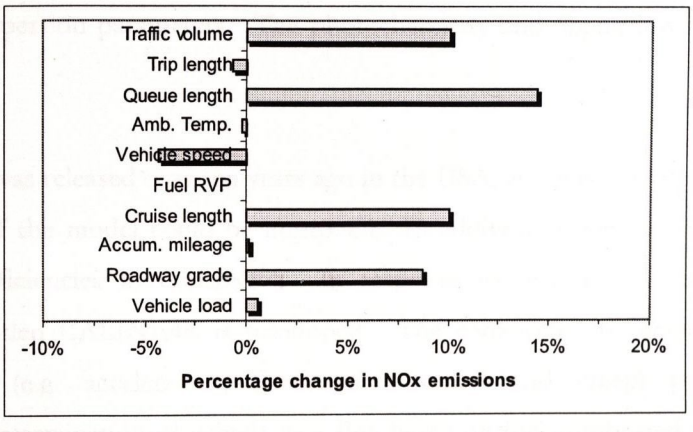


Figure 5.32: Sensitivity analysis of primary inputs for NO_x estimation

5.6 SUMMARY

This Chapter has outlined the translation of the conceptual MVEIM (described in Chapter three) into a functional software program. Each of the modules and sub-modules are described in detail using entity diagrams and process flow charts. The salient features of the MVEIM were presented. Finally, a sensitivity analysis is performed on the MVEIM. The results show that the model is most sensitive to queue length, followed by traffic volume and cruise length. Other parameters such as vehicle accumulated mileage and vehicle load appear to have a lesser affect.

The air dispersion model, CALINE4R that employs traffic emissions along with site topography and local meteorology to estimate ambient roadside pollutant concentrations will be described in the next Chapter.

6. DEVELOPMENT OF POLLUTANT DISPERSION MODEL

6.1 INTRODUCTION

This Chapter describes the dispersion model employed in this study. As already stated in Chapter two, CALINE4 was chosen for use in this project. The Chapter begins with an introduction into the history of CALINE4. Next, the algorithms employed in CALINE4 are described, along with the Gaussian line formulation, mixing cell concept, horizontal and vertical dispersion parameters. The photochemistry and deposition sub-modules are described also.

As CALINE4 was released over ten years ago in the USA, an objective of the research was to investigate if the model could be improved. In addition, a literature review reveals a number of deficiencies in CALINE4. In response to this, an enhanced version of CALINE4 entitled CALINE4R is developed. The enhancements include modules for traffic modal (e.g. acceleration, deceleration, cruise and creep) predictions near intersections, determination of vehicle heat flux based on fuel combusted, flexible output, increased number of receptors and links, calculation of settling velocity, use of NWS data, improved dispersion parameters, incorporation of photochemical reactions and pollutant decay. CALINE4R should be thought of as an expanded and updated version of CALINE4.

6.2 BACKGROUND TO CALINE4

As the name suggests, CALINE4 is the fourth in a generation of models developed for predicting carbon monoxide concentrations. In addition various hybrid versions have been developed.

6.2.1 CALIFORNIA LINE SOURCE MODEL

A mathematical approach generally known as the 'California Line Source Model' was developed in 1972 by the California Department of Traffic and widely used to estimate highway (project-level) impact on air quality [Beaton, 1972]. The approach was developed

to estimate inert gaseous pollutant concentrations from traffic on highways. It comprised a series of tables and nomographs and a modified form of the Gaussian point source plume dispersion equation along with a mixing cell concept. While the model was validated against a very limited dataset of measurements, the results were inconclusive.

6.2.2 CALINE2

This original mathematical model was replaced by a second-generation model, CALINE2 [Winter, 1976]. CALINE2 is based on the generalised Gaussian dispersion theory, and simulates the dispersion of pollutants from a uniform line source [Ward and Ranzieri, 1975]. It was developed to estimate concentrations of carbon monoxide downwind from roadways. Details of the theory and development of CALINE2 are contained elsewhere [Ward et al., 1977]. This model was written in the FORTRAN programming language for implementation on IBM 360/65 computers [Jones, 1977]. The computational algorithms in the CALINE2 model are extracted and assembled in a series of subroutines contained in a controlling subroutine called CAL2 [Jones and Wilbur, 1976].

The Alabama State Highway Department [Treadway et al., 1978] produced a graphical procedure by which 'desk-top' estimates of carbon monoxide concentration levels could be made using a minimum of calculations. The procedure used families of curves based on CALINE2, and employed selected low-altitude vehicle emission factors based on the US-EPA's mobile source emission factors. Using this procedure, a 'first pass' carbon monoxide analysis could be done in a matter of minutes.

The performance of CALINE2 was evaluated in several studies [Bemis et al., 1977], [Benson and Squires, 1979], [Noll et al., 1977; 1978], [Noll and Claggett, 1979], [Rodden et al., 1982]. It was found that the model over-estimated during stable atmospheric conditions and when the prevailing wind was parallel to the highway. A major limitation to CALINE2 was that emission source strength or surface roughness couldn't be specified [Ward and Ranzieri, 1976]. Another evaluation study of CALINE2 [Green and Bullin, 1982] found that the model was inaccurate because it neglected the change in wind speed with height and because it incorrectly represents transport processes when the wind angle to the roadway differs from ninety-degrees.

6.2.3 CALINE3

The limitations of CALINE2 led to the development of a third generation line source air quality model called CALINE3 [Benson, 1979]. The background to the development of CALINE3 is documented elsewhere [Benson, 1980]. CALINE3 kept the basic Gaussian dispersion formulation, but the virtual point source methodology was replaced with an equivalent finite-line source concept. The model employs a mixing zone to characterise pollutant dispersion over the roadway. For horizontal dispersion, coefficients from Turner [1969] are employed with adjustments for roughness length and averaging-time. For vertical dispersion, empirical coefficients as defined by Pasquill [1974] are used. Initial traffic-induced dispersion is handled implicitly by plume size parameters. The dispersion coefficient is adjusted for averaging time using a power law formulation.

The purpose of the model is to assess air quality impacts near traffic facilities (highways and arterial streets) in what is known as the micro-scale region. It can be applied to determine air pollution concentrations at receptor locations downwind of 'at-grade', 'fill', 'bridge', and 'cut section' highways located in relatively uncomplicated terrain. Given emission source strength, local meteorology, site geometry, site characteristics, and traffic volume, the model can reliably predict carbon monoxide concentrations for receptors located within 150 meters of the roadway. The model contains an algorithm for deposition and settling velocity so that particulate concentrations can be predicted.

Details of sensitivity, evaluation and verification analyses of CALINE3 have been documented elsewhere [Benson and Baishiki, 1980], [Bianconi, 1993], [Rao and Visalli, 1985], [Olmstead, 1982], [Dresnack and Golub, 1994], [Dabberdt, 1975], [Hlavinka and Bullin, 1988]. Rao et al. [1986] compared CALINE3, HIWAY2, and ROADWAY using the tracer data from the General Motors Sulfate Dispersion Experiment. Experimental studies [Benson, 1980] indicated that the Gaussian distribution employed in CALINE3 adequately represents the vertical distribution of emissions from traffic at the edge of the roadway. In addition, the height of this initial vertical spread is positively correlated with pollutant emissions residence time over the roadway. The effects of vehicle induced turbulence were investigated and it was concluded that vehicle induced turbulence is a significant effect in cases of neutral to stable atmospheric conditions. The model was initially released to run on a mainframe computer [Mersch, 1989] but was subsequently upgraded so that it could be used on microcomputers [US-EPA, 1992b] and compiled using Microsoft FORTRAN version 4.1. Cohn and Gaddipati [1984] developed an interactive graphics display to plot model results from CALINE3. Hlavinka et al. [1987]

developed TEXIN2, which consisted of CALINE3 and an emission rate model, MOBILE3.

The FDOT developed a graphical procedure to estimate carbon monoxide concentrations near an at-grade four-way intersection in either an urban or rural area. The procedure is known as COSCREEN [Cooper, 1991]. This screening model is based on CALINE3 and emission factors are derived from MOBILE4 [US-EPA, 1991b]. As the screening procedure is based on a number of very conservative assumptions, if the project fails the screening procedure, more detailed computer modelling is required (i.e. the use of CALINE3).

'Appendix W to part 51 - Guideline on Air Quality Models' [US-EPA, 1998] recommends that CALINE3 is appropriate for the following applications:

- Highway (line) sources;
- Urban or rural areas;
- Simple terrain;
- Pollutant transport distances less than 10 km; and
- One-hour to twenty-four hour averaging times.

In general, for analyses of highways characterised by uninterrupted traffic flows, CALINE3 is recommended.

6.2.4 CAL3QHC

A special version of CALINE3 was developed specifically for air quality modelling at intersections called CAL3QHC [Schattanek and Kahng, 1992]. CAL3QHC enhances CALINE3 by incorporating methods for estimating queue lengths and the contribution of emissions from idling vehicles. The model predicts the total pollution concentration levels due to both moving and idling vehicles. However, it does not permit the direct estimation of the contribution of emissions from idling vehicles to the total predicted concentration. As the idle emissions account for a substantial portion of the total emissions at an intersection, the model is relatively insensitive to average vehicle speed. On congested urban roadways, this traffic activity parameter can prove difficult to estimate accurately without a substantial data collection effort [US-EPA, 1992c]. CAL3QHC requires all the inputs required for CALINE3, plus signal timing data, idling emission rates and the

number of 'moving lanes' in each approach link. A second version of the model, CAL3QHC2 has been released [Eckhoff, 1995]. The main difference between CAL3QHC and CAL3QHC2 relates to the determination of intersection capacity, queue length, and vehicle delay [Zandi, 1997]. CAL3QHC2 includes three new traffic variables, namely, saturation flow rate (number of vehicles per hour per lane departing from a stop line infinite green) signal type (pre-timed, actuated, or semi-actuated), and arrival rate (the rate of vehicle progression for each queue link). These variables allow a more precise specification of the operational characteristics of an intersection than in the original CAL3QHC model [Eckhoff, 1995]. Wholley and Michaud [1995] developed a GUI for CAL3QHC entitled CAL3QHC-AC to facilitate the modelling process and reduce common modelling errors by allowing air quality analysts to operate the model in a user-friendly graphical format (AutoCAD). CAL3QHC has been modified to process hourly meteorological data [Schattanek et al., 1995], [Eckhoff and Braverman, 1996].

Details of sensitivity, evaluation and verification analyses of CAL3QHC have been documented elsewhere [Akeredolu et al., 1994], [Dabberdt et al., 1998], [Guldberg, 1990; 1991], [Lindemann, 1995], [Moseholm et al., 1996], [O'Neal, 1991], [Rossi, 1990] and [Spitzak et al., 1995]. The NYCDEP and Parsons Brinckerhoff (the consultant firm that assisted the US-EPA in the development of CAL3QHC) also performed a study evaluating the sensitivity of predicted carbon monoxide levels to changes in traffic conditions at numerous types of congested intersections in New York City [Petsios et al., 1993]. The study found that changes in traffic characteristics and physical configurations of intersections could substantially affect predicted carbon monoxide concentrations.

A study carried in Tuscon, Denver, and near Washington D.C. [Carr et al., 1996] provided substantial evidence that air from moving traffic near intersections is dragged along in the direction of the moving traffic. The study [Carr et al., 1996] stated that "algorithms in current regulatory roadway intersection dispersion models (CAL3QHC, CALINE3) appear appropriate under unstable conditions; however, under neutral and stable conditions propagation of vehicle-induced turbulent wake effects, spatial variability in the horizontal flow field, and vehicle exhaust effects that are not included in most of the current models become important".

The FDOT has updated their screening graphical procedure called COSCREEN98 [Cooper and Keely, 1999]. This updated version is based on CAL3QHC2 [Eckhoff, 1995] and it employs emission factors from MOBILE5a [US-EPA, 1993].

The 'Guideline for Modelling Carbon Monoxide from Roadway Intersections' [US-EPA, 1992d] recommends that CAL3QHC should be used for analysing carbon monoxide impacts at roadway intersections.

6.2.5 CALINE4

CALINE4 is the latest version in the series of California Line Source models available. It represents a refinement and extension of the capabilities contained in CALINE3 rather than a new generation model [Benson, 1992]. The user manual is available from CALTRANS [Benson et al., 1989].

CALINE4 contains an algorithm for air quality intersection modelling but does not include a traffic model component. CALINE4 also has incorporated algorithms for the thermal and mechanical turbulence caused by moving vehicles. A full description of CALINE4 is given later in this Chapter.

The 'Guideline on Air Quality Models' [US-EPA, 1998] also suggests that in areas where the use of CALINE4 has previously been established, its use may continue. Effectively, CALINE3 and CAL3QHC, which are recommended by US-EPA guidance for highways and intersection modelling respectively, are employed in most states in the USA except in the state of California, where the use of CALINE4 model is recommended [O'Connor et al., 1993].

6.3 PREVIOUS STUDIES USING CALINE4

This section summarises previous studies performed using the CALINE4 dispersion model.

6.3.1 EVALUATION AND VALIDATION OF CALINE4

A number of studies have been carried out to validate CALINE4 with measured data and consequently evaluate its performance. For example, [Benson et al., 1986], [Nokes and Benson, 1985], [Benson et al., 1985], and [Benson, 1988], [US-EPA, 1992a], [Ireson and Mahoney, 1986]. CALINE4 was initially verified and evaluated with results from five separate field studies. These were:

1. CALTRANS Sacramento Intersection Study [Benson, 1980];
2. CALTRANS Highway-99 SF_6 Tracer Experiment [Benson, 1984];
3. General Motors Sulfate Dispersion Experiment [Cadle, 1976], [Cadle et al., 1977], [Eskridge et al., 1979], [Eskridge and Hunt, 1979], [Chock, 1976; 1977a, 1977b];
4. Illinois EPA Freeway/Intersection Study [Noll and Claggett, 1979], [Claggett and Miller, 1979]; and
5. US-EPA NO_2/O_3 Sampler Siting Study [Rhodes and Holland, 1979].

The accuracy of prediction for CALINE4 in respect to the General Motors and Caltrans SF_6 tracer studies is reflected in correlation coefficients between observed and predicted concentrations of 0.87 and 0.51 respectively. Eighty-five percent of the predictions fall within a factor-of-two envelope of observed values (with 85% of these being over-estimates). It was observed that CALINE4 over-estimated (12-15%) more frequently than under-estimated (1-7%) when concentrations differed by more than a factor-of-two. It is worth noting that CALINE4 over-estimated 95% of the measurements taken when the prevailing wind was parallel to the roadway (with 80% of these inside the factor-of-two envelope). This is due to the fact that CALINE4 is sensitive to the assumption of steady-state homogenous wind flow during parallel wind conditions. The performance of CALINE4 deteriorates as wind speed decreases. For example, when the wind speed was greater than 1 m/s, 90% of the predictions fell within the factor-of-two envelope, whereas when the wind speed was less than 1 m/s, only 75% of the predictions fell within the factor-of-two envelope. CALINE4 performed similarly for both intersection and highway sites.

It was found that the performance of CALINE4 in the NO_2/O_3 Sampler Siting Study was better for NO_2 than for SF_6 or CO. However, only a very limited data set was employed in this study. In addition, the lowest average wind speed was 1.4 m/s, and the prevailing wind angle was perpendicular to the roadway during the experiment. CALINE4 performs best under these conditions of wind speed and direction.

Various groups have also carried out independent validation and evaluation studies on CALINE4, as well as sample applications. These include [Anderson, 1988], [Carpenter and Barboza, 1988], [Chan et al., 1988], [Dames and Moore, 1987], [Gondwe, 1998], [Held et al., 1998], [Hlavinka, 1995], [Hung et al., 1991], [Ionel et al., 1999], [Johnson et al., 1987; 1988; 1989], [Lamoree and Turner, 1999], [Metallo et al., 1995], [Shenouda, 1994], [Singh et

al., 2000], [Singh and Colls, 1998], [Sokhi et al., 2000], [Velzy, 1995] and [Washington et al., 1994] amongst others.

These studies showed that CALINE4 adequately estimates pollutant concentrations during non-worst case scenarios (i.e. wind speeds greater than 1m/s and non-parallel winds). The model was found to provide good approximations of peak values and trends over time. However, care must be taken with the emission factors employed in the model. For example, many emission factor models only give emission factors in g/km. These emission factors were designed for regional inventories and were never intended to be used at a local level.

CALINE4 tends to over-estimate near the edge of the roadway and under-estimate at background sites. During low pollutant concentrations, CALINE4 tends to under-estimate. The model exhibits better agreement with measured data for longer-term averages (e.g. monthly and annually) than for shorter-term. In general, the above studies reported that most of the paired data points (observed and measured) fall within the factor-of-two envelope. However, the model is capable of predicting the extreme concentrations. The studies also show that "once the model has been validated, this approach, compared with the traditional approach involving a large amount of measurements, has the merits of being reliable and economical" [Metallo et al., 1995].

6.3.2 Integration of CALINE4 with Environmental Models

Consistent with the approach employed in this project, CALINE4 has been incorporated into or combined with a number of other traffic and emission rate models. For example:

1. Carr [2000] developed an integrated roadway intersection model – HYROAD, which incorporates CALINE4.
2. Fisher and Sokhi (1998) developed a screening model entitled GRAM based on algorithms in CALINE4.
3. Härkönen et al. [1997] developed an operational model for predicting pollution from a road, which incorporates components of CALINE4.
4. Hlavinka [1995] integrated the 1985 Highway Capacity Manual, MOBILE5a and CALINE4 into an air quality model entitled TEXIN3.

5. Lamoree and Turner [1999] developed a particulate emissions prediction model comprised of PART5 and CALINE4 to estimate emissions emanating from limited access highways.
6. Namdeo and Colls [1996] developed a suite of models for the prediction of pollution concentrations from vehicles in urban areas, which consisted of an emissions rate model ROADFAC and a dispersion model NOTLINE (a hybrid version of CALINE4).
7. Randall [1989] developed an integrated suite of air quality analysis tools, which includes CALINE4 and EMFAC (an emissions factor model used in the state of California).
8. Shenouda and Schmidt [1997] combined a Power-Based Exhaust Emissions Model with CALINE4.
9. Singh et al. [2000] combined a realtime microscale automobile emission factor model for carbon monoxide (MicroFacCO) with CALINE4.
10. Singh and Colls [1997] combined a vehicle particulate emissions model, PMFAC with CALINE4.
11. Sjodin et al. [1994] developed a model to estimate pollutant concentrations close to roadways, which incorporates components of CALINE4.
12. Yedlin et al. [1998] developed an 'Integrated Air Quality Intersection Computer Model' that comprises the TRAF-NETSIM traffic simulation model, the MOBILE emission rate model and CALINE4.

6.3.3 Comparison of CALINE4 to other Dispersion Models

A number of comparison studies between CALINE4 and other models have been carried out. The studies reviewed are summarised in Table 6.1. All comparative studies reported here included model validation with the exception of the comparisons performed by Sculley [1989] and Dabberdt et al. [1995]. Model validation is accomplished by comparing observed pollutant measurements with concentrations estimated by the model. In addition to pollutant concentration measurements, model validation is obtained by field observations of local meteorological and traffic conditions.

Overall, it was found that CALINE4 compares well to other available Gaussian based line source dispersion models for distances less than 500m from the source.

Table 6.1: Summary of reviewed comparison studies of CALINE4

Study	Pollutant	Models compared to	Country	Study Site
Benson et al., 1986	CO	CALINE3 [Benson, 1979]	USA	Arterial
Benson, 1991	SF_6	CALINE3 [Benson, 1979]	USA	Highway
Braverman & DiCristofara, 1992; Zamurs, 1990, 1991;	CO	CAL3QHC [Schattanek & Kahng, 1992] EPAINT [PEI, 1988] FHWAINT [PEI, 1988] GIM [EMI, 1985] IMM [NYS-DOT, 1982] TEXIN2 [Hlavinka et al., 1987] VOLUME9 [US-EPA, 1978]	USA	Urban intersection
Burden & Whitnell, 1997; Burden et al., 1997; Courthold 1998	NO_2	DMRB [UK-DOT, 1993]	UK	Motorway intersection
Chan et al., 1995	NO_2 CO	APRAC [Simmon et al., 1981] GZE [Chan et al., 1995] PWILG [Chan et al., 1995]	China	City-center streets
Courthold & Whitnell, 1988	NO_2	ADMS Urban [McHugh et al., 1997b]	UK	Motorway intersection
Dabberdt et al., 1995	C_2H_6	HIWAY2 [Petersen, 1980] Stör.lag [Schorling, 1989] ESSCO [Hoydysh & Dabberdt, 1994]	USA	Urban-canyon intersection
Datz, 1994	CO	FLINT [Cooper, 1997] CALINE3 [Benson, 1979] CAL3QHC [Schattanek & Kahng, 1992]	USA	Intersection
Heidorn et al., 1989, 1990	SF_6	HIWAY2 [Petersen, 1980] RWDI [Murphy & Davis, 1988]	USA	Highway, Wind Tunnel
Kunzli et al., 1994	CO	PREDCO [TRRL, 1983]	UK	Highway
Leung et al., 1996, 1997	CO	SMIGS [Waterfield & Hickman, 1982]	China	Urban intersection
Loranger et al., 1995	Mn_3O_4 CO	ISC3 [US-EPA, 1995a]	Canada	Highway
Manini et al., 1996	CO	CPB3 [Yamartino & Weigand, 1986] GEM [Lanzani & Tamponi, 1995] Johnson [Johnson et al., 1973]	Italy	Canyon, highway & side-street
Martínez et al., 1999	CO	HIWAY2 [Petersen, 1980] PAL2 [Petersen & Rumsey, 1987]	Colombia	Urban road
Min-Jung, 1999	NO_2	OMG [Kono & Ito, 1990] CALINE3 [Benson, 1979] HIWAY2 [Petersen, 1980]	Korea	Street canyon
PEI, 1990; Schewe, 1989	CO	CAL3Q [Smith, 1985] EPAINT [PEI, 1988] FHWAINT [PEI, 1988] GIM [EMI, 1985] IMM [NYS-DOT, 1982] TEXIN2 [Hlavinka et al., 1987] VOLUME9 [US-EPA, 1978]	USA	Urban Intersection
Sculley, 1989	CO	IMM [NYS-DOT, 1982] MICRO2 [Griffin, 1983] TEXIN2 [Hlavinka et al., 1987]	USA	N/A
Shenouda, 1994; Williams et al., 1994a;	NO_x CO HC CO_2	HIWAY2 [Petersen, 1980]	Australia	Highway
Smallbone, 1998	NO_2	DMRB [UK-DOT, 1993] CAR-Int. [denBoeft et al., 1996] CALINE3 [Benson, 1979]	UK	Roadside
Sokhi et al., 1996	NO_2	CAR [Eerens et al., 1993] DMRB [UK-DOT, 1993]	USA	Dual carriageway
Sokhi, 1998b; Sokhi et al., 1998	CO NO_2 PM_{10}	GRAM [Fisher and Sokhi, 1998] ADMS-urban [McHugh et al., 1997b]	UK	Motorway & street

All the models were reasonably accurate in predicting ground level concentrations. Most Gaussian models seem to predict well close to the source with the correlations decreasing

when the distance from the source is increased. The models tend to over-predict concentrations a lot more as the distance between source and receptor increases. Many of the studies indicate that the accuracy of the models was influenced by vehicular composition and associated emission factors. The accuracy of the models also depends on atmospheric conditions. For example, many models perform poorly for wind speeds less then 1m/s, whereas model accuracy in most cases increases with the angle between the wind and the road. Even the best models over- and under-estimate by more than a factor-of-two in the many cases.

This literature review revealed comparisons of CALINE4 with 32 different models developed all over the world. As CALINE4 performed better in some situations and worst in others, even within the same study, it cannot be concluded that CALINE4 is substantially better or worst than any other model. CALINE4 performed much better than less sophisticated screening models. In addition, CALINE4 also performed marginally better than CALINE3 and produced only slight improvements in the accuracy of predictions. However, some specialised street canyon models performed better than CALINE4. In general, it was found that CALINE4 overestimated in street canyons.

A state-of-the-art review of air quality dispersion models currently employed in Europe [Moussiopoulos et al., 1996] did not include CALINE4. However, a literature review reveals that CALINE4 is employed in Ireland [Sweetman, 2000], UK [Sokhi, 1998b], France [Sacre et al., 1995], Italy [Corti and Carnevale, 2000], and Romania [Ionel et al., 1999]. For example, a recent survey of all local authorities in the UK [Beattie et al., 1998] found that 11% of them are either currently using CALINE4 or intend to use it in the next year for local dispersion modelling. The UK-DETR included CALINE4 in its guidelines on selection and use of dispersion models [UK-DETR, 1998b].

6.3.4 Predicting Non-regulatory Pollutants with CALINE4

The CALINE series of models was developed primarily to predict ambient concentrations of carbon monoxide due to local road traffic. Later, modifications were made to the model to predict nitrogen dioxide and particulate matter. The model has been successfully employed to predict pollutants other than these (see Table 6.2). CALINE like many other Gaussian models treat other pollutants (such as benzene) as inert gases. This is a reasonable assumption since the distance from source to receptor is relatively short (i.e. metres) for roadside pollution estimation.

Table 6.2: Studies where CALINE was used to estimate non-regulatory pollutants

Pollutant	Source Study	Country	Study Site
VOC	Jones et al., 1998	UK	Urban intersection
Hydrocarbons	Sacre et al., 1995	France	Urban area
	Williams et al., 1994b	Australia	Highway
	Shenouda, 1997	Australia	Highway
PAHs	Sacre et al., 1995	France	Urban area
SO_2	Tino and Siple, 1998	USA	Airport
	Metallo et al., 1995	Italy	Urban area
CO_2	Shenouda and Schmidt, 1997	Australia	Highway
	Williams et al., 1994b	Australia	Highway
1,3-butadiene	Bloom, 1991	USA	Urban intersection
Formaldehyde	Bloom, 1991	USA	Urban intersection
Odour	Chadder, 1999	Canada	Car park
Benzene	Sacre et al., 1995	France	Urban area
	Bloom, 1991	USA	Urban intersection
	Jones et al., 1998	UK	Urban intersection

Although a literature review revealed a limited amount of published material on the use of the CALINE series of models to model pollutants other than CO, NO_2 and PM, it is felt that there is sufficient evidence to justify the use of CALINE4 in this way. In addition, the US-EPA [Atkinson, 1999] stated that CALINE4 could be employed to predict pollutants (other than CO, NO_2 and PM) as long as the user realises that the model assumes that the pollutants do not react after being emitted.

6.4 CALINE4 MODEL DESCRIPTION

This section describes the CALINE4 model. Much of the information provided is taken from the CALINE4 User Manual [Benson et al., 1989] and other sources that describe the model, for example [Benson, 1988; 1991; 1992; 1997] and [Wayson, 1999]. CALINE4 is based on the Gaussian plume formulation for a line source of finite length, together with concepts of a box model. The model employs traffic volume, emission factors, local meteorological data, and site geometry to estimate pollutant concentrations within 500 meters of the roadway. The model can predict carbon monoxide, nitrogen dioxide, and particulate emissions from mobile sources. Options for modelling near intersections, parking lots, elevated or depressed freeways, and within canyons are available. Example input files for the implementation of each of these options are given in the CALINE4 User Manual [Benson et al., 1989]. In addition, the model includes a simple modal emissions model developed for traffic at intersections.

6.4.1 FINITE LINE SOURCE GAUSSIAN FORMULATION

Each roadway is modelled as a series of links having constant width, altitude, traffic volume and composite vehicle emission factor as illustrated in Figure 6.1. The location of the link is defined by two sets of endpoint co-ordinates. The location of a receptor is defined in terms of a uniform co-ordinate system. It is worth noting that CALINE4 has two co-ordinates system (one local and one global). The location of the links and receptors are defined in the global co-ordinate system, which can be linked to national co-ordinates.

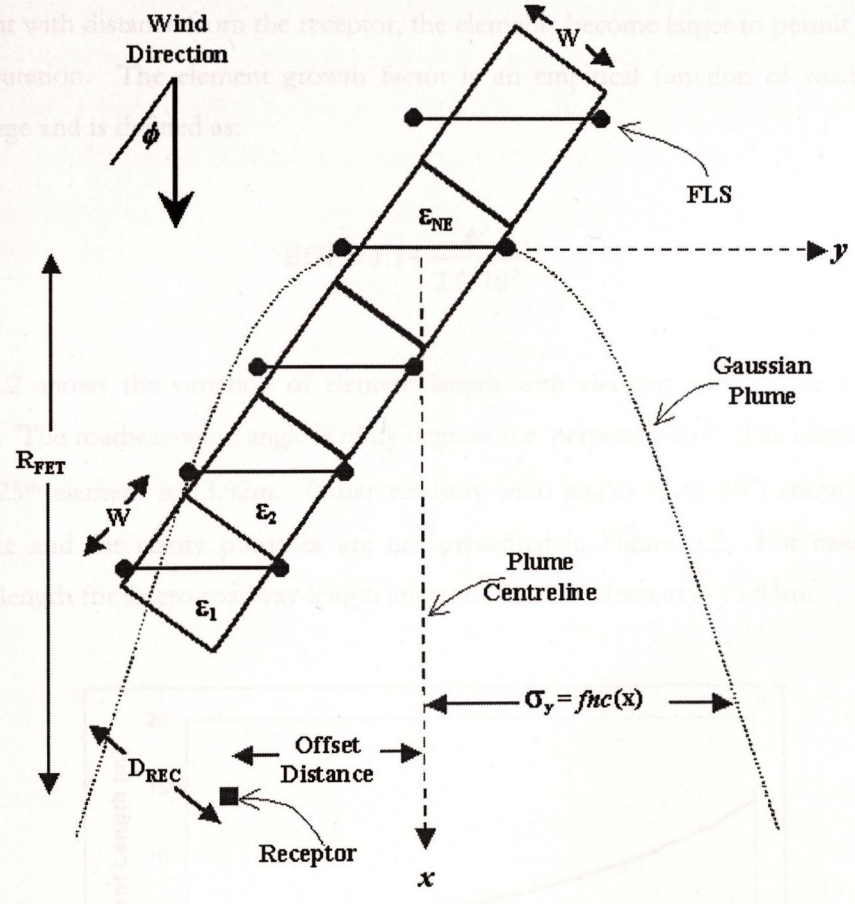


Figure 6.1: Roadway geometry and dispersion calculation in CALINE4 [source: adapted from Benson, 1989]

CALINE4 divides each link into a series of elements or parallelograms for processing purposes. The receptor-link distance, D_{REC}, is measured along a perpendicular distance from the receptor point to the link centreline. The first element is formed at this point as a square with sides equal to the highway or link width. The lengths of subsequent elements are described by the following empirical formula:

$$EL = W \cdot EGF^{NE} \qquad 6.1$$

where: EL is the element length;
W is the highway width;
NE is the element number; and
EGF is the element growth factor.

Where ϕ is the roadway-wind angle (in degrees). As element resolution becomes less important with distance from the receptor, the elements become larger to permit efficiency in computation. The element growth factor is an empirical function of roadway-wind angle range and is defined as:

$$EGF = 1.1 + \frac{\phi^3}{2.5 \cdot 10^5} \qquad 6.2$$

Figure 6.2 shows the variation of element length with element number for a 3m wide roadway. The roadway-wind angle is ninty degrees (i.e. perpendicular). The element length for the 25th element is 13.92m. Other roadway-wind angles (0 to 90°) show very little difference and for clarity purposes are not presented in Figure 6.2. For example, the element length for a zero roadway-length angle for the 25th element is 13.84m.

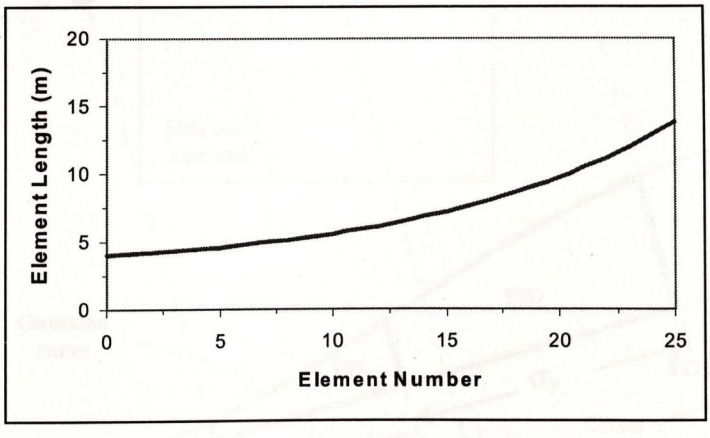


Figure 6.2: Variation of element length with element number

A wind-orientated local x-y coordinate system originating at the element midpoint is defined for each element. Each element is then modelled as an equivalent FLS positioned perpendicular to the wind direction and centred at the element midpoint (see Figure 6.1).

This FLS is always perpendicular to the wind direction and thus its alignment changes with changing wind direction. All emissions resulting from each element are assumed to be released along the FLS representing that element and dispersed downwind (i.e. along the local x-axis) according to the Gaussian formulation. Emissions are distributed within each element by partitioning each element into three sub-elements, namely a central sub-element and two peripheral sub-elements. The geometry of the sub-elements is a function of the element size and the roadway-wind angle as can be seen from Figure 6.3. For example, when the roadway-wind angle is zero or ninty degrees (i.e. the wind is parallel to the roadway), there is only a central sub-element (with no side sub-elements). In addition, the width of the central sub-element is directional proportional to the width of roadway. The emission rate in the central sub-element is assumed uniform across the sub-element along the FLS. Emissions for the two peripheral sub-elements are assumed to decay linearly along the FLS from the emission rate at the elements interface to zero at the end of the FLS.

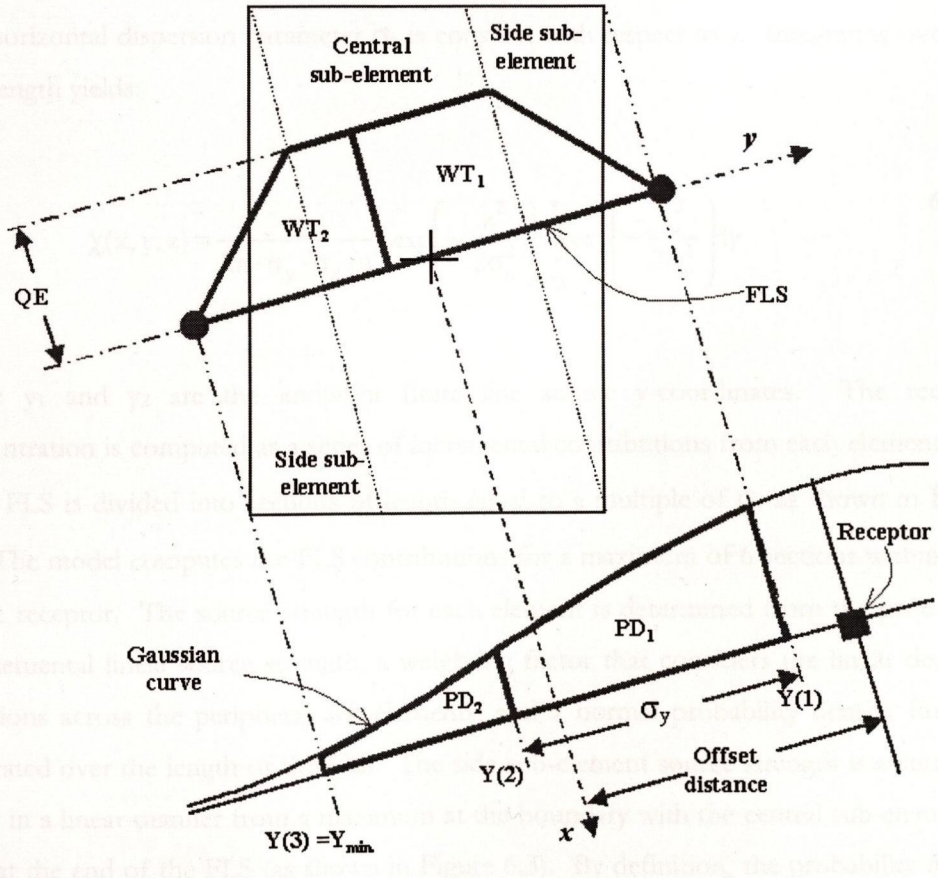


Figure 6.3: Illustration of FLS sub-element source strength and division into sections σ_y long [source: adapted from Benson, 1989]

The crosswind FLS Gaussian formulation computes downwind pollutant contributions from each element. For example, the receptor concentration attributable to an infinitesimal FLS section of length dy, as illustrated in Figure 6.3 is:

$$d\chi(x,y,z) = \frac{q \cdot dy}{2\pi \cdot u \cdot \sigma_y \cdot \sigma_z} \cdot \exp\left(-\frac{y^2}{2\sigma_y^2} - \frac{z^2}{2\sigma_z^2}\right) \qquad \textbf{6.3}$$

where: $d\chi(x, y, z)$ is the incremental concentration;

q is the line source strength;

dy is the length of the sub-element FLS;

u is the wind speed; and

σ_y is the horizontal Gaussian dispersion parameter; and

σ_z is the vertical Gaussian dispersion parameter.

The horizontal dispersion parameter σ_z is constant with respect to y. Integrating over the FLS length yields:

$$\chi(x,y,z) = \frac{q}{2\pi \cdot \sigma_y \cdot \sigma_z \cdot u} \cdot \exp\left(-\frac{z^2}{2\sigma_z^2}\right) \cdot \int_{y_1}^{y_2} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) dy \qquad \textbf{6.4}$$

where y_1 and y_2 are the endpoint finite line source y-coordinates. The receptor concentration is computed as a series of incremental contributions from each element FLS. Each FLS is divided into sections of length equal to a multiple of σ_y as shown in Figure 6.3. The model computes the FLS contributions for a maximum of 6 sections within $\pm 3\sigma_y$ of the receptor. The source strength for each element is determined from the product of the elemental lineal source strength, a weighting factor that considers the linear decay of emissions across the peripheral sub-elements, and a normal probability density function integrated over the length of the FLS. The side sub-element source strength is assumed to decay in a linear manner from a maximum at the boundary with the central sub-element to zero at the end of the FLS (as shown in Figure 6.3). By definition, the probability density function is the area under the normal curve with standard deviation σ_y. Horizontal dispersion effects are determined by the normal probability density function.

The model also allows for reflection of pollutants from the ground and for the influence of a finite mixing height or inversion layer, which is larger than the release height. Assuming repeated multiple reflections of pollutants from the ground and at the mixing layer height, the total receptor concentration from a roadway is:

$$\chi(x,y,z:H)=\frac{1}{\sqrt{2\pi}\cdot u}\sum_{i=1}^{Ne}\left\{\frac{1}{\sigma_{z_i}}\sum_{k=-CNT}^{CNT}[A]\cdot\sum_{j=1}^{6}\left[WT_j\cdot QE_i\cdot PD_{i,j}\right]\right\} \qquad 6.5$$

where:

$$A=\exp\left(\frac{-(z-H+2kL)^2}{2\sigma_{z_i}^2}\right)+\exp\left(\frac{-(z+H+2kL)^2}{2\sigma_{z_i}^2}\right) \qquad 6.6$$

$$PD_{i,j}=\frac{1}{\sqrt{2\pi}}\int_{Y_j/\sigma_{y_i}}^{Y_{j+1}/\sigma_{y_i}}\exp\left(-\frac{p^2}{2}\right)dp \qquad 6.7$$

and:

CNT is the total number of reflections;

i, j, and k are counters;

H is the height of the emission source above the roadway (m);

N_e is the number of elements;

L is the mixing height or inversion layer height (m);

σ_{z_i} is the vertical dispersion parameter as a function of downwind distance for the i^{th} element;

σ_{y_i} is the horizontal dispersion parameter as a function of downwind distance for the i^{th} element;

QE_i is the central sub-element lineal source strength for the i^{th} element;

WT_j is the source strength-weighting factor for the j^{th} FLS section (accounts for linear decay of emissions across the peripheral sub-elements);

Y_j and Y_{j+1} are the receptor offset distance from the plume centreline for the j^{th} FLS segment;

$PD_{i,j}$ is the normal probability distribution function; and

$p = y/\sigma_y$.

In CALINE4, the total receptor concentration is calculated as three separate factors. The first factor accounts for dilution and vertical dispersion by including the effects of wind speed and σ_z. The second factor accounts for the horizontal dispersion of the FLS plume. The third factor contains multiple reflection terms, which account for restricted mixing height. These terms are represented by the non-zero k indices (k is a counter in Equation 6.5 for multiple reflections).

6.4.2 MIXING CELL CONCEPT

CALINE4 employs a mixing cell concept (see Figure 6.4) to determine near field vertical mixing based on wind speed, direction, and roadway geometry. The mixing cell is defined as the volume of air above the travelled roadway plus 3m (approximately two vehicle widths) on either side. The 3m on either side accounts for initial horizontal dispersion caused by the added mechanical turbulence generated by moving vehicles. For queue links, no additional width should be added [US-EPA, 1992d], since idling vehicles are stationary and consequently they don't generate any mechanical turbulence around them.

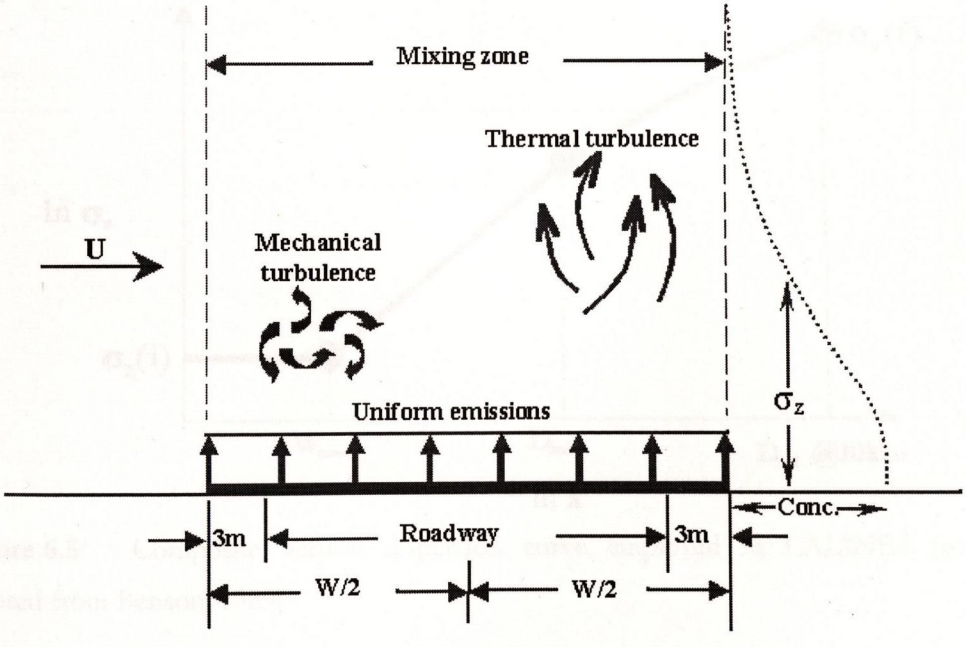


Figure 6.4: CALINE4 mixing cell concept [source: adapted from Benson, 1989]

The mixing cell concept was developed to account for the initial pollutant dispersion caused by the mechanical (generated by moving vehicles) and thermal (generated by the emission of hot vehicle exhaust) turbulence above a roadway and is considered a zone of constant turbulence and emissions. The sources of thermal and mechanical turbulence are

assumed to be important dispersion mechanisms within the mixing cell [Dabberdt, 1981], [Eskridge and Rao, 1983]. Independent studies by Benson and Squires [1979] suggest that this is a reasonable assumption. Hargreaves [1997] states that the "turbulence from the movement of the vehicles is by far the dominant process for mixing close to the lanes of traffic".

6.4.3 VERTICAL DISPERSION COEFFICIENTS

CALINE4 employs a modified version of the Pasquill-Smith vertical dispersion curves [Pasquill, 1974] to incorporate the thermal effects of vehicular emissions. This modified version evolved from an earlier model [Benson, 1982]. CALINE4 defines the vertical dispersion coefficients at two positions as illustrated in Figure 6.5. The first position, W_{mix}, is located at the edge of the mixing cell and is known as the initial vertical dispersion coefficient. The second position is located at a reference distance D_{ref}, (defined as being 10 km downwind from the roadway). The equations to compute the vertical dispersion coefficients σ_z are presented in Figure 6.5 for the various distances from the mixing cell.

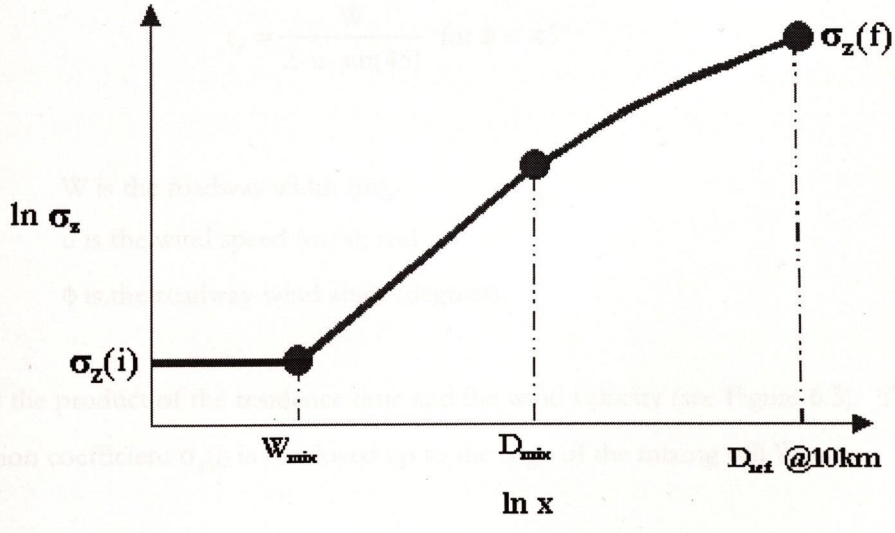


Figure 6.5: Composite vertical dispersion curve employed in CALINE4 [source: adapted from Benson, 1989]

The initial vertical dispersion coefficient $\sigma_z(i)$, is assigned a value based on roadway geometry, wind speed and direction. It is independent of surface roughness and atmospheric stability class. CALINE4 assumes a linear relationship between the initial vertical dispersion $\sigma_z(i)$ at the edge of the mixing cell and the time the air remains in the

mixing cell. An empirical equation relating this initial dispersion and residence time derived from the General Motors Sulphate Experiment database [Chock, 1977b] is:

$$\sigma_z(i) = 1.5 + \frac{t_r}{10} \qquad \textbf{6.8}$$

where: $\sigma_z(i)$ is the initial vertical dispersion (m) and

t_r is the residence time of the air in the mixing cell (s).

The residence time depends on the average wind speed and wind direction (with respect to the roadway) and is computed as [Benson, 1989]:

$$t_r = \frac{W}{2 \cdot u \cdot \sin(\phi)} \quad \text{for } \phi \geq 45° \qquad \textbf{6.9}$$

$$t_r = \frac{W}{2 \cdot u \cdot \sin(45)} \quad \text{for } \phi < 45° \qquad \textbf{6.10}$$

where: W is the roadway width (m);

u is the wind speed (m/s); and

ϕ is the roadway-wind angle (degrees).

W_{mix} is the product of the residence time and the wind velocity (see Figure 6.5). The initial dispersion coefficient $\sigma_z(i)$ is employed up to the edge of the mixing cell W_{mix}.

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]:

$$\sigma_z = P_{z_1} \cdot R_{FET}^{P_{Z2}} \qquad \textbf{6.11}$$

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 crosswind line drawn through the centre of an element (as shown in Figure 6.1).

The downwind reference distance D_{ref} of 10 km was selected because at that distance, an active emissions release (roadway release) is indistinguishable from a passive release (i.e. the type of release has little effect on the vertical extent of the plume) [Benson, 1989]. In addition, it is the maximum distance suggested by Pasquill [1974] for power-curve approximations to the vertical dispersion coefficients. Furthermore, it is greater than the distance usually required for local dispersion modelling.

CALINE4 also accounts for the impact of thermal energy from exhaust gases on the vertical dispersion of pollutants by employing a modified stability class. This modified stability class is determined from Smith's atmospheric stability nomograph [Smith, 1972] using an estimated upward sensible heat flux, the wind speed measured at 10m, and either the incoming solar radiation (day time) or the cloud coverage (night time). The incoming solar radiation takes into account implicitly the cloud cover; while at nighttime there is no incoming solar radiation only outgoing radiation from the Earth. The sensible heat flux is calculated as the product of a heat flux factor (kJ/m) and the traffic volume (vehicles/hour), divided by the mixing cell width (m) W_{mix} as shown in Figure 6.5. The same units for heat flux are employed in the nomograph developed by Smith [1972]. A heat flux factor of 2.46 kJ/m per vehicle is employed [Benson, 1989].

CALINE4 uses this new modified stability class to estimate a modified dispersion coefficient at the downwind reference distance. Since the downwind reference dispersion coefficient is modified, the power-curve approximation used to estimate the dispersion coefficient between the mixing cell and the downwind reference distance is altered also. The thermal turbulence algorithm will have only a very slight effect on the plume spread surrounding the mixing cell, because the algorithm only modifies the dispersion coefficient at the downwind reference distance and not the initial dispersion coefficient at the edge of the cell. The vertical dispersion of the plume is assumed to follow the modified stability curve for a specific distance D_{mix}, downwind of the FLS. The location of D_{mix} may be defined as the distance downwind when more than 50% of the plume mass falls outside the mixing zone width. Beyond this point, the decreasing effect the mixing cell turbulence has on the plume spread is dealt with by returning the modified vertical dispersion curve back to the Pasquill-Smith value at the reference distance (as illustrated in Figure 6.5). This is

accomplished by adding a term to Equation 6.11, which has the functional form [Benson, 1989]:

$$\sigma_z = P_{z_1} \cdot R_{FET}^{P_{Z2}} \cdot \left(\frac{R_{FET}}{D_{mix}} \right)^{P_{Z_3} \cdot \ln\left(\frac{R_{FET}}{D_{mix}}\right)} \qquad 6.12$$

where P_{z_3} is a power curve coefficient.

6.4.4 HORIZONTAL DISPERSION COEFFICIENTS

The horizontal dispersion coefficients are computed using an adapted algorithm originally formulated by Draxler [1976]. Essentially, the algorithm consists of a general equation derived from data collected during field experiments. The study found that the horizontal dispersion coefficient depends on the horizontal wind angle standard deviation, the downwind distance, and the diffusion time. The equation takes the functional form of [Draxler, 1976]:

$$\sigma_y \approx \sigma_\theta \cdot R_{FET} \cdot f_1 \cdot \frac{t_{diff}}{t_{lagr}} \qquad 6.13$$

where: σ_θ is the horizontal wind angle standard deviation (in radians);
R_{FET} is the downwind distance (m);
f_1 is an function of diffusion time t_{diff}; and
t_{lagr} is the Lagrangian time scale (s).

The diffusion (or travel) time t_{diff} (s) is determined from:

$$t_{diff} = \frac{R_{FET}}{u} \qquad 6.14$$

where u is the wind speed (m/s). The lagrangian time can be determined from:

$$t_{lagr} = \int_0^{R_{FET}} R(\xi)d\xi \qquad 6.15$$

where $R(\xi)$ is an autocorrelation function of the wind velocity fluctuations. The Lagrangian time incorporates random motion (see Equation 6.15) while the diffusion time assumes linear motion (see Equation 6.14). The function f_1 is computed as follows:

$$f_1 = \frac{1}{1+0.9\sqrt{\frac{t_{diff}}{t_i}}} \qquad 6.16$$

where t_i is the diffusion time (seconds) required for f_1 to equal 0.5. When t_{diff} is less than 550 seconds, a value of 300 seconds is employed for t_i [Benson, 1989]. When t_{diff} exceeds 550 seconds, the following formula is used [Benson, 1989]:

$$t_i = 0.001 \cdot t_{diff}^2 \qquad 6.17$$

The standard deviation of the horizontal wind angle may be derived by direct measurement. Alternatively, various methods have been developed to estimate it [Hanna, 1983], [Yamartino, 1984]. One of the major advantages of this method is that it can account for site-specific conditions and unique meteorological regimes (e.g. low wind speed directional meander). However, the standard deviation of the horizontal wind angle σ_θ must be given as input to CALINE4.

6.4.5 Deposition and Settling Velocities

CALINE4 incorporates a method by which estimated concentrations may be adjusted for pollutant settling and deposition. The deposition and settling effects are accounted for in the vertical term of the Gaussian formulation employed in CALINE4. The method has been adapted from a model developed by Ermak [1977]. The deposition flux is defined as the quotient of the deposition velocity and the area under the plume. The mass of pollutant removed from the atmosphere can be calculated from the deposition flux.

Deposition velocity is a measure of the rate at which a pollutant can be absorbed or assimilated by a surface. It involves a molecular, not turbulent diffusive process through the laminar sub-layer covering the surface. The deposition velocity depends upon such factors as the type and size of the pollutant particles, the roughness of the terrain, the type of ground cover and the meteorological conditions. A survey of deposition velocities for a number of pollutants over a variety of ground conditions is given by McMahon and Denison [1979] and by Rasmussen et al. [1975].

Settling velocity (v_s) is the rate at which a particle falls with respect to its immediate surroundings. It is the actual velocity of the particle in the downward direction. The effects of settling velocities can be modelled by including an extra term in the Gaussian equation.

6.4.6 PHOTOCHEMISTRY

The chemical transformation of nitrogen dioxide is modelled using the discrete parcel method. In this method, air parcels are considered in which emissions and the background air are uniformly mixed. The discrete parcels are dispersed across the FLS plume in accordance with Gaussian methodology. Chemical reactions take place within the parcels at rates governed by the initial mixing zone concentrations and independent of the dispersion mechanism. It is assumed that emissions and ambient reactants are fully mixed within the mixing zone to a height of 3.5m. The parcel nitrogen dioxide concentrations are computed separately for each element-receptor combination to account for the variable travel times involved.

Nitrogen dioxide is a product of the reaction between nitrogen monoxide and ozone. However, ozone itself is formed as a result of sunlight acting on nitrogen dioxide. The amount of nitrogen monoxide transformed to nitrogen dioxide and the rate of reaction depend on the concentration of nitrogen monoxide to be oxidised and the available ozone. The basic reactions of nitrogen monoxide, nitrogen dioxide, oxygen and ozone are:

$$NO + O_3 \xrightarrow{k_f} NO_2 + O_2 \qquad 6.18$$

$$NO_2 + h_v \xrightarrow{k_r} NO + O \qquad 6.19$$

$$O + O_2 + M \rightarrow O_3 + M \qquad 6.20$$

where: h_v represents an interacting photon of light;

NO is nitrogen monoxide;

NO_2 is nitrogen dioxide;

O_3 is ozone;

k_r is a photo-oxidation (photolysis) rate constant (1/s);

k_f is a photo-oxidation (photolysis) rate constant (1/ppb-s); and

M is an unspecified catalytic agent.

The initial tailpipe NO_x emissions are assumed to consist of 92.5% nitrogen monoxide and 7.5% nitrogen dioxide by mass.

6.4.7 STREET CANYON

An algorithm suggested by Turner [1969] has been integrated into CALINE4 to handle canyon situations. The algorithm calculates the effect of single or multi-horizontal reflections for each plume in a similar manner as mixing height reflections are handled. CALINE4 handles the bluff and canyon situations by reflecting the plume at distances specified on one or both sides of the mixing zone. The horizontal topography boundary (barrier) and wind direction are assumed to be parallel to the roadway.

6.5 DEFICIENCIES IN CALINE4

An extensive literature review revealed a number of deficiencies in the CALINE4 model. For example, Washington and Guensler [1995] suggested that a number of improvements could be made to the model. They proposed two types of improvements, namely, short- to medium-term and long-term. In the short- to medium term, the study recommended that CALINE4 be revised to "incorporate individual emission rates into its emission estimation algorithms" and "update the modal activity algorithms to cover all modelling scenarios". CALINE4 does contain a modal emissions algorithm to convert carbon monoxide composite emission rates into modal emission factors for acceleration, deceleration, idle and cruise, and hence can estimate air quality around junctions [Benson, 1997]. CALINE4 contains simple algorithms to calculate the distance required for a vehicle to accelerate or decelerate. However, the creep mode of vehicle operation, which represents the

movement of a vehicle queuing at an intersection or roundabout, whereby it progressively approaches the junction through a number of stop-starts, is not taken into account. The model also employs a disaggregated analytical approach to estimate the quantity of pollutants emitted during each mode of vehicle operation. As this algorithm is based on emissions measurements for the USA [Kunselman et al., 1974], [Griffin, 1980], it is not applicable in Ireland.

Furthermore "there has been a growing concern that some of the algorithms built into CALINE4, implemented to perform intersection analyses, are not appropriate for today's vehicle fleet" [Brown and Caldwell, 1998]. An earlier study of CALINE4 [Sculley, 1989] also warned that "the emissions adjustment procedures in CALINE4 must be used with caution" when combining them with emission rate models. Brown and Caldwell [1998] suggest using a modelling technique that combines CALINE4 with a speed dependent emission factor to analyse intersections.

An evaluation of intersection models [Zamurs and Conway, 1991] found that "models, on average, under-predicted observed concentrations, with only those that separate composite emissions into their more discrete components indicating a potential for approaching or over-predicting observed carbon monoxide levels".

An evaluation study of CAL3QHC [Guldberg, 1991] found that errors in model predictions were partially due to the model under-estimating queue lengths (up to 8%) at congested junctions (i.e. a volume-to-capacity ratio greater than 1.3). A sensitivity study [Rossi, 1990] of CAL3QHC on various types of intersections found that the queue length played the key role in determining the worst predicted air quality. Rossi, [1990] further suggests that the total number of vehicles approaching an intersection, by itself, is not a reliable indicator of the relative magnitude of predicted air quality impacts from different traffic scenarios. An evaluation study of queuing algorithms [Al-Deek et al., 1997] found that "the predicted queue lengths of CAL3QHC were too long for over-saturated cases".

The US-EPA [1999] recommends the use of the line source treatment in ISC3 [US-EPA, 1995a] where deposition is of concern because ISC3 contains an advanced deposition algorithm.

6.6 DEVELOPMENT OF CALINE4R

As already stated, an extensive literature review revealed a number of deficiencies in the existing CALINE4 model. In light of the above observations, it was decided to modify current version CALINE4 and produce an enhanced model called CALINE4R. Under the license agreement, the source code for this new version is returned to CALTRANS (the developers of CALINE4) for independent evaluation and validation.

6.6.1 VEHICLE MODAL EMISSIONS

CALINE4R allows a more accurate prediction of modal emissions to be performed by (a) dividing each lane into a number of segments reflecting the areas in which vehicles are most likely to be in cruise or creep mode, and (b) employing modal emissions factors derived from European data rather than US data.

Washington and Guensler [1995] suggested that as a long-term improvement to CALINE4 "vehicle simulation models be used to estimate vehicle activity". This implies using a traffic model or real-time data to estimate traffic activity, rather than depending on the simple algorithms incorporated in CALINE4. This is achieved by the integration of the dispersion algorithms of CALINE4R with the MVEIM and the SATURN & SATCHMO traffic model [Willumsen et al., 1993].

6.6.2 VEHICLE HEAT FLUX

Brown and Caldwell [1998] stated that "there has been a growing concern that some of the algorithms built into CALINE4, implemented to perform intersection analyses, are not appropriate for today's vehicle fleet".

For example, the HFF of 2.46 kJ/m per vehicle currently employed in CALINE4 was developed for motor vehicles in the USA. The HFF is computed as:

$$HFF = \frac{SE \cdot \eta_c}{FE} \qquad 6.21$$

where: HFF is the heat flux factor;

SE is the specific energy of fuel (J/litre);

FE is average fuel economy per vehicle (km/litre); and

η_c is the conversion efficiency of thermal energy to specific heat.

The HFF employed in CALINE4 is based on an assumed average fleet fuel economy of 8.5 km/litre, a 60% conversion efficiency of thermal energy to specific heat, and a specific energy of 3.48 x 10^7 J/litre of fuel. Dabberdt [1981] modified the HFF on the basis of time extrapolated US-DOT fuel consumption curves [Cope, 1973] and obtained a value of 3.46 kJ/m per vehicle. In addition, Dabberdt [1981] assumed that the conversion efficiency of thermal energy to specific heat was 85%. Yamartino and Weigand [1986] modified the HFF to reflect European vehicles and obtained a value of 3.1 kJ/m per vehicle.

As the MVEIM estimates the average fuel consumption for each link, it is employed along with a conversion efficiency of 60%, to compute the HFF in CALINE4R using the above equation. The average specific energy of petrol and diesel is 3.19 x 10^7 J/litre and 3.56 x 10^7 J/litre of fuel respectively [Reynolds, 1996a].

6.6.3 Improved Dispersion Coefficient

Williams et al. [1994b] suggested a different formulation for the vertical dispersion coefficient. The formulation proposed for the coefficient is a function of the plume travel time, t:

$$\sigma_z = c_1 + c_2 \cdot t^m \qquad \textbf{6.22}$$

where: c_1 is the wake induced vertical dispersion coefficient (≈ 4m);

c_2 is the atmospheric stability coefficient (e.g. 0.55. for stable, 1.1 for neutral, and 2.2 for unstable);

m is an exponent (≈ 0.5); and

t is the plume travel time.

When modelling the dispersion of surface releases, Venkatram [1992] recommends a value of m = 0.5 for the exponent. This value should be valid for distances up to approximately 100m from the edge of the roadway.

6.6.4 Output Flexibility

As the concentrations of some pollutants (e.g. benzene and 1,3-butadiene) are much lower than those of the more traditional pollutants (e.g. carbon monoxide), the output from CALINE4R is changed from parts-per-million to parts-per-billion for these pollutants.

Considering the fact that some air quality standards are given in parts-per-million and others are in micrograms-per-cubic-metre, CALINE4R outputs concentrations in both units for all pollutants.

6.6.5 Expanded Capabilities

CALINE4 was originally designed to compute pollutant concentrations from a single highway or junction, and the maximum number of receptors or links is twenty. However, in urban areas, the distance from one junction to the next can be short and consequently, emissions from one junction will have an effect on pollutant concentrations at another junction. To provide for adequate modelling, therefore, the maximum number of links in CALINE4R is one hundred. This allows the modelling of adjacent traffic junctions that interact with each other within a short distance.

In addition the number of receptors in CALINE4R is also one hundred. This allows for pollution contours for an area to be computed with sufficient accuracy.

6.6.6 Pollutant Decay

All gaseous pollutants with the exception of carbon monoxide and nitrogen dioxide are modelled in CALINE4 as inert gases. In reality, pollutants are subject to chemical reactions after they are released. It is beyond the scope of a practical model to incorporate all the chemical reactions for every pollutant [McHugh et al, 1996]. Therefore a simple exponential decay scheme has been incorporated in CALINE4R to expand the use of the Gaussian plume formulation to reactive species [US-EPA, 1995b]. Bell and Reynolds [1995] also suggest that instantaneous emissions will completely disperse over a longer period (e.g. fifteen minutes) and that the decay is an exponential function. The exact rate of decay will depend on geographical layout and meteorology. The implemented exponential scheme is a simple means of accounting for pollutant removal by physical or chemical process. It takes the functional form of :

$$R_d = \exp\left(-\psi\frac{x}{u}\right) \qquad 6.23$$

where: R_d is the decay term;

ψ is the decay coefficient (sec^{-1});

x is downwind distance (m); and

u is wind speed (m/s).

A value for ψ can be obtained from the following:

$$\psi = \frac{0.693}{t_{1/2}} \qquad 6.24$$

where $t_{1/2}$ is the pollutant half-life in seconds. The default value for the decay term is 1.0, unless a value for the decay coefficient is specified. As an example, a decay half-life of 4 hours (i.e. a decay coefficient equal to 0.0000481 sec^{-1}) is assigned for sulphur dioxide when modelled in urban areas.

6.6.7 NWS METEOROLOGICAL DATA

Burden et al. [1997] suggested that "a modification of the programme needs to be made to enable automated multiple runs". To this end, CALINE4R has been modified to allow time-series calculations to be determined automatically using NWS data. The required meteorological data is stored in an hourly database. The model requires the data for input in the format as shown Table 6.3.

Table 6.3: CALINE4R meteorological data input format

Variable	Format	Columns
Year (last two digits)	I2	1-2
Month	I2	3-4
Day	I2	5-6
Hour ending	I2	7-8
Wind flow vector (deg.)	F9.4	9-17
Wind speed (m/s)	F9.4	18-26
Ambient temperature (K)	F6.1	27-32
Stability class (A=1, F=6)	I2	33-34
Rural mixing height (m)	F7.1	35-41
Urban mixing height (m)	F7.1	42-48

6.6.8 TREATMENT OF CALMS

Treatment of calm or light and variable wind poses a special problem in Gaussian models where the calculated concentration is inversely proportional to wind speed. As concentrations become unrealistically large when wind speeds less than 1 m/s are employed, CALINE4 uses an empirical relationship to handle wind speeds as low as 0.5 m/s. A procedure has also been developed by the US-EPA [1984a] to prevent the occurrence of extremely conservative concentration predictions during periods of calms. This procedure acknowledges that Gaussian plume models are not reliable during calm conditions, and disregards any individual hours identified as calm. The hour is treated as missing and a convention for handling missing hours is recommended.

Many pre-processing meteorological programs substitute a 1.0 m/s wind speed and the previous direction for the calm hour. The treatment of calms in these models attempts to identify the original calm cases by checking for a 1.0 m/s wind speed coincident with a wind direction equal to the previous hour's wind direction.

In CALINE4R, calm wind conditions (< 0.5 m/s) are processed according to US-EPA guidance [US-EPA, 1984a]. When a calm wind condition exists, the hourly concentrations are set to zero, and the hourly ambient background concentrations are not used in any computations for that hour. The annual mean is computed from the quotient of the sum of each valid (non-calm) one-hour mean concentration and the total number of non-calm hours or 75% of the total number of hours, whichever is greater.

6.6.9 SETTLING VELOCITY

An algorithm was developed for implementation in CALINE4R to automatically compute gravitational settling velocity. The algorithm employed was originally developed for another dispersion model – ISC3 [US-EPA, 1995a] and is applicable for particles less than 80 micrometers in size (aerodynamic diameter), having a Reynolds number less than 2.0 and a low velocity.

The settling velocity, the product of a modified version of Stoke's law and a slip correction factor, is computed as:

$$v_g = \frac{(\rho_p - \rho_{air}) g \cdot d_p^2 \cdot 10^{-8}}{18\mu_{air}} S_{CF} \qquad 6.25$$

where: v_g is the settling velocity (cm/s);

ρ_p is the particle density (g/cm^3);

ρ_{air} is the air density ($\approx 1.2 \times 10^{-3}$ g/cm^3);

g is acceleration of gravity ($\approx$ 981 cm/s^2);

d_p is the particle diameter (μm);

μ_{air} is the absolute viscosity of air ($\approx 1.81 \times 10^{-4}$ g/cm/s);

S_{CF} is the slip correction factor, which is computed as:

$$S_{CF} = 1 + \frac{0.1634 + 0.052 \cdot \exp -(8.462 \cdot d_p)}{d_p} \qquad 6.26$$

The slip correction factor accounts for molecular slip, which occurs when the size of the particle is of the same magnitude as the distance between gas molecules. The particle no longer moves as a continuum in the gas, but as a particle among discrete gas molecules thereby reducing the drag force.

As can be seen from Figure 6.6, the slip correction factor is significant for particles in the air with actual diameters of 0.1 micrometer and less.

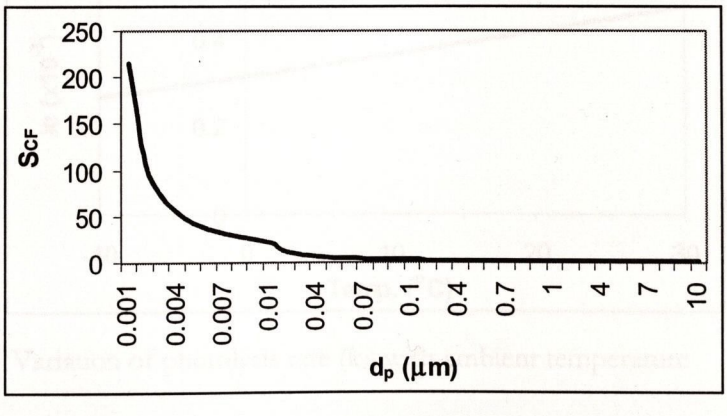


Figure 6.6: Variation of slip-correction-factor (S_{CF}) with particle size (d_p)

6.6.10 PHOTOCHEMISTRY REACTION RATES

In CALINE4, the photolysis rate (k_r) is inputted directly for each run. The reaction rates k_f and k_r employed in the photochemistry algorithm are functions of temperature and solar radiation intensity. Stanhill [1998] analysed the long-term trends in solar irradiances at eight stations in Ireland and found significant increases at Dublin airport. For annual averages, the temperature and solar radiation intensity will vary substantially throughout the year. Therefore, an algorithm is developed and implemented in CALINE4R to automatically compute both photolysis rates. They are calculated as [Seinfeld, 1986], [Hertel and Berkowicz, 1989]:

$$k_f = \frac{16.133}{T} \exp\left(-\frac{1430}{T}\right) \qquad \textbf{6.27}$$

$$k_r = 0.8 \cdot 10^{-3} \cdot \exp\left(-\frac{10}{Q_R}\right) + 7.4 \cdot 10^{-6} \cdot Q_R \qquad \textbf{6.28}$$

where: T is the ambient temperature (K); and
Q_R is the solar radiation intensity (W/m^2).

The variation of photolysis rate (k_f) with ambient temperature is presented in Figure 6.7.

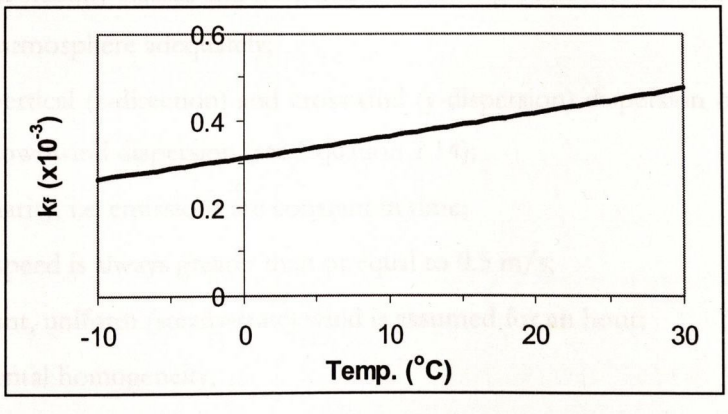


Figure 6.7: Variation of photolysis rate (k_f) with ambient temperature

The solar radiation intensity can be obtained from the meteorological hourly database or from an atmospheric stability nomograph, for example Smith [1972]. Alternatively, Middleton [1976] presents a nomograph to calculate incoming solar radiation (in mW/cm^2)

on a cloudless day as a function of time-of-the-day and month-of-the-year. A supplementary table of correction factors for cloudy conditions is provided by Middleton [1976] also. Figure 6.8 presents the variation of photolysis rate (k_r) with incoming solar radiation.

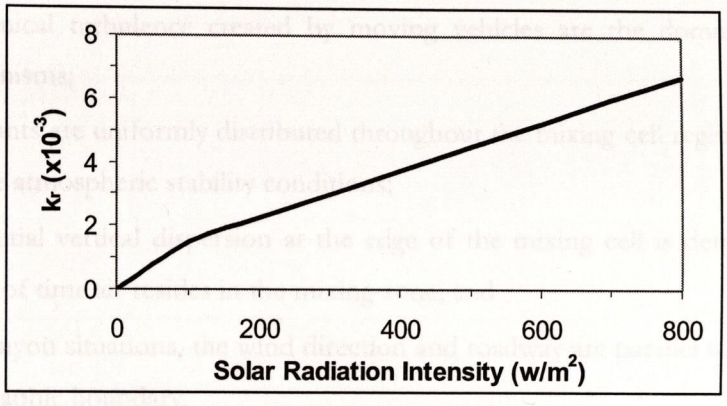


Figure 6.8: Variation of photolysis rate (k_f) with solar radiation intensity

6.7 INHERENT ASSUMPTIONS IN CALINE4R

Like any air dispersion model, CALINE4R possesses a number of inherent assumptions and constraints. The primary assumptions are:

- Pollutants disperse in a Gaussian manner downwind from the source to a maximum distance of 10 km;
- Pasquill stability classes and modified dispersion parameters describe the turbulence of the atmosphere adequately;
- Only vertical (z-direction) and crosswind (y-dispersion) dispersion occurs i.e. there is no downwind dispersion (see Equation 2.14);
- Stationarity, i.e. emissions are constant in time;
- Wind speed is always greater than or equal to 0.5 m/s;
- Constant, uniform (steady-state) wind is assumed for an hour;
- Horizontal homogeneity;
- The heat release rate for each vehicle is 24.6 J/cm;
- When the plume intersects the ground surface, perfect plume reflection occurs;
- Roadways are modelled as finite line sources;
- For each of the segments of a link, the assigned emission factor is constant and continuous over the length of the link segment;

- Meteorological variables (e.g. temperature, atmospheric stability, wind speed and direction) are homogenous and constant in the modelled area. In addition, the variance in the wind direction is normally distributed about the mean.;
- Surface roughness is reasonably uniform throughout the study area;
- Within the mixing cell, the thermal turbulence created by vehicle exhaust and the mechanical turbulence created by moving vehicles are the dominant dispersive mechanisms;
- Pollutants are uniformly distributed throughout the mixing cell region regardless of surface atmospheric stability conditions;
- The initial vertical dispersion at the edge of the mixing cell is determined by the length of time air resides in the mixing zone; and
- For canyon situations, the wind direction and roadway are parallel to the horizontal topographic boundary.

6.8 INPUT DATA REQUIREMENTS FOR CALINE4R

The input data requirements of CALINE4R can be generally categorised into five types, namely:

- Site geometry and topography;
- Traffic activity;
- Emission rates;
- Meteorological data; and
- Receptor locations.

Due to limitations in CALINE4R, which also exist in CALINE4, the queue segment of a link is modelled as a free flow segment using a method developed by Hallmark and O'Neill [1996]. The emission source strength is converted to line source strength so that the dispersion elements of CALINE4R can process it as a free-flow link. Total emissions are calculated by multiplying creep-emission factors by the total amount of delay in the queue segment. To model as a free-flow segment, an emission factor in g/km is assumed, and total emissions are divided by this factor to give an adjusted traffic volume for the queue segment. The queue segment is then specified as the physical length of the roadway.

Table 6.4 gives a description of input variables required for CALINE4R, while Table 6.5 gives the ranges (limits) for the input variables. Table 6.6 presents typical surface roughness coefficients for various urban land-uses [Myrup and Ranzieri, 1976].

Table 6.4: Description of input variables for CALINE4R [source: adapted from Benson, 1989]

Record N°	Input Variable	Units	Description
1	JOB		Job title
2	PTYP	1 to 4	Pollutant type (CO, NO_2, inert gas or PM)
	Name		Pollutant name
3	Z0	Cm	Aerodynamic roughness coefficient
	MOWT	n/a	Molecular weight
	VS	cm/s	Settling velocity
	VD	cm/s	Deposition velocity
	NL and NR		No. of links and receptors respectively
	SCAL	M/?	Scale factor
	LC and RC		Link and receptor title option respectively
	ALT		Altitude above sea level
4	RCP		Receptor name
5	XR, YR, ZR		X, Y, Z receptor co-ordinates
6	LNK		Link name
7	TYP	1 to 6	Link Type (at grade, depressed, fill, bridge, parking lot or intersection)
	XL1, YL1		Co-ordinates of link end point 1
	XL2, YL2		Co-ordinates of link end point 2
	HL	m	Roadway height
	WL	m	Mixing zone width
	MIXWR & MIXWL	m	Mixing width (right and left respectively)
	CC	1 or 2	Continuation code
9	RTYP	1 to 4 or 9	Run type (standard, multi-run, worst case run angle, multi-run/worst case hybrid, last run)
	VPHCOD		Traffic volume code
	EFLCOD		Emission factor code
	INTCOD		Intersection parameter code
	METCOD		Meteorology code
	RUN		Run title
10	VPHL	vph	Hourly traffic volume by segment
11	EFL	gm/veh-km	Composite emission factor by segment
13	BRG	deg.	Wind direction bearing
	U	m/s	Wind speed
	CLAS	A=1 to G =7	Atmospheric stability class
	MIXH	M	Mixing height
	SIGTH	deg.	Wind direction standard deviation
	AMB	ppm, ppb or $\mu g/m^3$	Ambient background concentration
	TEMP	°C	Temperature
	O3	ppm	Ambient O_3 concentration
	NOA	ppm	Ambient NO concentration
	NO2A	ppm	Ambient NO_2 concentration
	KR	sec^{-1}	NO_2 photolysis rate constant

Table 6.5: Ranges for input variables employed by CALINE4R [source: adapted from Benson, 1989]

Variable	Explanation	Limits	Comments
Z_o	Surface Roughness	$3 \leq Z_o \leq 400$ cm	15% of average canopy height or see Table 6.6 for general values
V_s	Settling Velocity	$V_s \geq 0$	$V_s=2.98 \times 10^5 D_{ar}^{-2}$ where D_{ar} is aerodynamic resistance diameter (cm)
V_D	Deposition Velocity	$V_D \geq 0$	
U	Wind Speed	$U \geq 0.5$ m/s	Measured at 5m (localised sources and nearby receptors) to 10m (for diffuse sources and distant receptors)
CLAS	Stability Class	$1 \leq CLAS \leq 7$	Modified Pasquill stability class scheme.
SIGTH	Directional Variability	$5^o \leq SIGTH \leq 60^o$	Measure at 4 to 10m or assume worst case
MIXH	Mixing Height	MIXH ≥ 5m (algorithm is deactivated if MIXH is set to 1000m or greater)	MIXH = 0.185 x U x k/(ln(Z/Zo) x f) U is wind speed (m/s) Z is height U measured at (m) Z_o is surface roughness (m) k is von karman constant (0.35) f = Coriolis parameter $= 1.45 \times 10^{-4} \cos \theta$ (rad/sec) $\theta = 90^o$ – study site latitude
TEMP	Temperature		January mean minimum plus time period adjustment
KR	Photolysis Rate	$KR \geq 0$	
BRG	Wind Direction	$0 \leq BRG \leq 360$	Wind azimuth bearing measured relative to positive y-axis
W	Mixing Zone Width	WL ≥ 10m	Minimum of 1 lane plus 3m per side of link (except for a parking lot)
LL	Link Length	$WL \leq LL \leq 10$km	Link length needs to be greater or equal to the mixing zone width for proper element resolution and less than 10km to stay within the range of validity for the vertical dispersion algorithm.
H	Source Height	$-10 \leq HL \leq 10$m	Limits of verified model performance
Z	Receptor Height		Gaussian plume reflected at air-surface interface; model assumes plume transport over horizontal plane. For depressed sections $Z \geq H$ (where H is negative) is permitted for receptors within the section
MIXWR	Mixing Width Right	MIXWR ≥ WL/2	An assigned value of zero is interpreted as no horizontal obstruction.
MIXWL	Mixing Width Right	MIXWL ≥ WL/2	An assigned value of zero is interpreted as no horizontal obstruction.

Table 6.6: Surface roughness for various urban land uses [source: Myrup and Ranzieri, 1976]

Type of Surface	Z_0 (cm)
Single family residential	108
Suburban	108
Park	127
Office Block	175
Central Business District	321
Apartment residential	370

6.9 SUMMARY

A line source dispersion model, CALINE4R, which is an enhancement of CALINE4 has been described. CALINE4R is a Gaussian model designed for the assessment of traffic emissions from roads. Given emission source strength, local meteorology, site geometry, and site characteristics, CALINE4R can reliably predict pollutant concentrations for receptors located within 200 meters of the roadway. It can model junctions, street canyons, parking lots, bridges and underpasses. CALINE4R is designed to handle near-saturated and/or over capacity traffic conditions and complex junctions. Each link to be modelled is subdivided into two segments depending on whether vehicles are more likely to be cruising or queuing mode. It includes a photochemistry module to predict downwind concentrations of $N0_2$ from NO emitted by vehicle exhausts and a pollutant decay module for other pollutants. It also includes pollutant settling velocity and chemical reaction rate modules. CALINE4R estimates one-hour mean concentrations and therefore is useful for investigating episodes of high pollutant concentrations. Either discrete or continuous hourly meteorological conditions can be employed. CALINE4R requires details on ambient NO_2, NO and ozone levels for the photochemistry simulations. The model can handle up to 100 road links and 100 receptors.

A limited validation of the combined MVEIM along with the CALINE4R dispersion model in three different European cities has been performed and these will be described in the next Chapter.

7. VALIDATION OF AIR QUALITY MODEL

7.1 INTRODUCTION

The previous four Chapters have described an AQMS developed for traffic related pollution in urban areas. An objective of any project, which results in the development and implementation of a computer software model, is to falsify it with measured data. Therefore, the AQMS is applied and validated at a heavily trafficked junction within the centre of Dublin. Previous studies have found that emissions are higher near junctions with the maximum occurring in the queuing area of each link [Claggett et al., 1981], [Lee, 1983], [Matzoros, 1988; 1990], [Namdeo and Colls, 1995]. A further objective of this research is to assess the transferability of the AQMS to other European urban areas. Consequently, the model is validated at Melton Mowbray in the UK using traffic data collected by the SCOOT urban traffic control system [Hunt et al., 1981]. This data is supplied by the Institute of Transport Studies at the University of Leeds.

TRAPOS compare methods for estimating air pollutant concentrations in a street canyon on the basis of the usually available input data. The study site selected is a street canyon in Hannover, Germany. The author participates in this study and consequently the validity of the AQMS is demonstrated in Germany.

7.2 VALIDATION IN DUBLIN

This section describes the application and validation of the AQMS in Dublin. Since the complete urban area model can be considered as an amalgamation of similar junctions and links, such local assessments of accuracy provide a platform for assessing the validity of the emissions inventory and dispersion model as a whole.

One of the major advantages of MVEIM and CALINE4R is that they are developed as separate and independent components of the overall AQMS. Consequently, each component can be validated. In this study in Dublin, traffic activity and fleet composition observations are compared with traffic module results, and measured ambient pollutant concentrations are compared with dispersion module predictions.

7.2.1 SURVEY SITE

The survey site was at an arterial four-way signalised controlled junction in the heart of Dublin City, which is characterised by high local congestion. It is one of the busiest signalised intersections in the city, with in excess of forty thousand vehicles traversing the junction daily.

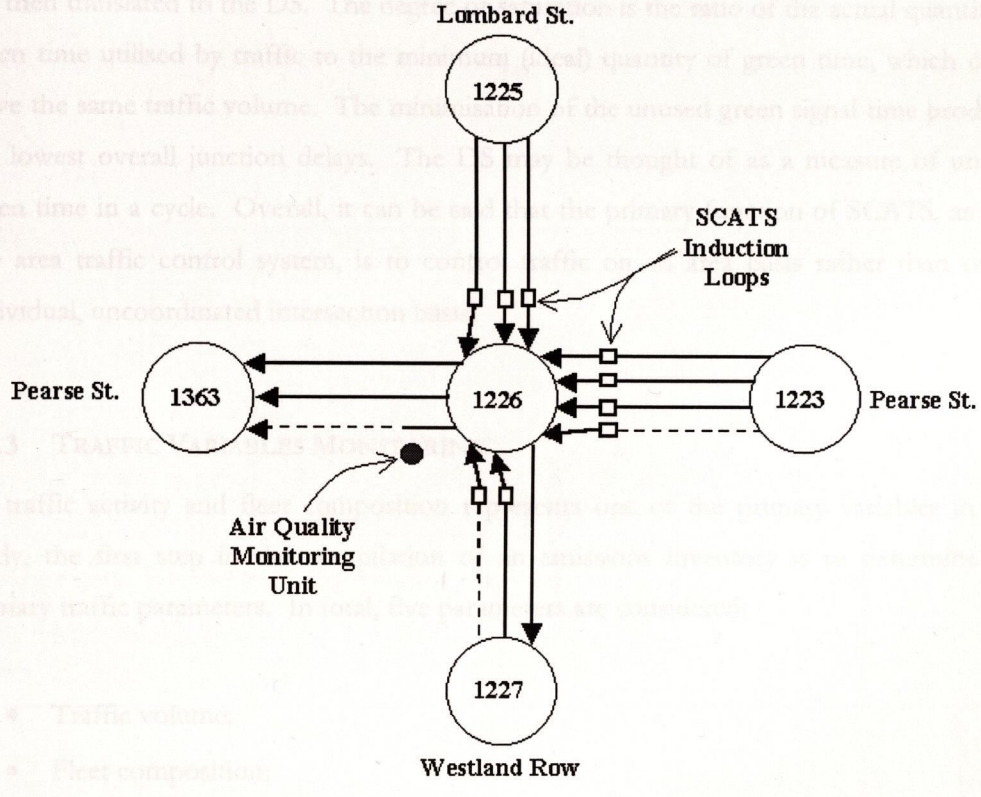


Figure 7.1: Schematic representation of intersection at survey site in Dublin

The junction geometry is depicted in Figure 7.1, in which the direction of traffic flow through the junction is indicated, and the dashed lines represent bus lanes. Lombard Street consists of a one-way three-lane roadway, while Westland Row has one lane going in either direction. Pearse Street has four lanes travelling in the same direction. The numbers of the junctions are assigned in the traffic module. For completeness, they are shown here. In addition, the location of the air quality monitoring unit is depicted. The location of the SCATS traffic induction loops is presented also.

7.2.2 SCATS URBAN TRAFFIC CONTROL SYSTEM

The junction is controlled by the SCATS urban traffic control system [Sim and Dobinson, 1980]. SCATS gathers data on traffic flows in real-time at each intersection. This data is transferred via the traffic control signal box to a central computer, which makes

incremental adjustments to traffic light timings based on minute-by-minute changes in traffic flow at each intersection. SCATS is a 'reactive' traffic control system [Gross, 1998]. Traffic patterns in a previous cycle are used to determine the proportion of green and red time. SCATS performs a vehicle count at each stop line, and also measures the gap between vehicles as they pass through each junction. These traffic volume counts and gaps are then translated to the DS. The degree of saturation is the ratio of the actual quantity of green time utilised by traffic to the minimum (ideal) quantity of green time, which could serve the same traffic volume. The minimisation of the unused green signal time produces the lowest overall junction delays. The DS may be thought of as a measure of unused green time in a cycle. Overall, it can be said that the primary function of SCATS, as with any area traffic control system, is to control traffic on an area basis rather than on an individual, uncoordinated intersection basis.

7.2.3 TRAFFIC VARIABLES MONITORING

As traffic activity and fleet composition represents one of the primary variables in this study, the first step in the compilation of an emissions inventory is to determine the primary traffic parameters. In total, five parameters are considered:

- Traffic volume;
- Fleet composition;
- Average vehicle speed;
- Average queue length; and
- Vehicle delay (both link and turn delay).

7.2.3.1 Traffic volume

Automatic traffic sensors measure the traffic volume passing through the junction and the distance between each vehicle, which is a measure of the level of congestion. These sensors consist of induction loops embedded beneath each traffic lane surface, a lead-in cable and an electronic detector module [Marsden, 1997b]. When a vehicle passes over the embedded induction loops, eddy currents generated within the passing vehicle reduce the inductance in the loop. This causes a change in the oscillator frequency of the circuit (i.e. loop and lead-in cable), which is detected by the electronic detector and subsequently sends a pulse to the signal controller or traffic counter.

The embedded induction loops can detect vehicles passing above, but cannot distinguish between various types of vehicles. Hence, only total traffic volume and degree of saturation may be recorded, this data being stored as aggregate values, per lane, and may be reported on a minute-by-minute basis. The boxes in Figure 7.1 show the position of the induction loops. The diurnal variation of traffic volume for a typical weekday is depicted in Figure 7.2. The sharp fall in flow close to 6 pm reflects severe traffic congestion during the evening peak demand period.

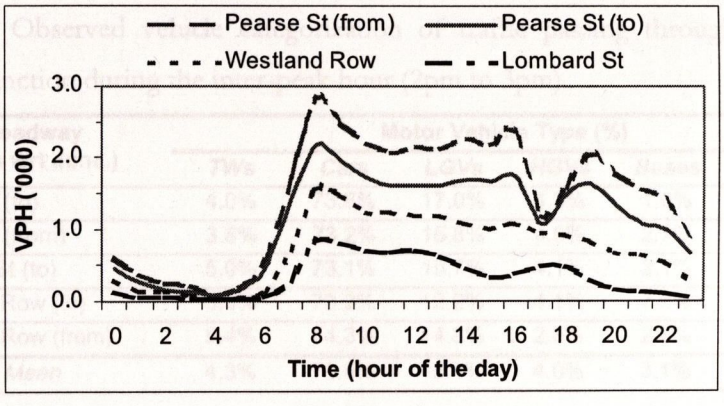


Figure 7.2: Diurnal variation of measured traffic volume traversing study junction for an average weekday in Dublin

7.2.3.2 Fleet composition

A video camera was employed to record morning peak hours (8am to 9am) and inter-peak hours (2pm to 3pm) at the junction so that more specific traffic parameters could be established. In this regard, a five-category motor-vehicle classification system is employed:

- Cars;
- LGVs;
- HGVs;
- Buses; and
- TWs.

The observed vehicle mix for peak and inter-peak hours, in terms of the percentage vehicle categorisation at the junction in question, is given in Table 7.1 and Table 7.2. Passenger cars are the most populated vehicle category in both peak (86.3%) and inter-peak (73.5%) hours. All other categories increase in the inter-peak hour.

Table 7.1: Observed vehicle categorization of traffic passing through Dublin city-centre study junction during the peak hour (8 am to 9 am).

Roadway (Dir'n wrt Junc.)	Motor Vehicle Type (%)					
	TWs	*Cars*	*LGVs*	*HGVs*	*Buses*	*TOTAL*
Pearse St (to)	1.2%	90.7%	4.8%	2.9%	0.4%	*2057*
Pearse St (from)	1.2%	88.3%	5.7%	2.8%	1.9%	*2898*
Lombard St (to)	3.8%	83.5%	9.3%	2.6%	0.8%	*1024*
Westland Row (to)	0.7%	84.2%	6.7%	1.9%	6.6%	*701*
Westland Row (from)	3.7%	85.1%	8.5%	1.9%	0.8%	*884*
Mean	2.1%	86.3%	7.0%	2.4%	2.1%	

Table 7.2: Observed vehicle categorization of traffic passing through Dublin city-centre study junction during the inter-peak hour (2pm to 3pm).

Roadway (Dir'n wrt Junc.)	Motor Vehicle Type (%)					
	TWs	*Cars*	*LGVs*	*HGVs*	*Buses*	*TOTAL*
Pearse St (to)	4.0%	73.8%	17.0%	4.3%	1.0%	*1608*
Pearse St (from)	3.8%	73.2%	15.8%	4.5%	2.7%	*2477*
Lombard St (to)	5.0%	73.1%	15.7%	4.1%	2.1%	*813*
Westland Row (to)	3.3%	73.2%	12.2%	4.1%	7.2%	*691*
Westland Row (from)	5.4%	74.3%	14.8%	2.8%	2.7%	*635*
Mean	4.3%	73.5%	15.1%	4.0%	3.1%	

7.2.3.3 Traffic activity

To obtain an accurate estimate of the space-mean-speed over one-hour periods, traffic speeds were determined using camera recordings. A sample of travel time data was collected using the 'chase car' method to verify data collected from the video recordings. The 'chase-car' method involves driving along the link in traffic and recording the time it takes (i.e. finish time less start time). The space-mean-speed is then computed from the quotient of the link length and the time taken to traverse that link. It was not feasible in this study to measure the time-mean-speed, acceleration or deceleration of the vehicles travelling through the traffic junction. Space-mean-speeds are associated with a given length of roadway, while time-mean-speeds are associated with a specified point along the roadway and are calculated by averaging spot speeds [Turner et al., 1998].

The required sample size for vehicle speed and traffic volume needs to consider errors resulting from speed measurements. Errors can arise due to both the sample size and the precision of the measurement [Bennett, 1994]. However, the required size of the sample is dependent on the distribution of speeds, the precision of the measurement, and the chosen confidence intervals. The minimum acceptable sample size can be estimated from the following relationships [Pan, 1995].

$$n_{min} = \left(\frac{\sigma_s \cdot K}{E_L} \right)^2 \qquad 7.1$$

$$\sigma_S = \frac{\sqrt{\sum_{i=1}^{n_{min}} (S_i - S_{avg})^2}}{n_{min} - 1} \qquad 7.2$$

$$S_{avg} = \sum_{i=1}^{n_{min}} \left(\frac{S_i}{n_{min}} \right) \qquad 7.3$$

where: n_{min} is the minimum acceptable sample size;

σ_s is the standard deviation of the speed measurements;

K is the normal distribution factor;

E_L is the error limit due to chance;

S_{avg} is the mean observed speed for all traffic on a link (km/hr); and

S_i is the individual vehicle mean-space-speed (km/hr).

If a confidence interval of 95% is chosen and vehicle speeds are assumed to be normally distributed, then the K factor has a value of 1.96. E_L has a value of two when the standard deviation of the sample is in the range of 8 to 12 km/hr [Bennett, 1994]. The minimum sample size is then in the range of 65 to 140. As in the surveys, all vehicles passing through the junction were included, the sample size employed was much bigger than this.

The delay experienced by a vehicle is the difference between the time a vehicle crosses the stop-line and the time that it initially came to a stop at the back of a queue. If the vehicle does not come to a complete stop, its delay time is zero. The average vehicular delay is computed as the sum of the individual vehicle delays, divided by the total number of vehicles as follows:

$$D_{avg} = \frac{1}{n_{samp}} \sum_{i=1}^{n_{samp}} (t_{out} - t_{in}) \qquad 7.4$$

where: D_{avg} is the average vehicular delay (sec.);

n_{samp} is the sample size;

t_{in} is the time a vehicle came to a stop at the back of a queue; and

t_{out} is the time a vehicle crosses the stop-line.

The queue length at any point in time is the number of vehicles idling at a junction. The average queue length is computed as the sum of the individual queue lengths, divided by the number of observations as follows:

$$Q_{avg} = \frac{1}{n_{obs}} \sum_{i=1}^{n_{obs}} Q(t) \qquad 7.5$$

where; Q_{avg} is the average queue length (pcu);

n_{obs} is the number of observations; and

Q(t) is the queue length at time t.

Table 7.3 and Table 7.4present the observed average speeds for the junction during peak and inter-peak hours. The average queues, link delays, and turn delays are also presented.

Table 7.3: Observed traffic characteristics at Dublin city-centre study junction during the peak hour (8 am to 9 am).

Roadway (Dir'n wrt Junc.)	Mean Queue (pcu)	Link Delay (sec.)	Turn Delay (sec.)	Mean Speed (km/hr)
Pearse St (to)	5	17	12	9.5
Pearse St (from)	0	0	N/A	9.4
Lombard St (to)	6	37	28	12.7
Westland Row (to)	4	N/A	39	9.6
Westland Row (from)	0	0	N/A	11.5

Table 7.4: Observed traffic characteristics at Dublin city-centre study junction during the inter-peak hour (2 pm to 3 pm).

Roadway (Dir'n wrt Junc.)	Mean Queue (pcu)	Link Delay (sec.)	Turn Delay (sec.)	Mean Speed (km/hr)
Pearse St (to)	3	10	8	11.3
Pearse St (from)	0	0	N/A	10.7
Lombard St (to)	4	27	31	9.1
Westland Row (to)	3	N/A	37	8.5
Westland Row (from)	0	0	N/A	11.7

The daily traffic volume can be determined using updated expansion factors for short period traffic counts developed by the National Roads Authority [Devlin, 1978].

The daily traffic volume for each link in the Dublin road network can be computed from the sum of 3.95 times the peak hour volume plus 11.35 times inter-peak hour volume [McCabe, 1998]. The traffic volume for either Saturday or Sunday is the product of the inter-peak hour volume and a constant, 15.3 [McCabe, 1998].

Alternatively, the annual traffic volume can be computed from the sum of 1,442 times the peak hour volume plus 4,143 times the inter-peak hour volume [Motherway, 2000].

7.2.4 TRAFFIC MODULE RESULTS

Table 7.5 and Table 7.6 present the results of the peak hour and inter-peak hour traffic module simulations in terms of the percentage vehicle classification at the junction in question.

Table 7.5: Predicted vehicle categorization of traffic passing through Dublin city-centre study junction during the peak hour (8 am to 9 am).

Roadway (Dir'n wrt Junc.)	Motor Vehicle Type (%)			
	LDVs	*HGVs*	*Buses*	*TOTAL*
Pearse St (to)	95.7%	3.8%	0.5%	*1311*
Pearse St (from)	93.5%	4.2%	2.3%	*2019*
Lombard St (to)	95.4%	3.1%	1.5%	*1072*
Westland Row (to)	81.2%	8.1%	10.8%	*372*
Westland Row (from)	94.0%	3.8%	2.2%	*733*
Mean	91.9%	4.6%	3.5%	

Table 7.6: Predicted vehicle categorization of traffic passing through Dublin city-centre study junction during the inter-peak hour (2 pm to 3 pm).

Roadway (Dir'n wrt Junc.)	Motor Vehicle Type (%)			
	LDVs	*HGVs*	*Buses*	*TOTAL*
Pearse St (to)	99.3%	0.1%	0.6%	*772*
Pearse St (from)	91.9%	6.1%	2.0%	*1568*
Lombard St (to)	87.2%	10.1%	2.7%	*631*
Westland Row (to)	73.2%	18.6%	8.3%	*327*
Westland Row (from)	76.3%	12.4%	11.3%	*151*
Mean	85.6%	9.5%	5.0%	

The predicted time delays (both link and turn depending on which is applicable), average queue, and average vehicle speed are shown in Table 7.7and Table 7.8. SATURN & SATCHMO specifies average queue lengths in pcus.

Table 7.7: Predicted traffic characteristics at Dublin city-centre study junction during the peak hour (8 am to 9 am).

Roadway (Dir'n wrt Junc.)	Mean Queue (pcu)	Link Delay (sec.)	Turn Delay (sec.)	Mean Speed (km/hr)
Pearse St (to)	5	14	17	13
Pearse St (from)	0	0	N/A	11
Lombard St (to)	6	21	20	15
Westland Row (to)	2	N/A	18	10
Westland Row (from)	0	0	N/A	24

Table 7.8: Predicted traffic characteristics at Dublin city-centre study junction during the inter-peak hour (2 pm to 3 pm).

Roadway (Dir'n wrt Junc.)	Mean Queue (pcu)	Link Delay (sec.)	Turn Delay (sec.)	Mean Speed (km/hr)
Pearse St (to)	2	11	17	15
Pearse St (from)	0	0	N/A	35
Lombard St (to)	5	30	40	10
Westland Row (to)	0	N/A	12	13
Westland Row (from)	0	0	N/A	31

7.2.5 Comparison of Predicted and Observed Traffic Variables

SATURN & SATCHMO has been extensively calibrated and validated against independent traffic surveys across Dublin [McCabe, 1998]. In this study, measured traffic parameters are used to validate simulated parameters as an assurance that these traffic variables are an adequate basis on which to base an emissions inventory whenever direct measurements are not available.

Table 7.1, Table 7.2, Table 7.5 and Table 7.6 show the modelled and measured traffic volume and percentage mix for the junction. The observed vehicle flow rates and percentage traffic composition agree reasonably well with those predicted by SATURN & SATCHMO considering the fact that the model was calibrated in 1996 and the observations were collected in 1998 by the author. At peak hour, the total predicted flow through the junction is 73% of that observed. This difference is slightly greater for the off-peak simulation. Overall, the model over-estimates the proportion of HGVs and buses within the traffic stream. For example, 99 HGVs were observed to pass through the junction during the peak hour, while the model predicts 113. This may be due to the fact that SATURN & SATCHMO was set-up for 1996 and the survey was conducted in 1998. In addition, SATURN & SATCHMO does not take account of motorcycles, further affecting the volume composition.

For both peak and off-peak hours, the average queue length and link delay parameters are well predicted, but turning delays are not.

Average vehicle speeds were observed to be slightly lower than predicted with the exception of Westland Row (from) during the peak hour and both Pearse St. (from) and Westland Row (from) during the inter-peak hour.

Overall, SATURN & SATCHMO generally under-predicts traffic volume and congestion and over-predicts vehicle speed. This discrepancy may be due, in part, to the fact that certain journeys are not incorporated within the trip matrix (e.g. private buses, taxis, and out-of-town visitors) and therefore are not included in the assignment module.

It is felt that these discrepancies are indicative of the overall ability of SATURN & SATCHMO to predict actual on-street traffic conditions and, as such, to act as the basis of an emissions inventory.

7.2.6 Source Strength at Study Intersection in Dublin

The emissions inventory for all roadways leading to and from the study junction is computed in by MVEIM and presented in Table 7.9.

Table 7.9: Emissions inventory for all traffic passing through the study junction in Dublin as computed by MVEIM

Pollutant	Pearse St (to) (kg/day)	Pearse St (from) (kg/day)	Lombard St (to) (kg/day)	Westland Row (to) (kg/day)	Westland Row (from) (kg/day)
PM_{10}	0.38	0.53	0.28	0.41	0.11
NO_2	6.41	8.56	4.46	6.82	1.82
CO	68.97	76.49	47.99	40.90	21.23
VOC	7.87	8.98	5.59	5.07	2.44
C_4H_6	0.14	0.16	0.09	0.10	0.04
C_6H_6	0.35	0.39	0.23	0.20	0.10

7.2.7 Air Quality Monitoring in Dublin

On-line kerbside monitoring of pollutant concentrations was carried out using a mobile air-monitoring laboratory. The location of the monitoring laboratory is shown in Figure 7.1, with the sampling air inlet located 3m from the roadside. The layout of the mobile air-monitoring laboratory is given in Figure 7.3.

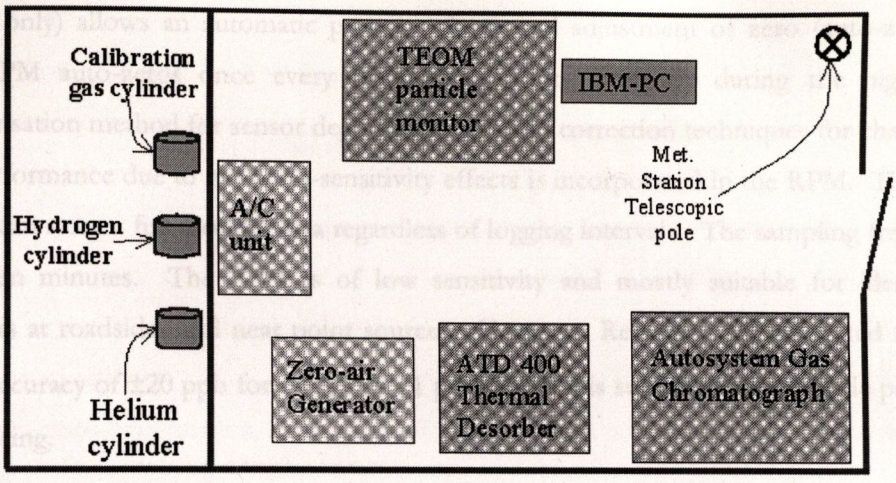


Figure 7.3: Layout of main equipment in mobile air quality monitoring unit

The equipment is capable of sampling and analysing each of the pollutants identified in Table 7.9, as well as recording meteorological conditions (such as temperature, relative humidity, and wind speed and direction). The laboratory, which also contains air conditioning and data logging/processing equipment, is operable at any location where standard electricity supply is available. This unit was used to measure a wide variety of pollutants including carbon monoxide, nitrogen dioxide, particulate matter and volatile organic compounds.

7.2.7.1 NO_2 and CO measurement

These more traditional pollutants have been the subject of study for many years. Consequently, a wide variety of well established monitoring equipment is available, normally based on conventional gas sampling and analysis techniques. The nitrogen dioxide and carbon monoxide analysers used in this study are installed in a RPM originally developed under ITEMMS [Bell et al., 1996c].

The RPM consists of an electro-chemical sensor, a pump and a filter. Air is continuously drawn at a constant flow rate of two litres-per-minute through a filter, purmapure humidity exchanger and valve system to the electrochemical cells. These sensor cells contain a chemical, which reacts with a target pollutant and consequently produces a small electric current. This current generated by the sensor is proportional to the target pollutant concentration. The cells are temperature stabilised over the ambient temperature from 10°C to +30°C using a peltiér device. At temperatures outside this range, some degradation due to temperature variations in the cells may occur. However, this is minimised by an advanced sensor design. An integral charcoal scrubber (on the NO_2

sensor only) allows an automatic periodic check and adjustment of zero (auto-zeroing). The RPM auto-zeros once every twenty-four hours, normally during the night. A compensation method for sensor degradation and also correction techniques for changes in cell performance due to gas cross-sensitivity effects is incorporated in the RPM. The data-logger can store a full months data regardless of logging intervals. The sampling frequency is fifteen minutes. The RPM is of low sensitivity and mostly suitable for identifying hotspots at roadsides and near point sources. However, Reynolds [1996b] noted that the RPM accuracy of ±20 ppb for NO_2 and ±1 ppm for CO is sufficient for kerbside pollution monitoring.

7.2.7.2 PM_{10} measurement

Particulate matter of aerodynamic diameter less than 10 microns (PM_{10}) are monitored using an R&P TEOM 1400a monitor [Patashnick and Rupprecht, 1989; 1991], [Rupprecht et al., 1992]. A schematic diagram of the monitor is shown in Figure 7.4. The monitor incorporates an inertial balance. It measures the mass collected on an exchangeable filter cartridge by monitoring the corresponding frequency changes of a tapered element. The electronics feedback system maintains the tapered element in oscillation. A precision frequency counter in the electronics feedback control unit measures the frequency of oscillation.

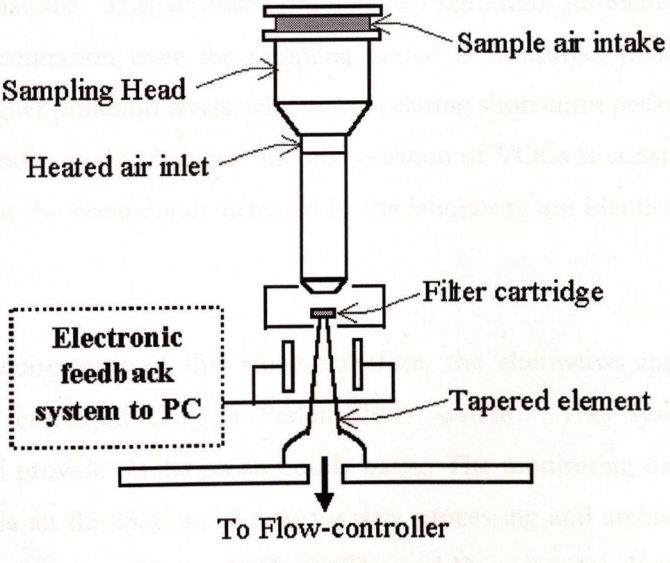


Figure 7.4: Schematic diagram of the TEOM ambient particle monitor

The TEOM detector is capable of operating with flowrates between 0.5 and 5 litres-per-minute. The flow rate depends on the requirements of the sampling head selected. With

the PM_{10} sampling head, a flow rate of 16.7 litres-per-minute is used. A flow splitter, and a second flow controller are used to bypass 13.7 litres-per-minute to maintain the mass detector within its operating range. The remaining sample flow (3 litres-per-minute) passes through the filter, where particulate matter collects, and then continues through a hollow tapered element on its way to an electronic flow control system and vacuum pump. The inlet of the sampler is kept at 50°C (i.e. above dew point) to eliminate the effect of water droplets, associated with hygroscopic salts, on the measurements. As more mass collects on the exchangeable filter, the tube's natural frequency of oscillation decreases. A microprocessor converts the vibration frequency to mass concentrations. The instrument is isolated from external vibrations through the use of shock absorbers.

The tapered element technology enables highly precise and accurate mass determinations, providing more resolution than conventional microbalances. The equipment is capable of automatically recording atmospheric concentrations at short intervals, making it ideally-suited to investigating diurnal changes in particulate concentrations. In this case, a sampling frequency of fifteen minutes was employed.

7.2.7.3 VOC measurement

Conventional VOC monitoring is carried-out with the use of desorbtion tubes, which collect and store the pollutant over a period of weeks, after which they are taken to a laboratory and analysed. This approach presents two significant problems. Firstly, as only the average concentration over the sampling period is measured, it is not possible to determine the higher pollution levels, which occur during short-term peaks such as those at rush-hour. Secondly, as the character and composition of VOCs is constantly changing; it is not certain that the compounds detected in the laboratory are identical to those in the open air.

To meet the requirements of this study therefore, the alternative approach of online measurement is employed using a Perkin-Elmer system. This system can operate continuously and provide results on an hourly basis. The monitoring data is downloaded to a computer via an RS-232C serial port for data processing and archiving. The system comprises an AutoSystem GC, an ATD-400 Thermal Desorber fitted with peltiér electric cooling of the cold trap, an auxiliary air sampler and a Nafion dryer. A schematic diagram of the system is shown in Figure 7.5.

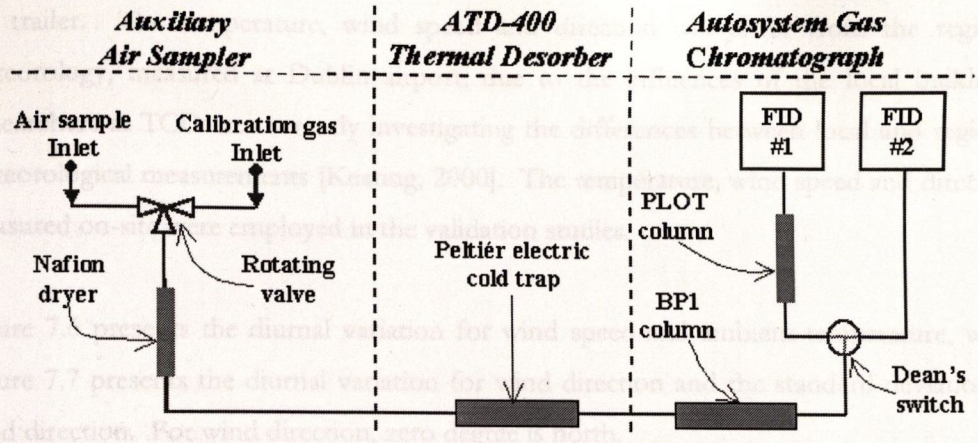


Figure 7.5: Schematic diagram of the Perkin-Elmer ambient VOC monitor

A sample of air (0.6 litres in total) is drawn into the trap at a flow rate of 15 ml/min. over a period of forty minutes through the Nafion dryer. This dries the air sample, thus preventing the build-up of ice in the cold trap. The trap is cooled to -30°C to retain any volatile organic carbon compound except methane, and then heats very rapidly to +400°C. The carrier gas (helium) flow is then reversed to back-flush the hydrocarbons from the trap through a heated transfer line to the AutoSystem GC. The AutoSystem GC is equipped with a BP1 capillary column (50m x 0.22 mm id, 1.0 μm film thickness) connected to a FID. Hydrogen and zero-air (pure air) are the combustion gases for the FID. Analysis in the AutoSystem GC takes forty-eight minutes, and twenty minutes after the AutoSystem GC analysis begins, the next sample can be collected. Zero-air is used in the Nafion dryer (i.e. to dry the sampled air), to power certain pneumatic processes in the ATD-400, and to purge the peltier-cooled trap. Calibration is performed using a reference gas mixture supplied by the National Physical Laboratory in the UK.

Twenty-seven different VOCs (in the range C_1 to C_9) are analysed each hour, including 1,3-butadiene and benzene, but excluding methane. Primarily petrol engine vehicles emit C_1 to C_9 hydrocarbons, while diesel engine vehicles emit a high percentage of semi-volatile hydrocarbons (i.e. C_{10} to C_{20}) [Zielinska et al., 1996].

7.2.7.4 Meteorological measurement

A meteorological station is also installed in the air quality-monitoring unit. This station comprises an anemometer and a wind vane for measuring wind speed and direction. In addition, it consists of two probes that measure relative humidity and temperature. These sensors are attached to a telescopic pole and are connected to a data-logger located within

the trailer. The temperature, wind speed and direction will differ from the regional meteorology, measured at Dublin airport, due to the influences of the local buildings. Researchers at TCD are currently investigating the differences between local and regional meteorological measurements [Keating, 2000]. The temperature, wind speed and direction measured on-site were employed in the validation studies.

Figure 7.6 presents the diurnal variation for wind speed and ambient temperature, while Figure 7.7 presents the diurnal variation for wind direction and the standard deviation of wind direction. For wind direction, zero degree is north.

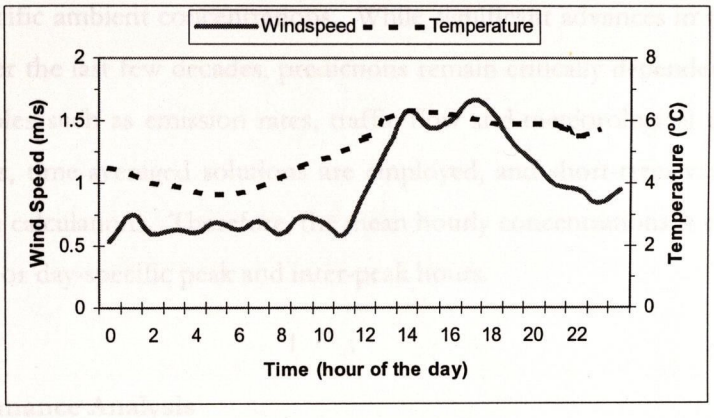


Figure 7.6: Diurnal variation of wind speed and temperature in Dublin

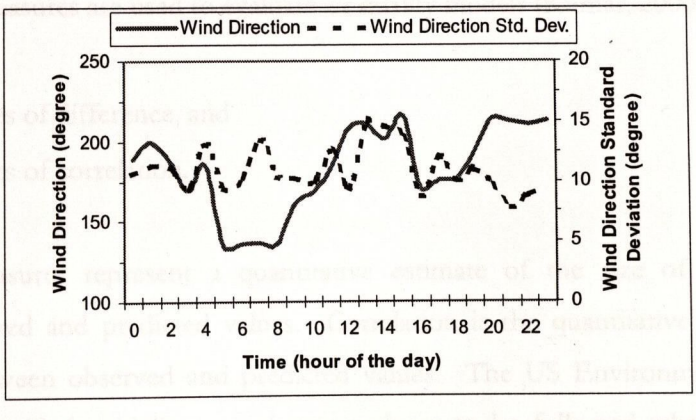


Figure 7.7: Diurnal variation of wind direction and wind direction standard deviation in Dublin

7.2.8 Comparison of Predicted and Observed Concentrations

Observed kerbside pollution concentrations display large short-term (e.g. minute-by-minute) variations and are highly sensitive to the exact monitoring location employed. This

results in a signal to noise ratio so low that direct time-series comparison between pollution concentration and passing traffic flows is almost meaningless [Penn et al., 1996]. However previous studies have shown that good correlations can be achieved between observed and predicted pollutant concentrations when these are averaged over longer periods of time, e.g. hourly, daily, monthly or annually.

CALINE4R was used to predict the mean hour-by-hour pollutant concentrations over a weekday using mean hour-by-hour traffic data recorded over a week. These predicted concentrations are compared to average hour-by-hour observed concentrations measured over a month. It should be noted that dispersion modelling does not attempt to predict exact time-specific ambient concentrations. While significant advances in techniques have been made over the last few decades, predictions remain critically dependent on a number of input variables such as emission rates, traffic flow and meteorological conditions. On account of this, time-averaged solutions are employed, and short-term variations are not reflected in the calculations. Therefore, the mean hourly concentrations is employed rather that individual or day-specific peak and inter-peak hours.

7.2.8.1 Performance Analysis

Several parameters are employed to evaluate pairs of data. However, two primary types of performance measures are used to evaluate air quality models [Kumar, 2000]:

- Measures of difference, and
- Measures of correlation.

Difference measures represent a quantitative estimate of the size of the differences between observed and predicted values. Correlation is the quantitative measure of the association between observed and predicted values. The US Environmental Protection Agency has provided guidelines on the procedures to be followed when evaluating air quality models [US-EPA 1984b; 1987], as has Wilmott [1982; 1985], Kumar [2000] and the EEA [Van Aalst et al., 1998]. From these works, a number of statistics for model evaluation were chosen such as bias, fractional bias, normalized mean square error, and correlation coefficient.

Bias is the mean error that is defined as the mean observed value of pollutant concentration $\overline{C}_o$ less the mean predicted value $\overline{C}_p$. The expression for the bias is given by:

$$\text{Bias} = \overline{C}_o - \overline{C}_p \qquad 7.6$$

The bias is normalized to make it non-dimensionless. This FB varies between -2 and +2 and has a value of zero for a perfect model. It is given by:

$$\text{FB} = \frac{2.(\overline{C}_o - \overline{C}_p)}{\overline{C}_o + \overline{C}_p} \qquad 7.7$$

This NMSE emphasises the scatter in the entire data set. The normalization by the mean product C_o (observed concentration) and C_p (predicted concentration) assures that the NMSE will not be biased towards models that over predict or under predict. Smaller values of NMSE denote better model performance. It is written in symbolic form as:

$$\text{NMSE} = \frac{\overline{(C_o - C_p)^2}}{\overline{C_o}.\overline{C_p}} \qquad 7.8$$

The correlation coefficient (R) gives a quantitative relationship between observed and predicted parameters. A value of correlation coefficient close to unity implies good model performance. In equation form it is represented as:

$$R = \frac{\overline{(C_o - \overline{C}_p)(C_o - \overline{C}_p)}}{\sigma_o.\sigma_p} \qquad 7.9$$

where σ_o is the standard deviation of the measured data; and

σ_p is the standard deviation of the predicted data;

The percentage of two (P-2) is defined as the percentage of the predicted pollutant concentrations within a factor of two of the observed values. The ideal value for the factor of two should be 1 (i.e. 100%). It is written in symbolic form as:

$$P-2 = 0.5 \leq \frac{C_P}{C_o} \leq 2.0 \qquad 7.10$$

These performance measurements are summarised in Table 7.10 for observed and predicted pollutant concentrations in Dublin.

Table 7.10: Statistical analysis of diurnal hour-by-hour observed and diurnal hour-by-hour predicted ambient pollutant kerbside concentrations in Dublin

Statistic	PM_{10}	NO_2	CO	VOC	C_4H_6	C_6H_6
$\overline{C}_o$	37.93	0.025	1.91	38.58	0.40	1.88
σ_o	13.42	0.008	1.28	17.61	0.21	1.04
$\overline{C}_P$	31.8	0.027	2.5	43.1	1.0	4.1
σ_p	17.9	0.012	1.3	25.8	0.6	2.4
Bias	6.18	-0.002	-0.54	-4.52	-0.57	-2.19
NMSE	0.10	0.103	0.16	0.09	1.09	0.76
R	0.81	0.86	0.80	0.89	0.84	0.84
FB	0.18	-0.067	-0.25	-0.11	-0.84	-0.74
P-2	71%	71%	71%	75%	29%	42%

As already stated, a perfect model will have both the FB and NMSE equal to zero. However, real world models are seldom perfect. To determine the reliability of a model, Kumar [2000] suggests that the NMSE is less than one-half (i.e. NMSE < 0.5) and that the FB is greater than minus one-half and less than plus one-halt (i.e. -0.5 < FB < +0.5). In addition, the percentage of two should be greater that two-thirds (i.e. P-2 > 0.67). CALINE4R meets Kumar's criteria for all pollutants with the exception of benzene and 1,3-butadiene (see Table 7.10). This observation may be due to the fact that the dispersion model does not incorporate any chemical reaction sinks for these pollutants. However, total volatile organic compounds are modelled as inert gases and the predicted and observed results agree more closely. Consequently, the poor prediction for benzene and 1,3-butadiene may be attributed to the fact that the emission factors employed for these compounds are based on a very limited data set.

The overall results show a negative bias between the observed and predicted observations with the exception of PM_{10}. This means that the model generally over-predicts kerbside

concentrations. Muir [2000] states that "the UK Department of the Environment, Transport and the Regions has advised Local Authorities that to compare TEOM data with the European limit value, the TEOM data should be multiplied by a factor of 1.3". Over two-thirds of the predicted values for PM_{10}, NO_2, CO, and VOC are within a factor-of-two of the observed values.

The model tends to under-predict at low concentrations (i.e. during the night when the traffic volume traversing the intersection is low) and over-predict at higher concentrations (i.e. during the day when the traffic volume traversing the intersection is high). At low concentrations, the accuracy of some of the measurement equipment is questionable.

A fractional bias close to zero indicates a good model. The fractional bias of -0.74 for benzene denotes 74% over-prediction of the mean of the estimated values for all hours over the mean of the observed values for all hours.

The NMSE indicates the value of the error produced by the model. The normalisation assures that NMSE will not bias towards models that under- or over-predict. For example, the bias for PM_{10} is relatively large (6.2), while the NMSE is relatively small (0.1).

7.2.8.2 Regression Analysis

Scatter diagrams and correlation coefficients are widely employed by researchers to report the performance of their models [Kumar, 2000]. Figure 7.8 to Figure 7.13 show the scatter plots for the mean diurnal hour-by-hour predicted (collected over a week) pollutant concentrations with the mean diurnal hour-by-hour measured (collected over a month) pollutants concentrations. This gives a total of twenty-four pairs of data (i.e. one pair for each hour of the day).

A linear regression analysis was performed between the observed and predicted data sets for each pollutant and this is depicted in Figure 7.8 to Figure 7.13 also.

In addition, dashed lines show the envelope for the percentage of predicted pollutant concentrations within a factor of two of the observed values.

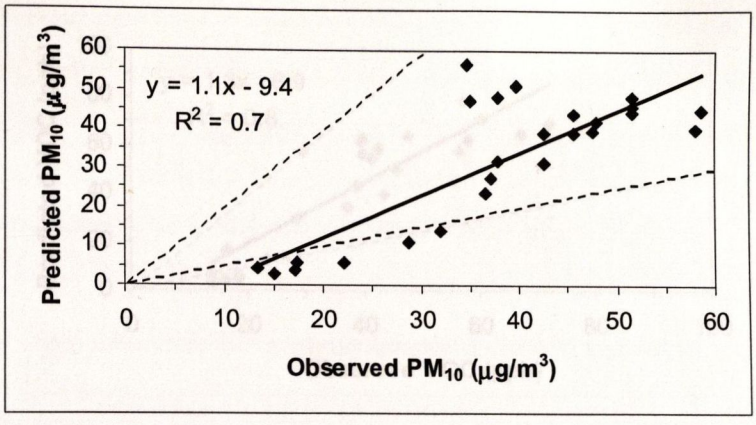


Figure 7.8: Diurnal hour-by-hour predicted versus diurnal hour-by-hour observed particulate-matter concentrations in Dublin

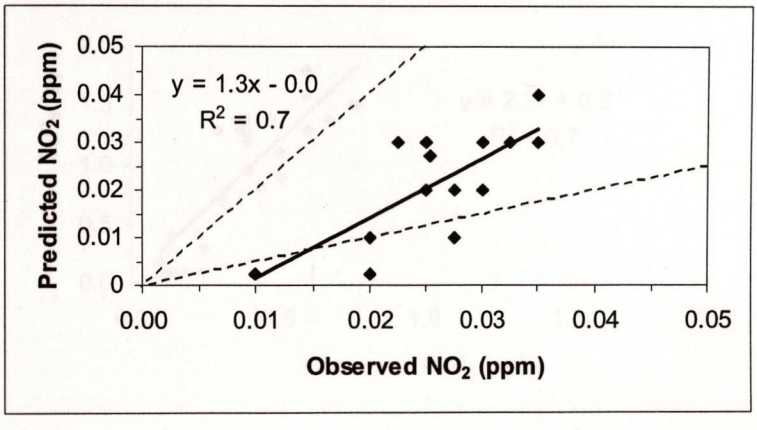


Figure 7.9: Diurnal hour-by-hour predicted versus diurnal hour-by-hour observed nitrogen dioxide concentrations in Dublin

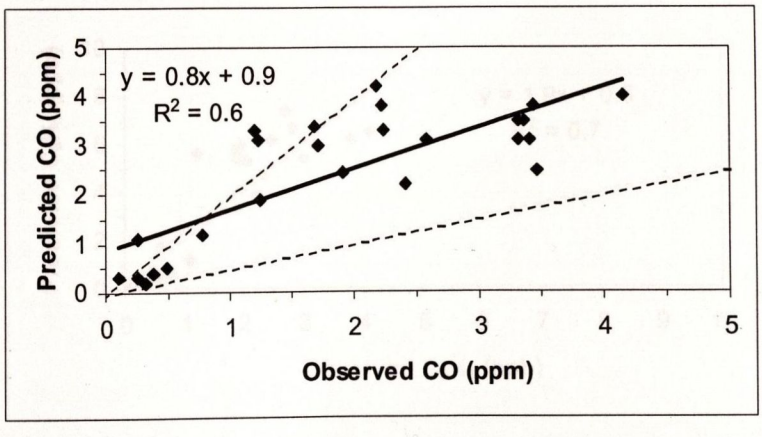


Figure 7.10: Diurnal hour-by-hour predicted versus diurnal hour-by-hour observed carbon monoxide concentrations in Dublin

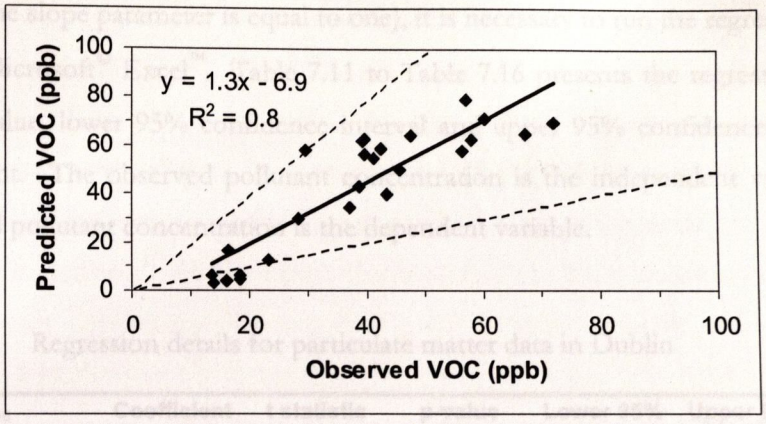


Figure 7.11: Diurnal hour-by-hour predicted versus diurnal hour-by-hour observed volatile organic compounds concentrations in Dublin

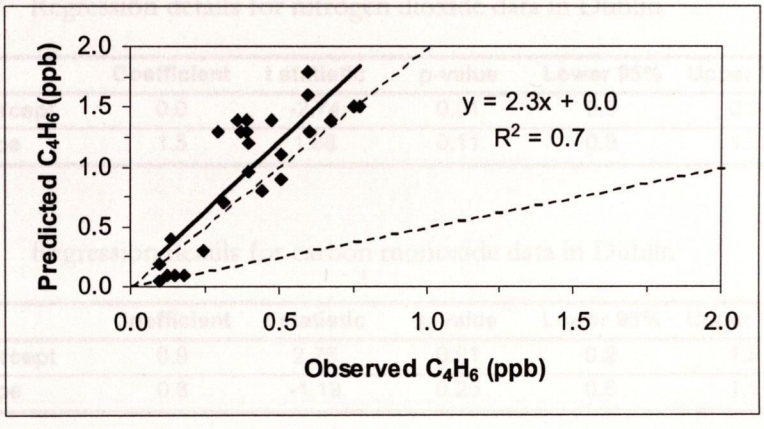


Figure 7.12: Diurnal hour-by-hour predicted versus diurnal hour-by-hour observed 1,3-butadiene concentrations in Dublin

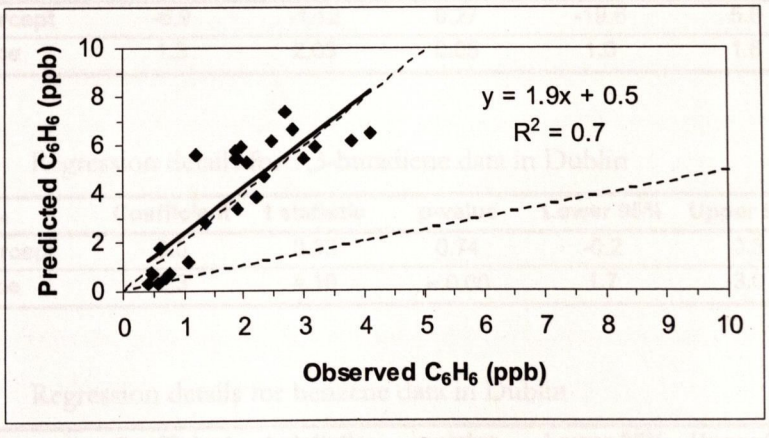


Figure 7.13: Diurnal hour-by-hour predicted versus diurnal hour-by-hour observed benzene concentrations in Dublin

The slopes and intercepts of the regression lines (presented in Figure 7.8 to Figure 7.13) are different for each pollutant. To ascertain whether or not the intercept parameter is equal

to zero (or the slope parameter is equal to one), it is necessary to run the regression analysis toolpak in Microsoft© Excel™. Table 7.11 to Table 7.16 presents the regression details (t statistic, p-value, lower 95% confidence interval and upper 95% confidence interval) for each pollutant. The observed pollutant concentration is the independent variable, while the predicted pollutant concentration is the dependent variable.

Table 7.11: Regression details for particulate matter data in Dublin

PM_{10}	Coefficient	t statistic	p-value	Lower 95%	Upper 95%
Intercept	-9.4	-1.42	0.17	-23.2	4.4
Slope	1.1	0.52	0.61	0.7	1.4

Table 7.12: Regression details for nitrogen dioxide data in Dublin

NO_2	Coefficient	t statistic	p-value	Lower 95%	Upper 95%
Intercept	0.0	-2.74	0.01	0.0	0.0
Slope	1.3	1.66	0.11	0.9	1.6

Table 7.13: Regression details for carbon monoxide data in Dublin

CO	Coefficient	t statistic	p-value	Lower 95%	Upper 95%
Intercept	0.9	2.76	0.01	0.2	1.5
Slope	0.8	-1.19	0.25	0.6	1.1

Table 7.14: Regression details for volatile organic compounds data in Dublin

VOC	Coefficient	t statistic	p-value	Lower 95%	Upper 95%
Intercept	-6.9	-1.12	0.27	-19.6	5.8
Slope	1.3	2.03	0.05	1.0	1.6

Table 7.15: Regression details for 1,3-butadiene data in Dublin

C_4H_6	Coefficient	t statistic	p-value	Lower 95%	Upper 95%
Intercept	0.0	0.33	0.74	-0.2	0.3
Slope	2.3	4.10	≈ 0.00	1.7	3.0

Table 7.16: Regression details for benzene data in Dublin

C_6H_6	Coefficient	t statistic	p-value	Lower 95%	Upper 95%
Intercept	0.5	0.87	0.39	-0.7	1.7
Slope	1.9	3.38	≈ 0.00	1.3	2.5

The intercept is not statistically significantly different from zero (at the 95% significant level) for PM_{10}, VOC, C_4H_6 and C_6H_6, as zero is in between the lower and upper 95%

confidence limits for each of these pollutants. This means that the true line can pass through the origin for PM_{10}, VOC, C_4H_6 and C_6H_6. The corresponding p-values greater than 0.05 (for PM_{10}, VOC, C_4H_6 and C_6H_6) confirm this. Conversely, the intercept is statistically significantly different from zero (at the 95% significant level) for CO and NO_2, as zero is not in between the lower and upper 95% confidence limits for each of these pollutants. The extremely small p-values (for both CO and NO_2) confirm this. The slope is not statistically significantly different from one (at the 95% significant level) for PM_{10}, NO_2, CO, and VOC as one is in between the lower and upper 95% confidence limits for each of these pollutants. The corresponding p-values greater than 0.05 (for PM_{10}, NO_2, CO, and VOC) confirm this. Conversely, the slope is statistically significantly different from one (at the 95% significant level) for C_4H_6 and C_6H_6, as one is not in between the lower and upper 95% confidence limits for each of these pollutants. The extremely small p-values (for both C_4H_6 and C_6H_6) confirm this

7.3 VALIDATION IN HANNOVER

Numerous methods are employed for the estimation of vehicle-induced air pollution concentrations in urban areas. On one level, a large range of atmospheric dispersion model formulations can be identified, including Gaussian, Semi-empirical, Eulerian, Lagrangian, Chemical Mass Balance, Receptor, and Stochastic. On another level, significant variations arise in the compilation of emissions inventories, the pre-processing of meteorological data and the computation of background concentrations. To assess these differences, a model inter-comparison workshop was held as part of the 6th International Conference on 'Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes', at which selected participants applied their method of pollutant concentration estimation to a specific street canyon in Hannover, Germany. Street canyons are building configurations near a road, which extend in height much more than the spacing between the walls of facing buildings on the two sides of the street.

Model results were submitted prior to the conference. The objective of the exercise was to determine the variation in calculated concentrations arising due to:

- The use of different pollutant dispersion models;
- The particular application of the same pollutant dispersion model by different users;
- The use of different procedures for pre-processing the available input-data; and

- The use of different methods for post-processing air quality model output.

The observed ambient concentrations in the street canyon were not available to the participants prior to the submission of their modelled results. The primary objective of the exercise was not to rank the pollutant dispersion models but to compare the different methods being used.

7.3.1 EXERCISE PARTICIPANTS

In total fifteen participants took part, using twelve different dispersion models, including the model described herein. The other eleven models were:

- A Wind Tunnel [Lohmeyer, 1999];
- ADMS-urban [McHugh et al., 1997b];
- AUTOMOD [Hesek, 1992];
- CPB3 [Friedrich and Schierbaum, 1997];
- MIMO [Goetting et al., 1997];
- MISKAM [Beckroge, 1998];
- OSPM [Berkowicz et al., 1996];
- PROKAS_B [Bösinger, 1998];
- CD model [Craig et al., 1999];
- Street Box model [Pfeifer et al., 1995]; and
- ZONE model [Lohmeyer, 1999].

The models can be divided into different types, namely physical (i.e. the Wind Tunnel), quasi-Gaussian (ADMS-urban and PROKAS_B), combined plume and box (OSPM and CALINE4R), three-dimensional Eulerian (AUTOMOD, and MISKAM), and finite-volume (MIMO and CD model). No information was available on the 'Wind Tunnel' or ZONE models. Some participants employed the same models.

7.3.2 SURVEY SITE

The area under consideration, the Lister Platz and surroundings, is shown in Figure 7.14. The point of interest is at the front of N° 5 Podbielski Strasse. This site is a five-storey building with an estimated height of 25m (including the roof). The building facades along

the street are covered with open and closed balconies. Podbielski Strasse consists of a two-way, three-lane roadway, with two lanes going towards Lister Platz and one-lane going away from Lister Platz.

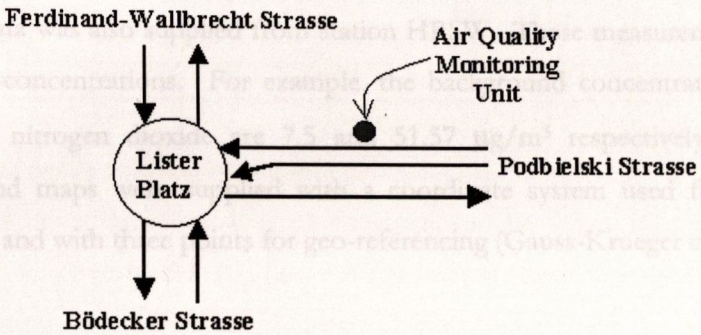


Figure 7.14: Location of study site in Hannover

7.3.3 DATA SUPPLIED

Traffic volume, meteorological data (wind speed and direction), and background concentrations were supplied by the organisers of the exercise.

A traffic count was conducted by the Tiefbauamt Hannover between 1987 and 1995 during the hours between 6:30 am and 6:30 pm. No information on heavy-duty traffic was available as only passenger cars and light-duty vehicles were monitored. Traffic lights located at the Lister Platz junction are demand-controlled (i.e the traffic lights change in response to the volume of traffic and consequently the ratio of green to red is not constant but varies from cycle to cycle). Public transport vehicles on Bödecker Strasse and Ferdinand-Wallbrecht Strasse have priority in controlling the traffic lights (i.e. when a public transport vehicle approaches the junction, the traffic lights change to 'green' to allow the vehicle traverse the junction with the minimum of delay). This causes increased traffic queues on Podbielski Strasse. The total number of vehicles in the time period 6:30 am to 6:30 pm in the direction towards and from Lister Platz is 9,200 and 7,300 vehicles respectively. An independent count by the organisers of the exercise yielded a total traffic flow of 16,345 per day. This gives an average hourly traffic flow of 681 vehicles per hour.

A meteorological station (name: HRSW) is located on a flat roof of the building of the Niedersaechsisches Landesamt fuer Oekologie, Goettinger Strasse, Hannover, about 4 km south-west of the Podbielski Strasse. The wind anemometers are at a height of 42m above the ground and 10m above roof level. Half-hourly means of wind speed and wind

direction were supplied for each day during the period 1989 to 1998. The participants were required to compute the annual average hourly wind speed (3.7 ± 1.1 m/s), wind direction (200° ± 39°, assuming 0° is North) and their corresponding standard deviations.

Air pollution data was also supplied from station HRSW. These measurements were used as background concentrations. For example, the background concentration of nitrogen monoxide and nitrogen dioxide are 7.5 and 51.57 $\mu g/m^3$ respectively. In addition, photographs and maps were supplied with a coordinate system used for definition of receptor points and with three points for geo-referencing (Gauss-Krueger co-ordinates).

7.3.4 Source Strength at Street Canyon in Hannover

The emissions source strength for traffic traversing the study junction at Melton Mowbray was computed by MVEIM. Composite emission factors can be formulated, since the traffic composition travelling along Podbielski Strasse is assumed homogenous and constant throughout the day and for all lanes. These composite emission factors given in Table 7.17 are calculated based on traffic composition data (for all of Germany) given by Kyriakis et al. [1998].

Table 7.17: Composite emission factors for traffic travelling along Podbielski Strasse in Hannover as computed by MVEIM

Pollutant	CEF (g/km)
CO	5.05
Benzene	0.11
Soot	0.02
NO_2	2.88

7.3.5 Comparison of Predicted and Observed Concentrations

At the workshop, Mueller [1999] presented annual average hourly measurements made in the street canyon. CALINE4R was employed to estimate the annual average hourly pollutant concentrations in the street canyon using the annual average hourly values of traffic volume (681 vehicles per hour), along with the composite emission factors in Table 7.17.

A comparison of the average annual observed and average annual predicted pollutant concentrations are given in Table 7.18.

Table 7.18: Annual average observed pollutant concentrations measured in the street canyon and the corresponding annual average predicted concentrations.

Pollutant	Observed ($\mu g/m^3$)	Predicted ($\mu g/m^3$)	P/O
CO	928.0	1356.0	1.46
Benzene	16.2	19.4	1.20
Soot	3.0	3.9	1.29
NO_2	95.5	131.1	1.37

A comparison of prediction and measurement results indicates that while the AQMS over-estimated the pollutant concentrations, its predictions all lay within a factor-of-two of the measured data. The over-prediction may have arisen because a worst-case meteorological scenario was assumed, since stability height and temperature were not supplied with the original input data. In addition, CALINE4R has not been designed specifically for street canyons. However, it can be employed in street canyons by limiting the horizontal dispersion of pollutants.

Overall, it can be concluded that the combined MVEIM and CALINE4R models can be applied in street canyons with some degree of confidence. However, it must be remembered that this comparison was performed on the basis of annual average hourly values of traffic and pollution concentrations, masking some errors and uncertainties, which may be arise in shorter-term predictions. As there was only one predicted concentration value and one observed concentration value for each pollutant, a statistical analysis could not be performed.

7.3.6 Comparison of Results from Exercise Participants

The workshop participants were required to estimate pollutants at a five locations along the street canyon. For a practical comparison of the dispersion models the estimation of a non-dimensional concentration (c*) under well-defined conditions of emission is necessary. This difference in c* values represents the differences in the dispersion modelling and is defined as:

$$c^* = \frac{c \cdot u \cdot H}{q} \qquad 7.11$$

where: c* is the non-dimensional concentration at the receptor point;

c is the concentration at the receptor point (g/m^3);

u is the wind speed at a reference height (m/s);

q is the emission density (g/m-s); and

H is the average building height (m).

To preserve anonymity, the individual results from each participant are not available [Lohmeyer, 1999]. Therefore, a direct comparison between CALINE4R and the other models employed is not possible. Instead Lohmeyer [1999] presented the coefficient of variation (defined as the standard deviation divided by the sample mean) for each pollutant. The coefficient of variation for wind speed, emission factor, non-dimenaional concentration, background concentration, additional concentration due to traffic, and total concentration are presented in Table 7.19. Only pollutant concentrations for benzene, nitrogen dioxide and soot were sought in the exercise.

Table 7.19: Coefficient of variation between workshop participants [source: Lohmeyer, 1999]

Parameter	Benzene	Soot	NO_2
Wind speed (u)	0.05	0.05	0.05
Emission density (q)	0.3	1.08	0.62
Non-dimensional concentration (c*)	0.6	0.6	0.6
Background concentration	0.22	0.48	0.16
Additional concentration due to traffic	0.54	0.21	0.5
Total concentration (c)	0.3	0.14	0.3

Table 7.19 gives an indication of the possible variations involved in estimating concentrations in a street canyon. The half-hourly wind speed was given for the past ten years. However, different participants got different annual hourly averages. This discrepancy was due to the method of averaging. For example, some participants included missing values as zero, other participants removed the zero values, while others used interpolation to approximate the missing values. It is worth noting that two pairs of participants used the same models independently (MISKAM and OSPM). However, all participants obtained different c* values (again, to preserve anonymity, the individual results from each participant are not available) [Lohmeyer, 1999]. This difference in c* indicates that even when modellers employ the same model, they may obtain different results. The primary reason for this is that different modellers make different assumptions. The most common conclusion concerning the results is the variation in the results of single steps (e.g. the determination of emission factors) is comparatively high but the variation in the estimated total concentration is comparatively low. For example, the coefficient of

variation for soot emission factors is 1.08 while the coefficient of variation for the estimated soot concentrations is 0.14.

7.4 VALIDATION IN MELTON MOWBRAY

The Institute of Transport Studies at the University of Leeds supplied data with which the AQMS could be validated at a site in the UK. Researchers at University of Nottingham have previously studied the temporal variations in pollutant levels at this junction over a number of years [Boddy, 1999]. In addition, researchers at the University of Leeds are currently developing an ETEM using traffic activity data from SCOOT and pollutant measurements from a RPM located at this site [Jalihal, 2000].

7.4.1 SURVEY SITE

The survey site was at an arterial four-way signalised controlled junction between the A606 and Norman Way. The A606 is the primary road between Nottingham and Melton Mowbray. The area is a mix of commercial buildings and residential properties. A schematic representation of the junction is depicted in Figure 7.15. It is a four-way signalised controlled intersection, with all arms possessing lanes going both directions to and from the intersection. The numbers at the junctions identify the intersections in the SCOOT system. The location of the RPM is also shown in Figure 7.15.

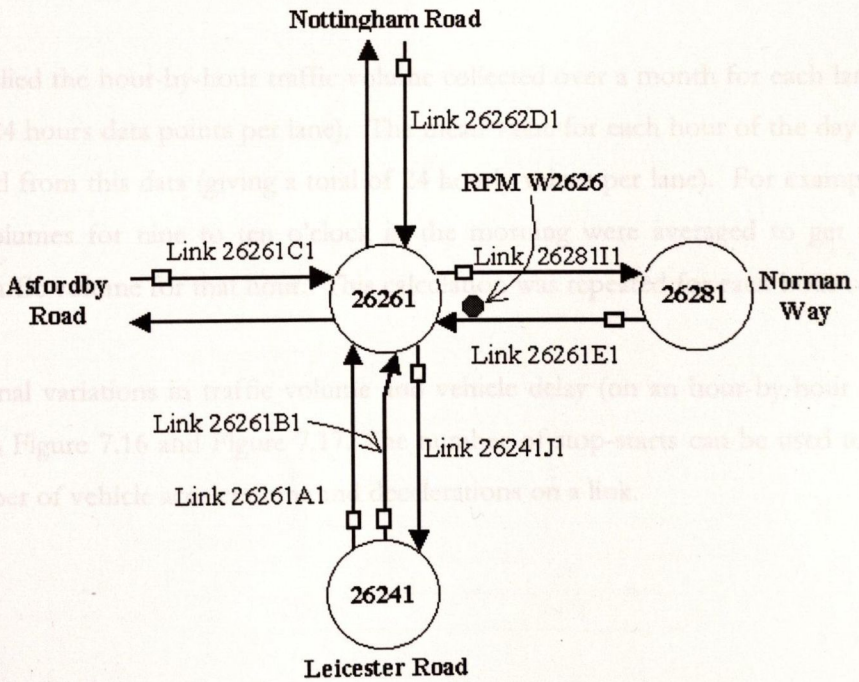


Figure 7.15: Schematic representation of intersection at Melton Mowbray

7.4.2 SCOOT URBAN TRAFFIC CONTROL SYSTEM

The traffic traversing the junction is controlled by the SCOOT urban traffic control system. The SCOOT employs inductive loop vehicle detectors located on the approaches to the junction [Day, 1998]. This data is processed by a central computer, which may decide to alter the green split, cycle time or offset at any controlled signalised junction. The green split is the percentage of cycle time that a traffic signal is green, while the cycle time is the total time period taken to complete a green, amber and red light sequence. The offset is the difference between the commencement of a cycle at one intersection and the commencement of a cycle at the next intersection upstream.

Signal splits change incrementally based on current demand obtained from the traffic detectors every four seconds, while offsets and cycle times are adjusted gradually every few minutes. The response to incidents depends on the adaptive logic of the SCOOT system. Further information is given elsewhere, for example, Bell et al. [1996b].

7.4.3 TRAFFIC ACTIVITY AND FLEET COMPOSITION

The SCOOT urban traffic control system measures traffic volume. In addition, its internal model makes frequent estimates of other traffic variables such as vehicular delay and number of stop-starts per vehicle.

ITS supplied the hour-by-hour traffic volume collected over a month for each lane (i.e. 31 days by 24 hours data points per lane). The mean value for each hour of the day was then computed from this data (giving a total of 24 hourly values per lane). For example, all the traffic volumes for nine to ten o'clock in the morning were averaged to get the mean hourly traffic volume for that hour. This calculation was repeated for each hour of the day.

The diurnal variations in traffic volume and vehicle delay (on an hour-by-hour basis) are shown in Figure 7.16 and Figure 7.17. The number of stop-starts can be used to estimate the number of vehicle accelerations and decelerations on a link.

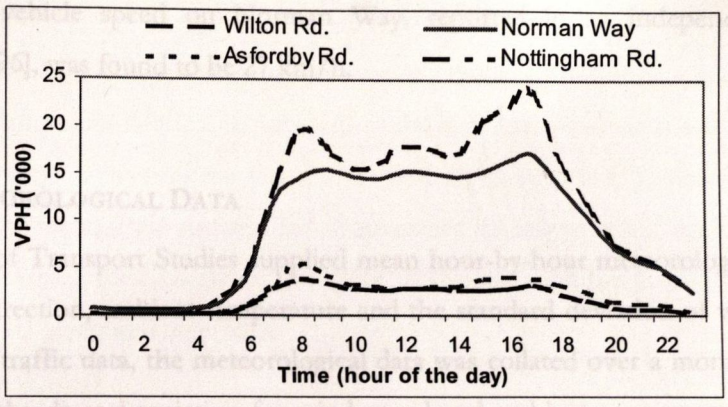


Figure 7.16: Diurnal variation (hour-by-hour) of traffic volume traversing junction in Melton Mowbray

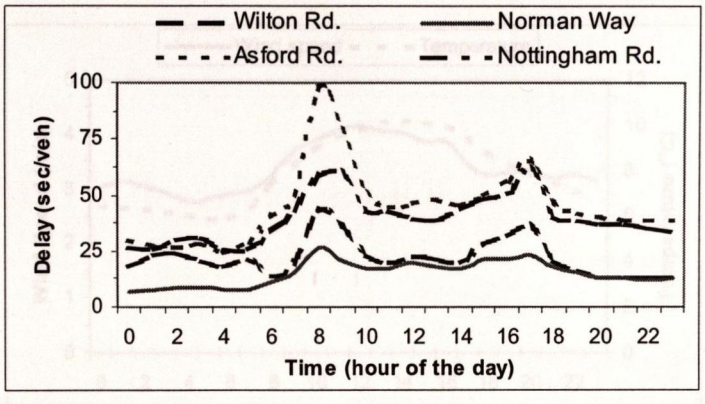


Figure 7.17: Diurnal variation (hour-by-hour) of vehicle delay at study junction in Melton Mowbray

The vehicle category distribution for all lanes and all hours of the day is assumed constant and is presented in Table 7.20. ITS supplied this data also.

Table 7.20: Vehicle category distribution for traffic traversing study junction in Melton Mowbray

Vehicle Category	Distribution
Petrol cars	74%
Diesel cars	6%
Petrol LGVs	2%
Diesel LGVs	9%
Buses	1%
HGVs	8%
TOTAL	100%

The average vehicle speed on Norman Way, reported in an independent study by Goodman [1996], was found to be 27 km/h.

7.4.4 METEOROLOGICAL DATA

The Institute of Transport Studies supplied mean hour-by-hour meteorological data (wind speed, wind direction, ambient temperature and the standard deviation of wind direction). Similar to the traffic data, the meteorological data was collated over a month also. Figure 7.18 presents the diurnal variation for wind speed and ambient temperature, while Figure 7.19 presents the diurnal variation for wind direction and the standard deviation of wind direction. For wind direction, zero degree is north.

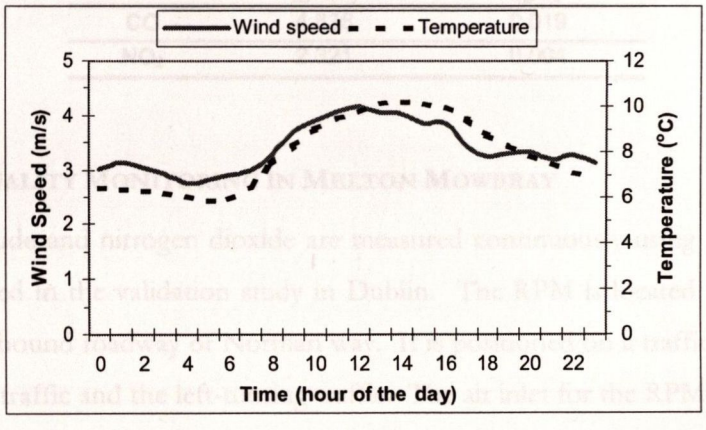


Figure 7.18: Diurnal variation (hour-by-hour) of wind speed and temperature in Melton Mowbray

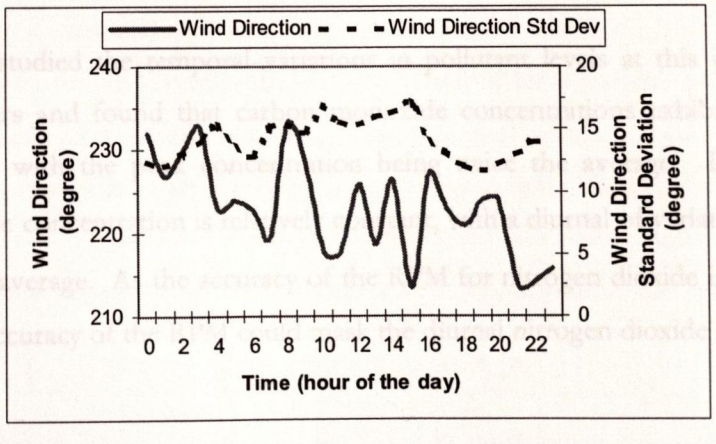


Figure 7.19: Diurnal variation (hour-by-hour) of wind direction and wind direction standard deviation in Melton Mowbray

7.4.5 Source Strength at Intersection in Melton Mowbury

The emissions source strength for traffic traversing the study junction at Melton Mowbray were computed by the MVEIM. Composite emission factors can be formulated, since the traffic composition traversing the junction in Melton Mowbray is assumed homogenous and constant throughout the day and for all roadways leading to/from the junction. These composite emission factors given in Table 7.21 are calculated based on the fleet composition data given in Table 7.20.

Table 7.21: Composite emission factors for traffic traversing study junction in Melton Mowbray as computed by MVEIM

Pollutant	Cruise CEF (g/km)	Queue CEF (g/s)
CO	4.836	0.019
NO_2	2.321	0.004

7.4.6 Air Quality Monitoring in Melton Mowbray

Carbon monoxide and nitrogen dioxide are measured continuously using an RPM similar to that employed in the validation study in Dublin. The RPM is located by the stop-line facing the westbound roadway of Norman way. It is positioned on a traffic island between the straight-on traffic and the left-turning traffic. The air inlet for the RPM faces the traffic travelling straight-ahead towards the junction [Boddy, 1999]. A data cleaning procedure developed by Bell and Boddy [1998] was employed to remove faulty data and negative readings.

Boddy [1999] studied the temporal variations in pollutant levels at this junction over a number of years and found that carbon monoxide concentrations exhibit morning and evening peaks, with the peak concentration being twice the average. In contrast, the nitrogen dioxide concentration is relatively constant, with a diurnal of variation of only ±10 ppb about the average. As the accuracy of the RPM for nitrogen dioxide is only ±10 ppb, the relative inaccuracy of the RPM could mask the diurnal nitrogen dioxide variation.

7.4.7 Comparison of Predicted and Observed Concentrations

CALINE4R was used to predict the mean hour-by-hour diurnal pollutant concentrations using mean traffic and meteorological data recorded over a month. These are compared to average hour-by-hour observed pollutant concentrations measured over the same month.

The inputs to CALINE4R include traffic volume (given in Figure 7.16), vehicle delay (given in Figure 7.17), and the composite emissions factors (given in Table 7.21) for each hour of the day. CALINE4R was 'run' a total of twenty-four times for each pollutant to generate the diurnal hour-by-hour predicted concentrations for that pollutant.

7.4.7.1 Performance Analysis

The statistical parameters employed to compare the predicted and observed data at the validation site in Dublin are used here as well. These performance statistics are summarised in Table 7.22.

Table 7.22: Statistical analysis of measured and predicted ambient pollutant kerbside concentrations in Melton Mowbray

Statistic	CO	NO_2
$\overline{C}_o$	1.16	60.45
σ_o	0.69	6.02
$\overline{C}_p$	1.20	49.24
σ_p	0.83	19.83
Bias	-0.03	11.21
NMSE	0.04	0.06
R	0.92	0.84
FB	-0.03	0.20
P-2	100%	79%

The model meets Kumar's [2000] performance criteria for both pollutants. In particular, the model performs exceptionally well for carbon monoxide. For example, all predicted values lie within a factor-of-two of the measured values, and both the bias and FB are nearly zero. The nitrogen dioxide data shows a relatively large positive bias (11.21) which means that the model is under-predicting. However, the NMSE is relatively small (0.06). Boddy [1999] noted that there appears to be no relationship between average nitrogen dioxide concentration levels and average total vehicular flow levels, and concluded that a factor or factors other than traffic appear to be affecting the nitrogen dioxide concentration levels.

Jalihal [2000] also found a weak correlation between nitrogen dioxide and traffic flows at the junction, and suggested that this was probably due to the chemical reactivity of the nitrogen dioxide.

7.4.7.2 Regression Analysis

A linear regression analysis carried out between the observed and predicted data sets is depicted in Figure 7.20 and Figure 7.21. In addition, dashed lines show the envelope for the percentage of predicted pollutant concentrations within a factor of two of the observed values.

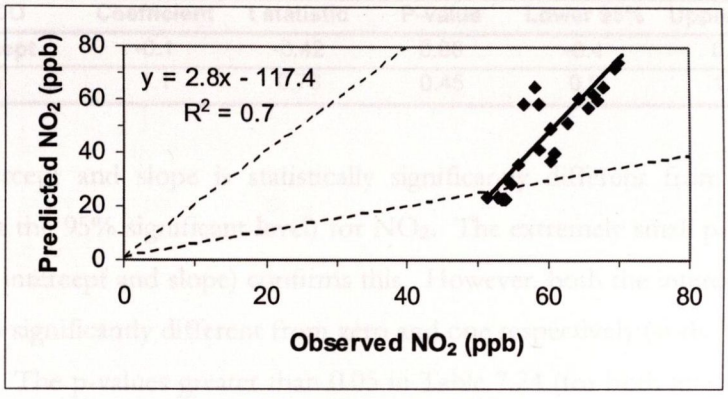


Figure 7.20: Diurnal hour-by-hour predicted versus hour-by-hour measured nitrogen dioxide concentrations in Melton Mowbray

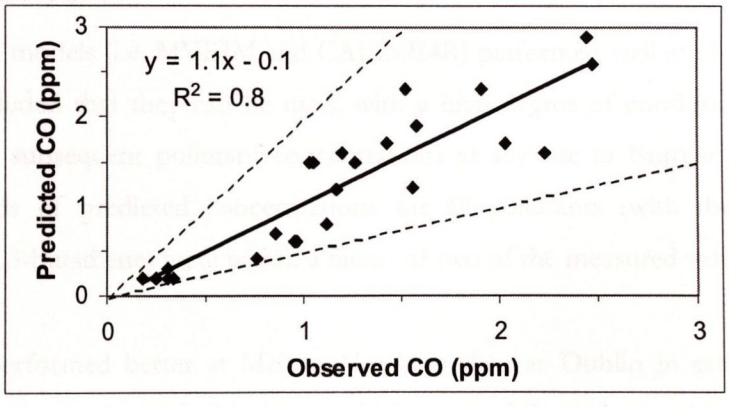


Figure 7.21: Diurnal hour-by-hour predicted versus hour-by-hour observed carbon monoxide concentrations in Melton Mowbray

A similar regression analysis to that carried out on the Dublin pollution data is performed on the Melton Mowbray pollution data. Table 7.23 and Table 7.24 present the regression details for both pollutants. Again, the observed pollutant concentration is the independent variable, while the predicted pollutant concentration is the dependent variable.

Table 7.23: Regression details for nitrogen dioxide data in Melton Mowbray

NO_2	Coefficient	t statistic	P-value	Lower 95%	Upper 95%
Intercept	-117.4	-5.02	0.00	-165.9	-68.8
Slope	2.8	4.56	0.00	2.0	3.6

Table 7.24: Regression details for carbon monoxide data in Melton Mowbray

CO	Coefficient	t statistic	P-value	Lower 95%	Upper 95%
Intercept	-0.1	-0.42	0.68	-0.4	0.2
Slope	1.1	0.76	0.45	0.9	1.3

Both the intercept and slope is statistically significantly different from zero and one respectively (at the 95% significant level) for NO_2. The extremely small p-values in Table 7.23 (for both intercept and slope) confirms this. However, both the intercept and slope is not statistically significantly different from zero and one respectively (at the 95% significant level) for CO. The p-values greater than 0.05 in Table 7.24 (for both intercept and slope) confirms this.

7.5 DISCUSSION

The combined models (i.e. MVEIM and CALINE4R) performed well at all three test sites, and it is concluded that they can be used, with a high degree of confidence, to estimate emissions and subsequent pollutant concentrations at any site in Europe. For example, over two-thirds of predicted concentrations for all pollutants (with the exception of benzene and 1,3-butadiene) were within a factor of two of the measured values.

The AQMS performed better at Melton Mowbray than at Dublin in estimating carbon monoxide. For example, both the slope and intercept of the carbon monoxide regression line were not statistically significantly different from one and zero respectively in Melton Mowbray (see Table 7.13), while in Dublin the intercept of the carbon monoxide regression line was statistically significantly different from zero (see Table 7.24). The slope of the carbon monoxide regression line in Dublin was not statistically significantly different from one. This AQMS performance difference may be due, in part, to the fact that traffic activity data was measured over over month at Melton Mowbray as compared to over one week in Dublin. In addition, traffic congestion was recorded through the day by SCOOT in Melton Mowbray, while it was estimated in Dublin from video-recordings for peak and inter-peak hours only. Each hour of the day was then categorised as peak (8 am to 9 am

and 5 to 6pm), inter-peak (7 am to 8 am, 9 am to 5 pm, and 6 am to 8 pm) or free-flow (8 pm to 7 am).

7.6 SUMMARY

The Chapter has described the application of the combined MVEIM and CALINE4R models to three test sites. The first was located in a city centre at a heavy trafficked signalised controlled junction (Dublin). The second site was located midway along a street canyon (Hannover, Germany). The third was located on an arterial suburban route at a traffic intersection (Melton Mowbray, UK). Traffic activity data and pollutant concentrations were measured at all three sites. In addition, local meteorology was supplied or measured.

The next Chapter will describe the use of the MVEIM to compile an emission and fuel consumption inventory for the greater Dublin area. The inventory is compiled for a base year (1991), a present year (1996) and two future years (2006 and 2016). The following Chapter (i.e. Chapter nine) employs both the MVEIM and CALINE4R to determine ambient concentration at a number of potential pollutant hot-spot locations in Dublin. The model was not validated at these locations.

8. EMISSIONS INVENTORY FOR ENTIRE DUBLIN AREA

8.1 INTRODUCTION

An objective of this project is to develop an emissions and fuel consumption inventory for the entire Dublin area. Traffic emission inventories can be compiled using two different methods, namely top-down and bottom-up. In general, the top-down approach is calculated on an annual basis for an entire area, while the bottom-up approach is calculated for each section of roadway on an hourly basis and aggregated to an annual average. This Chapter describes the compilation of an emissions inventory using both approaches. The MVEIM is employed to compile the bottom-up emissions inventory using traffic data from SATURN & SATCHMO, while COPERT III [Ntziachristos et al., 1999] is employed to compile the top-down emissions inventory using vehicle licensing records and AAKT. The two methods are then compared. As the emissions inventory is heavily dependent on statistical data, potential sources are given. Comparing the corresponding fuel consumption inventory against retail fuel sales data indirectly validates the emissions inventory. A further objective of this research was to investigate the potential of alternative fuels to reduce overall emissions of certain pollutants. Consequently, a number of scenarios involving alternative fuels are simulated using the MVEIM.

The Chapter begins with a historical review of emission inventories compiled previously for Dublin. The shortfalls in these preceding emission inventories are identified.

8.2 REVIEW OF EMISSIONS INVENTORIES FOR DUBLIN

The first urban emissions inventory compiled in Ireland was for Dublin in 1978 [Bailey and Walsh, 1980a]. This divided sources into four primary categories, namely industrial, commercial, domestic and power-generation. Mobile sources were not considered. Emissions were computed for sulphur dioxide and black smoke on a 1 x 1 km grid over the study area. The inventory identified the importance of domestic sources in contributing to the overall smoke levels in the city.

The 1978 emissions inventory was updated for the year 1981 [Bailey, 1983]. Mobile sources were included and nitrogen oxide was computed in addition to sulphur dioxide and black smoke. Emission estimates for traffic were computed from national fleet and fuel statistics. It was estimated that road traffic emitted 1,800 and 2,200 tonnes-per-annum of sulphur dioxide and black smoke respectively.

Emissions inventories for 1989 and 1991 were prepared as part of the initial Air Quality Management System for the Dublin region [EOLAS, 1992]. Mobile sources, were included but emission estimates were once again based on national vehicle, energy and fuel sales statistics. The study area was divided into sixty heterogeneous squares. The diurnal variation in emissions was included in the inventory to reflect the change in emissions throughout the day.

An emission inventory for TSP was compiled in 1993 for the greater Dublin area [DGE, 1993]. The inventory was employed in a dispersion model. Emission factors utilised in previous emission inventories, in addition to those from the CORINAIR working group [Eggleston et al, 1989], were used in the compilation.

An emissions inventory for nitrogen dioxide, volatile organic compounds, carbon monoxide and particle matter was compiled for 1996 as part of the Dublin Air Quality Management Plan [ENVIROCON, 1997]. The inventory included traffic on all arterial roads in the conurbation and the majority of city streets. Vehicles were classified into two types (LDV and HDV). The emission factors were based on average speeds for different zones in the city. For example, a typical driving speed of 25 km/hr was assumed for the inner city, 40 and 60 km/hr for the suburbs and 100 km/hr for the motorway routes. The emission factors used were derived from the UK Department of Transport. Even though this emissions inventory was the most comprehensive so far, it suffered from a number of major limitations. No allowance was made for evaporative emissions or cold-starts, when emissions are much greater than after the engine/catalyst has warmed up. No account was taken of vehicle queuing at junctions. Vehicles were classified into two categories only and the age of the fleet was not taken into account explicitly. The emissions inventory was compiled on a gridded basis and therefore is of no use in calculating roadside concentration levels or investigating potential 'hot-spots'.

An energy balance was compiled by CODEMA [1999]. The primary objective of the study was to estimate the total annual energy consumption for Dublin and consequently estimate

the total carbon dioxide emissions for 1996. The study categorised carbon dioxide emissions into three types, namely, transport, commercial and residential. Unfortunately, the study did not give a spatial breakdown of carbon dioxide emissions. In addition, it covered Dublin city centre (between the canals) only and not the suburbs.

8.3 DATA REQUIRED FOR EMISSIONS INVENTORY

As already stated, the fundamental methodology for compiling a mobile source emissions inventory is relatively straightforward. It is the product of an emissions rate and a travel activity factor that is representative of the level of emission-producing activity [Meyer, 1997], [Holman, 1999]. However, in reality emission inventory compilation is a very complex process [Meyer, 1997], [Guensler, 1993], and the general methodology used in the compilation of an emissions inventory for the entire Dublin area can be divided into five steps:

1. Quantify emission producing vehicle activities through a traffic model or other means of estimation;
2. Collate data on vehicle, fuel, operating and environmental parameters;
3. Develop vehicle activity-specific emission rates for the relevant vehicle, fuel, operating and environmental conditions;
4. Multiply activity estimates by corresponding activity-specific emission rates; and
5. Sum the estimated emissions emanating from all activities.

The derivation of the required emissions factors has been described in Chapter four. The method for estimating travel activity is described in Chapter three. In the following sections, the compilation of the emissions inventory is described. First, the actual travel activity factors employed are described.

8.3.1 TRAFFIC MODULE OUTPUTS

A summary of the parameters generated by the traffic module is given in Table 8.1 for the years 1991, 1996, 2006 do minimum (do-min), 2006 do strategy (do-str), 2016 do minimum, and 2016 do strategy. The values for VKT and VHT are calculated as annual average hourly values. The VHT within a traffic network is a useful indicator of overall system performance, reflecting traffic delay on a broader scale, as opposed to junction

delay, which measures delay on a single junction or specific approach. The link delay, turn delay, link speed, link queue and free-flow time are average values for all links.

The data in Table 8.1 shows that VKT is increasing at a significant rate. For example, it increases by over 60% (from 225,478 to 366,937) in 25 years (1991 to 2016 do-str). It is worth noting that in the 2006 do-strategy scenario, the VKT is higher than in the 2006 do-minimum scenario. A partial explanation for this is that in the 2006 do-strategy scenario, more drivers are using new infrastructure (e.g. the M50) and consequently are taking longer routes but experiencing less delay on these routes. This analysis is substantiated by the fact that the VHT for 2006 do-minimum scenario is much greater (approximately one-quarter) than for the 2006 do-strategy scenario. By increasing the number of vehicle trips and VHT, new infrastructure may cause increased emissions. Such increases could to some extent counterbalance the emission benefits obtained from improved vehicle technology, enhanced traffic operations and a more effective traffic system [Ostria and Lawrence, 1994].

Table 8.1: Summary of traffic activity data from SATURN & SATCHMO

Parameter	1991	1996	2006 do-min	2006 do-str	2016 do-min	2016 do-str
VKT (per hr)	225,478	271,671	312,023	336,815	434,349	366,937
VHT (per hr)	15,663	20,473	26,575	20,417	26,460	25,411
Ratio VKT to VHT (km/hr)	14.4	13.3	11.7	16.5	16.4	14.4
Mean link delay (sec.)	36.3	42.6	54.1	45.1	35.9	55.2
Mean turn delay (sec.)	34.4	42	53.9	44.6	40.6	54.6
Mean link speed (km/hr)	33.7	33	32.9	35.5	32.3	34.9
Mean vehicle queue (pcu)	4	5	6	5	6	6
Mean free-flow time (sec.)	52.2	53.7	53.9	51.8	53.3	52.6
Total links (#)	3,264	3,264	3,328	3,531	3,328	3,531
Total lanes (#)	6,262	6,262	6,366	6,819	6,366	6,819
Free-flow driving (%)	14.8%	14.2%	13.8%	11.8%	13.8%	11.2%
Congested driving (%)	3.9%	4.6%	4.2%	3.5%	6.7%	4.9%
Free-flow Links (%)	46.2%	40.6%	39.7%	42.7%	24.8%	40.9%
Congested Links (%)	7.0%	10.5%	13.4%	10.4%	18.9%	12.8%

The ratio of VKT to VHT is a quasi-indication of roadway efficiency (i.e. it is analogous to the average vehicle speed for the entire Dublin area). The higher the VKT to VHT ratio, the further a driver travels in a specified amount of time. For example, the VKT to VHT ratio is 11.7 km/hr in the 2006 do-minimum scenario, and 16.5 km/hr in the 2006 do-strategy scenario. This indicates that the road network is used much more inefficiently in the 2016 do-minimum scenario when compared to the 2006 do-strategy scenario because the VKT to VHT ratio is 4.8 km/hr less. The analysis is supported by the observation that

the average link delay in the 2006 do-minimum scenario (54.1s) is much greater than that in the 2006 do-strategy scenario (45.1s). The average turn delay shows a similar trend. Increases in delay suggest increased local congestion, and emphasise the need to include vehicle-operating mode in any emission inventory calculation, if the environmental benefits of transport network improvements are to be quantified.

The average vehicle queue remains relatively constant as does the average link free flow time. SATURN & SATCHMO estimates that the average link speed in the 1996 scenario is 33 km/hr. An independent European study [Kyriakis et al., 1998] estimated the average urban speed for passenger cars in Ireland in 1995 to be 30 km/hr. The same study [Kyriakis et al., 1998] estimated that all other vehicles (excluding motorcycles) have an average urban speed of 20 km/hr.

The one-hour volume-to-capacity (per link) ratio reflects local traffic conditions. One set of ranges that define free-flow and congestion links are 0.0-to-0.1 and 0.975-to-1.0 respectively [Cottrell, 1992]. On this basis, SATURN & SATCHMO results show that nearly one fifth of links in the Dublin network are congested in 2016 do-minimum scenario. Consequently only one-quarter of the links are free flowing, compared to all the other scenarios where the percentage is close to or more than 40%.

A study of European driving conditions for emission modelling purposes [André, 1997] defines congested driving as vehicles travelling with average speeds between 10 and 16 km/hr, and free flowing urban driving as vehicles travelling at average speeds between 26 km/hr and 32 km/hr. For comparison purposes, these statistics are calculated for the case scenarios given above. Congested driving conditions were found to account for between 3.5 and 4.9% of the total VKT, while free flow driving ranges from 11.2 to 14.8%. It is acknowledged that traffic statistics computed for the entire Dublin area will vary enormously from area to area (for example, congestion is far greater in the city centre as compared to the suburbs). However, they can prove very useful when comparing different cities. For example, André [1997] found that 5.9% of the total urban mileage travelled in the European Union occurs in congested conditions, while only 5.1% occurs in free flow conditions. This suggests that there is slightly less congestion and considerably more free flowing traffic in the greater Dublin area than in the average European city. It is also worth noting that the do-strategy options for both 2006 and 2016 show significant improvements over the do-minimum scenarios.

The changes in the variables described in Table 8.1 indicate that evaluating road network usage efficiency in terms of pollutant emissions is a complex issue. It is not adequate to compute one or even two variables for the purposes of road network usage efficiency, as traditionally has been the case. In addition, the approach of globally analysing a complete network does not account for the spatial distribution of traffic parameters. A study in the USA [Cottrell, 1992] found that even when the total VKT change in a sizeable metropolitan area is insignificant, local variations of average vehicular velocity can result in much more significant changes in a wide range of VKT related impacts, including air quality and fuel consumption.

Another parameter employed to assess road network efficiency is LOS. This is defined by the TRB [1995] as "... a measure of driver discomfort, frustration, fuel consumption, and lost travel time. Specifically, level-of-service criteria are stated in terms of average stopped delay...". LOS may be defined as the average vehicle delay. TRB characterises six levels of service (i.e. A through F).

Table 8.2: Level-of-service in the entire Dublin road network

Level of Service Category	1991	1996	2006 do-min	2006 do-str	2016 do-min	2016 do-str
A (*< 5 sec.*)	49.2%	47.2%	46.0%	43.9%	42.3%	42.7%
B (*5.1 to 15 sec.*)	20.5%	20.8%	20.8%	23.7%	20.5%	23.5%
C (*15.1 to 25 sec.*)	14.2%	13.8%	13.4%	14.5%	12.5%	14.0%
D (*25.1 to 40 sec.*)	9.4%	9.1%	9.0%	9.2%	10.2%	9.2%
E (*40.1 to 60 sec.*)	1.7%	1.8%	1.9%	1.9%	2.6%	1.9%
F (*> 60 sec.*)	5.0%	7.3%	8.8%	6.8%	11.8%	8.7%

The LOS for each junction in the network was determined from the SATURN & SATCHMO results. Table 8.2 shows the percentage of vehicles in each category. In all scenarios, nearly two-thirds of junctions experience a LOS of either A or B with the most populated category being LOS A. An interesting point is that the percentages in categories B to E all remain relatively constant. However, a worrying factor is that the percentage of vehicles in category F increases from 1991 to 2006, regardless of the traffic strategies, while the percentage in category A declines. This means that overall congestion is increasing all the time. The LOS represents an important parameter for emission inventory calculations, because as the LOS decreases, volume-to-capacity ratios increase, the progression of vehicles through the junction decreases, longer vehicle queues occur, and idle emissions increase [Cottrell, 1992]. The US-EPA employs intersection LOS as one of its primary criteria for identifying potential carbon monoxide hot-spots [Meng and Niemeier, 1998].

Intersections operating at LOS A, B, or C are automatically eliminated as potential carbon monoxide hotspots, whereas intersections operating at LOS D or worse must undergo detailed carbon monoxide concentration analysis. On this basis, the proportion of junctions, which can be considered potential hotspots, would rise from 18.2% in 1996 to 24.0% in 2016, if the do-minimum approach were followed, but to only 19.8% if the do-strategy were completed. However, intersections can often operate at the same LOS but produce different levels of estimated carbon monoxide concentrations. For example, a five-lane approach operating at LOS D will produce substantially higher carbon monoxide emissions than a two-lane approach also operating at LOS D [Meng and Niemeier, 2000]. This is due to the fact that LOS does not take into account explicitly the total number of vehicles travelling on a roadway, only the average vehicle delay. For example, fifty vehicles delayed for thirty seconds will produce much more emissions than ten vehicles (also delayed for thirty seconds). Therefore, LOS alone is not sufficient to determine if an intersection is a potential hotspot.

8.3.2 VEHICLE CLASSIFICATION

As pollutant emissions are vehicle dependent, a detailed vehicle classification is required for accurate emissions predictions. One such classification system is suggested by the MEET project [Hassel and Weber, 1997b]. This categorises vehicles by transport mode, engine size or the vehicle weight, engine technologies, emission standards and fuels used. The total number of vehicles and relative percentages in each sub-category (as defined in the EECT module of the MVEIM) is shown in Table 8.3. The fleet age profile for vehicles in the greater Dublin area is given in Figure 8.1. This information was obtained from the licensing records of the Department of the Environment [DOE, 1999].

When examining link-by-link emissions, if active vehicle fleet information is collected by the SCATS urban traffic control system, this data can be input directly into the EECT module. Alternatively, passive information collated during manual counts/surveys may also be input into the EECT module. However, currently available CCTV technology can only distinguish between four or five categories of vehicles and cannot identify a number of other parameters such as size of engine and type of fuel. Therefore, a detailed classification must be defined from the Dublin average vehicle fleet.

Table 8.3: Total number of vehicles and relative percentages for the greater Dublin area in 1998 [source: DOE, 1999]

Total 392,559 100%								
Cars 343,775 87.57%								
Petrol 320,707 93.29%			**Diesel** 22,823 6.64%			**LPG** 245 0.07%		
<1.4l 209,913 65.45%	**1.4-2.0l** 100,736 31.41%	**>2.0l** 10,058 3.14%	**<1.4l** 771 3.38%	**1.4-2.0l** 18,637 81.66%	**>2.0l** 3,415 14.96%	**<1.4l** 107 43.67%	**1.4-2.0l** 97 39.59%	**>2.0l** 41 16.73%
LGVs 31,173 7.94%								
Petrol 1,302 4.18%			**Diesel** 29,850 95.76%			**LPG** 21 0.07%		
HGVs 6,313 1.61%								
Petrol 59 0.93%			**Diesel** 6,251 99.02%			**LPG** 3 0.05%		
3.5-7.5t 29 49.15%	**7.5-16t** 29 49.15%	**>16t** 1 1.69%	**3.5-7.5t** 2,788 44.60%	**7.5-16t** 3,357 53.70%	**>16t** 106 1.70%	**3.5-7.5t** 2 66.67%	**7.5-16t** 1 33.33%	**>16t** 0 0.00%
Buses 2253 0.57%								
<16s 291 12.92%			**16-35s** 371 16.47%			**>35s** 1591 70.62%		
MC 8976 2.29%								
<50cc 2717 30.27%		**50-250cc** 3631 40.45%			**250-750c** 1953 21.76%		**>750cc** 675 7.52%	
Mopeds 69 0.02%								

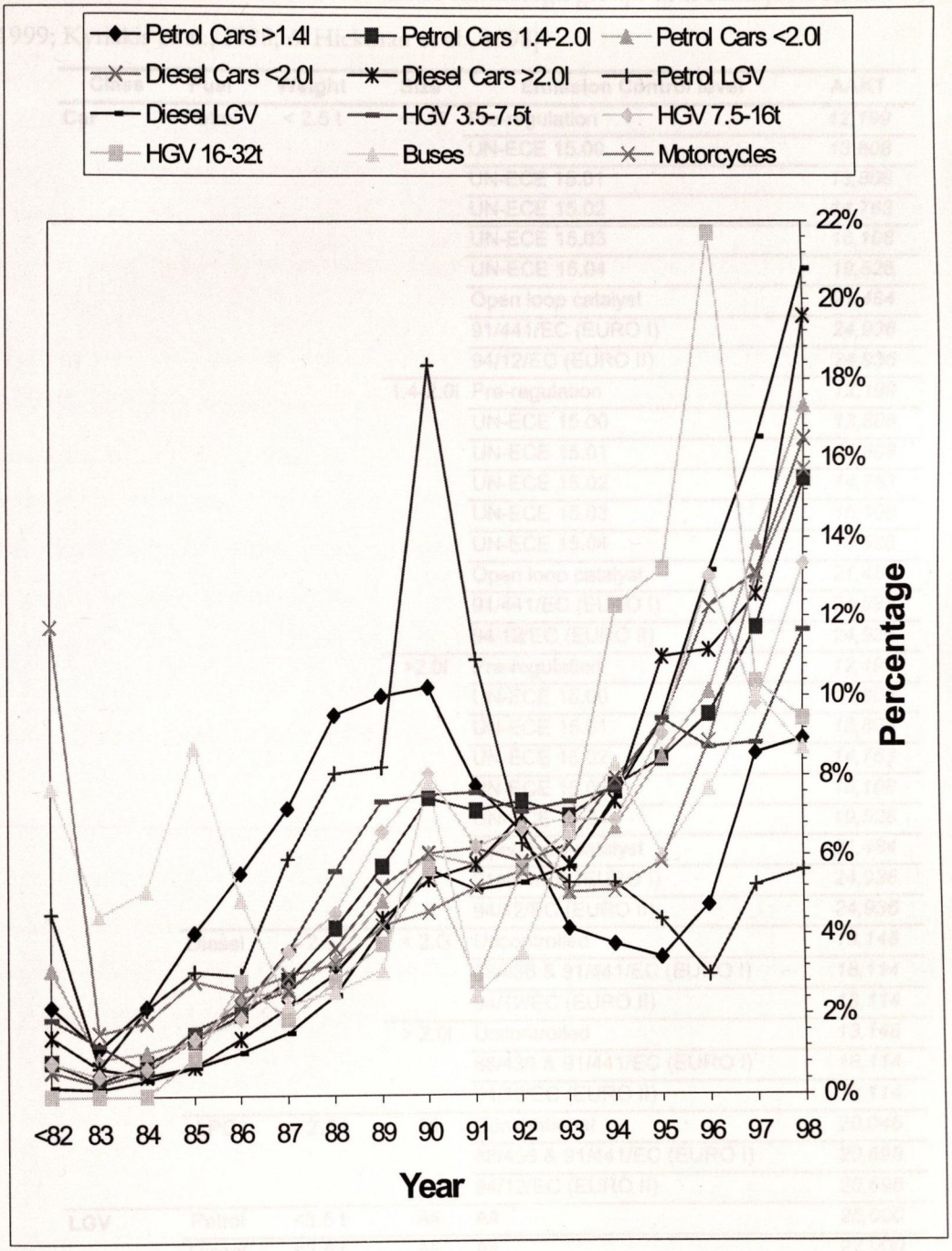


Figure 8.1: Age profile of vehicular fleet in the greater Dublin Area in 1998 [source: DOE, 1999]

Table 8.4: AAKT for various vehicle technologh groups in Dublin [source: DOE, 1999; Kyriakis et al., 1998; & Hickman et al., 1998]

Class	Fuel	Weight	Size	Emission Control level	AAKT
Car	Petrol	< 2.5 t	<1.4l	Pre-regulation	*12,199*
				UN-ECE 15.00	*13,808*
				UN-ECE 15.01	*13,808*
				UN-ECE 15.02	*14,763*
				UN-ECE 15.03	*16,108*
				UN-ECE 15.04	*19,528*
				Open loop catalyst	*21,484*
				91/441/EC (EURO I)	*24,936*
				94/12/EC (EURO II)	*24,936*
			1.4-2.0l	Pre-regulation	*12,199*
				UN-ECE 15.00	*13,808*
				UN-ECE 15.01	*13,808*
				UN-ECE 15.02	*14,763*
				UN-ECE 15.03	*16,108*
				UN-ECE 15.04	*19,528*
				Open loop catalyst	*21,484*
				91/441/EC (EURO I)	*24,936*
				94/12/EC (EURO II)	*24,936*
			>2.0l	Pre-regulation	*12,199*
				UN-ECE 15.00	*13,808*
				UN-ECE 15.01	*13,808*
				UN-ECE 15.02	*14,763*
				UN-ECE 15.03	*16,108*
				UN-ECE 15.04	*19,528*
				Open loop catalyst	*21,484*
				91/441/EC (EURO I)	*24,936*
				94/12/EC (EURO II)	*24,936*
	Diesel	< 2.5 t	< 2.0l	Uncontrolled	*13,148*
				88/436 & 91/441/EC (EURO I)	*18,114*
				94/12/EC (EURO II)	*18,114*
			> 2.0l	Uncontrolled	*13,148*
				88/436 & 91/441/EC (EURO I)	*18,114*
				94/12/EC (EURO II)	*18,114*
	LPG	< 2.5 t	All	Conventional	*20,046*
				88/436 & 91/441/EC (EURO I)	*20,698*
				94/12/EC (EURO II)	*20,698*
LGV	Petrol	<3.5 t	All	All	*25,000*
	Diesel	<3.5 t	All	All	*27,000*
HGV	Diesel	3.5 - 7.5 t	All	All	*30,000*
		7.5 - 16 t	All	All	*30,000*
		16 - 32 t	All	All	*40,000*
Bus	Diesel	Buses	All	All	*48,136*
		Coaches	All	All	*48,136*
TW	Petrol	Mopeds	All	All	*15,000*
		Motorcycles	All	All	*15,000*

This approach was employed in Chapter seven, when the model was validated at specific sites. However, it is not feasible (either practically or economically) to measure traffic at every junction, and traffic fleet information must be obtained from the traffic module. It is difficult to calculate emissions from traffic model data alone, because the SATURN & SATCHMO only classifies the vehicle fleet into three broad categories (LDV, HGV and bus). A further breakdown of the fleet is defined based on statistical data for the greater Dublin area. The statistical data includes engine technology and capacity, type of fuel used (petrol, diesel or LPG), gross vehicle weight, and the age profile of the fleet.

Various sub-categories of vehicles have different AAKT. It has been found that average mileage is highly dependent on vehicle age [Bourdeau, 1998] [Kyriakis et al., 1998]. For example, the annual mileage for ten-year old vehicles is about half the mileage of a new vehicle [Henriksson, 1994]. This decrease in AAKT with increasing vehicle age is incorporated in the model, as suggested by Holman [1999], by employing vehicle AAKT as a weighting factor in determining fleet composition. Unfortunately, information on AAKT is difficult to obtain and must be partially estimated. The source data for determining AAKT could be improved by collecting data at vehicle inspections introduced in January 2000. This method has been utilised successfully in Sweden [Henriksson, 1994].

The AAKT for each vehicle sub-category is given in Table 8.4. For LPG cars, the European average AAKT is employed, as Irish data is insufficient. Other data sources for AAKT information include the World Road Statistics [IRF, 1994], which give an average annual mileage of 35,909 for buses in Ireland in 1992, which is equivalent to an AAKT of 57,454. This is higher than the value (48,136 km) given in Table 8.4 for buses in 1995.

8.4 EMISSIONS DATA EMPLOYED

As described in Chapter four, MEET emission factors are used in the emission inventory calculations because they are the only source that provides comprehensive data for each vehicle sub-category, at various speeds, and which are applicable to Ireland. In addition, the emission factors can be used to determine emissions during queuing, as described in Chapter three. Unfortunately, reliable emission factors for acceleration and deceleration are not currently available. However, it has been shown that emission estimation based on the use of simple procedures employing traffic flow characteristics such as travel time on a link, delay and stops is often sufficient [Chaudhary, 1995], because emissions due to accelerations and decelerations are intrinsically included in average speed emission factors.

The emission factors employed consist of three types, namely, hot stabilised, start-up and evaporative [Baldasano, 1998]. These have been described in detail in Chapter three. In the following sections, the driving statistics (e.g. trip length) and other data (e.g. ambient temperature) required by the MVERA module are detailed. Some of the information required was not directly available for the greater Dublin area and had to be sourced elsewhere (e.g. European or UK average values).

8.4.1 Hot Stabilised Emissions

Hot stabilised vehicle emissions are affected by a number of parameters including vehicle category and technology, mean speed or driving patterns, road gradient, vehicle load, and emission deterioration factors, etc. These hot stabilised emissions are further divided into average speed and creep emissions.

As emissions are measured for different vehicle categories and technologies, but the traffic module only classifies vehicles into three categories, a vehicle type mapping is required. This mapping translates the traffic data into a form suitable for use with the MEET emission factors. The EECT module of the MVEIM carries this out task.

To make full use of the MEET data, information on average vehicle speed is required from the traffic module. This module also provides the information on link/turn delay and the number of vehicles being delayed so that emissions due to vehicle creep can be calculated. The product of average vehicle delay (either turn or link) and the number of vehicles on a given link gives the total creep for that link.

Roadway gradient also affects emissions. Ideally, the gradient information should be available for all segments of a link. In the absence of such information, the Workbook on Emission Factors for Road Transport Explanatory Notes [FEA, 1995] suggests using either average gradient over a road link or homogeneous sections of a road link, or a network. For this purpose, the average link gradients were obtained from a GIS of the greater Dublin area.

Vehicle loading also affects fuel consumption and pollutant emissions [André et al, 1998]. In the UK [HMSO, 1996], loading factors (the ratio of the actual load to the potential capacity) vary between 0.4 and 0.5, and the proportion of empty mileage for all goods

vehicles is approximately 29%. In France [OEST, 1992], goods vehicles are loaded 75% of the time. Empty mileage for urban buses in France is of the order of 8% of the total mileage [OEST, 1992]. In Sweden [André et al., 1998], load factors are quite low ranging from 0.26 to 0.46 (depending on the goods vehicle category). Unfortunately, data on vehicle loading for Dublin could not be obtained. Therefore, following the recommendation of the German/Swiss handbook [SAEFL, 1995], where a partly loaded category is proposed, a goods vehicle loading of 50% is assumed.

8.4.2 START-UP EMISSIONS

Start-up over-emissions are a function of vehicle technology and type, mean speed (during the thermal transient operation), trip length, ambient temperature, and engine temperature at the start of a trip [Sérié and Joumard, 1997], [Hammarström and Edwards, 1997]. To allow these to be determined, the vehicle technology and typology are classified, and the average speed of the vehicles is obtained from the traffic module on a link-by-link basis.

Kyriakis et al. [1998] notes that one of the more important factors affecting emissions is the average trip length per engine start, because of its influence on cold-start emissions. Other researchers agree with this finding [Eggleston, 1992]. There are two primary methods of collecting trip length data, the first is by survey or questionnaire and the second is by instrumented vehicles or chase cars [André, 1998]. A study in France in the early eighties [Vallet et al., 1982] compared trip length distribution collected with on-board instrumentation (35 private cars in 1983-'85) and by diary survey (600 to 1000 vehicles during three different periods in 1981-'82). The study found that 40 to 50% of the trips less than one-kilometre are not taken into account in a diary survey, leading to large variations in assumed and actual trip data. One reason given for this discrepancy is that the diary survey considered trip purpose, while the instrumented study recorded all vehicle start-ups. Another contributing factor is that people have difficulty in quantifying short distances [André et al., 1998].

In this project, it was not feasible to collect trip length by instrumented vehicle. Instead survey trip length data was employed instead. The trip length distributions for private cars in the four Boroughs that make up the greater Dublin area are given in Table 8.5 [CSO, 1996]. This information is required to calculate the emissions due to vehicle start-up. It is used to determine the CMP on each link (i.e. the fraction of vehicles with cold engines).

Table 8.5: Relative percentages of distance travelled by vehicles in the four Dublin Boroughs [source: CSO, 1996]

Trip Length (miles)	Dublin Co. Borough	Dublin Belgard	Dublin Fingal	Dun Laoghaire/ Rathdown	Greater Dublin Area
< 1	0.54%	0.25%	0.33%	0.67%	0.47%
1 to 2	23.89%	12.75%	9.45%	14.47%	16.51%
3 to 4	33.55%	23.76%	12.57%	23.61%	25.18%
5 to 9	32.28%	46.66%	39.88%	44.17%	39.76%
10 to 14	6.82%	12.45%	24.95%	12.57%	12.73%
15 to 29	2.15%	3.48%	11.65%	3.72%	4.53%
30 to 49	0.48%	0.40%	0.81%	0.47%	0.52%
> 50	0.29%	0.25%	0.35%	0.31%	0.30%

One surprising statistic from Table 8.5 is that less than 0.5% of trip lengths are less than 1.6 km (1 mile). Studies in other countries (e.g. Switzerland [SAEFL 1995], and France [Vallet et al., 1982]) found that approximately 5 to 11% of the total trips are less than one kilometre. A separate study in France in 1994 [André et al., 1997] found that 25% of trips were less than one kilometre. A European study [André, 1997] in which eighty private cars were instrumented in four different countries (i.e. France, Germany, UK and Greece) found that 19 to 27% of trips do not exceed one kilometre. A separate survey in the UK [Royles, 1995] found that approximately 33% of journeys are less than 5 miles in length and are made by car. It was also found that the average journey was between 20 and 25 minutes [Royles, 1995].

It is evident from Table 8.5 that in the Greater Dublin area as a whole, 42% of trip lengths are less than 6.4 km (4 miles) and nearly 82% of trip lengths are less than 14.4 km (9 miles). The most populated category is the 8 to 14.5 km (5 to 9 miles) distance, with nearly 40% of trips in the greater Dublin area within this range. The average trip length for the greater Dublin area is 10.87 km (≈ 6.79 miles). The average trip length can vary due to its sensitivity to very long trips. However, in the greater Dublin area, this group (greater than 50 miles) accounts for a very small percentage of the total passenger car trips (i.e. less than 0.5%).

An independent European study [Andrias et al., 1994] estimated the average urban trip length to be 14 km/hr in 1990 in Ireland. Another European study [André, 1997] found that the average trip length in four countries (i.e. France, Germany, UK and Greece) is in the range of 7 to 10 km, while median values vary between 3.1 and 3.4 km. André et al. [1998] noted the strong influence of season, day of the week and type of trip on trip length distribution. For example, Sunday-trips are significantly longer than during the week. The

observed trends are coherent according to the investigation methods (diary survey or vehicle instrumentation). Various other factors including location and availability of facilities, sex, familial and professional status also have an effect on trip length [Tarry, 1992], [UK-AA 1992].

Very little data exists on trip lengths for goods vehicles and buses. The primary reason for this is that the goods transported and their flow (tonnes x km) are studied more than the vehicles and trip lengths themselves [André et al., 1998]. In the UK, the average length of a haul for HGV is about 90 km and ranges from 30 to 130 km depending on the HGV type [HMSO, 1996]. Concerning buses, one study in France [OEST, 1995] found that the average trip length of an urban bus was 9.2 km, while the average trip length of a school bus was 22.0 km.

Another factor that affects start-up emissions is ambient temperature [Holman, 1999], [Sérié and Joumard, 1997]. The annual average temperature for the greater Dublin area is approximately 10°C.

When calculating emissions based on areas, then the number of starts per vehicle is important. However, in this study, emissions are calculated on a link-by-link (or part of) basis. Using the CMP approach, a certain proportion of vehicles on any given link are assumed to be travelling under start-up (either hot or cold) conditions. Statistical analysis of trip length data collected during the European Union sponsored MODEM project [Jost et al., 1992] found that 41.9% of trips are started with a fully warmed-up engine for passenger cars, while approximately 19% of the trips are started with a cold engine [André et al., 1997]. Sérié and Joumard [1997] also found that approximately 20% of all passenger car trips are started with an intermediate engine temperature (i.e. a temperature between ambient and a fully warmed-up engine).

The fraction of VKT with cold engines is called the CMP. Two methods of estimating CMP based on either measured or estimated trip lengths were proposed in Chapter three. In this case, the MVERA module employs the estimated trip length definition. However, if measured trip length data becomes available in the future, it can be employed since both methods are incorporated within the MVERA module.

By using an average ambient temperature of 9.8 °C (computed from data in Figure 8.2) and an average trip length of 10.9 km (computed from data in Table 8.5), it is estimated that

31.6% of all journey distances in the entire Dublin area are driven with cold-engined vehicles. The traffic module calculates an average trip length from the O-D matrices of 12.3 and 11.7 km for the morning peak hour (8 to 9 am) and the afternoon inter-peak hour (2 to 3 pm) respectively.

8.4.3 Evaporative Emissions

Evaporative emissions occur whenever fuel is exposed to the atmosphere [Watkins, 1991]. These are emitted while the vehicle is stationary (diurnal or daily losses), during vehicle usage (running losses) and after operation (hot soak losses) [André et al., 1998], as described in Chapter three. When calculating emissions on a link-by-link basis, running losses are of primary importance. The other three types of evaporative emissions occur when a vehicle is stationary, and hence are calculated as background emissions. In the case of refuelling losses, these are generally calculated as stationary sources because they occur at fuel handling locations.

Evaporative emissions depend on four major factors [Samaras et al., 1997] [Hickman et al., 1997]:

- Vehicle technology (either equipped or not with a carbon canister);
- Ambient temperature and daily variation;
- Gasoline volatility (depending on the temperature variation); and
- Driving conditions (average trip length, parking time, etc.).

Vehicle technology is dealt with earlier in this Chapter in the section on vehicle classification.

As evaporative emissions are affected by diurnal temperature changes, the maximum and minimum temperatures on a month-by-month basis are required. Figure 8.2 presents the monthly values of temperature (average, standard deviation, average maximum and average minimum). The average annual temperature is 9.8 °C, while the annual average maximum and minimum is 24.8 °C and –3.7 °C respectively. Monthly averages are always positive for the year ranging from 5.3 °C in February to 15.5 °C in July. The average monthly maximum temperature of 28.5 °C occurs in August and the average monthly minimum of –7.3 °C occurs in December.

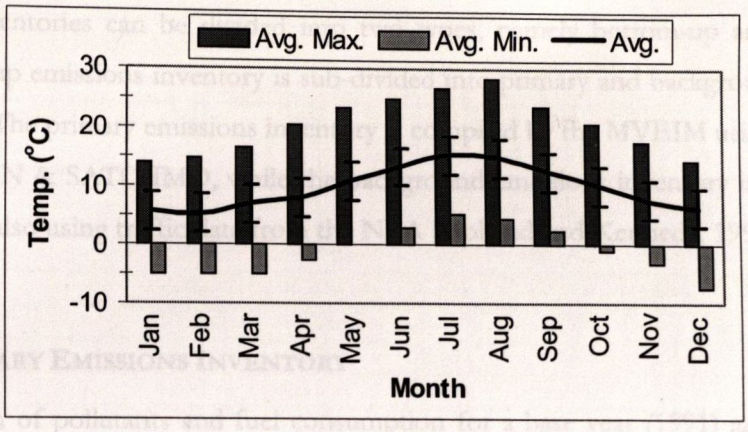


Figure 8.2: Mean monthly temperatures in Dublin

Fuel properties are also required to quantify the fuel volatility, a measure of which is given by the RVP. Fuel volatility varies from country to country and even from season to season. The RVP minimum and maximum limits in the greater Dublin area for summertime are 45 to 80 kPa respectively, while the wintertime limits are and 65 to 100 kPa respectively [Harrington, 1998].

The number of trips (LDV, HGV and bus) in an average weekday morning is shown in Table 8.6 [McCabe, 1998].

Table 8.6: Average number of morning trips for three primary categories of vehicles [source: McCabe, 1998]

No. Trips	LDV Trips	HGV Trips	Bus trips
1991	80,055	5,333	830
1996	115,428	5,333	920
2006 do-min	144,075	5,333	1,150
2006 do-str	132,814	5,333	1,350
2016 do-min	170,647	5,333	1,150
2016 do-str	154,500	5,333	1,550

Again due to lack of specific data for the greater Dublin area, cold start-up conditions are assumed in the morning and hot start-up conditions are assumed for the remainder of the day. A fully warmed-up vehicle vehicle in the morning will not have completely cooled down by evening.

8.5 BOTTOM-UP EMISSIONS INVENTORY

Emission inventories can be divided into two types, namely bottom-up and top-down. The bottom-up emissions inventory is sub-divided into primary and background emissions inventories. The primary emissions inventory is compiled by the MVEIM using traffic data from SATURN & SATCHMO, while the background emissions inventory is compiled by the MVEIM also using traffic data from the NRA [Holland and Kennedy, 1997].

8.5.1 PRIMARY EMISSIONS INVENTORY

An estimation of pollutants and fuel consumption for a base year (1991) and the relative percentage increase/decrease for the present (1996) and two future years (2006 and 2016) are presented in Table 8.7 as determined by the MVEIM.

It is recalled that the emission inventory for 1990 and 1996 employs historical statistical data, while the future emission inventories are predictions.

The forecasts of growth in 'trip-making' for future years have been made using various land-use scenarios, which incorporate several factors affecting transport demand. These include population growth, gross domestic product, number of households, population age, employment, car ownership, passenger throughput at Dublin airport, and Dublin Port freight traffic.

Likewise, the emissions factors used for future years were modified to take into account already agreed and adopted legislation, anticipated improvements in engine emission technology and fleet turnover, amongst others. These future emissions rates are subject to considerable uncertainty.

The modified emissions factors are used as the basis for forecasting the likely future inventories if no further measures were taken (i.e. a do-minimum strategy). In contrast, the 'do-strategy' option takes account of various traffic initiatives to be implemented in Dublin such as Quality Bus Corridors.

Table 8.7: Relative change in emission and fuel consumption levels with respect to the base year 1991 as calculated by the MVEIM using traffic data from SATURN & SATCHMO

Pollutant/ FC (ton)	1991	1996	2006 do-min	2006 do-str	2016 do-min	2016 do-str
Fuel consumption	*291,439*	+41.6%	+99.4%	+103.2%	+145.9%	+129.9%
CO	*65,335*	-10.1%	-63.2%	-68.3%	-78.2%	-80.3%
NM-VOC	*7,373*	-10.5%	-77.1%	-80.8%	-91.1%	-92.1%
PM_{10}	*335*	-4.9%	-55.4%	-60.1%	-68.8%	-70.2%
CO_2	*806,855*	+49.2%	+120.0%	+124.6%	+173.2%	+155.6%
1,3-butadiene	*121*	+5.6%	-56.7%	-63.6%	-82.0%	-84.1%
Benzene	*356*	-13.2%	-83.7%	-86.3%	-96.3%	-96.9%
$PM_{2.5}$	*23*	-4.9%	-55.4%	-60.1%	-68.8%	-70.2%
SO_2	*151*	+29.1%	-61.5%	-60.8%	-52.5%	-55.6%
Methane	*297*	-3.3%	-59.5%	-63.2%	-79.2%	-80.2%
NO_x	*8,217*	-6.2%	-51.3%	-53.9%	-67.6%	-69.7%

The MVEIM results allow transport planners to objectively evaluate the environmental effects of these different strategies. As an example, CO_2 is seen to increase by 155.6% by the year 2016 in the 'do-strategy' option, as compared to 173.2% in the 'do-minimum' option. However the results show that improved transport policies do not necessarily ensure lower emissions. For example, in the year 2006, CO_2 increases by 120.0% in the 'do-minimum' option and by 124.6% in the 'do-strategy' option. It is also worth noting that while some emissions increase, others decrease. For example, emissions of NM-VOC decrease all the time (from 1991 to 1996 to 2006 to 2016), but CO_2 emissions increase.

Fuel consumption increases from 1991 to 1996 to 2006 to 2016 due to the increase VKT and VHT as presented in Table 8.1, while emissions of all pollutants except CO_2 decrease. This decrease in emissions is due to tighter restrictions on emissions levels from new vehicles. However, catalysts convert CO and hydrocarbons to CO_2, thus resulting in an increase in CO_2. The emissions of SO_2 are directly related to sulphur content in the fuel. Sulphur will be reduced dramatically in 2005 (see Table 4.3 and Table 4.4).

Emissions are calculated as hot stabilised, start-up and evaporative. The relative percentage of each of these types of emissions is given in Table 8.8. Evaporative emissions only concern NM-VOC, 1,3-budatiene and benzene and the relative percentages are quite small. Only running and diurnal losses are included as calculations are performed on a link-by-link basis. The other types of evaporative emissions (hot soak and refuelling) are included as background stationary sources.

Table 8.8: Relative percentages of the various components of pollutants as calculated by the MVEIM using traffic data from SATURN & SATCHMO

Pollutant/FC	1991	1996	2006 do-min	2006 do-str	2016 do-min	2016 do-str
			Hot (cruise)			
Fuel consumption	54.8%	61.3%	62.9%	69.9%	73.2%	67.1%
CO	34.2%	30.0%	25.4%	28.8%	33.0%	27.3%
NM-VOC	40.1%	35.5%	33.2%	36.3%	51.1%	43.3%
PM_{10}	57.1%	57.3%	51.7%	57.7%	65.6%	55.0%
CO_2	57.0%	63.7%	64.7%	71.9%	75.2%	68.9%
1,3-butadiene	41.0%	36.9%	33.9%	37.0%	51.1%	43.7%
Benzene	39.2%	33.8%	28.4%	31.0%	40.6%	35.6%
$PM_{2.5}$	57.1%	57.3%	51.7%	57.7%	65.6%	55.0%
SO_2	57.0%	61.1%	61.4%	68.5%	72.5%	65.6%
Methane	57.0%	58.2%	58.5%	65.1%	78.6%	70.5%
NO_x	67.3%	64.0%	60.6%	65.8%	70.7%	61.2%
			Hot (creep)			
Fuel consumption	38.5%	31.3%	29.4%	22.3%	18.8%	25.1%
CO	35.6%	30.0%	27.3%	24.0%	19.5%	25.3%
NM-VOC	36.7%	30.9%	31.4%	28.4%	23.3%	33.3%
PM_{10}	41.2%	41.1%	46.6%	40.5%	32.4%	43.0%
CO_2	38.4%	31.1%	29.8%	22.6%	19.2%	25.6%
1,3-butadiene	37.9%	31.7%	31.3%	28.3%	22.5%	32.7%
Benzene	35.6%	29.4%	26.0%	23.3%	12.2%	17.9%
$PM_{2.5}$	41.2%	41.1%	46.6%	40.5%	32.4%	43.0%
SO_2	37.6%	32.7%	32.0%	24.8%	20.6%	27.7%
Methane	43.0%	41.8%	41.5%	34.9%	21.4%	29.5%
NO_x	31.3%	31.2%	33.4%	28.1%	23.6%	33.3%
			Start-up			
Fuel consumption	6.7%	7.4%	7.7%	7.8%	7.9%	7.8%
CO	30.2%	40.0%	47.3%	47.2%	47.5%	47.4%
NM-VOC	23.2%	33.5%	35.0%	34.8%	24.2%	22.2%
PM_{10}	1.7%	1.6%	1.8%	1.8%	2.0%	2.0%
CO_2	4.6%	5.2%	5.5%	5.5%	5.6%	5.6%
1,3-butadiene	21.1%	31.2%	34.3%	34.1%	23.9%	21.8%
Benzene	25.2%	36.7%	45.2%	45.1%	43.4%	43.6%
$PM_{2.5}$	1.7%	1.6%	1.8%	1.8%	2.0%	2.0%
SO_2	5.4%	6.1%	6.5%	6.6%	6.9%	6.7%
Methane	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
NO_x	1.4%	4.8%	6.0%	6.1%	5.7%	5.5%
			Evaporative			
NM-VOC	0.1%	0.1%	0.4%	0.5%	1.5%	1.3%
1,3-butadiene	0.1%	0.1%	0.6%	0.7%	2.5%	1.8%
Benzene	0.1%	0.1%	0.5%	0.6%	3.8%	2.9%

The relative percentages for start-up emissions can be significant. For example, between 30.2% (in 1991) to 47.3% (in 2016 do-strategy) of CO are emitted during the warm-up period for an engine. In contrast, only about 2% of PM_{10} emissions are produced during the start-up phase.

8.5.2 Background Emissions Inventory

The background emissions inventory accounts for emissions from traffic not included in the traffic module. The NRA [Holland and Kennedy, 1997] provides an independent estimate of the total VKT in the greater Dublin area. The NRA estimates are based on automatic and manual traffic counts carried out during the year. Future estimates do not exist, and estimates for the greater Dublin area were not available for 1991.

The residual VKT between the NRA estimate and the traffic module output is assumed to be equal to the traffic on side-streets, which is not included in the traffic module. Table 8.9 compares the total roadway length used in both methods and the corresponding VKT (millions) for 1996. The Traffic module covers 93.7% of the total road network. Therefore, side-streets are assumed to make up the remaining 6.3% of the road network. The VKT estimated by the NRA includes motorcycles, cars, LGV, HGV, buses, and miscellaneous vehicles. Miscellaneous vehicles comprise any vehicles that are not included in the other categories. Unfortunately, a percentage breakdown for the greater Dublin area is not available. However, the motorcycles and miscellaneous categories are estimated to contribute 88 and 10 million VKT respectively [Holland and Kennedy, 1997]. This means that the other vehicles (cars, LGVs, HGVs, and buses) travelled 3,185 million vehicle-km in 1996.

The residual between this VKT and that estimated by the traffic module is the traffic that travelled on the side-streets and minor-roads. Therefore, it is reasonable to assume that this traffic comprises primarily of LDVs.

Table 8.9: Comparison of roadway length and VKT from SATURN & SATCHMO and NRA for 1996

Parameter	NRA	Traffic Module	Difference
Length (km)	2,525	2,366	*6.3%*
VKT ($x10^6$)	3,283	2,752	*13.6%*

The background emissions inventory was calculated for the entire greater Dublin area using a top-down approach, and presented in Table 8.10.

Table 8.10: Background emissions inventory and fuel consumption in the greater Dublin area for LDVs in 1996 as calculated by the MVEIM using NRA traffic data

Pollutant/FC	Hot	Start-up	Evap.	Total
Fuel consumption	90.9%	9.1%	--	*45,600*
CO	59.3%	40.7%	--	*9,192*
NM-VOC	63.1%	36.8%	0.1%	*977*
PM_{10}	95.1%	4.9%	--	*16*
CO_2	93.5%	6.5%	--	*134,404*
1,3-butadiene	63.0%	36.8%	0.2%	*18*
Benzene	63.1%	36.8%	0.1%	*50*
$PM_{2.5}$	95.1%	4.9%	--	*1*
SO_2	90.9%	9.1%	--	*20*
Methane	100.0%	0.0%	--	*46*
NO_x	90.8%	9.2%	--	*549*

The background emissions inventory for motorcycles is estimated using the MVERA module, and presented in Table 8.11. Unfortunately, there are no emissions factors available for either start-up or running loss (evaporative) activity for either mopeds or motorcycles. Therefore, the emissions inventory includes hot-stabilised emissions only.

Table 8.11: Total emissions inventory for motorcycles in the greater Dublin area in 1996 as calculated by the MVEIM using traffic data from the NRA

Pollutant/FC	Total
Fuel consumption	3,010
CO	1,939
NM-VOC	343
PM_{10}	N/A
CO_2	7,246
1,3-butadiene	N/A
Benzene	N/A
$PM_{2.5}$	N/A
SO_2	1
Methane	18
NO_x	8

The methodology used for establishing urban emission inventories is usually a combination of 'top-down' and 'bottom-up' approaches [Loibl et al., 1993]. Researchers in Portugal [Borrego et al., 1999] also used a combination of top-down and bottom-up methodologies for the compilation of an emissions inventory for Lisbon. Similarily, the combination of Table 8.7, Table 8.10 and Table 8.11 gives the total emissions inventory due to motor vehicle activity in the greater Dublin area in 1996. This inventory may be termed a 'combined bottom-up inventory'.

8.6 TOP-DOWN EMISSIONS INVENTORY

Table 8.12 shows the top-down emission inventory for the greater Dublin area as calculated by COPERT III [Ntziachristos et al., 1999]. COPERT III was developed to estimate emissions from road traffic on a macro-scale level, not only by the fifteen member states of the European Union but also by most countries of Central and Eastern Europe [Zachariadis and Samaras, 1999]. It is an updated version of COPERT II, and is designed to produce, in a short time, a complete annual emission data set from road transport. COPERT III is a self-driven methodology, meaning that once a user starts the package, the software will lead one through the necessary steps until the end of the program. A special feature of the program is that it checks constantly the data entry and informs the user about incorrect or illegal actions. This can certify that the results will be reasonable, but cannot guarantee their accuracy.

Table 8.12: Emissions inventory for the greater Dublin area (1996) based on the COPERT III top-down approach

Pollutant/FC	Hot	Start-up	Evap.	TOTAL
Fuel consumption	91.1%	8.9%	--	*764,724*
CO	60.0%	40.0%	--	*89,379*
NM-VOC	70.9%	27.5%	1.6%	*10,082*
PM_{10}	85.2%	14.8%	--	*400*
CO_2	91.2%	8.8%	--	*2,324,832*
1,3-butadiene	N/A	N/A	N/A	*309*
Benzene	N/A	N/A	N/A	*1,019*
$PM_{2.5}$	N/A	N/A	--	*N/A*
SO_2	91.8%	8.2%	--	*309*
Methane	100.00%	0.00%	--	*844*
NO_x	94.2%	5.8%	--	*10,857*

The total VKT data required was obtained as the product of the number of vehicles registered in the greater Dublin area and the average annual mileage per vehicle category.

An average urban speed of 30 km/hr was assumed for cars and LDVs and 20 km/hr for HGVs and buses as recommended by Hickman et al. [1998]. Motorcycles and mopeds were also assumed to have a mean speed of 30 km/hr.

8.7 COMPARISON OF TOP-DOWN AND BOTTOM-UP APPROACHES

A methodological approach for comparing top-down and bottom emission inventories was developed by Samaras et al. [1995]. Samaras et al. suggest three calibration or comparison points, namely VKT, start-up conditions and emission factors. In this case, the same base

emission factors and start-up conditions were used in both inventories. Therefore, the major differences lie in the VKT data employed, and the way in which the emission factors are applied. For example, the top-down approach uses a mean average speed for all vehicles in the study domain, while the bottom-up approach uses an average link speed. The VKT data are compared in the next section. The combined bottom-up approach is taken to be the base-case for all comparisons.

8.7.1 Comparison of VKT Employed

Table 8.13 compares the VKT data employed in the top-down and bottom-up approaches. The VKT data in the top-down approach is the product of the AAKT and the number of vehicles in each category for 1996 registered in the greater Dublin area. The total VKT calculated using this method is over twice that of the combined bottom-up approach. In addition, the ratios of the different vehicle categories are also different. For example, the VKT by cars estimated using the top-down approach is 2.66 times that estimated using the combined bottom-up approach, while the top-down approach for estimating HGV and bus VKT under-predicts the bottom-up approach by approximately a factor of 2 and 3 respectively.

These differences in VKT could be explained by the fact that a substantial number of vehicles registered (i.e. Dublin license plates) in Dublin are owned by people living outside Dublin. Conversely, the number of vehicles owned by people in Dublin but registered outside Dublin is thought to be small. In addition, the top-down approach takes no account of daily commuters.

Table 8.13: Comparison of VKT for the greater Dublin area in 1996 from top-down and bottom-up approaches

VKT (millions)	Bottom-up	Top-down	Ratio
Total	3,283	7,473	*2.28*
Cars	2,415	6,429	*2.66*
LGVs	212	710	*3.35*
HGVs	408	185	*0.45*
Buses	151	44	*0.29*
Motorcycles	88	106	*1.20*
Misc.	10	0	*N/A*

Since, the VKT calculated using the top-down approach is more than twice that of the bottom-up approach, a corresponding difference in overall emissions can be expected.

8.7.2 COMPARISON OF TOTAL EMISSIONS

Table 8.14 compares the total emissions inventory as estimated using the bottom-up and combined bottom-up approach. COPERT III does not estimate the $PM_{10}/PM_{2.5}$ emissions ratios hence it is not included in the top-down approach.

Table 8.14: Comparison of top-down and bottom-up emissions inventories and fuel consumption for the greater Dublin area in 1996

Pollutant/FC	Top-down	Bottom-up	Ratio
Fuel consumption	764,724	461,316	*1.66*
CO	89,379	69,861	*1.28*
NM-VOC	10,082	7,922	*1.27*
PM_{10}	400	334	*1.20*
CO_2	2,324,832	1,345,478	*1.73*
1,3-butadiene	309	146	*2.12*
Benzene	1,019	359	*2.84*
$PM_{2.5}$	N/A	23	*N/A*
SO_2	309	216	*1.43*
Methane	844	351	*2.40*
NO_x	10,857	8,261	*1.31*

In general, the top-down approach estimates a larger inventory for all pollutants and fuel consumption. As the same set of emission factors were used to estimate both emissions inventories, the discrepancy is attributable to the traffic activity and composition data. In addition, the top-down approach does not take into account traffic congestion.

8.8 VALIDATION OF FUEL CONSUMPTION INVENTORY

Singer [1998] suggests "fuel-based estimates should be used to validate or adjust official vehicle emission inventories before society embarks on new, more costly air pollution control programs". Therefore, the fuel consumption module is validated macroscopically through comparison with total fuel deliveries for the greater Dublin area. The total retail fuel (petrol and diesel) deliveries to filling stations for 1996 was 364,191 tonnes [Harrington, 1998]. The predicted fuel consumption for LDVs as estimated under the top-down and combined bottom-up approach was 707,254 and 378,640 tonnes respectively in 1996. As HGVs and buses tend to refuel at depots, these are not included in the predicted fuel consumption for validation purposes. The percentage differences for the top-down and combined bottom-up approaches are therefore 94.0% and 3.9% respectively. As the combined bottom-up approach is very close to the actual retail fuel sales, it must be considered that that this is the more accurate approach.

One reason for the discrepancy between the predicted and actual fuel deliveries is that there can be a significant difference between fuel deliveries and actual fuel consumption. Most available statistics relate to fuel deliveries, which in many cases, relate closely to consumption. Nevertheless, there may be significant geographical differences between the point of delivery and that where the fuel is used.

8.9 ALTERNATIVE FUELS

Among the strategies available for reducing emissions is the use of alternative fuels. Alternative fuels offer a major potential for improvements in air quality, particularly for depot-based diesel vehicles with high travel kilometres. To this end, and as an example of the issues to which an emission inventory model can be applied, an abatement strategy to reduce total emissions from mobile sources involving the use of alternative fuels in depot-based vehicles is evaluated. The primary interest is in determining what relative changes in emissions could be achieved.

Although alternative fuels offer promising solutions to traffic related air pollution, timely and effective implementation remains a major challenge. While there are an infinite number of options that could be examined regarding the use of alternative fuels, only realistic scenarios are considered here. Holman [1999] states "the fuels considered most likely to make a major impact in the short term are CNG and LPG". Other studies agree, citing LPG and CNG as the most likely alternative fuels [Henderson, 1992]. Armstrong [1999] categorised LPG and CNG as realistic alternative fuels. From an economic prospective, LPG and CNG seem the most feasible alternative fuels, with LPG offering overall vehicle operating costs similar to petrol or diesel [Gover et al., 1996a]. However, LPG powered vehicles are banned from using underground car parks and tunnels in several European countries, because of the higher perceived risk they pose [TNO, 1998]. The NSCA [1998] conclude that "the most likely alternative fuels to be widely used in the near future are the gaseous fuels – CNG and LPG". In addition the NSCA [1998] stated "cleaner fuels will be most effective if used in cities with pollution hot-spots, and particularly where diesel vehicle fleets (buses, taxis and delivery vans) currently make a large contribution to urban pollution". Poulton [1994] concludes that CNG and LPG will gradually start to penetrate the market in ten years with urban buses and local fleets being the most likely candidates. Joumard [1999] also concludes that alternative fuels show an important potential for the reduction of emissions especially from diesel engines. Even new diesel vehicles emit relatively high levels of NO_x and $PM_{2.5}$. Greene and DeCicco

[2000] believe that emissions control breakthroughs or acceptable replacements for diesel engines are crucial research needs. The AIP [2000] found that "CNG is the fuel which is most likely to penetrate into the transport fuel market in the near future, as city bus fleets are progressively replaced by CNG powered versions in order to reduce particulate emissions". Buses are most likely to use alternative fuels because, despite statistics to the contrary, the public still believes that fossil-fueled transit buses contribute to the pollution problem rather than alleviate it [Dockendorf et al., 2000]. CONCAWE [1996] believe that "natural gas and LPG are particularly suitable for consideration as fuels for buses in city centre use" because "the potential environmental improvement is at its greatest, limited range is less of a problem, and fleet-refuelling facilities at depots is a practical proposition".

Taking the above into account, the realistic scenarios chosen for investigation are the conversion of public transport vehicles (e.g. buses and taxis) and local authority vehicles (e.g. refuse trucks) to CNG or LPG. The NSCA [1998] believe that local authority fleets and bus operators in particular have a duty to lead the development of strategies to improve air quality.

The primary reason why these two conversion scenarios (LPG and CNG) are realistic is that they are mass-market segments where mass-market conditions do not have to be met. The vehicles are depot based and the distribution of alternative fuel is limited to depots rather than being citywide. In addition, both public transport and local authority vehicles are more-controlled by regulatory measures than other vehicle types.

8.9.1 Alternative Fuel Testing in Ireland

Within the European Community, the potential for alternative fuels is significant and their exploitation and development is promoted through various initiatives of DG XVII (Directorate General with Responsibility for Energy in the EU) such as ALTENER and JOULE-THERMIE [TPRI, 1996]. However, there is limited use of alternative fuels in Ireland.

As part of the ALTENER initiative, Cork County Council tested bio-diesel in four sets of three vehicles over a period of twelve months [O'Sullivan and Barrett, 1998]. Each set of vehicles included a refuse truck, a lorry, a van and a transit pick-up. One vehicle from each set was fuelled by RME, one by SME, and one by mineral diesel. Some of the vehicles were tested on a chassis dynamometer in two different laboratories employing regulatory

driving cycles selected to portray typical urban conditions. As the vehicles were used in normal everyday operation for the 12 months, it was not feasible to measure emissions with on-board instrumentation.

Compared to diesel, the emission tests for RME showed average increases in CO, CO_2, NO_x, and PM_{10} of 5%, 3%, 13% and 6% respectively, and an average decrease in VOC of 46%.

In the case of SME, the emission tests show average decreases in CO and CO_2 of 1.8% and 4.8% respectively, and an average increase in NO_x of 10.6%.

As part of the JOULE-THERMIE initiative, Bus Átha Cliath in association with local gas supplier Bord Gáis are measuring real-world pollutant emissions from both CNG-fuelled and diesel-fuelled Volvo B10L buses operating on high frequency route (N° 3) in Dublin over a period of 3 years [Kerr, 1999]. As there has been considerable debate over how representative the regulatory test cycles are of real driving conditions, this project measures the emissions on both buses using on-board instrumentation.

The emission tests for CNG show average decreases in CO, NM-VOC and NO_x of 41%, 51.8%, and 54.1% respectively, and an increase in CO_2 of 3.4%.

8.9.2 Scenario using CNG/RME as an Alternative Fuel

The MVEIM is used to demonstrate that the conversion of all local authority vehicles to RME, and the conversion of the urban bus fleet to CNG would result in a significant reduction in many pollutants in Dublin.

Emission factors from JOULE-THERMIE [Kerr, 1999] and ALTENER [O'Sullivan and Barrett, 1998] as well as MEET data were employed in this investigation.

Table 8.15 compares these results to the base calculations using diesel and petrol only. For example, under the scenario described above, SO_2 emissions are estimated to be 17.9% lower in the year 2006 do-minimum projection than if conventional fuels are employed. However, it should be noted that methane emissions would increase by 129.8% in the year 2016 do-strategy option if CNG/RME scenario were implemented.

Table 8.15: Relative percentage change in pollutant emissions under CNG/RME scenario as compared to business as usual scenario

Pollutant	2006 do-min	2006 do-str	2016 do-min	2016 do-str
SO_2	-17.9%	-17.5%	-13.3%	-16.3%
NO_X	-14.6%	-14.8%	-12.1%	-14.5%
CO_2	-2.5%	-2.3%	-1.8%	-2.1%
CO	-6.6%	-6.5%	-4.7%	-5.3%
Methane	+119.9%	+125.7%	+98.6%	+129.8%
NM-VOC	-5.9%	-5.8%	-3.9%	-4.8%
PM_{10}	-15.6%	-15.8%	-12.4%	-15.3%

8.9.3 Scenario using LPG as an Alternative Fuel

The MVEIM also has been used to demonstrate that the conversion of all local authority vehicles, and the entire public transport fleet to LPG would result in a significant reduction in pollutants in Dublin. Table 8.16 shows the relative decrease in pollutant emissions under the LPG scenario described, as compared to using regular fuels (diesel and petrol). As reliable emission factors were not available for all the pollutants listed in Table 8.16, only some pollutants were calculated. When improved emission factors become available, they can be incorporated into the Emission Factor database. It is evident from Table 8.16 that there is a relative decrease in the emissions of all the pollutants listed. For example, 10.5% less CO will be produced under the LPG scenario with the year 2016 do-strategy option. As most of the local authority and public transport vehicles have diesel engines, there is a large reduction in SO_2 and PM_{10}. For example, 24.5% less PM_{10} will be produced for the year 2006 do-strategy option.

Table 8.16: Relative percentage decrease in pollutant emissions levels under LPG scenario as compared to business as usual scenario

Pollutant	2006 do-min	2006 do-str	2016 do-min	2016 do-str
SO_2	-18.2%	-17.4%	-13.5%	-16.2%
NO_x	-10.8%	-11.4%	-5.6%	-7.7%
CO_2	-4.5%	-4.1%	-3.3%	-3.8%
CO	-11.7%	-12.9%	-9.4%	-10.5%
NM-VOC	-8.7%	-8.5%	-4.5%	-5.1%
PM_{10}	-25.0%	-24.5%	-13.0%	-14.9%

8.10 SUMMARY

This Chapter has described the compilation of a bottom-up traffic related emission and fuel consumption inventory for the greater Dublin area for a base year (1990) and the

relative percentage increase/decrease for the present (1996) and two future years (2006 and 2016). Sample emission inventory results were presented for a set of transport policies (e.g. quality bus corridors) currently being implemented in Dublin. The fuel inventory was successfully validated macroscopically against retail fuel sales data. An abatement strategy to reduce total emissions involving the use of alternative fuels was evaluated and showed promising results. The MVEIM was employed to compile the bottom-up emissions inventory, while COPERT III was employed to compile the top-down emissions inventory. A comparison of both revealed substantial discrepancies. However, the bottom-up inventory is much more accurate.

9. AMBIENT POLLUTANT CONCENTRATIONS

9.1 INTRODUCTION

In the previous Chapter, the air pollutant emissions inventory for the entire Dublin area was compiled. However, emissions are only one of the factors that affect ambient concentrations. Other factors such as local topography and meteorology also influence air quality. In this Chapter, the local air quality in Dublin is described in detail. An objective of this research is to investigate potential pollutant hotspots in urban areas. The CALINE4R dispersion model is employed to estimate pollutant concentration at three sites (potential pollutant hotspots) in Dublin. The first of these has the heaviest traffic volume in the city, while the second has the greatest level of congestion. The third site is located in the centre of the circular area of greatest emissions production, identified using a moving buffer zone. This approach has the capacity to incorporate the contributions to ambient concentrations from all emission sources in the intermediate vicinity. A further objective of this research is to develop a method to aggregate different pollutant emissions (e.g. CO and NO_x). Consequently, indices of air emissions and air pollutants are formulated.

9.2 THE GREATER DUBLIN AREA

The GDA is located on the eastern side of Ireland along the Irish Sea (latitude 53.2° N and longitude 6.05° W). To the south lie the Dublin Mountains and the rest of the city is surrounded mainly by flat land. The city is primarily level.

The GDA has a population of 952,692 people with a population density of 4,098 people per square kilometre [CSO, 1996]. The entire GDA includes the city and county of Dublin and parts of counties Kildare, Meath and Wicklow. All of the built-up area of Dublin is included. The GDA represents the Dublin journey to work area as defined by the DTO [SDG, 1994].

There is little difference between the city centre and the suburbs in terms of aerodynamic roughness. For example, the average building in the city-centre is four stories and the suburbs are generally two stories.

9.3 AIR QUALITY IN DUBLIN

Local air quality is monitored primarily by Dublin Corporation. In addition several independent monitoring campaigns have been carried out including that employed in this study. The following sections describe the air quality in Dublin since records began.

9.3.1 LOCAL AUTHORITY MONITORING NETWORK

Dublin Corporation has a limited network of monitoring stations located around the city [Dublin Corporation, 1998]. The primary pollutants monitored are SO_2 (at 14 sites), smoke (at 14 sites), lead (at 8 sites), NO_x (at 1 site), CO (at 1 site), PM_{10} (at 5 sites), and $PM_{2.5}$ (at 1 site). The EPA operates separate NO_x and ozone sites also.

9.3.2 HISTORICAL REVIEW OF AIR QUALITY IN DUBLIN

The earliest accounts of air pollution in Dublin go back to World War Two [Leonard et al., 1940; 1941; 1950]. In the 1960's, the Department of Local Government published information on air pollution measurements [Dawson, 1963; 1964; 1966]. The Air Quality Monitoring and Noise Control Unit of Dublin Corporation has produced an annual report on atmospheric pollution in Dublin since 1974, for example Dublin Corporation [1998]. The EPA publishes Reports on NO_x measurements at one site in Dublin, for example O'Donnell [1989].

In addition, numerous publications have reviewed the general position in Dublin regarding air pollutant emissions and air quality [Bailey, 1981b; 1983; 1984; 1988], [Bailey et al., 1978; 1986], [Bailey and Walsh, 1980b], [Cabot, 1985], [Delaney and Dowding, 1998], [ENFO, 1992], [ENVIROCON, 1995], [Flanagan et al., 1988], [Kelly, 1993], [McGettigan and O'Donnell, 1995], [McGettigan et al., 1993], [McManus and Reilly, 1976], [McManus, 1975; 1998], [Nolan, 1979], [Reilly, 1986], [Richter and Williams, 1998], [Spanton and McInnes, 1993] [Stapleton, 1996], [Sweeney, 1991], [Tarrant, 1999], [Walsh, 1976; 1988], and [Williams et al., 1983].

A number of studies also linked health and air pollution in Dublin including [Chapman, 1965], [deWytt and Kevany, 1971], [Dean, 1988], [Sinclair, 1997], [Dockery, 1999], [Goodman et al., 1999], [Kelly and Clancy, 1984], [Kevany et al., 1975] and [Ward et al., 1978].

The above studies were largely based on measurements of pollutants made by Dublin Corporation, Dublin County Council, Forbairt and ESB who all at some stage operated monitoring stations in the GDA. Discrepancies exist in the average concentration levels reported by different agencies due to the different number of sites, locations and samples at each site included in the analysis. In addition, different methods (e.g. diffusion tubes and electrochemical sensors) were used to measure the pollution. The following summaries give indicative values for average annual pollutant concentrations.

9.3.2.1 Smoke

Mean annual concentrations of smoke showed a downward trend from 1963 to 1978. For example, the annual average smoke concentration was approximately 128 $\mu g/m^3$ in 1963 but had dropped to approximately 27 $\mu g/m^3$ by 1978. Measurements in the 1980's show a dramatic increase in smoke levels. This was due to the increased use of coal for domestic heating following an international oil crisis. The daily smoke concentrations limit of 250 $\mu g/m^3$ as set out by the EU Directive 80/779/EC [Murley, 1999] was breached on a number of occasions. There was also a sharp increase in the winter of 1981/82 where the average annual concentration rose to approximately 60 $\mu g/m^3$. This high level was due to temperature inversions associated with anti-cyclone weather systems and stable air. The level of smoke has fallen dramatically since 1990 due to two reasons. Firstly, the marketing, sale and distribution of 'smokey fuels' (e.g. bituminous coal) are prohibited in the Dublin since September 1990. Secondly, natural gas is now widely used for domestic heating instead of solid fuel. The maximum-recorded smoke concentration in 1997/98 was 88 $\mu g/m^3$ as compared to a maximum level of 1,545 $\mu g/m^3$ recorded in November 1988. The mean annual concentration of smoke in 1998 was 12 $\mu g/m^3$. Reilly and Duggan [1978] estimated that the annual concentration of smoke in 1990 would be 65 $\mu g/m^3$. In comparison, the actual 1990 annual average value was only 27 $\mu g/m^3$.

9.3.2.2 Sulphur dioxide

Mean annual concentrations of SO_2 increased from 63 $\mu g/m^3$ in 1963 to 100 $\mu g/m^3$ in 1971, but then declined to 45 $\mu g/m^3$ in 1984. However, during the severe winter of 1981/82 there was a significant increase in mean concentration to approximately 65 $\mu g/m^3$. SO_2 levels continued to decline during the 1980's (with the exception of 1986/87). The fall in SO_2 concentrations in the 1980's may be attributed to the change over from oil

to natural gas by ESB Poolbeg power plant, and some factories and hospitals. The annual average concentration continued to decline in the early 1990's (to approximately 20 $\mu g/m^3$), increasing slightly in the late 1990's. Although some of the smokeless solid fuels being sold in the Dublin have considerably higher sulphur contents than the bituminous coal they replaced, no consequent increase in SO_2 concentrations was apparent. The annual average concentration of SO_2 in 1998 was 26 $\mu g/m^3$. Reilly and Duggan [1978] estimated that the annual concentration of SO_2 in 1990 would be 75 $\mu g/m^3$, whereas in 1990 the actual annual average concentration was only 26 $\mu g/m^3$.

9.3.2.3 Lead

Initial measurements of lead concentrations began in 1974 at a city-centre site. During the 1970's the annual average lead concentration varied between 2.2 and 3.1 $\mu g/m^3$. In 1978 the maximum content of lead in petrol was reduced 0.4 g/l to 0.15 g/l. Since 1982 concentrations of lead in air have been monitored by Dublin Corporation at eight sites representing both city-centre and suburban locations. The annual mean values of lead concentrations at some sites frequently approached 2 $\mu g/m^3$ in the early 1980's, but concentrations have been decreasing since the mid-1980's. For example, the annual average concentration of lead declined from 0.5 $\mu g/m^3$ in 1988 to 0.13 $\mu g/m^3$ in 1997. This trend can be attributed to a number of reductions in the lead content of petrol. In addition, since 1989 there has been a significant increase in the share of unleaded petrol (as a percentage of total petrol sales). For example, in 1989 unleaded petrol accounted for approximately 7% of total petrol sales in the GDA. This ratio has risen dramatically to 74% in 1997. The sale of leaded petrol has been banned in Ireland since January 2000.

9.3.2.4 Nitrogen dioxide

In 1975, Dublin Corporation measured NO and NO_2 at a number of locations in a once off study. Dublin Corporation has measured NO_2 at a city centre site since 1988. The average annual concentration of NO_2 in 1988 was 58.38 $\mu g/m^3$ and this level declined to 47 $\mu g/m^3$ in 1990. However, between 1990 and 1995 the concentration increased to 90 $\mu g/m^3$. The average annual concentration of NO_2 in 1997 was 83 $\mu g/m^3$. It is worth noting that a busy bus-stop is located close to Dublin Corporation's city-centre monitoring site in College Green. Since the buses burn diesel, this has an affect on the NO_2 levels measured. Since 1988, the EPA has also measured NO_2 at an independent site along one

of the major commuter routes between the city-centre and the suburbs. The annual average level recorded in 1988 was 38 $\mu g/m^3$. This level remained relatively constant up to 1994, but declined to 18 $\mu g/m^3$ in 1995. The primary reason for this change was the repositioning of the station inlet approximately 10m above ground level and well back from the kerbside. Overall, the levels appear to be on the increase. The NO_2 levels recorded at Rathmines are consistently lower than those at College Green, reflecting lower NO_x emissions due to a lower traffic density. The ESB also operate a continuous NO_2 monitor at Howth Head. The site is located on a bleak headland on the north side of Dublin bay and as such is relatively remote from the city-centre. The daily average NO_2 levels recorded in 1997 were 10 $\mu g/m^3$.

9.3.2.5 Carbon monoxide

Dublin Corporation measured CO at a number of locations in 1975 in a once off study. Since 1996, CO is measured in the city-centre at the same site as NO_2. The average annual value of CO in 1996 and 1997 was 1.95 and 2 ppm respectively.

9.3.2.6 Particulate matter

PM_{10} is measured at five sites throughout the city. In 1998, the average annual concentrations at the two city centre sites were 43 $\mu g/m^3$ and 41 $\mu g/m^3$. The average annual concentrations at the suburban sites were 21 $\mu g/m^3$ and 22 $\mu g/m^3$, while the concentration at the background site was 17 $\mu g/m^3$.

$PM_{2.5}$ is measured at one city centre site. The average concentration of $PM_{2.5}$ was 33 $\mu g/m^3$. A comparison was carried out between PM_{10} and $PM_{2.5}$ measured at the same site. Analyses of the measurements show that the concentration of $PM_{2.5}$ is always lower than PM_{10} by between 7 and 31 percent. The average difference between PM_{10} and $PM_{2.5}$ concentrations is 20%.

9.3.3 Independent Studies of Air Quality in Dublin

A number of independent studies on air quality in the GDA have also been carried out over the past few years. The main findings from each study are outlined.

A baseline study on the concentrations of VOCs and PM_{10} in Dublin city was carried out over a 13-month period (from January 1st 1996 to January 31st 1997) [Henderson et al., 1997] [Keary et al., 1998]. The study was divided into two components, namely PM_{10} [Keary, 1997] and VOC [Shanahan et al., 1997]. PM_{10} was measured at six sites in the city. Four sites were located within 6m of the side of the roadway while the other two were situated 150 and 250m from the roadway. The annual average mass concentrations at the two inner city sites (i.e. College Green and Merchants Quay) were 44 and 40 $\mu g/m^3$. Average PM_{10} concentrations in wintertime exceed concentration levels in summertime by 40 to 50% for all six sites. In addition, it was evident that PM_{10} concentrations increase significantly during the early morning with maximum concentrations occurring between 8:00am and 10:00am. The study observed a correlation between traffic counts and particulate concentration levels at the College Green site. VOCs were measured at twenty sites using passive diffusion tubes over a forty-two week period. All but three of the sites were located within 6m of the roadway. The average annual concentrations of benzene, toluene, p-xylene, and m-, o-xylene were 4.97 $\mu g/m^3$, 11.70 $\mu g/m^3$, 11.84 $\mu g/m^3$ and 14.88 $\mu g/m^3$ respectively.

A study carried out by the Environmental Research Unit in TCD [Healy and Dowling, 1997, 1998] investigated the level of PM_5 in Dublin city centre. PM_5 was measured using a monitor attached to a bicycle over the summer months of 1997. The measurement apparatus consisted of a portable pump and particulate matter cyclone sampling head. The study showed that people in traffic experienced higher levels of pollution than averaged background values. For example, the measured PM_5 concentration levels were consistently twice as high as the PM_{10} levels measured by Dublin Corporation. Exposure concentrations between 23 and 96 $\mu g/m^3$ were measured, with an average value of 57 $\mu g/m^3$. Significantly higher concentrations were measured in periods of dry sunny weather with easterly winds. This is could be indicative of the role of secondary pollutants and long-distance pollutant transport. An estimation of the effect of monitored pollutant concentrations on mortality risk was carried out using established epidemiological associations. The study showed that mortality rates for those living in the centre of Dublin are 26% higher than in the less polluted suburbs.

As part of the Dublin Air Quality Management Plan [ENVIROCON, 1996], intermittent kerbside concentrations of NO_2 were measured using diffusion tubes at one hundred locations in the city-centre on a weekly basis between 1994 and 1996. The weekly

concentration levels of NO_2 measured along heavily trafficked streets varied between 40 and 50 ppb. Background concentration levels measured in Trinity College and on pedestrianised streets varied between 20 and 30 ppb. Maximum concentrations in the order of 75.9 to 84.3 ppb were recorded at Fleet Street. A lot of buses frequent this street hence the high concentration of NO_2. NM-VOC kerbside concentrations of benzene, toluene and xylene were also measured at fifty-one sites as part of the same study. The sites were chosen along heavily trafficked streets. The average minimum concentrations of benzene, toluene and xylene were 1.5, 6.8 and 0.3 ppb respectively, while the average maximum concentrations were 5.0, 13.0 and 7.8 ppb respectively. Carbon monoxide was also measured but the values detected were typically in the order of 2 ppm, which is close to the detection limit of the diffusion tube.

As already stated, air quality has been monitored at the junction of Pearse Street and Lombard Street from August 1997 to January 1999. Pollutants monitored include CO, NO_2, PM_{10}, 27 different VOCs including benzene and butadiene. The full list of VOCs monitored is given in Table 9.1 along with the average concentrations for each. These pollutant data were analysed by researchers at Trinity College [Keating et al., 1998; 1999], [Marnane et al., 1998; 1999a; 1999b]. A brief summary of their findings is given here.

Table 9.1: Average VOC concentrations in Dublin (ppb)

Compound	Concentration	Compound	Concentration
1,2,4-Trimethylbenzene	0.76	**Isopentane**	2.16
1,3,5-Trimethylbenzene	0.41	**Isoprene**	0.16
1,3-Butadiene	0.29	**m+p-Xylene**	1.66
1-Butene	0.15	**n-Butane**	2.88
2-Methylpentane	0.35	**n-Heptane**	0.17
3-Methylpentane	0.31	**n-Hexane**	0.48
Acetylene	2.12	**n-Pentane**	0.75
Benzene	1.71	**o-Xylene**	0.62
Cis-2-Butene	0.15	**Propane**	1.62
Cis-2-pentene	0.12	**Propylene**	1.71
Ethane	3.28	**Toluene**	3.13
Ethylbenzene	0.53	**Trans-2-Butene**	0.16
Ethylene	3.97	**Trans-2-Pentene**	0.19
iso-Butane	1.08	**Average VOC**	1.15

Analysis of the VOCs concentrations revealed that different patterns were exhibited for different days of the week, reflecting variations in traffic volume flow traversing the intersection. In addition, different patterns were exhibited for different months of the year reflecting variations in meteorological conditions. Within an individual day, three different types of diurnal variations were identified for the VOCs:

1. Relatively constant (ethane and propane);
2. Double peaked diurnal pattern with a maximum peak during the morning rush hour (iso-butane and n-butane).
3. Double peaked diurnal pattern with a maximum peak during the afternoon rush hour (other 23 VOCs);

Correlations between individual VOCs and meteorological conditions (e.g. temperature, wind speed and direction) were very poor and virtually non-existent on an hourly basis. This was attributed to the masking effect of variations in the traffic volume traversing the intersection. Summer VOC concentrations are lower on average than winter concentrations. A very strong correlation was found between the majorities of the individual VOCs even for short-term one-hour values. This strong correlation is largely due to the dominance of a common emission source (i.e. traffic). Overall, traffic variations and consequently emissions variations have a much stronger influence on ambient VOCs than local meteorological conditions.

Non-VOC pollutants (CO, NO_2 and PM_{10}) exhibit characteristic diurnal trends with double peaks on weekdays corresponding to traffic flow traversing the junction. These characteristic double peaks are absent during the weekend, with average pollutant levels similar to the non-peak levels during the week. CO, NO_2 and PM_{10} exhibited characteristic diurnal patterns. Mean weekday concentrations are higher that than those of the weekend, with a ratio of weekend to weekday for CO, NO_2 and PM_{10} of 0.85, 0.95 and 0.85 respectively. The daily means recorded for CO, NO_2 and PM_{10} were 0.5 ppm, 0.03 ppm and 15 $\mu g/m^3$ respectively. The correlation coefficient for twenty-four averages between wind speed and CO, NO_2 and PM_{10} were 0.83, 0.78 and 0.85 respectively.

9.4 CLIMATOLOGY OF THE GREATER DUBLIN AREA

Air quality depends not only on emissions but also on local climatology [Shahgedanova, 1998], [Reynolds, 1993]. Meteorological factors such as wind speed and direction, air temperature, and the mixing layer height all have a direct affect on the dispersion of pollutants. CALINE4R has been adapted to use chronological meteorological data. For future estimates, it is recommended that ten years of data be employed. This implies that the standard dispersion field has to be calculated for up to 87,648 data sets for each pollutant, which may result in long computational times. In order to speed up the model,

an analysis was performed on the meteorological data collected at Dublin Airport form 1986 to 1995, to determine if pre-classified categories or combinations of data could be used to represent the full range of possible weather conditions. Consequently, the number of standard dispersion fields could be reduced dramatically.

The analysis showed that it is extremely difficult to employ average weather conditions to represent ten years of data as the weather in Dublin is highly variable. For example, the ambient temperature varies between 25 °C and -4 °C. Therefore, the full ten years of data are used when estimating future pollutant concentrations. This should give a more accurate result. However, as an initial estimate of pollutant concentration, worst case meteorology and traffic conditions (e.g. morning peak hour) should be used because this involves one 'run' of CALINE4R. Subsequently, the model should be 'run' 87,648 times to get a more accurate result.

9.5 AIR QUALITY STANDARDS

Current air quality standards are defined over different time periods for different pollutants. For example, pollutants such as benzene, 1,3-butadiene and lead have air quality standards expressed as long-term averages (e.g. annual means), while pollutants such as carbon monoxide, nitrogen dioxide, PM_{10} and sulphur dioxide, have air quality standards defined as short-term averages (e.g. one-hour means). In addition, some air quality standards (e.g. SO_2 in the UK) are expressed as a 99.9^{th} percentile [Murley, 1999], implying that the highest 35 concentration levels out of 35,040 fifteen-minute intervals in a year may exceed the stated limit value.

It is not possible to directly compare the predicted concentrations for all pollutants directly with air quality standards as these standards are defined over different time periods. Most dispersion models usually output pollutant concentrations as average hourly values because meteorological conditions are likely to remain relatively constant over this period. However, statistics may be employed to convert from one averaging period to another.

The one-hour mean is the normal output from most dispersion models [UK-DETR, 1998b]. The fifteen-minute mean and the eight-hour mean are less usual averaging periods. There are two primary methods used to convert estimated concentration levels to other averaging periods.

The first is to model the different time periods according to the air quality standard. However, quite often data (e.g. traffic) does not exist for eight-hours or twenty-four-hours. The SATURN & SATCHMO traffic module only predicts traffic data for peak and inter-peak hours in the entire Dublin area. Previous measurements by the author indicate that traffic activity and composition varies over the day. In addition, estimating concentrations from every hour of the year involves considerable computer processing, expensive meteorological data, and running a model over 8.5 thousand times to generate an annual hourly concentration. It worth noting that empirical relationships could be used to estimate eight-hour or twenty-four-hour traffic activity averages.

The second method is the use of empirical relationships, more commonly known as persistence factors, which convert one-hour averages to other time-period averages [Cooper, 1988a, 1988b, 1989], [Cooper et al., 1989]. This persistence factor method has the advantage over modelling sequential hours of data in that it includes the effects in both traffic and meteorological conditions. The US-EPA [Schewe and DiCristofaro, 1992] suggests using persistence factors to convert between one-hour maximum concentrations and other values. For example, the US-EPA [Schewe and DiCristofaro, 1992] recommends using a persistence factor of 0.7 to convert 1-hour carbon monoxide concentrations to 8-hour concentrations for many regions in the USA. Cooper et al. [1992] however, recommends using a persistence factor of 0.55 to convert 1-hour carbon monoxide concentrations to 8-hour concentrations in Orlanda, Florida. This value is based on a comprehensive statistical analysis of ten years of meteorological data, coupled with detailed hourly modelling results. The US-EPA [1992e] recommends using a persistence factor of 0.08 to convert 1-hour PM_{10} concentrations to annual average concentrations.

The UK-DETR [1998b] state, that the maximum 8-hour mean for carbon monoxide within urban areas is unlikely to exceed the air quality objective of 10 ppm if the maximum 1-hour concentration is less than 12 ppm. This is equivalent to a conservative persistence factor of approximately 0.83. The UK-DETR [1998b] also state that the 15-minute mean for sulphur dioxide within urban areas is approximately 1.36 times the 1-hour mean, and that the air quality objective for PM_{10} (50 $\mu g/m^3$ as the 99th percentile of running 24-hour means) is unlikely to be exceeded where the annual mean concentration is less than about 18 $\mu g/m^3$.

The UK-DETR [1998b] is currently developing empirical relationships to estimate compliance with the air quality standards in the UK. In addition, current research at

Trinity College is developing persistence factors for a range of pollutants [Keating et al., 1999].

9.6 PREDICTING AIR QUALITY HOTSPOTS

Traditionally, air quality modelling has been carried out at locations where conditions are thought to be the most conductive to high concentration impacts. In urban areas, pollutant concentrations may be high near locations where traffic has a tendency to build-up, slow-down, and idle for a period of time, such as at a junction. The extent of this problem is a function of the number of vehicles present, their operating mode, their movement, and the length of delay. Therefore the pollutant distribution across an urban area is not only a function of the distribution and density of development in the area, but also of individual junctions, roadways and traffic characteristics [Haynie, 1996].

Schewe and DiCristofaro [1992] give a junction selection procedure to identify junctions that could cause high pollutant concentrations. They suggest investigating the top-ranked junctions based on highest traffic volumes and worst LOS [Schewe and DiCristofaro, 1992]. The LOS is defined in terms of vehicle delay time. It is related to both the physical characteristics of the junction and to various operating conditions that occur when variable traffic volumes are traversing a junction [Garber, 1988]. Schewe and DiCristofaro [1992] assume that if the junctions selected based on the above criteria do not exceed air quality standards, neither will any other. In this study, the investigation of vehicle emission impacts in Dublin therefore starts by modelling the junctions with the heaviest traffic volume and the greatest congestion, bearing in mind that the highest concentrations would be expected during the morning peak hour of traffic.

9.6.1 CALINE4R INPUTS FOR WORST CASE ANALYSIS

CALINE4R requires a number of inputs as described in Chapter five. A worst-case scenario was modelled, as this gives the highest concentrations [Nokes and Benson, 1985]. The generic nature of the inputs required for worst-case scenario is described in the following sections.

9.6.1.1 Maximum link length

The AQTAN [Benson et al., 1988] recommend an approach or departure link length of 150 metres. The US-EPA's Guidelines [Schewe and DiCristofaro, 1992] recommend

modelling a roadway from the junction of interest to the next junction or up to a maximum distance, of 300m away. However, previous studies and modelling experiments [Chiquetto, 1995b] have shown that emission contributions become negligible when road segments are situated at distances of more than 200m from the receptor. In addition, deHoogh [1999] when estimating exposure to traffic related pollution using CALINE3, only modelled sources within a 200m distance of a receptor. Consequently it was decided to model traffic emissions within 200m of the receptor, or to the next junction.

9.6.1.2 Receptor location

As a rule, receptors should be located where the maximum concentration is likely to occur and where the general public is likely to have access [US-EPA, 1978]. However, some restrictions may apply to these criteria. For example, if estimated concentrations are to be compared to air quality standards, then the receptor should be located according to the standard guidelisnes. In addition, the dispersion model may have limitations, and importantly, Gaussian models, by their nature, cannot predict concentrations at the source.

The US-EPA has established a policy whereby receptors should be located at least 3m from the nearest traffic lane, and at a height of 1.8m [Schewe and DiCristofaro, 1992]. The 3m receptor distance is the nearest distance for which predicted concentrations are considered valid in CALINE4 [Benson et al., 1988], and corresponds to the edge of the 'mixing zone' above and surrounding the travelled roadway. The 1.8m receptor height represents the 'breathing zone'. In addition, the receptors should be located at 25m and 50m away from the junction corner [Schewe and DiCristofaro, 1992].

A proposed European Union Directive [Murley, 1999] requires sampling inlets for benzene and carbon monoxide to be located at heights between 1.5m and 4m. In addition, the Directive suggests that the sampling inlet for all pollutants should be at least 25m from the edge of major junctions and at least 4m from the centre of the nearest traffic lane. For carbon monoxide, inlets should also be located less than 5m from the kerbside.

Accordingly, to model worst-case conditions, the CALINE4R receptors were located at a height of 1.8m, a distance of 25m from the junction and at a distance of 3m from the nearest traffic lane edge beside all roadways. For a typical four-way junction, eight receptors are required – two along each arm. In each analysis, the receptor with the highest

concentration is identified. It is worth noting that this may vary depending on the wind direction and total emissions produced.

These receptor locations comply with all of the above guidelines and agree with the limitations of the dispersion model.

9.6.1.3 Meteorological inputs

The generalised worst-case meteorology for the estimation of maximum 1-hour pollutant concentrations is given in Table 9.2.

Table 9.2: Generalised worst-case meteorology for the estimation of maximum 1-hour pollutant concentrations

Variable	Value
Wind speed (m/s)	0.5
Wind direction (degree)	Worst
Wind direction standard deviation (degree)	5°
Atmospheric stability class (A to G)	G
Mixing height (m)	1,000
Temperature (°C)	3.9°

Even though measurements exhibited wind speeds of less than 0.5 m/s, the minimum worst-case wind speed was set to this value because it represents the lowest available value in the CALINE4R model.

The worst-case wind direction gives the highest concentration. This can be found by calculating the pollution level for every 10° of wind direction from 0° to 350° (or a total of 36 directions). The actual wind direction (to a degree) is then calculated by repeating the exercise between the two highest 10° wind directions. It is worth noting that this value varies from site to site.

Variability of wind direction is explicitly defined as the standard deviation (σ_θ) of the measured wind directions. It is a measure of atmospheric turbulence. As presented in Table 6.5, it can vary from 5° (representing clam conditions) to 60° (representing turbulent conditions). Again this was set to the lowest value available in CALINE4R, which reflects conditions during an atmospheric inversion (i.e. very calm conditions).

Schewe and DiCristofaro [1992] advise employing a mixing height of 1,000m. Coe et al. [1998] state that "reasonable values for the worst case mixing height rarely have a significant impact on CALINE4 model results".

Since Stability Class G reflects very stable atmospheric conditions, for obvious reasons this was employed.

For worst-case analysis, Benson et al., [1988] suggest using the lowest January mean temperature over a representative 3-year period. Schewe and DiCristofaro [1992] suggest using the average January temperature. In this study the lowest January mean temperature over ten years was employed.

9.6.2 JUNCTION WITH HIGHEST TRAFFIC VOLUME

SATURN & SATCHMO computed that the junction with the highest traffic volume in Dublin (denoted as #4320) is located at the main entrance to UCD on the Stillorgan dual carriageway. Figure 9.1 shows a schematic representation of the junction and the location of the receptors. The roadway (a dual carriageway) is a primary artery to Dublin from the South and also carries a significant volume of traffic from the citycentre to the University. The roadways are all modelled as individual links.

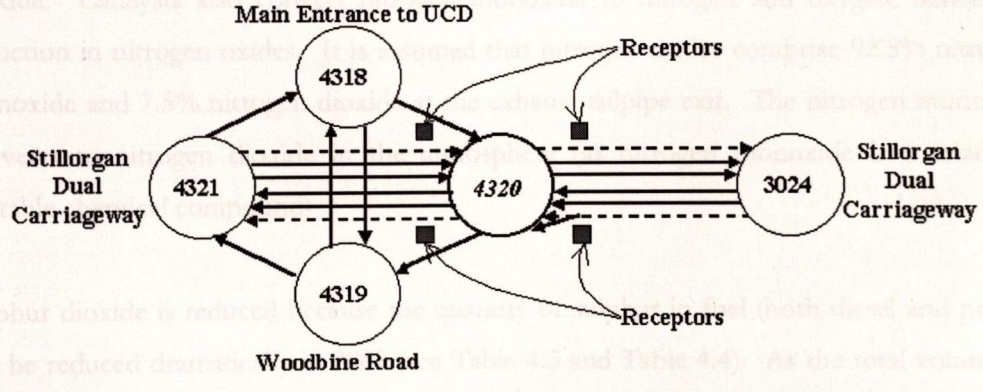


Figure 9.1: Schematic representation of intersection with highest traffic volume in Dublin (#4320)

For the purpose of this exercise, SATURN & SATCHMO computed the peak hour VKT and VHT for the links shown in Figure 9.1 only. These values are presented in Table 9.3 for the base year (1991) and the relative percentage increase/decrease for the present

(1996) and two future years (2006 and 2016). The VKT and VHT increase every year except for the 2006 do-strategy option in which both are predicted to decrease slightly.

The average vehicle queue is zero for all years and all scenarios, as the junction contains exit/on-ramps from/to the dual carriageway (instead of traffic lights). Consequently, all emission factors employed by the MVEIM are speed-dependent only.

Table 9.3: VKT and VHT (as computed by SATURN & SATCHMO) for junction with highest traffic volume in Dublin

Year	1991	1996	2006 do-min	2006 do-str	2016 do-min	2016 do-str
VKT	*1,540*	+8.7%	+21.3%	-1.9%	+31.3%	+11.2%
VHT	*31*	+6.4%	+20.2%	-0.2%	+45.5%	+16.2%

The MVEIM is employed to compute the emissions source strength for a base year (1991) and the relative percentage increase/decrease for the present (1996) and two future years (2006 and 2016). These values are presented are in Table 9.4.

The emissions of all pollutants decrease with the exception of carbon dioxide and sulphur dioxide (in 1996). The increase in carbon dioxide concentrations is due in part to catalysts being fitted on all vehicles in future years. The function of the catalytic converter is to convert carbon monoxide and hydrocarbons (e.g. 1,3-butadiene and benzene) into carbon dioxide. Catalysts also convert nitrogen monoxide to nitrogen and oxygen, hence the reduction in nitrogen oxides. It is assumed that nitrogen oxides comprise 92.5% nitrogen monoxide and 7.5% nitrogen dioxide at the exhaust tailpipe exit. The nitrogen monoxide converts to nitrogen dioxide in the atmosphere (as nitrogen monoxide is a relatively unstable chemical compound)

Sulphur dioxide is reduced because the quantity of sulphur in fuel (both diesel and petrol) will be reduced dramatically in 2005 (see Table 4.3 and Table 4.4). As the total volume of traffic increases, the number of diesel vehicles will also increase. This causes an increase in sulphur dioxide emissions in 1996 as diesel contains much more sulphur that petrol. In addition, the number of buses travelling along the route increases.

Table 9.4: Relative change in peak hour emission inventory with respect to base year 1991 (as computed by the MVEIM) at the junction with highest traffic volume in Dublin

Pollutant (g/hr)	1991	1996	2006 do-min	2006 do-str	2016 do-min	2016 do-str
CO	*13,729*	-32.9%	-80.0%	-83.6%	-86.4%	-90.2%
NM-VOC	*1,707*	-28.3%	-85.6%	-88.4%	-96.0%	-96.8%
PM_{10}	*56*	-12.3%	-69.4%	-75.7%	-77.7%	-81.7%
CO_2	*203,035*	+89.0%	+202.1%	+137.5%	+227.5%	+172.5%
1,3-butadiene	*26*	-14.3%	-72.2%	-77.6%	-92.2%	-93.7%
Benzene	*88*	-30.6%	-88.6%	-90.7%	-97.9%	-98.4%
$PM_{2.5}$	*4*	-12.3%	-69.4%	-75.7%	-77.7%	-81.7%
SO_2	*33*	+56.6%	-39.8%	-52.7%	-34.8%	-45.8%
Methane	*63*	-18.8%	-69.4%	-76.1%	-87.3%	-88.9%
NO_x	*2,424*	-21.0%	-71.5%	-78.3%	-84.4%	-86.8%

CALINE4R is employed to compute the maximum pollutant concentrations for the base year (1991) and the relative percentage increase/decrease for the present (1996) and two future years (2006 and 2016). The values are presented in Table 9.5 and give an indication as to whether the pollutant concentrations at that junction are increasing or decreasing. The concentrations of all pollutants decrease with the exception of carbon dioxide. Sulphur dioxide increases in 1996 due to the increased volume of traffic. However, it reduces in future years due to the decrease of sulphur in fuel.

Table 9.5: Relative change in maximum 1-hour concentrations with respect to base year 1991 (as computed by CALINE4R) at the junction with highest traffic volume in Dublin

Pollutant	1991	1996	2006 do-min	2006 do-str	2016 do-min	2016 do-str
CO (ppm)	*9.5*	-35.8%	-78.9%	-83.2%	-83.2%	-89.5%
NM-VOC (ppb)	*435.0*	-32.0%	-86.9%	-87.8%	-96.1%	-96.4%
PM_{10} ($\mu g/m^3$)	*37.8*	-10.1%	-72.2%	-73.5%	-73.8%	-78.3%
CO_2 (ppm)	*72.7*	+63.1%	+157.6%	+128.6%	+178.5%	+147.2%
1,3-butadiene (ppb)	*9.2*	-21.7%	-76.1%	-78.3%	-99.0%	-99.0%
Benzene (ppb)	*21.5*	-35.8%	-87.4%	-94.0%	-99.0%	-99.0%
$PM_{2.5}$ ($\mu g/m^3$)	*1.9*	-15.8%	-99.0%	-99.0%	-99.0%	-99.0%
SO_2 (ppb)	*8.3*	+20.5%	-50.6%	-57.8%	-45.8%	-51.8%
Methane (ppb)	*79.2*	-23.5%	-74.2%	-79.0%	-89.9%	-90.0%
NO_x (ppb)	*185.6*	-5.3%	-27.3%	-29.0%	-35.0%	-36.4%

9.6.3 JUNCTION WITH GREATEST TRAFFIC CONGESTION

SATURN & SATCHMO computed that the junction with the greatest traffic congestion in Dublin (denoted as #2077) is located at the intersection of Kilbarrack and Howth Roads. Figure 9.2 shows a schematic representation of the junction and the location of the

receptors. The roadway is a primary artery in to Dublin from the North. In addition, there is only one lane travelling in each direction. The roadways were modelled as individual links, with each link being divided into two segments representing the areas where vehicles are most likely to be queuing or cruising.

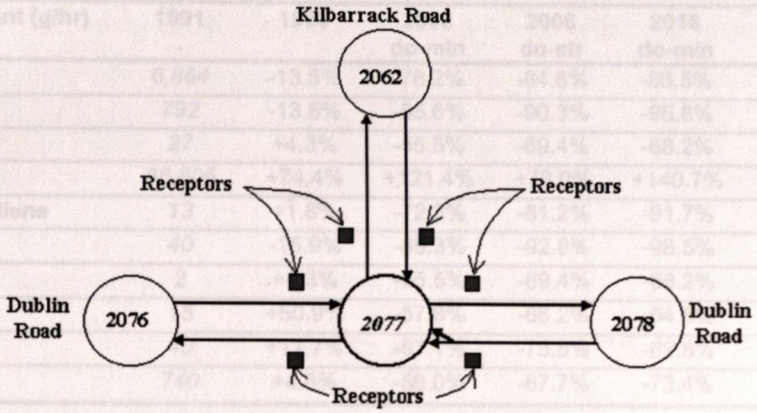


Figure 9.2: Schematic representation of junction with greatest traffic congestion in Dublin (#2077)

For the purpose of this exercise, SATURN & SATCHMO computed the peak hour VKT and VHT for the links shown in Figure 9.2 only. These values are presented in Table 9.6 for the base year (1991) and the relative percentage increase/decrease for the present (1996) and two future years (2006 and 2016). The VKT increases every year. The VHT decreases every year except in the 2016 do-minimum strategy where it is projected it will increase by nearly 10%. Only queues on the approach links to the junction are taken into account in the calculation of VHT, along with the time it takes for the total number of vehicles to traverse the 200m buffer distance. It is assumed that there are no vehicle queues on the departure links.

Table 9.6: VKT and VHT (as computed by SATURN & SATCHMO) for junction with the greatest congestion in Dublin

Year	1991	1996	2006 do-min	2006 do-str	2016 do-min	2016 do-str
VKT	*590*	+40.4%	+50.3%	+20.8%	+61.4%	+23.2%
VHT	*154*	-5.3%	-3.9%	-66.2%	+9.5%	-53.0%

The MVEIM is employed to compute the peak hour emissions source strength for a base year (1991) and the relative percentage increase/decrease for the present (1996) and two future years (2006 and 2016). These values are presented in Table 9.7. Again, carbon dioxide emissions increase for all future scenarios due to increased numbers of vehicles. In

1996, many pollutant emissions (e.g. methane and nitrogen oxide) increase, while other emissions (e.g. benzene and carbon monoxide) decrease.

Table 9.7: Relative change in peak hour emission inventory with respect to base year 1991 (as computed by MVEIM) at the junction with the greatest congestion in Dublin

Pollutant (g/hr)	1991	1996	2006 do-min	2006 do-str	2016 do-min	2016 do-str
CO	*6,864*	-13.5%	-76.2%	-84.6%	-86.5%	-91.2%
NM-VOC	*792*	-13.8%	-85.6%	-90.3%	-95.8%	-97.2%
PM_{10}	*27*	+4.3%	-55.5%	-69.4%	-68.2%	-78.4%
CO_2	*86,805*	+74.4%	+121.4%	+78.0%	+140.7%	+82.9%
1,3-butadiene	*13*	+1.8%	-72.3%	-81.2%	-91.7%	-94.5%
Benzene	*40*	-15.9%	-89.3%	-92.8%	-98.5%	-99.0%
$PM_{2.5}$	*2*	+4.3%	-55.5%	-69.4%	-68.2%	-78.4%
SO_2	*15*	+50.9%	-57.8%	-66.2%	-54.5%	-65.5%
Methane	*40*	+11.7%	-67.1%	-75.8%	-89.8%	-92.1%
NO_x	*740*	+4.6%	-56.0%	-67.7%	-73.4%	-80.9%

CALINE4R is employed to compute the pollutant concentrations for a base year (1991) and the relative percentage increase/decrease for the present (1996) and two future years (2006 and 2016). These values are presented in Table 9.8. As expected, the concentrations of all pollutants decrease for the future scenarios with the exception of carbon dioxide. In 1996, $PM_{2.5}$ along with carbon dioxide and sulphur dioxide increase while the rest decrease.

Table 9.8: Relative change in maximum 1-hour concentrations with respect to base year 1991 (as computed by CALINE4R) at the junction with greatest congestion in Dublin

Pollutant	1991	1996	2006 do-min	2006 do-str	2016 do-min	2016 do-str
CO (ppm)	*12.7*	-22.8%	-78.0%	-81.1%	-88.2%	-89.8%
NM-VOC (ppb)	*543.4*	-24.6%	-87.5%	-88.9%	-96.7%	-97.1%
PM_{10} ($\mu g/m^3$)	*53.8*	-3.9%	-56.5%	-72.5%	-61.5%	-76.0%
CO_2 (ppm)	*94.5*	+33.5%	+53.8%	+29.6%	+60.7%	+37.4%
1,3-butadiene (ppb)	*11.8*	-11.9%	-71.2%	-84.7%	-99.0%	-99.0%
Benzene (ppb)	*25.6*	-26.6%	-89.8%	-91.1%	-99.0%	-99.0%
$PM_{2.5}$ ($\mu g/m^3$)	*3.9*	+21.6%	-99.0%	-99.0%	-99.0%	-99.0%
SO_2 (ppb)	*10.7*	+21.5%	-66.4%	-71.0%	-65.4%	-70.1%
Methane (ppb)	*123.8*	-7.9%	-73.6%	-76.7%	-93.9%	-93.9%
NO_x (ppb)	*155.0*	-5.5%	-32.8%	-37.7%	-45.0%	-46.8%

It is worth noting that a direct correlation between emissions and concentrations does not exist. For example, emissions of nitrogen oxides increased by 5%, while ambient concentrations of nitrogen oxides decreased by 6%.

9.6.4 Alternative Method to determine Potential Hotspot

One of the primary drawbacks of the above selection criteria for junctions is that they both only take one junction into account. The criteria rank junctions according to traffic volume or vehicular delay. While a relationship does exist between traffic volume and vehicular delay, other factors such as junction geometry and surrounding topography are also important. In addition, in urban areas, junctions may be located quite close to each other. In view of the above, a more general approach is required to determine the location where the highest ambient concentrations are likely to occur. The approach used here employs the link-by-link emissions data calculated by the MVEIM to determine the area where the greatest total emissions are produced. This approach is based upon the principle that pollutant concentrations at any location are a function of all the emission sources in the near vicinity, while beyond a certain distance the effects of emissions become negligible.

The DMRB contains a model, which is used to assess the environmental impact of proposed roads and bridges in the UK [UK-DOT, 1993]. The DMRB employs a maximum distance of 200m from the centre of a roadway as a cut-off point in the model for rural roads. When assessing the environmental impact of roads, Li et al. [1999] recommend analysing the distribution of pollutant concentrations in the scope of 200m from road centrelines. Wrobel et al. [2000] found that the traffic contribution in the coarse particle size fraction was approximately 80% up to 150m from the road; it dropped abruptly over a distance of 150 to 200m. Collins [1988] noted that line dispersion models can only accurately model pollution levels close to the emissions sources, for example, up to a distance of 200m in the case of CALINE4. In addition, deHoogh [1999] found that, "it is widely accepted that dispersion models such as CALINE are relatively inaccurate at distances greater than this". Therefore, moving circular buffer zones with a radius of 200m across were employed in the study domain. This radius of 200m reflects the area of influence around a receptor. This approach therefore assumes that concentration at any location is a function of its distance from a roadway.

All roadways that start and finish inside the circular buffer zone are included in the total. Roadways that are partially inside a buffer zone are added to the total on a pro-rata basis (see Figure 9.3). This is performed by automatically searching for all nodes within 200m of a receptor point (h, k). Roadways are identified by a start (x_1, y_1) and finish node (x_2, y_2), and are assumed to be connected by a straight line. All the roadways that traverse the buffer zone boundary limit are identified. Then using trigonometry, the point (x_i, y_i) of

intersection of the circle and line is found, and the length of the roadway segment inside the buffer zone is calculated and added to the total.

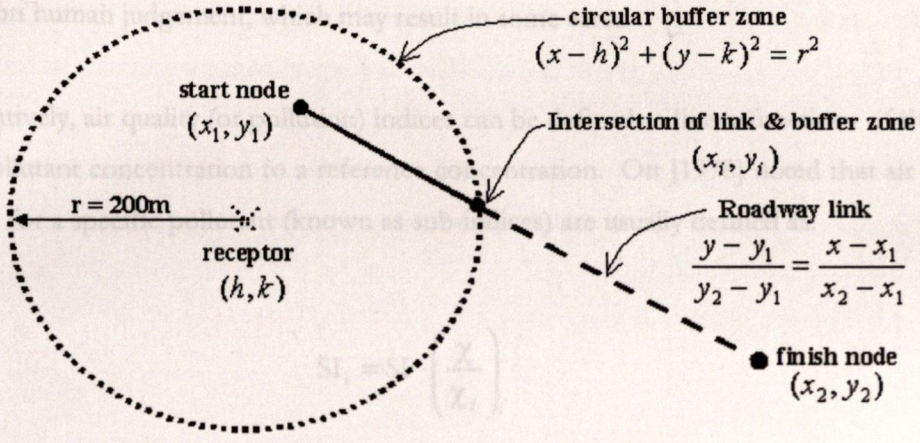


Figure 9.3: Geometry of moving buffer and roadway link

The computed value at the centre of the buffer zone is a function of the local road network density, traffic volume and delay, fleet composition, and corresponding emissions produced. The direction of the link is also checked as queuing only occurs on approach links to junctions. The buffer zone with the highest total emission rate is selected as the potential most polluted area. It should be noted that the effect of buildings is not taken into account in this approach.

9.6.5 Formulation of an Air Emissions Index

The MVEIM calculates eight different pollutant emissions and two greenhouse gases (CO_2 and CH_4). However, to identify the worst potential hotspot, it is not sufficient to simply determine the total amount of each pollutant emitted (on a mass basis). For example, one buffer zone may release more benzene than another, but less particulate matter depending on the ratio of petrol to diesel engined vehicles traversing the roadways in the buffer zone. In addition, the environmental effect of 1kg/m^2 of carbon dioxide emissions is far less than 1kg/m^2 of 1,3-butadiene emissions (with all other things being equal).

A number of methods to determine air quality (or pollution) indices have been developed to compare pollutant levels. For example, Sengupta et al. [1996] proposed a comparison matrix of three pollutants (SO_2, NO_x, and TSP) formed on a priority scale of their reactive toxicity to human health. The 'weightages' for SO_2, NO_x, and TSP were 71%, 21% and 8% respectively. Sharma [1999] formulated a method to calculate air quality indices based

on various physical and chemical characteristics of suspended particulate matter, such as particle size distribution, chemical (elemental) properties and parameters governing the acidity of precipitation. However, a major drawback of these methods is that they are based on human judgement, which may result in some error.

Alternatively, air quality (or pollution) indices can be defined as linear functions of the ratio of a pollutant concentration to a reference concentration. Ott [1978] noted that air quality indices for a specific pollutant (known as sub-indices) are usually defined as:

$$SI_i = SF \cdot \left(\frac{\chi}{\chi_r} \right)_i \qquad \textbf{9.1}$$

where: SI_i is the sub-index for a pollutant i;

SF is a scaling factor;

χ is the observed pollutant concentration; and

χ_r is a reference pollutant concentration.

The US-EPA [1994] employs a scaling factor of one hundred, while Bezuglaya et al. [1993] used a scaling factor of one in Russia. The sub-indices are then aggregated together using a variety of techniques, including linear-sum, root-mean-square, maximum-operator, and arithmetic-mean amongst others.

Trozzi et al. [1999] employed a maximum operator as an aggregation function and a scaling factor of one hundred in determining an overall air quality index, that is:

$$AQI = \text{Maximum}\{SI_i\} = \text{Maximum}\left\{ 100 \cdot \left(\frac{\chi_i}{S_i} \right)_{i=1}^{N_p} \right\} \qquad \textbf{9.2}$$

where: AQI is the overall Air Quality Index for all pollutants;

χ is the hourly concentration for NO_2, CO and O_3, while it is the rolling 24-h concentration for SO_2 and PM_{10}; and

S_i is the 'attention state' pollutant concentration value (similar to an air quality standard);

N_p is the number of pollutants.

The US-EPA employ a maximum operator as an aggregration function in reporting air quality also. However, this approach neglects the role of synergism between the individual pollutants in affecting air quality and health [Wark and Wong, 1999].

Bezuglaya et al. [1993] formulated a technique to determine the index of air pollution with several pollutants, using a linear aggregation method, that is:

$$AQI = \sum_{i=1}^{N_p} \left(\frac{\chi_i}{MPC_i} \right)^{C_i} \qquad 9.3$$

where: χ is the measured ambient concentration of pollutant i;

MPC_i is the Maximum Permissible Concentration for pollutant in Russia (similar to an air quality standard);

C_i is a four-tiered danger level degree exponent for each pollutant relative to sulphur dioxide (ranging from 0.9 to 1.7).

Swamee and Tyagi [1999] state that the "maximum operator aggregation does not consider change in the remaining pollutants", whereas other aggregation methods such as "linear sum and root-sum suffer from ambiguity". In response, Swamee and Tyagi [1999] proposed an aggregated (i.e. root-sum-power) AQI (that is free from ambiguity) as:

$$AQI = \left[\sum_{i=1}^{N_{SI}} (SI_i)^{1/m} \right]^m = \left[\sum_{i=1}^{N_{SI}} \left(\frac{\chi}{\chi_s} \right)_i^{1/m} \right]^m \qquad 9.4$$

where: N_{SI} is the number of sub-indices; and

SI_i is the i^{th} Sub-Index;

χ is the measured ambient concentration of pollutant i;

χ_s is a standard concentration of pollutant i (e.g. air quality standard);

m is an exponent.

It is worth noting that as the exponent m approaches infinity, the root-sum-power aggregation method employed by Swamee and Tyagi [1999] is approximately equal to the maximum aggregation method.

The UK Environment Agency [Ridley, 1999] developed the VIM to determine the 'greenest' vehicle available. The VIM uses the vehicle pollutant mass release rate over a regulatory driving cycle (the specific vehicle's EURO3 emission data) instead of the measured ground level concentration as defined by Ott [1978]. A linear sum is employed as an aggregation function and a scaling factor of 50 and 90 for rural and urban areas respectively. The air quality effect of a motor vehicle is calculated as:

$$AQE_v = SF\sum_{i=1}^{N_p}\left(\frac{ME_i}{NAQS_i}\right) \qquad \textbf{9.5}$$

where: AQE_v is the Air Quality Effect of vehicle v;
N_p is the number of pollutants; and
ME_i is the Mass Emission of pollutant i (in g/km or g/s);
$NAQS_i$ is the National Air Quality Standard for pollutant i (in $\mu g/m^3$).

A major disadvantage of this AQE_v index is that different denominator time-scale units are mixed (i.e. the denominator varies for different pollutants while the numerator remains constant). For example, benzene has an air quality standard expressed as an annual average while carbon monoxide has an air quality standard defined as a one-hour average.

During this research, an integrated AEI was formulated to determine the combined environmental effect of an emissions inventory in a targeted study area. Similar to the VIM, the AEI employs an emissions inventory instead of the measured pollutant concentration level, a root sum square aggregation function, and a scale factor of one. The AEI is calculated as:

$$AEI = \sqrt{\sum_{p=1}^{N_p}\left(\frac{MRR_p}{AQS_p}\right)^2} \qquad \textbf{9.6}$$

where: AEI is the air emissions index;

MRR_p is the Mass Release Rate of pollutant p emitted in the study area (in kg/hr or equivalent);

AQS_p is the Air Quality Standard for pollutant p (in $\mu g/m^3$) and

N_p is the total number of pollutants.

The units of the AEI are $(kg/hr)/(\mu g/m^3)$ or equivalent. One of the primary advantages of this definition of an AEI is that the ambient air quality for a pollutant can be taken into account by subtracting it from the AQS for that pollutant. This biases the AEI towards pollutants that have high measured concentrations.

$$AEI = \sqrt{\sum_{p=1}^{N_p} \left(\frac{M_p}{AQS_p - AMC_p} \right)^2} \qquad 9.7$$

where AMC_p is the Ambient Measured Concentration of pollutant p (in $\mu g/m^3$). Background pollutant concentrations may also be employed in the AEI instead of ambient pollutant concentrations as:

$$AEI = \sqrt{\sum_{p=1}^{N_p} \left(\frac{M_p}{AQS_p - BMC_p} \right)^2} \qquad 9.8$$

where BMC_p is the Background Measured Concentration of pollutant p (in $\mu g/m^3$). The AEI not only represents the integrated influence from multi-pollutant emissions on the environment, but also puts stress on the damage from severe air pollutants as well.

A major drawback of the AEI is that it does not take into account meteorological conditions. Consequently, an API is formulated. The API is computed from the quotient of the AEI and the volume of air in which the emissions are mixed (known as the control volume). The control volume is computed from the product of the mean wind speed, the width of the emissions area perpendicular to mean wind speed and the mixing height. The unit of the control volume is m^3/s or equivalent. The API is written in symbolic form as:

$$API = \frac{AEI}{CV} \qquad 9.9$$

where: API is the air pollutant index (in s/m^3 or equivalent); and

CV is the control volume above the emitted pollutants (in m^3/s or equivalent).

The API takes two meteorological conditions (i.e. wind speed and mixing height) into account. Therefore, it may be employed to compare the relative severity of emissions produced in different geographic areas and for different years.

9.6.6 Potential Highest Polluted Location

The buffer zone with the highest AEI is located in the city centre on Custom House Quay. Figure 9.4 illustrates the intersections in the buffer zone.

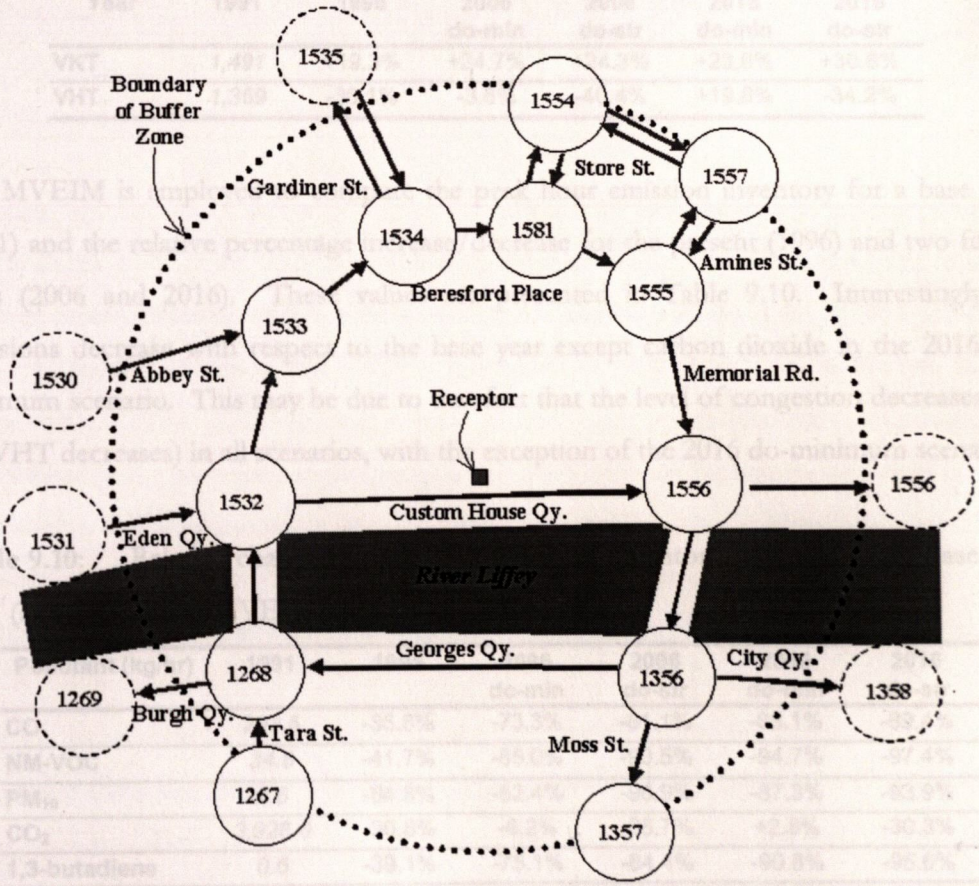


Figure 9.4: Schematic representation of moving buffer zone with highest emissions in Dublin

For clarity, only the direction of traffic is shown between the junctions in Figure 9.4. The buffer zone boundary is depicted using a dotted line. Junctions located outside the buffer zone are shown with dashed circles. The receptor is located along Custom House Quay in the centre of the buffer zone as illustrated in the diagram.

For the purpose of this exercise, SATURN & SATCHMO computed the peak hour VKT and VHT for the links shown in Figure 9.4 only. These values are presented in Table 9.9. The VKT increases all the time with respect to the base year regardless of the scenario being implemented (i.e. do-minimum or do-strategy). However, the VHT decreases in all years except the 2016 do-minimum scenario. Therefore, while more vehicles are travelling in the buffer zone, they are expected to take less time. The increase in VHT in the 2016 do-minimum scenario indicates that congestion is increasing.

Table 9.9: VKT and VHT (as computed by SATURN & SATCHMO) for buffer zone surrounding receptor on Custom House Quay

Year	1991	1996	2006 do-min	2006 do-str	2016 do-min	2016 do-str
VKT	*1,491*	+19.3%	+24.7%	+24.3%	+23.6%	+30.8%
VHT	*1,369*	-30.1%	-3.6%	-40.4%	+19.8%	-34.2%

The MVEIM is employed to compute the peak hour emission inventory for a base year (1991) and the relative percentage increase/decrease for the present (1996) and two future years (2006 and 2016). These values are presented in Table 9.10. Interestingly, all emissions decrease with respect to the base year except carbon dioxide in the 2016 do-minimum scenario. This may be due to that fact that the level of congestion decreases (i.e. the VHT decreases) in all scenarios, with the exception of the 2016 do-minimum scenario.

Table 9.10: Relative change in peak hour emission inventory with respect to base year 1991 (as calculated by MVEIM) on Custom House Quay

Pollutant (kg/hr)	1991	1996	2006 do-min	2006 do-str	2016 do-min	2016 do-str
CO	*293.6*	-35.8%	-73.3%	-81.1%	-85.1%	-89.4%
NM-VOC	*34.6*	-41.7%	-85.0%	-90.5%	-94.7%	-97.4%
PM_{10}	*2.6*	-64.8%	-82.4%	-90.9%	-87.3%	-93.9%
CO_2	*3,928.6*	-30.6%	-6.2%	-35.7%	+2.8%	-30.3%
1,3-butadiene	*0.6*	-39.1%	-75.1%	-84.4%	-90.8%	-95.6%
Benzene	*1.5*	-35.9%	-88.1%	-91.5%	-98.3%	-98.8%
$PM_{2.5}$	*0.2*	-64.8%	-82.4%	-90.9%	-87.3%	-93.9%
SO_2	*0.8*	-42.5%	-85.1%	-89.7%	-83.8%	-89.0%
Methane	*1.2*	-32.5%	-73.1%	-82.7%	-88.8%	-94.7%
NO_x	*41.0*	-55.2%	-75.0%	-86.3%	-82.9%	-91.6%

CALINE4R is employed to compute the maximum one-hour concentrations for worst-case meteorology conditions. These values are presented in Table 9.11. The pollutant concentrations at the receptor site are much higher than at either of the junctions investigated above. This shows that while the effect of emissions from individual junctions may not exceed air quality standards, combinations of junctions in close proximity can.

Table 9.11: Relative change in maximum 1-hour concentrations with respect to base year 1991 (as computed by CALINE4R) on Custom House Quay for worst-case meteorology conditions

Pollutant	1991	1996	2006 do-min	2006 do-str	2016 do-min	2016 do-str
CO (ppm)	*20.7*	-2.9%	-64.7%	-67.6%	-77.3%	-84.1%
NM-VOC (ppb)	*1054.5*	-48.2%	-87.7%	-90.1%	-95.0%	-97.5%
PM_{10} ($\mu g/m^3$)	*93.3*	+51.6%	-35.4%	-58.6%	-49.4%	-74.6%
CO_2 (ppm)	*261.5*	-31.7%	-16.8%	-32.0%	+2.9%	-34.5%
1,3-butadiene (ppb)	*31.6*	-29.1%	-74.4%	-79.1%	-89.6%	-93.4%
Benzene (ppb)	*38.1*	-6.3%	-84.5%	-85.6%	-97.1%	-98.2%
$PM_{2.5}$ ($\mu g/m^3$)	*33.1*	-71.3%	-87.0%	-91.8%	-89.7%	-96.4%
SO_2 (ppb)	*41.6*	-46.4%	-88.0%	-89.7%	-84.9%	-90.9%
Methane (ppb)	*159.6*	-6.9%	-64.7%	-72.4%	-83.8%	-92.5%
NO_x (ppb)	*297.6*	-50.8%	-66.4%	-71.7%	-70.6%	-77.2%

Ambient concentrations due to traffic in the buffer zone decrease for all pollutants except carbon dioxide under the 2016 do-minimum scenario. This is a positive sign, even though some of these pollutants may exceed air quality standards. For example, in 1991 and 1996, nitrogen dioxide exceeds the WHO guideline of 104 ppb for maximum hourly concentration. The WHO guideline value of 25.8 ppm for carbon monoxide measured over 1-hour is not exceeded in any year. The UK-NAQS for carbon monoxide is 10 ppm as a running eight-hour average [Murley, 1999]. By applying a persistence factor of 0.7, the eight-hour average can be calculated from the peak hour value. The receptor would exceed the UK-NAQS in 1991 and 1996. However, it would reach attainment in all future years.

Since the worst-case pollutant estimates exceed some air quality standards, the next step is to perform a comprehensive analysis using measured weather data. For 1991 and 1996, the actual weather data from Dublin Airport for the respective years is employed by CALINE4R (i.e. CALINE4R was 'run' 8,760 times for each year). For future years, ten years of weather data (from 1986 to 1995) is employed by CALINE4R (i.e. CALINE4R was 'run' 87,648 times for each year and scenario).

Table 9.12 gives the resulting average pollutant concentrations as computed by CALINE4R. The pollutant concentrations are lower as expected. However, 1,3-butadiene exceeds the UK-NAQS of 1 ppb in 1991, 1996 and 2006 do-minimum scenario. In addition, benzene exceeds the UK-NAQS of 5 ppb in 1991. NO_x exceeds the UK-NAQS of 21 ppb in all years and scenarios. NO_x also exceeds the WHO guideline for Europe of 20.8 ppb in all years and scenarios.

Table 9.12: Relative change in annual average 1-hour concentrations with respect to base year 1991 (as computed by CALINE4R) on Custom House Quay

Pollutant	1991	1996	2006 do-min	2006 do-str	2016 do-min	2016 do-str
CO (ppm)	*2.9*	0.0%	-62.1%	-62.1%	-75.9%	-82.8%
NM-VOC (ppb)	*135.4*	-8.8%	-77.0%	-81.4%	-88.8%	-95.3%
PM_{10} ($\mu g/m^3$)	*11.3*	+83.2%	-6.2%	-47.8%	-24.8%	-67.3%
CO_2 (ppm)	*33.3*	-22.5%	7.8%	-16.5%	27.0%	-14.1%
1,3-butadiene (ppb)	*4.1*	-19.5%	-68.3%	-75.6%	-82.9%	-92.7%
Benzene (ppb)	*5.4*	-3.7%	-83.3%	-83.3%	-96.3%	-98.1%
$PM_{2.5}$ ($\mu g/m^3$)	*4.1*	-61.0%	-82.9%	-90.2%	-87.8%	-95.1%
SO_2 (ppb)	*5.3*	-37.7%	-84.9%	-86.9%	-81.1%	-88.7%
Methane (ppb)	*20.5*	+6.8%	-57.1%	-65.9%	-75.6%	-90.7%
NO_x (ppb)	*72.8*	-29.3%	-44.5%	-50.4%	-48.9%	-70.3%

9.7 DISCUSSION

It is worth noting that every application site is different and trends observed at one site are not necessarily noticed at other sites. Boddy [1999] came to a similar conclusion when performing a spatial and temporal analysis of pollutant levels at various sites in the UK. The relationship between traffic and pollutants is complex, and depends on traffic operating profiles, dispersion, local climate and turbulence, chemistry, site characteristics [Bell, 1999]. In the application sites, there is no direct correlation between emission inventory and ambient pollutant concentrations.

The results show a significant decrease in ambient concentrations between 1991 and 1996, yet there is no evidence that this has occurred, e.g. measurements by Dublin Corporation have not shown a decrease in NO_x concentration levels. For example, the annual average NO_2 concentrations measured at College Green show a consistent increase every year (from 1991 to 1996) [Dublin Corporation, 1998], while the annual average concentration predicted by the AQMS decreases (e.g. in Table 9.12 NO_2 concentrations decrease by 21%).

There are a number of reasons for these discrepancies. First, the traffic activity data was obtained from SATURN & SATCHMO. While, SATURN & SATCHMO was validated at a number of sites in Dublin both by the author (see Chapter seven) and Dublin Transport Office [McCabe, 1998], it was not validated at every location. Secondly, the fleet composition data was obtained from licensing records, which give the composition as registered in Dublin, not the actual composition on the individual streets. Thirdly, there are errors associated with the emissions factors employed. However, these are thought to be relatively low since the MVEIM was successfully validated.

The predictions for future years (2006 and 2016) exhibit even greater decreases in many pollutant concentrations. These predictions assume that all cars will be equipped with catalysts and that the catalysts will operate efficiently. Therefore, emissions of many pollutants and consequently ambient concentrations should decrease. There is no allowance made for 'tampering', 'malfunction of emission control equipment' or 'poor maintenance' of vehicles as this data does not exist currently in Ireland. Finally, as with any future projections, the emission factors employed are subject a high degree of uncertainty.

9.8 SUMMARY

This Chapter has described the application of the combined MVEIM and CALINE4R at three sites in Dublin. The first site is located at the junction with the highest peak demand hour traffic volume. The second site is located at the junction with the worst level of service. Finally, the third site is situated at the location with the greatest potential for elevated ambient pollutant levels. An emission inventory and pollutant concentrations were estimated at each site assuming worst-case meteorology. In addition, sequential meteorological data was employed at the third site.

The next Chapter will provide an overall summary of the work performed in this research project. In addition, the main conclusions drawn from this project and the tremendous scope for future work will be outlined.

10. CONCLUSIONS, MAJOR CONTRIBUTIONS AND FUTURE WORK

10.1 SUMMARY

The thesis has described the development and application of an urban AQMS. The AQMS can be subdivided into two primary models, namely an emission inventory model (i.e. MVEIM) and a pollutant dispersion model (i.e. CALINE4R).

The MVEIM comprises of a number of modules, namely a traffic (SATURN & SATCHMO) module, an EECT module, a MVERA module, and a MVFC module. In addition, the MVEIMl also includes a database of relevant emission and fuel consumption factors. Real-time traffic data can be obtained from an urban traffic control system (e.g. SCATS and SCOOT). The EECT module estimates the vehicle technology distribution per vehicle category (e.g. LGV, HDV, and bus) for each link in the network.

The MVEIM predicts key motor vehicle emissions such as NO_x, SO_2, CO, CO_2, and PM_{10}. It can also predict less frequently-considered emissions such as CH_4, NM-VOC, C_4H_6, C_6H_6, and $PM_{2.5}$. Emissions are estimated as three types, namely hot-stabilised, start-up and evaporative on a link-by-link basis, with each link being divided into two segments, representing the areas that vehicles are most likely to be in either cruise or creep mode. The kernel of the MVERA module is a database of vehicle emissions factors (hot stabilised, start-up, and evaporative) for petrol, diesel and alternative fuels (such as LPG and CNG). Since limited emission factors are available specifically for Ireland, these are primarily derived from the MEET project, supplemented by others.

The dispersion module translates the pollutant emissions determined by the MVEIM into time and spatial patterns of the resulting states of the natural environment. The dispersion module takes into account traffic volume and associated emission rates at a specific location, along with meteorological conditions experienced, and the local topography specific geometry, to estimate ambient concentrations for each of the atmospheric pollutants identified above. A literature review revealed a number of deficiencies in present version of CALINE4; consequently, an enhanced version of CALINE4, named CALINE4R was developed.

The AQMS was validated at a heavy trafficked junction in Dublin city centre. Traffic activity and fleet composition data were measured at the site using CCTV and the SCATS urban traffic control system. Local meteorology and ambient kerbside pollutant concentrations were simultaneously measured also. In addition, the model was validated at two other sites, one in Melton Mowbray, UK and one in Hannover, Germany. The model performed acceptably well at all three sites. For example, over two-thirds of all predicted pollutant concentrations (with the exception of C_4H_6 and C_6H_6 in Dublin) are within a factor-of-two of the measured values. In addition, the AQMS meets Kumar's [2000] performance criterion for all predicted pollutant concentrations (again with the exception of C_4H_6 and C_6H_6 in Dublin).

An emission and fuel consumption inventory using a bottom-up approach was compiled for the greater Dublin area using the MVEIM for the past (1991), the present (1996) and two future years (2006 and 2016). Two different emission and fuel consumption inventories were compiled for do-minimum and do-strategy scenarios in both future years. The do-strategy scenario represents a set of transport policies currently being implemented in the Dublin area. In addition, a comparison of an emission and fuel consumption inventory compiled using a top-down approach and a combined bottom-up approach for 1996 was performed. The 1996 fuel consumption inventory was validated against retail fuel sales.

The AQMS was applied at three potential hotspots in Dublin. The first was located at the junction with the highest traffic volume, while the second was located at the junction with the greatest congestion. The third hotspot was situated at the location with the greatest combined potential for emissions and subsequent concentrations, this being identified on the basis of the emissions for each link.

10.2 CONCLUSIONS

The main conclusions are from this project are summarised in this section.

Traffic-related urban emissions inventories have been developed for decades in the United States, but the resulting methodologies and databases are not directly transferable to other countries due to a variety of technical, institutional and economical barriers. European states therefore require their own methodology for preparing and validating inventories of

traffic related air pollution emissions. Whereas the US approach relies extensively on expensive source testing, the AQMS has been verified through the separate validation of its individual components.

Even though the AQMS contains a number of uncertainties due to model limitations and assumptions, its estimations were reassuringly close to real world measurements. The model performed best for carbon monoxide at Melton Mowbray in the UK (i.e. both the slope and intercept of the regression line was not statistically significantly different from one and zero respectively). There are a number of reasons for this. For example, carbon monoxide is a relatively inert pollutant. In addition, the observed data (e.g. traffic activity) were collected over a month (as compared to a week in Dublin). Overall, it may be concluded that the AQMS gives sound predictions of local urban air quality.

Since the methodology employed in the MVEIM is generic, future improved emission factors can be readily incorporated into the database, as can factors relating to new alternative fuels such as methanol and ethanol.

The AQMS is designed to perform a worst-case analysis as well as a time series analysis using local meteorological data. This design also enables the model to be easily updated over time to include the latest research results.

One of the major advantages of AQMS is that it can employ either real-time traffic data from an urban traffic control system or passive traffic data from a traffic network module. This has been successfully demonstrated in Dublin using traffic data from the SCATS traffic control system and in Melton Mowbray using traffic data from the SCOOT traffic control system.

SCOOT traffic data is more complete for use with an emissions inventory models than SCATS traffic data. For example, SCOOT supplies traffic volume, number of stops, and vehicle delay, while SCATS supplies traffic volume and degree-of-saturation. An extensive literature review failed to uncover a direct relationship between degree-of-saturation and vehicle delay. Neither traffic control system differentiates between vehicle types, and consequently statistical data, CCTV and manual traffic surveys must be employed to estimate fleet composition.

In the emission inventory, emissions of all pollutants are decreasing with respect to the base year (1991), with the exception of carbon dioxide. This is due mainly to stricter emission limits on new vehicles and the use of three-way catalytic converters. However, catalysts will increase carbon dioxide emissions slightly.

At present, improvements in emission control technology appears to be one of the most effective ways in reduce traffic related emissions. However, alternative fuels also exhibit great potential in the reduction of emissions. The effect of employing alternative fuels such as CNG and LPG in high-travel depot-based diesel vehicles was investigated and showed promising results. In addition, transport management strategies currently being implemented in the Dublin area also exhibited a reduction in emissions.

Comparison of top-down and bottom-up urban emission inventories for 1996 revealed substantial differences. This was due to a major difference in the VKT data employed in either case. In addition, queuing is not taken into account explicitly in the top-down approach, and an average speed was assumed for the entire domain study area. The bottom-up fuel consumption inventory compared favourably with retail fuel sales, while the top-down exhibited a large discrepancy. This discrepancy highlights the dangers of employing a top-down approach in emission inventory compilation for urban areas.

Pollution hotspots are often considered to occur at junctions with the highest traffic volume or with the greatest congestion. However, a new method developed during the course of this research found that other areas are likely to experience higher ambient concentrations.

10.3 MAJOR CONTRIBUTIONS

This section provides a discussion on the scientific contributions of this research project to the field of 'air quality'.

First, this project brings together state-of-the-practice and state-of-the-art in traffic related air quality modelling. Frequently, many research models have proven very difficult, if not impossible, to implement on a large urban scale. To this end an AQMS has been developed that incorporates the latest traffic related air quality knowledge at a high level of spatial and temporal resolution (restricted only by data availability)

The AQMS can use traffic data from both a traffic model (SATURN & SATCHMO) and an urban traffic control system. The AQMS can incorporate real-time traffic data from both SCATS and SCOOT urban traffic control systems. These traffic control systems differ fundamentally in the traffic data that they provide. For example, SCATS computes traffic volume only, while SCOOT computes the traffic volume along with vehicular delay and number of stops on a link. While previous studies have implemented other air quality models with SCOOT, none have been implemented with both SCOOT and SCATS. The AQMS was successfully validated in Dublin with SCATS traffic data and in Melton Mowbray with SCOOT traffic data.

The most advanced vehicle emissions rate model currently in the world was developed by CE-CERT in the USA. The author worked on this project, and much of this experience is represented in the MVEIM described in this thesis. The ideal level of complexity for an traffic emissions model should lie between the most advanced vehicle emissions research efforts (e.g. CMEM) and the currently used speed dependent designated models (e.g. MOBILE6 and COPERT III). To this end, the MVEIM lies in between the precise (but extremely data intensive) microscopic approach and the inaccurate macroscopic approach. The MVEIM offers significant advantages over the forty-five emission rate models reviewed in Chapter two. For example, the MVEIM, as implemented can account for:

- Emissions of 6 pollutants (NO_x, SO_2, PM_{10}, $PM_{2.5}$, CO and NM-VOC), 2 greenhouse gases (CO_2 and CH_4) and 2 toxins (C_4H_6 and C_6H_6);
- Three different types of emissions (hot-stabilised, cold and evaporative);
- Five different types of fuels (petrol, diesel, LPG, CNG and bio-diesel);
- Ninety-four specific vehicle technology groups;
- The influence of vehicle load;
- The influence of vehicle accumulated mileage;
- Vehicle modal activity (i.e. explicit modelling of cruise/queue effects and implicit modelling of acceleration/deceleration effects);
- Three types of roadways (urban, rural and motorway);
- The influence of fuel RVP;
- The impact of ambient temperature; and
- The effect of roadway grade.

MEET emissions data (supplemented by other data) was employed in this project. The MEET project was undertaken to provide a basic, Europe-wide procedure for evaluating the impact of transport on air pollutant emissions and energy consumption. It brings together the most comprehensive and up-to-date information on vehicle emissions and activity statistics which, together, make it possible to estimate the emissions resulting from almost any transport operation. However, the MEET emissions data was developed for the estimation of emissions inventories on a national or regional scale and as such is not directly applicable to urban areas. This research has successfully adapted the emissions data for use at a local scale (i.e. high spatial resolution) in an urban area. The MVEIM is modular in design and therefore new and updated emissions data can be included as they become available. Consequently, an unlimited numbed of vehicle technology groups can be included in the MVEIM.

An extensive literature review revealed that one of the most commonly used pollutant dispersion models in the world currently is CALINE4. The current version of the model was developed by CALTRANS in the 1980s. However, a number of researchers and users have raised issues concerning the model (e.g. treatment of modal emissions, calculation of vehicle heat flux factor). To this end, CALINE4 has been reprogrammed and restructured, and an enhanced version known as CALINE4R has been developed. CALINE4R has expanded capabilities (increased number of links and receptors) and flexible input and output. In addition, CALINE4R contains new or improved algorithms that incorporate:

- Vehicle heat flux factors based on local fleet composition;
- Vehicle modal emissions at intersections;
- Treatment of calms (i.e. wind speed < 0.5 m/s);
- Computation of pollutant settling velocity;
- Improved description of dispersion process near roadways (i.e. new dispersion coefficients);
- National Weather Service data (e.g. allows annual averages to be computed);
- Pollutant decay; and
- Computation of photochemistry reaction rates.

Emissions inventories may be validated using remote sensing, on-board instrumentation and tunnel measurements. All methods involve the use of expensive equipment, which was not available during this research. Therefore, other methods were employed to

validate the MVEIM. As the fuel consumption factors and emissions factors were derived from the same source, the emission inventory was validated at a macroscopic level against retail fuel sales data in Dublin. In addition, the MVEIM was indirectly validated against ambient pollutant concentration measurements in Dublin, Hannover and Melton MowBray. Frequently, emissions inventories are not validated against measured data but against each other, for example [Seika et al., 1996], [Lindley et al., 2000].

The modular design of the AQMS allows an independent evaluation of the performance and precision of each of the individual components (e.g. traffic module, emissions rate module, and pollutant dispersion module). In addition, the ease of application and transferability of the MVEIM and CALINE4R means they have a wide range of academic and applied uses. The integration of individual well-accepted models (SATURN & SATCHMO traffic model, MEET emissions data, and the CALINE4 dispersion model) ensures that the new AQMS will be acceptable for regulatory purposes, including demonstrations of attainment with air quality standards, and environmental impact assessments.

As the environmental impacts of emissions are often as a result of a combination of pollutants, a novel air emissions index is formulated to compare different traffic related pollutants for air quality analysis purposes. It may be employed as an aid in determining the potential severity of air emissions within a fixed geographical area. The method consists of normalising the mass release rate of each pollutant in a specific domain by the corresponding air quality standard and the results are aggregated for all pollutants using the root-sum-square method. However, it does not take into account meteorological conditions. Consequently, an air pollutant index is formulated. The air pollutant index provides a general indication of a study domain's air pollution potential under specified conditions. In addition, the relative severity of areas may be ranked according to the pollutant index. It is envisaged that this approach will be used to compensate for the limited amount of pollutant measurement data available for some districts.

Air quality modelling and monitoring is usually carried out at locations where conditions are thought to be the most conductive to high concentration impacts. In urban areas, pollutant concentrations may be high near locations where traffic has a tendency to build-up, slow-down, and idle for a period of time, such as at a junction. Traditionally, monitoring has been performed at junctions with the highest traffic volume, the greatest level of congestion (i.e. worst LOS) or a combination of both. This method assumes that if

the area beside a junction selected based on the above criterion does not exceed air quality standards, neither will any other. However, recent research has shown that two junctions may have the same LOS, but produce different levels of emissions and resultant pollutant concentrations. In addition, a primary drawback of this selection criterion is that only one junction is taken into account (in urban areas, junctions may be located quite close to each other). In view of this, a more general approach is required to determine the location where the highest ambient concentrations are likely to occur. This approach, known as a 'moving buffer zone', employs the link-by-link emissions data to determine the location where the greatest total emissions are produced. The 'moving buffer zone' method is based upon the principle that pollutant concentrations at any location are a function of all the emission sources in the near vicinity, while beyond a certain distance the effects of emissions become less or negligible. The 'moving buffer zone' method may be used to locate ambient pollutant monitors.

10.4 RECOMMENDATIONS FOR FURTHER WORK

This research project performed over the past three years at Trinity College and described herein was ambitious, its goal being to establish an operational AQMS. Naturally, the scope for future work in this area is still tremendous. Some of the more important issues, which should be addressed, are as follows.

- Due to economic constraints, the validation of the AQMS has been limited to three sites and a small range of meteorological conditions. The AQMS should be further validated at other types of sites in Dublin and over longer periods of time.

- The PARAMICS traffic model is currently being set-up for the greater Dublin area. It would be advisable to compare traffic data from PARAMICS [Cameron and Duncan, 1996] with SATURN & SATCHMO and evaluate the resultant emissions inventories. However, although PARAMICS is a micro-simulation model and therefore, by definition, produces a higher spatial resolution of traffic activity, reliable and up-to-date emission factors are not yet available for this resolution.

- Persistence factors should be developed for Dublin to allow AQMS outputs to be compared with air quality standards and limits. This issue is being addressed in another research project currently being carried out at Trinity College [Keating et al., 1999].

- When reliable and up-to-date emission factors become available for acceleration and deceleration vehicle modes, it is suggested that these be incorporated into the EFD. The MVEIM can be easily upgraded to incorporate vehicle acceleration and deceleration.

- The level of uncertainty associated with the emissions inventory should be estimated using the various methods described in the literature review.

- Emissions factors should be measured from Irish vehicles and compared with MEET data.

- As researchers at the Institute of Transport Studies (UK) are currently using the ADMS-urban dispersion model to estimate ambient roadside pollution at Melton Mowbray, it would be very useful to compare the results obtained with those determined using CALINE4R.

- Ambient kerbside pollutant concentrations should be measured at the three potential hotspots identified in Dublin (i.e. the junction with highest traffic volume, junction with greatest traffic congestion, and the location with the greatest production of emissions). The EPA has commenced monitoring at the location identified as that with the greatest potential for production of emissions.

- The impact of the complete do-strategy scenario currently being implemented by DTO was evaluated together as it is modelled in the traffic module together. It is essential that environmental effects of individual components of the do-strategy scenario be evaluated separately.

APPENDIX A

The appendix contains a list of peered review publications and scientific communications produced during this research project.

JOURNALS:

Reynolds, A.W. and Broderick, B.M. Development of a GIS based urban air quality modelling system for transport related pollution. *International Journal of Environment and Pollution* (in press).

Reynolds, A.W. and Broderick, B.M. Emission and dispersion of NO_x from motor vehicles in Dublin. *Biology and the Environment* (in press).

Reynolds, A.W. and Broderick, B.M. (2000) Predicting real-time traffic-related PM_{10} and $PM_{2.5}$ emissions and concentrations in urban areas. *Journal of Aerosol Science* 31 (1), 250-252.

Reynolds, A.W. and Broderick, B.M. (2000) Development of an emissions inventory model for mobile sources. *Traffic Research: Part D – Transport and Environment* 5 (2), 77-101.

Reynolds, A.W. & Broderick, B.M. (1999) Air quality monitoring and modelling in Dublin. *Biology and the Environment* 99 (2), 125.

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Reynolds, A.W. and Broderick, B.M. (2001) A new method to identify potential traffic related pollutant hot-spots in urban areas. In: *Proceedings of 33rd Universities Transport Study Group (UTSG) Annual Conference*, Oxford, UK.

Reynolds, A.W. (2000) Influence and evaluation of meteorological parameters on urban air quality modelling using CALINE4R. In: *Proceedings of the 3rd Symposium on the Urban Environment*, San Diego, CA, USA, N° 15341.

Reynolds, A.W. (2000) Comparison of fuel-based macro-scale and micro-scale urban emission inventories. In: *Proceedings of the 93rd Air and Waste Management Association (AWMA) Annual Conference and Meeting – PhD Student Section*, Salt Lake City, Utah, USA, N° 54.

Reynolds, A.W. and Broderick, B.M. (2000) An air quality modelling system (AQMS) for traffic pollution in European cities. In: *Proceedings of 32nd Universities Transport Study Group (UTSG) Annual Conference*, Liverpool, UK, Vol. 3, N° D1.

Reynolds, A.W and Nolan, P.J. (2000) Development and implementation of an air quality model on a parallel computer. In: *Proceedings of Irish Society for Scientific and Engineering Computation (ISSEC) Annual Symposium*, Dublin, pp. 19.

Reynolds, A.W. and Broderick, B.M. (1999) Calculation of vehicle emissions and fuel consumption using modelled traffic data. In: *Proceedings of 8th International Symposium on Transport and Air Pollution / COST-319 Final Conference*, Graz, Austria, Vol. 76, Section III/4, pp. 15-24.

Reynolds, A.W. and Broderick, B.M. (1999) Air Pollution Monitoring and Modelling. In: *Proceedings of the 9th Irish Environmental Researchers' Colloquium*, Wexford, pp. 29.

Reynolds, A.W. (1999) Evaluating the environmental impacts of alternative-fuel public service vehicles. In: *Proceedings of the 92nd Air and Waste Management Association (AWMA) Annual Conference and Meeting – PhD Student Section*, St. Louis, MO, USA, N° DP104.

Reynolds, A.W. and Broderick, B.M. (1999) A GIS based transport and emissions model. In: *Proceedings of the 31st Universities Transport Study Group (UTSG) Annual Conference.* York, UK, Vol. 3, N° H1.

Reynolds, A.W. and Broderick, B.M. (1998) On-road motor vehicle emissions inventory models. In: *Proceedings of the 4th Urban Transport and the Environment for the 21st Century Conference*, Lisbon, Portugal, pp. 387-397.

TECHNICAL REPORTS:

Reynolds, A.W. (2000) *Development of a motor vehicle NO_x emission inventory.* ESB International, Dublin.

Reynolds, A.W. and Broderick, B.M. (2000) *TCD/ITS collaborative research project.* Draft Report for 'Enterprise Ireland', Dublin.

Reynolds, A.W. and Broderick, B.M. (1999) *Evaluating the environmental impacts of LPG-fuelled public service vehicles.* Report for 'Irish LPG Association', Dublin.

Reynolds, A.W. (1998) *Transient response analysis and data correction of measuremnets from nitrogen monoxide sensors.* Draft Report for the 'Centre for Environmental Research and Technology', Riverside, CA, USA.

Reynolds, A.W. and Broderick, B.M. (1998) *TCD/CE-CERT collaborative research project.* Report for 'Enterprise Ireland', Dublin.

INVITED PRESENTATIONS:

Reynolds, A.W. (2000) A fuel based motor vehicle emissions model. *Presented at the Seminar on 'Current Mechanical Engineering Research'*, Galway.

Reynolds, A.W. (1999) Air pollution and respiratory health in Dublin. *Presented at the Seminar on 'Activities in Bio-medical Engineering Research'*, Galway.

Reynolds, A.W. (1998) CE-CERT/TCD collaborative research project. *Presented at the Seminar on 'Road Traffic Impacts on Urban Air Quality'*, Dublin.

APPENDIX B

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- INRETS (French National Research Institute), Bron, France;
- Institute for Transport Studies (ITS), The University of Leeds, UK;

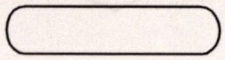
- Institute of Energy, London, UK;
- Institute of Environmental Science and Technology, Yokohama, Japan;
- Institute of Transport studies (ITS), University of California at Davis, CA, USA.
- Intergovernmental Panel on Climate Change (IPCC), Geneva, Switzerland;
- International Road Federation (IRF), Geneva, Switzerland;
- Irish LPG Association, Dublin;
- KLD Associates, Inc., New York, USA;
- Laboratory of Applied Thermodynamics (LAT), Thessaloniki, Greece;
- Lohmeyer Gmbh, Karlsruhe, Germany;
- London Research Centre (LRC), London, UK;
- Los Angeles City Department of Traffic, Los Angeles, CA, USA;
- Maricopa Association of Governments, Phoenix, Arizona, USA;
- Maxol Ltd., Dublin;
- McCann & Associates, Ottawa, Ontario, Canada;
- MET Eireann (the Irish Meteorological Service), Dublin;
- National Environmental Research Institute (NERI), Roskilde, Denmark;
- National Environmental Technology Centre (NETCEN), UK;
- National Renewable Energy Laboratory (NREL), Golden, CO, USA;
- National Roads Authority (NRA), Dublin;
- National Society for Clean Air (NSCA), Brighton, UK;
- New York State Department of Traffic, Albany, NY, USA;
- North Carolina State University, Raleigh, NC, USA;
- Norwegian Institute of Air Research (NILU), Kjeller, Norway;
- Oak Ridge National Laboratory, Oak Ridge, TN, USA;
- Observatoire Economique et Statistique des Tranports (OEST), Paris, France;
- Office of Mobile Sources, Ann Arbour, MI, USA;
- Radian Corporation, Austin, TX, USA;
- Roads and Traffic Authority (RTA), Haymarket, NSW, Australia;
- Rowan, Williams, Davies & Irwin Inc., Guelph, Ontario, Canada;
- Sarah J. Siwek & Assoc., Culver City, CA, USA;
- Scientific & Industrial Research for Australia (CSIRO), NSW, Australia;
- Service d'Etudes des transports (SET), Berne, Switzerland;
- Sigma Research Corporation, Concord, MA, USA;

- Society of Automotive Engineers (SAE), Warrendale, PA, USA;
- Sonoma Technology, Inc., Petaluma, CA, USA;
- South East Institute of Public Health (SEIPH), London, UK;
- Stanford Research Institute (SRI), San Francisco, CA, USA;
- Strategic Studies Department, ETSU, Harwell, UK;
- Swedish National Road and Research Institute, Linköping, Sweden;
- Swedish Road and Traffic Institute, Stockholm, Sweden;
- Swiss Agency for the Environment, Forests and Landscape, Berne, Switzerland;
- Systems Applications International, San Rafael, CA, USA;
- Technical University of Graz, Austria;
- Texas Traffic Institute (TTI), Austin, TX, USA;
- TNO, Schoemakerstraat, Delft, The Netherlands;
- Transport Research Laboratory (TRL), Crawthorne, Berkshire, UK;
- Traffic Research Board (TRB), Washington D.C., USA;
- TUV Rheinland, Cologne, Germany;
- University of Auckland, New Zealand;
- University of Central Florida, Orlando, FL, USA;
- University of Nottingham, Leicestershire, UK;
- University of Pennsylvania, Philadelphia, PA, USA; and
- World Health Organisation (WHO), Brussels, Belgium.

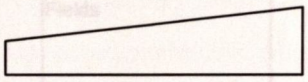
APPENDIX C

The appendix contains the legend for the process flowcharts and entity diagrams presented in Chapter five.

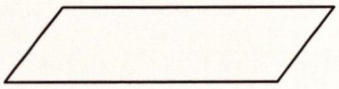
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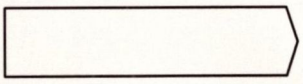
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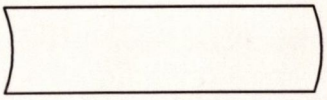
Output:



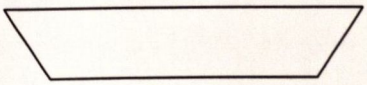
External data file:



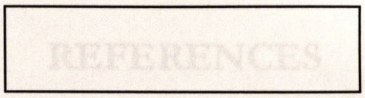
Internal (temporary storage) data file:



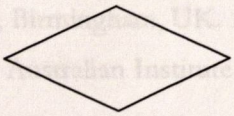
Manual or batch operation:



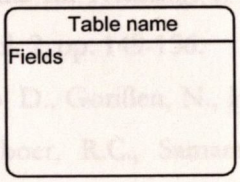
Process calculation



Decision:



Database table:



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