THE DEVELOPMENT & APPLICATION OF AN ADVANCED SCREENING MODEL TO PREDICT AIR QUALITY

by

IAIN COWAN

Submitted for the degree of Doctor of Philosophy

Department of Civil Engineering
School of Engineering
University of Surrey

September 2004

© Iain Cowan 2004
ABSTRACT

The aim of this research was to develop an advanced screening model that can be used quickly to identify areas of high pollution. The thesis describes the development of a new dispersion simulation that uses results from parametric studies of an existing advanced dispersion model. The output from the PARAmetrically Derived dispersion Simulation (PARADIS) is in the form of a receptor grid. This information may then be used in a Geographical Information System to produce pollutant contour maps.

The main objective of PARADIS was to assist Environmental Health Officers in their duty, under Part IV of the Environment Act 1995, in identifying areas that are likely to exceed Statutory Objectives for Air Quality within their area. PARADIS allows both manual and automated input through ESRI ArcMap®. These options permit the user to input data for each individual ‘road-link’ or import the data from a validated traffic model. The automated option vastly reduces the input time often required for dispersion models. PARADIS was further developed to include 3 additional tools that pinpoint locations where exceedences of the Air Quality Objectives are likely to occur.

PARADIS was validated through comparison with monitored data from both diffusion tubes and real-time units. The model was then used in several case-studies to examine the behaviour of traffic related pollutants in a variety of settings and future scenarios. These investigations were completed far more quickly than the methodology currently adopted by local authorities and other investigators.

Finally, some ideas to further develop PARADIS are presented. These included the identification of specific sensitive receptor locations, automated validation and links to external programs for transport planning and public knowledge.

The reduction of air pollution levels within the UK is a long-term Governmental Objective. The research undertaken in this thesis has demonstrated the need for a faster approach to determining air quality within a local area, such as that proposed by PARADIS.
For Anita...
ACKNOWLEDGEMENTS

Firstly, I would like to express my enormous gratitude, and thanks, to my supervisors Dr. Susan Hughes and Dr. Emma Hellawell. Thank you for the many hours of guidance, encouragement and assistance, in spite of enormous pressures of other work, and family commitments, including the births of Sophie, Toby and Nathan. Both of my supervisors have been a true inspiration, with whom it has been a pleasure to work.

A very special thank you to Mum and Dad for their continued support, thank you Mum for the many hours of proof reading. Thank you also to the rest of my family and friends, who have supported and encouraged me throughout this research. An enormous debt of gratitude to Ling Ling Lim and Matthew Lythe of the CivEng Air Quality Research Group, both for their friendship and technical assistance, which have made this research possible.

A special thank you to Phil Sivell of Surrey County Council for his support, suggestions and assistance throughout the research. I would also like to thank the Surrey County Air Quality Group, EPSRC and Surrey University School of Engineering for the financial assistance that allowed me to undertake this research degree.

Thank you to the 11 Boroughs of Surrey for the monitoring data and continued interest and support of this work. In addition, I would like to thank the Surrey County Council Transport Group (especially Helen Fanstone), the British Atmospheric Data Centre, the UK Meteorological Office, the UK Ordinance Survey and Cambridge Environmental Research Consultants for the various models and datasets used within this research.

Finally, I owe an enormous thank you to my wife, Anita. She has been my guiding light throughout this research. Her love, continuing support and many hours of encouragement have made the bad days good and the production of PARADIS possible.
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0 Introduction</td>
<td>1</td>
</tr>
<tr>
<td>1.1 Air Quality Issues</td>
<td>1</td>
</tr>
<tr>
<td>1.2 The Internal Combustion Engine</td>
<td>3</td>
</tr>
<tr>
<td>1.3 Research Aims</td>
<td>5</td>
</tr>
<tr>
<td>1.4 Thesis Outline</td>
<td>9</td>
</tr>
<tr>
<td>2.0 Background</td>
<td>11</td>
</tr>
<tr>
<td>2.1 Introduction</td>
<td>11</td>
</tr>
<tr>
<td>2.2 Air Quality Issues and Legislation</td>
<td>11</td>
</tr>
<tr>
<td>2.2.1 Oxides of Nitrogen (NOx)</td>
<td>12</td>
</tr>
<tr>
<td>2.2.2 Carbon Monoxide (CO)</td>
<td>13</td>
</tr>
<tr>
<td>2.2.3 Particulate Matter (PM)</td>
<td>14</td>
</tr>
<tr>
<td>2.2.4 European Legislation</td>
<td>16</td>
</tr>
<tr>
<td>2.2.5 The UK Air Quality Strategy</td>
<td>18</td>
</tr>
<tr>
<td>2.2.6 Problems in the Implementation of UK Legislation</td>
<td>22</td>
</tr>
<tr>
<td>2.3 Tools Used Within Air Quality Modeling</td>
<td>24</td>
</tr>
<tr>
<td>2.3.1 Transport Models</td>
<td>25</td>
</tr>
<tr>
<td>2.3.2 Emissions Inventories</td>
<td>29</td>
</tr>
<tr>
<td>2.3.3 Dispersion Models</td>
<td>33</td>
</tr>
<tr>
<td>2.3.4 GIS Software</td>
<td>46</td>
</tr>
<tr>
<td>2.4 Summary</td>
<td>47</td>
</tr>
<tr>
<td>3.0 Study Area</td>
<td>50</td>
</tr>
<tr>
<td>3.1 Introduction</td>
<td>50</td>
</tr>
<tr>
<td>3.2 Study Area Selection</td>
<td>52</td>
</tr>
<tr>
<td>3.3 Study Area Validation</td>
<td>54</td>
</tr>
<tr>
<td>3.3.1 Field Data</td>
<td>54</td>
</tr>
<tr>
<td>3.3.2 Airports</td>
<td>55</td>
</tr>
<tr>
<td>3.3.3 Suitability of Monitoring Data for Model Validation</td>
<td>57</td>
</tr>
<tr>
<td>3.3.4 Sparsely Distributed Data Across Surrey</td>
<td>59</td>
</tr>
<tr>
<td>3.4 Summary</td>
<td>62</td>
</tr>
<tr>
<td>4.0 Model Development</td>
<td>67</td>
</tr>
<tr>
<td>4.1 Introduction</td>
<td>67</td>
</tr>
<tr>
<td>4.2 Parameterisation</td>
<td>70</td>
</tr>
<tr>
<td>4.2.1 Description of the Pollution Field</td>
<td>71</td>
</tr>
<tr>
<td>4.2.2 Road Orientation</td>
<td>74</td>
</tr>
<tr>
<td>4.2.3 Configuration of 'Road-Links'</td>
<td>84</td>
</tr>
<tr>
<td>4.2.4 Traffic Configuration</td>
<td>88</td>
</tr>
<tr>
<td>4.3 Generation of 'Look-Up' Tables</td>
<td>91</td>
</tr>
</tbody>
</table>

An Advanced Screening Model to Predict Air Quality
List of Figures

Figure 2.1 Modern European Legislation ................................................................. 18
Figure 2.2 National Level Relationship between European and British Legislation... 19
Figure 2.3 Local Level Relationship between European and British Legislation ...... 20
Figure 2.4 Speed emission curves for petrol engine cars, with an engine size between 1.4 and 2 litres for various Euro classes ........................................ 30
Figure 2.5 Pollutant contribution with distance from road within DMRB model ........ 34
Figure 2.6 Normal Gaussian distribution .................................................................. 36
Figure 3.1 Schematic diagram representing developmental process ....................... 52
Figure 3.2 Location of real-time monitoring units within Surrey .............................. 55
Figure 3.3 Average weekday levels of CO in comparison to Christmas Day ............ 56
Figure 3.4 Average weekday levels of NO in comparison to Christmas Day .......... 57
Figure 3.5 Flight levels from Gatwick in comparison to NO pollution measured at Gatwick airport ...................................................................................... 59
Figure 3.6 Average weekday NO and PM_{10} concentration (April 2000 – April 2001) at three monitoring locations throughout the county .................... 60
Figure 3.7 Pollution levels recorded at Guildford Unit 1 April 1999 to January 2001 61
Figure 3.8 Spatially interpolated map of extrapolated data from real-time units with data from NO\textsubscript{2} diffusion tubes overlaid ......................................... 64
Figure 4.1 Schematic diagram representing developmental process ....................... 67
Figure 4.2 One day average of NO\textsubscript{x} with wind blowing from the Southwest all day.. 72
Figure 4.3 Annual average concentrations of NO\textsubscript{x} with statistical data set .......... 72
Figure 4.4 Wind direction from statistical weather data ........................................... 73
Figure 4.5 Transepts at various points along the same road ................................... 74
Figure 4.6 Road orientations and pollution fields .................................................... 78
Figure 4.7 Levels of pollutants at varying distances from road (minus numbers indicate distance to the left of road) ...................................................... 79
Figure 4.8 NO\textsubscript{x} concentrations vs. distance from road with curve fitting procedures superimposed – all distances ......................................................... 80
Figure 4.9 NO\textsubscript{x} concentrations vs. distance from road with curve fitting procedures superimposed – 0-10m from the road ..................................................... 81
Figure 4.10 NO\textsubscript{x} concentrations vs. distance from road with curve fitting procedures superimposed – 10-100m from the road ........................................ 82
Figure 4.11 NO\textsubscript{x} concentrations vs. distance from road with curve fitting procedures superimposed – >100m from the road ........................................ 82
Figure 4.12 The separation of carriageways by various central reservation widths .. 85
Figure 4.13 The separation of carriageways and the effect on predicted pollution levels ................................................................. 86
Figure 4.14 An increase in road width reduces average level of pollution.............. 87
Figure 4.15 NO₂ levels across an 8m wide road for varying traffic levels at 10kph with
10% HGV .......................................................... 89
Figure 4.16 Pollution concentration derived at the road centre for 500 vehicles at
various speeds ...................................................... 90
Figure 5.1 Schematic diagram representing developmental process .................... 97
Figure 5.2 Process of running PARADIS ............................................................... 98
Figure 5.3 PARADIS calculation program as an integral part of the system process 99
Figure 5.4 PARADIS GUIs surrounding the calculation program ....................... 104
Figure 5.5 Flow diagram for manual and automatic input methods and the link to the
calculation software ............................................. 106
Figure 5.6 Screen to choose road shapefile with associated database ................. 109
Figure 5.7 Screen for input of year and pollutant as well as background levels ......110
Figure 5.8 Choice of background raster maps ...................................................... 111
Figure 5.9 Manual input window for choices following input of road coordinates using
mouse ................................................................. 111
Figure 5.10 Selection of display type ................................................................. 114
Figure 5.11 Choice of raster map from which to determine levels ....................... 115
Figure 6.1 Schematic diagram representing developmental process .................... 119
Figure 6.2 Diffusion tube data compared to modeled output ................................. 123
Figure 6.3 PARADIS comparison with monitored data ........................................ 126
Figure 6.4 The mean level of various pollutants across modelled areas against
population density ............................................... 128
Figure 6.5 Annual average NO₂ pollution levels for 2002 in Guildford, calculated by
PARADIS ............................................................. 130
Figure 6.6 Annual average NO₂ levels in Figure 5.5 – Annual average NO₂ levels in
Woking for 2002, calculated by PARADIS ................................................. 131
Figure 6.7 Annual average NO₂ pollution in Godalming for 2002 calculated by
PARADIS ............................................................. 132
Figure 6.8 Annual average NO₂ pollutant levels in Horley for 2002, calculated using
PARADIS ............................................................. 133
Figure 6.9 Annual average NO₂ pollution for 2002 in Dorking, calculated by
PARADIS ............................................................. 135
Figure 6.10 Annual average NO₂ pollution in Haslemere for 2002, calculated by
PARADIS ............................................................. 136
Figure 6.11 Annual average NO₂ levels for Camberley in 2002 using PARADIS .... 138
Figure 6.12 Annual average NO₂ levels for Leatherhead in 2002 using PARADIS ...139
Figure 6.13 Annual average NO₂ levels for Weybridge & Walton on Thames in 2002
using PARADIS ............................................................. 140
Figure 6.14 Annual average NO₂ levels for Epsom & Ewell in 2002 using PARADIS ................................................................. 141
Figure 6.15 Annual average NO₂ levels for Reigate & Redhill in 2002 using PARADIS .................................................................. 143
Figure 6.16 Annual average NO₂ levels for Guildford & Woking in 2002 using PARADIS ................................................................. 145
Figure 6.17 Percentage reduction of NO₂ in various town sizes for 2002, 2005 and 2010 ................................................................. 146
Figure 6.18 Predicted annual average concentration of NO₂ in Guildford for 2005 (a) using the DMRB emission factors & (b) 80% of the expected emissions improvement included in plot (a) ......................................................... 148
Figure 6.19 Predicted annual average concentration of NO₂ in Guildford for 2010 ................................................................. 150
Figure 6.20 Predicted annual average concentration of NO₂ in Spelthorne for 2005 showing areas that are likely to exceed 21ppb ................................................................. 152
Figure 6.21 'Combination tool' used to define possible AQMAs by showing areas with a predicted annual average concentration greater than 21ppb in 2005 ................................................................. 153
List of Tables

| Table 1.1 | Important Acts of Parliament relating to air pollution during 19th Century... 1 |
| Table 2.1 | Health effects of NO₂........................................................................... 13 |
| Table 2.2 | UK and EU target values and dates.......................................................... 17 |
| Table 2.3 | History of the Surrey County Transportation Model.................................... 28 |
| Table 2.4 | Pasquill stability criteria and meteorological parameters.......................... 38 |
| Table 4.1 | $R^2$ values obtained from the trend lines fitted to the 3 distance datasets for NOₓ, PM and CO using the least squares method ........................................ 83 |
| Table 4.2 | Parameterised Road widths for varying speeds ........................................... 87 |
| Table 4.3 | Additional pollutant concentration 'c' for equation describing pollution on orthogonal line to road ................................................................. 91 |
| Table 4.4 | 'Look-up' table format............................................................................... 92 |
| Table 5.1 | Input values to PARADIS program and the definitions within the code........... 100 |
| Table 5.2 | Year Factors obtained from the DMRB emission factors and used within the PARADIS program ............................................................................. 101 |
| Table 5.3 | Data required and source for different input types....................................... 107 |
| Table 6.1 | Average level of NO₂ across Woking for 2002 at given and ±10% traffic flows from SCTM................................................................................... 121 |
| Table 6.2 | Annual average levels for the areas modeled around Guildford for 2005 and 2010 using DMRB predicted emission factors and a 20% increase.149 |
## List of Equations

<table>
<thead>
<tr>
<th>Equation</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1</td>
<td>The photodissociation of NO₂</td>
<td>4</td>
</tr>
<tr>
<td>1.2</td>
<td>Formation of hydrocarbon radicals</td>
<td>4</td>
</tr>
<tr>
<td>1.3</td>
<td>Formation of aldehyde peroxides and aldehyde peroxyacids</td>
<td>4</td>
</tr>
<tr>
<td>2.1</td>
<td>Endothermic nitrogen and oxygen reaction that occur in internal combustion engines</td>
<td>12</td>
</tr>
<tr>
<td>2.2</td>
<td>Equation used by DMRB to calculate contribution to ambient levels from traffic at distance (d) from source</td>
<td>34</td>
</tr>
<tr>
<td>2.3</td>
<td>Calculation to derive NO₂ from NOₓ</td>
<td>35</td>
</tr>
<tr>
<td>2.4</td>
<td>Gaussian dispersion equation including reflection at the boundary layer and ground</td>
<td>40</td>
</tr>
<tr>
<td>4.1</td>
<td>Chosen equation form for nest-fit lines for three distance bands</td>
<td>82</td>
</tr>
<tr>
<td>5.1</td>
<td>Empirical Correlation of NOₓ and NO₂</td>
<td>103</td>
</tr>
<tr>
<td>5.2</td>
<td>Formulae for the rotation of roads</td>
<td>108</td>
</tr>
</tbody>
</table>
## NOTATION

### Organisation:

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>AEAT</td>
<td>Atomic Energy Authority Technology plc</td>
</tr>
<tr>
<td>CALTRANS</td>
<td>CALifornia department of TRANSportation</td>
</tr>
<tr>
<td>CERC</td>
<td>Cambridge Environmental Research Consultants</td>
</tr>
<tr>
<td>DEFRA</td>
<td>Department for the Environment, Food and Rural Affairs</td>
</tr>
<tr>
<td>DETR</td>
<td>Department of the Environment, Transport and the Regions</td>
</tr>
<tr>
<td>EA</td>
<td>Environment Agency (United Kingdom)</td>
</tr>
<tr>
<td>EC</td>
<td>European Community</td>
</tr>
<tr>
<td>EEC</td>
<td>European Economic Community</td>
</tr>
<tr>
<td>EPAQS</td>
<td>Expert Panel on Air Quality Standards</td>
</tr>
<tr>
<td>EPSRC</td>
<td>Engineering and Physical Sciences Research Council</td>
</tr>
<tr>
<td>ESRI</td>
<td>Environmental Systems Research Institute</td>
</tr>
<tr>
<td>EU</td>
<td>European Union</td>
</tr>
<tr>
<td>EPA</td>
<td>Environmental Protection Agency (United States)</td>
</tr>
<tr>
<td>HMSO</td>
<td>Her Majesty's Stationery Office</td>
</tr>
<tr>
<td>SCC</td>
<td>Surrey County Council</td>
</tr>
<tr>
<td>TRL</td>
<td>Transport Research Laboratory</td>
</tr>
<tr>
<td>UK</td>
<td>United Kingdom</td>
</tr>
</tbody>
</table>

### Legislation:

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>AQS</td>
<td>Air Quality Strategy</td>
</tr>
<tr>
<td>AQMA</td>
<td>Air Quality Management Area</td>
</tr>
<tr>
<td>LAQM</td>
<td>Local Air Quality Management</td>
</tr>
<tr>
<td>EIA</td>
<td>Environmental Impact Assessment</td>
</tr>
<tr>
<td>NAQS</td>
<td>National Air Quality Strategy</td>
</tr>
</tbody>
</table>

---

An Advanced Screening Model to Predict Air Quality
Pollutant:

CH$_4$  Methane
CO  Carbon Monoxide
CO$_2$  Carbon Dioxide
COHb  Carboxyhaemoglobin
hv  Ultra-violet radiation
LPG  Liquefied Petroleum Gas
NO  Nitrogen Oxide
NO$_2$  Nitrogen Dioxide
NO$_x$  Oxides of Nitrogen usually NO and NO$_2$
O$^*$  Oxygen Radical
O$_2$  Oxygen
O$_3$  Ozone
PAN  Peroxyacylnitrate
PM  Particulate Matter
PM$_{10}$  Particulate Matter of less than 10µm aerodynamic diameter
ppb  Parts per billion
ppm  Parts per million
R$'$  Acetyl radical
SO$_2$  Sulphur Dioxide
Smog  Mixture of smoke and fog
TEA  Triethanolamine
µm  0.0001cm

Transport:

AADT  Annual Average Daily Traffic
CTM  County Transportation Model
DMRB  Design Manual for Roads and Bridges
HGV  Heavy Goods Vehicles
IC  Internal Combustion
kph  Kilometres per hour
LGV  Light Goods Vehicles
M25  London Orbital Motorway
PARADIS  PARAmetrically Derived dispersion Simulation
SCTM  Surrey County Transportation Model
TAZ  Traffic Analysis Zone
TNM  Town Near Motorway

Dispersion:
AERMOD  American meteorological Society/Environmental protection agency Regulatory MODel
AERMET  American meteorological Society/Environmental protection agency Regulatory METeorological pre-processor
ADMS  Atmospheric Dispersion Modeling System
ALR  Adiabatic Lapse Rate
CALINE  CAliifornia department of transportation LINE source model
ELR  Environmental Lapse Rate
GRS  Generic Reaction Scheme
H  Release height
H_{bi}  Height at top of boundary layer
LAEI  London Atmospheric Emissions Inventory
NAEI  National Atmospheric Emissions Inventory
Q  Source strength
q  Concentration at receptor
\( \sigma_y, \sigma_z \)  Standard deviations in x and y directions described by Pasquill stability classes
\( \bar{u} \)  Wind speed
x, y, z  Cartesian coordinates
X1, X2, Y1, and Y2  Original coordinates
X_{1(new)}, X_{2(new)}, Y_{1(new)} and Y_{2(new)}  Coordinates after rotation
X_{Centre} and Y_{Centre}  Coordinates of the centre point of the line
y = Cexp(mx)  y is pollutant concentration
C is the Y axis intercept
m is the growth factor
x is the distance from the road
\( \theta_{Rot} \)  Angle through which the road must be rotated

Miscellaneous:

DLL  Dynamic Link Language
GIS  Geographic Information System
GUI  Graphical User Interface
IDW  Inverse Distance Weighting
VB  Visual Basic
VBA  Visual Basic for Applications

An Advanced Screening Model to Predict Air Quality.
1.1 **Air Quality Issues**

In definitive terms, anthropogenic air pollution is the addition of chemical compounds to the atmosphere in quantities not naturally present. It is produced from many industrial, domestic and transportation sources and has existed since man discovered fire. Hand-in-hand with man’s production of air-borne pollutants has also been man’s counter-measures to control or reduce the quantity of contaminants released into the atmosphere.

Within the United Kingdom (UK), laws concerning air quality stem from 1273 when the use of coal was prohibited in London as it was thought to be damaging to health. The rise of the industrial revolution from 1750 onwards, saw a change from small to large scale air pollution. During this period, there was a greater need for energy to run the new machines, factories and smelters. This was produced through the burning of combustible materials, often fossil fuels, which in turn released more chemical pollutants into the atmosphere [Aric, 2004].

<table>
<thead>
<tr>
<th>Date</th>
<th>Act</th>
<th>Aims</th>
</tr>
</thead>
<tbody>
<tr>
<td>1863</td>
<td>Alkali Works Regulation Act</td>
<td>Mandatory to stop 95% of ‘offensive emissions’</td>
</tr>
<tr>
<td>1866</td>
<td>Sanitary Act</td>
<td>Powers to local sanitary authorities to take action in case of smoke nuisance</td>
</tr>
<tr>
<td>1875</td>
<td>Public Health Act</td>
<td>Reduction of smoke emissions, all modern legislation built on this act</td>
</tr>
</tbody>
</table>

Table 1.1 Important Acts of Parliament relating to air pollution during 19th Century
Thus, by the 19th century, the reliance on fossil fuels to power factories and heat domestic properties was already creating many air pollution problems. The combustion of the fuel itself released chemicals such as sulphur dioxide (SO\textsubscript{2}), carbon monoxide (CO) and oxides of nitrogen (NO\textsubscript{x}). During anticyclonic conditions, these oxides combined with fog to produce smog (a mixture of smoke particulates and fog) that results in particle loading and consequently a reduction in oxygen levels [Aric, 2004]. As well as reducing visibility in industrial and urban areas, the smogs or ‘pea-soupers’ as they were sometimes known were particularly detrimental to lung function in human health. Consequently, throughout the 19th Century, several acts of Parliament were passed concerning the release of these industrial gases into the atmosphere (Table 1.1) [Aric, 2004].

During the 20th century, the Clean Air Act of 1956 was the first major piece of legislation introduced, which consolidated and extended any previous acts of Parliament [UK Parliament, 1956]. This Act was primarily the response to the well-documented London Smog of 1952, when it was estimated that 4,000 people died as a result of poor air quality. This piece of legislation introduced for the first time smoke control areas and controlled chimney heights. The act also banned the emission of dark smoke from chimneys. The result was a dramatic improvement in urban air quality and the characteristic 'London' smogs of the past decades were abated [Aric, 2004].

The discovery and proliferation of electricity led to fewer and fewer factories needing their own power source. In addition, the new technology meant that energy could be transferred from area to area, and power stations could be located away from population centres. The reduction of the need for solid fossil
fuels to heat homes during the later half of the 20th century meant that pollution over urban areas began to decline [Environment Agency, 2004].

1.2 The Internal Combustion Engine
The brief respite in high air pollution levels in urban areas was ended by advances in engine technology and associated affordability, resulting in a rise in popularity of the motorcar as a method of transportation. The motor vehicle brought ease of movement to the population and a reduction in the cost of goods transportation. During the 1980s and 1990s, the environmental costs and health effects of the internal combustion engine were becoming more apparent. The escalation in vehicle numbers (which continue to increase within the UK at the rate of approximately 2% per annum) had a significant impact on local air quality [Borrego et al., 2000; Cowan et al., 2001 and Colls, 1997].

The internal combustion engine uses volatile fossil fuels, such as petrol and diesel. Upon combustion, it releases, amongst other pollutants, carbon monoxide (CO), nitrogen oxides (NOx) and particulate matter (PM). All of these are known to have detrimental effects on both the environment and human health, and are described in detail below.

The cocktail of pollutants, emitted from the internal combustion engine, react both with each other and with natural atmospheric components to form secondary pollutants such as carbon dioxide (CO2) and nitrogen dioxide (NO2). These simple oxidation reactions may be followed by further reactions and the reaction of more complex chemical compounds.

As an example, one such reaction sequence leads to the formation of a type of smog known as peroxyacylnitrate (PAN) first defined in Los Angeles [Colls,
1997. This may occur if photodisociation of NO₂ occurs resulting in the formation of ozone (O₃) or oxygen atoms (Equation 1.1).

**Equation 1.1 The photodisociation of NO₂**

\[
\begin{align*}
NO₂ + hν & \rightarrow NO + O^* \\
O^* + O₂ + M & \rightarrow O₃ + M \\
NO + O₃ & \rightarrow NO₂ + O₂ \\
hν & - \text{ultra-violet radiation} \\
O^* & - \text{oxygen radical}
\end{align*}
\]

These oxygen atoms are then able to react with hydrocarbons to form hydroxyl radicals, which in turn react with more hydrocarbons creating hydrocarbon radicals (Equation 1.2).

**Equation 1.2 Formation of hydrocarbon radicals**

\[
\begin{align*}
O^* + H₂O & \rightarrow 2OH^* \\
RH + OH^* & \rightarrow H₂O + R^* \\
R^* + O₂ & \rightarrow RO₂^* \text{ (Fast)} \\
RO₂^* + NO & \rightarrow NO₂ + RO^*
\end{align*}
\]

\[
\begin{align*}
R & - \text{Any compound} \\
RH & - \text{Any hydrocarbon compound} \\
^* & - \text{Radical}
\end{align*}
\]

Oxidation of the hydrocarbons produces aldehydes, which are in turn oxidised to form aldehyde peroxides and aldehyde peroxyacids (Equation 1.3). If a methyl compound is introduced in the final reaction, then PAN is formed.

**Equation 1.3 Formation of aldehyde peroxides and aldehyde peroxyacids**

\[
\begin{align*}
RO^* + O₂ & \rightarrow R'CHO + HO₂^* \text{ (Fast)} \\
R'CHO + OH^* & \rightarrow R'CO^* + H₂O \\
R'CO^* + O₂ & \rightarrow R'C(O)O₂^* \text{ (Fast)} \\
R'C(O)O₂^* + NO₂ & \rightarrow R'C(O)₂NO
\end{align*}
\]

\[
\begin{align*}
R'CO^* & - \text{an acyl radical} \\
R'C(O)O₂^* & - \text{an acylperoxy radical} \\
R'C(O)₂NO & - \text{an acylperoxy nitrate} \\
\text{When } R' & \text{ is a methyl (CH₃) pan is formed}
\end{align*}
\]
This reaction sequence is one of many that occur, dependant upon the levels of various chemical compounds within the atmosphere at any given time, and the amount of insolation that occurs.

Such long reaction sequences may not occur in all locations, or at all times of the year, due to the lack of one or more necessary constituents. More frequent are short oxidation and photodisociation reactions, such as that highlighted in Equation 1.1 [Colls, 1997].

1.3 Research Aims
Current UK legislation requires local councils to assess air pollution within their administrative area, and to predict air quality for future years. This includes pollutants from many different sources within urban areas, however, the internal combustion (IC) engine is the major contributor to air pollution [Aric, 2004; Environment Agency, 2004; Borrego et al., 2000; Colls, 1997]. Consequently, an understanding of the emission and dispersion patterns of pollutants emitted from the IC engine is a key part of this assessment process and of particular importance in the long-term objective for improving air quality in a region.

Methods of understanding emission/dispersion of pollutants from IC engines include real-time monitoring and theoretical modelling. For many local councils, accurate monitoring with a sufficient grid size to cover a borough is prohibitively expensive and there is often a lack of technical/computational expertise in the subject area to perform the required numerical modelling. As a consequence of this, the majority of air quality assessments are outsourced to external consultants at additional expense.
In order to perform the required assessments, several types of emission/dis\ndispersion models exist. These divide into two basic categories, namely screening models and (advanced) dispersion models. In terms of functionality, the basic screening models such as the the Design Manual for Roads and Bridges (DMRB) allow the calculation of pollutant concentrations at single sensitive point receptors [DMRB, 2003]. At the top end of the range, sophisticated dispersion models, such as ADMS-Urban, model pollutant dispersion from multiple sources and present pollution concentration levels over adaptive grids to allow spatial interpolation with Geographic Information Systems (GIS) software [CERC, 2001].

The main advantages of screening models are that they are relatively easy to use and therefore have a useful role simply as a screening tool that may be used by ‘non-experts’. However, screening models are also limited in that:

- the input is often manual and, therefore, ‘user intensive’;
- the road modeling generally is simplistic;
- key parameters such as meteorology are usually omitted;
- calculations are typically for single point receptors, making graphical representation meaningless; and
- they do not meet the criteria for current air quality assessments.

Whilst advanced dispersion models overcome many of the problems inherent to screening models, there are often prohibitive aspects to their use by local councils. For example, they may:

- be difficult to set up in terms of input;
- require expert users (in both IT terms and in the subject area itself);
- have long run times; and
have high computational demands in terms of processing.

The aim of this thesis is to investigate the dispersion of traffic related pollutants in the local environment. This will be achieved through the development and application of an intermediate screening model. This new model would be more sophisticated than currently available screening models, but less complex than advanced dispersion models. This research would enable further investigation into modelling air pollution and would involve examining aspects relating to emissions, dispersion and modelling techniques such as:

- vehicle flow;
- speed;
- percentage of Heavy Goods Vehicles (HGV);
- road width;
- meteorology;
- grid size; and
- interpolation techniques.

Road transport is responsible for the majority of NO\textsubscript{x}, PM\textsubscript{10} and CO generation in the UK [NAEI, 2003]. The number of vehicles using a road is therefore crucial in determining emissions generated along the road. Theoretically, doubling the number of vehicles should double the emissions and consequently the concentrations of pollutants at distance from the road. This supposition does not take into account a variation in speed, percentage of HGV, road width or meteorology all of which have an influence on either emissions, dispersion or both. These issues are investigated through the use of an existing advanced dispersion model to understand the relationship between these factors and pollutant concentrations at distance from a road source.
In terms of model output, the size of grid is crucial in determining an appropriate result. Air pollution concentrations change rapidly over short distances due to chemistry, dilution and dispersion. The grid, over which pollutant concentrations are calculated, needs to have a resolution which can detect these changes without having an excessive number of data points to calculate. An appropriate grid size is, therefore examined and discussed through the trial of a variety of grid sizes on the impact on model output.

The interpolation method used to discern values between data points can alter the observed pollution pattern within the results. The choice of the correct method is therefore an important issue. Three main types of interpolation routines exist, namely:

- Inverse Distance Weighted (IDW);
- Spline; and
- Kriging.

Each method is examined for its merits and downsides, and the appropriate method for air quality modelling selected.

The methodology used to achieve the above aims and objectives was:

1. Carry out a detailed literature review examining existing methodologies of emissions estimation, field measurements and dispersion theory
2. Review existing screening and advanced dispersion models
3. Develop a prototype advanced screening model
4. Test and validate the prototype using measured data
5. Apply the new intermediate model to several case studies.
1.4 Thesis Outline

This thesis has been divided into 7 chapters, and follows the process through which the idea, technique and screening model were developed.

Chapter 2 describes the background to the development of PARADIS with reference to both European / British legislation and the effects of various pollutants on human health. The tools currently used in determining air quality are also discussed as well as relevant studies to the development of PARADIS.

Chapter 3 investigates the need for the choice of a study area prior to the development of PARADIS. Various criteria for a suitable study area are listed, and data from within the selected study area is used to assess its suitability.

Chapter 4 details the parametric studies undertaken with the chosen dispersion model, ADMS-Urban to determine the pollution fields generated around a road. Consideration is given to how these results may be broken down into simple algorithms for faster calculation of pollution concentrations at distance from a road source.

Chapter 5 describes the development of the calculation program from the results of the parametric studies. This is followed by the development of Graphical User Interfaces (GUIs) within and ArcGIS extension for the use of PARADIS.

Chapter 6 addresses validation of the screening model against monitored data, with reference to present and future case studies. In addition the model is used to investigate various case studies including the effect of town size / type on pollution levels. Additional tools developed to ascertain current and future compliance with legislation are also discussed with reference to case studies.
Chapter 7 concludes the thesis and brings together the developmental process for the parameterisation of an advanced dispersion model. Further development ideas for PARADIS are discussed alongside how the model could be used by local authorities in place of existing techniques.
Chapter 2 - Background

2.1 Introduction
Chapter 2 deals with background issues relating to the development of the advanced screening model - PARADIS. In the first section, traffic related pollutants, NOx, CO and PM10 are discussed along with their effects on human health and the European and UK legislation that has resulted from epidemiological studies of these pollutants. The second section deals with four important tools namely, transport models, emissions inventories, atmospheric dispersion models and geographic information systems, which are used to determine, predict and display ambient air quality concentrations. Each of these tools has been used in the development of the advanced screening model - PARADIS. As such, alongside a general discussion on each tool is an investigation into the use of a specific tool in the developmental process.

2.2 Air Quality Issues and Legislation
Concern has been raised by governments and organisations worldwide on the deteriorating quality of air in many major cities. As a result, research has been undertaken to understand the physiological effect of poor air quality. This section deals with the health effects of the 3 main traffic related pollutants, namely NOx, PM10 and CO and the European and UK legislation that has subsequently been introduced.
2.2.1 Oxides of Nitrogen (NOx)

Combustion from vehicle fuels produces both NO and NO2 in approximately the mass ratio 9:1 (NO:NO2). Since NO will quite readily oxidise to NO2, the two are often put together and termed NOx in spite of being both physically and chemically different [Colls, 1997]. An estimated 51% of NOx produced within the United Kingdom is attributable to traffic [Colls, 1997]. Fuel for the internal combustion engine is generally low in nitrogen, meaning that most NO from the engine is produced thermally following Equation 2.1. These reactions are highly endothermic, and occur, therefore, in the hottest part of the engine taking both the majority of nitrogen and all of the oxygen from the air rather than the fuel. Typically petrol contains approximately 0.5-1.5% nitrogen, meaning that a small proportion of the nitrogen used in Equation 2.1 does originate from the fuel. Upon release, the mixture of NOx rapidly undergoes oxidation to form NO2 [Vautard, 2000].

Equation 2.1  Endothermic nitrogen and oxygen reaction that occur in internal combustion engines

\[ N_2 + O \rightarrow NO + N \]
\[ N + O_2 \rightarrow NO + O \]

Effects on human health

NOx emissions have been linked with environmental and health impacts due to the various compounds and derivatives that result, including nitrogen dioxide, nitric acid, nitrous oxide, nitrates, and nitric oxide [DEFRA1, 2004]. NO2 has a much higher toxicity than NO, and due to its limited solubility, it may penetrate deep into the lung, leading to direct effects on the respiratory system [Colls, 1997].

The effects on the respiratory system are dependent on the level of NO2 within the local environment, as shown in Table 2.1. Recent studies have concluded...
that individuals with asthma have an increased susceptibility to stimuli after exposure to NO$_2$ levels at 200ppb [DEFRA$^1$, 1998]. Acute effects of high level NO$_2$ exposure have been shown during episodes of accidental work-related incidents. Such exposures are indicative of severe and rapid damage to the lung resulting in pulmonary diseases and even death [DEFRA$^1$, 1998].

Table 2.1 Health effects of NO$_2$ (adapted from Colls, 1997)

<table>
<thead>
<tr>
<th>NO$_2$ Concentration (ppb)</th>
<th>Short term effects</th>
</tr>
</thead>
<tbody>
<tr>
<td>0-200</td>
<td>no obvious effects on health</td>
</tr>
<tr>
<td>100-200</td>
<td>odour detected</td>
</tr>
<tr>
<td>200-1000</td>
<td>metabolic effects detected</td>
</tr>
<tr>
<td>1000-2000</td>
<td>change in respiratory rate</td>
</tr>
<tr>
<td>2000-5000</td>
<td>deterioration of lung tissue</td>
</tr>
<tr>
<td>&gt;5000</td>
<td>severe damage to lung tissue</td>
</tr>
</tbody>
</table>

The risks of longer term exposure to NO$_2$ are unknown although it is thought that there are probable accumulative health effects. An approach to reduce the annual average levels of NO$_2$ has, therefore, been adopted with the hope of minimising any risks [DEFRA, 2004].

2.2.2 Carbon Monoxide (CO)

The complete combustion of any fossil fuel results in the release of carbon dioxide (CO$_2$), however, the internal combustion engine is approximately 32% efficient [Ferreira, 1998]. Of all the pollutants emitted from the internal combustion engine CO is emitted in the greatest quantities; in 1993 90% of all CO emitted in the United Kingdom was attributed to road transport [Colls, 1997].

Upon release, most of the carbon is only partially oxidised to CO; the rest is emitted directly, as partially burned hydrocarbons in to the atmosphere where they are rapidly oxidised to form CO and CO$_2$ [Colls, 1997]. CO$_2$ may then combine with water to form a weak carbonic acid. This weak acid has detrimental effects on both the built and natural environments.
Effects on human health

Carbon monoxide also has a detrimental effect to human health at high concentrations. As emitted from the internal combustion engine, CO will combine with haemoglobin 200 times more readily than oxygen, which severely reduces the amount of oxygen carried (from the lungs) around the body [Colls, 1997]. Concentrations of carbon monoxide in the blood are measured as a percentage, with the level of carboxyhaemoglobin (COHb) dependant on the concentration in the air, the length of exposure and the depth of breathing [DEFRA, 1998]. Since CO restricts the level of oxygen that may be transported around the body, organs that are dependant on a high level of oxygen in the blood, namely the heart and the brain, are most at risk from high CO levels.

A blood COHb level of around 1.3% would result in headaches and a reduction in mental performance. Such a level may occur from exposure to 30ppm of CO for 1 hour or 9ppm for 8 hours (calculations by WHO [Colls, 1997]). High levels that cause severe physical harm may be found within city centres on days of extreme pollution, but are rarely found within the United Kingdom.

2.2.3 Particulate Matter (PM)

Particulate matter (PM) is produced both within the combustion engine and 'naturally' through the erosion of roads, pavements and soils. 46% of all black smoke emissions, that contain high proportions of particulates, are produced from traffic within the UK (1990). Particles are produced from both petrol and diesel engines, however, diesel engines are the largest source accounting for 40% of all black smoke emissions (1990) [Colls, 1997]. Particles produced by the internal combustion engine are often very fine (<2μm in diameter) due to the high temperature environment in which they are formed [Harrison et al., 2001]. 'Natural' road dusts are usually coarser in nature (>2μm in diameter) as they are...
the result of erosion processes rather than incomplete combustion [Harrison et al., 2001]. Fine particles often have heavy metals and chemicals associated with them as they are formed in the combustion process, whilst larger particles act as nuclei for heavy metals from exhaust fumes.

All of these particulates have mass, and are deposited on the surrounding area. The passage of vehicles results in the deposited particles becoming resuspended in the lower troposphere increasing the load of particles in the air. Work in Kraków, Poland, has suggested that close to a road source (<150m) approximately 80% of PM$_{10}$ (particulate matter of less than 10µm) is attributable to road vehicles. This drops by a factor of two over a further distance of 150-200m [Wróbel et al., 2000]. These figures describing dispersion of PM$_{10}$ are, however, misleading as they suggest that particles come directly from the exhaust of the vehicle. In reality, approximately half is new PM whilst the other half is due to “vehicle-induced resuspension” [Harrison et al., 2001].

**Effects on human health**

Particles <10µm have the ability to penetrate the human respiratory system and cause damage to the lungs [Colls, 1997 and Harrison et al., 2001]. It is known that particles of size between 2-10µm may penetrate as far as the bronchiole, and particles smaller than this may infiltrate the alveoli.

Particles often act as nuclei for heavy metals found within the exhaust fumes, and these may cause a variety of effects on the human system. Epidemiological studies have concluded that overall, an increase in the level of PM results in a rise the incidence of both respiratory and cardiac diseases. Published studies concerning the effects of particulate matter on health have resulted in estimations
by the WHO that the daily mortality rate will increase by 5% for a 50μg m⁻³ change in average daily concentration of PM₁₀ [Air Quality Expert Group, 1995].

In order to tackle health problems associated with high concentrations of air pollutants, described above, both the European and UK Parliaments have passed legislation to reduce pollution levels. The United Kingdom's membership of the European Economic Community (EEC) in 1972 led the UK's air quality legislation to be intertwined with European Directives and Daughter Directives. Modern air quality legislation within the European Union and the UK has been based upon epidemiological studies and expert panel reviews on the short and long term effects of varying concentrations of pollutants in the air that we breathe. The aim of the legislation is to reduce the amount of pollution over time, to attain 'safer' levels in the future.

2.2.4 European Legislation

European Legislation on air pollution from motor vehicles first came to fruition on 20 March 1970 with an amalgamation of the laws of member states regarding pollution from positive-ignition engines of motor vehicles. The directive (70/220/EEC) concluded that it was against common market interests to have different targets across Europe, so a common policy was created. The common policy has continued with 35 additional directives and their associated daughter directives limiting pollution emissions from motor vehicles [Council of the European Union, 2004].

In general, EU legislation regarding air pollution has been governed towards reducing the amount of emissions per vehicle [Colvile et al., 2001]. The earliest directives concentrated on reducing emissions from engines by pressing the car manufacturing industry, through legislation, for improvements in engine
technology. Throughout the 1990s this process led to standards for emissions from engines known as Euro Classes. This meant that an engine with certain emission characteristics was a member of Euro Class I, II or III. Currently, Euro Class III engines are being produced with Euro Class IV due to come on line in January 2006 [Highways Agency, 2004].

<table>
<thead>
<tr>
<th>Pollutant</th>
<th>Target Level (Measurement Period (Exceedences allowed per year))</th>
<th>UK date</th>
<th>EU date</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO</td>
<td>10mgm⁻³ (8.6ppm) (8hr running mean)</td>
<td>31/12/2003</td>
<td>01/01/2010</td>
</tr>
<tr>
<td>NO₂</td>
<td>200µgm⁻³ (105ppb) (1hr mean (18))</td>
<td>31/12/2005</td>
<td>01/01/2010</td>
</tr>
<tr>
<td></td>
<td>40µgm⁻³ (21ppb) (Annual Mean)</td>
<td>31/12/2005</td>
<td>01/01/2010</td>
</tr>
<tr>
<td>PM₁₀</td>
<td>50µgm⁻³ (24hr running mean (35))</td>
<td>31/12/2004</td>
<td>01/01/2010</td>
</tr>
<tr>
<td></td>
<td>40µgm⁻³ (Annual mean)</td>
<td>31/12/2004</td>
<td>01/01/2010</td>
</tr>
<tr>
<td></td>
<td>50µgm⁻³ (24hr running mean (7))</td>
<td>31/12/2010</td>
<td>01/01/2010</td>
</tr>
<tr>
<td></td>
<td>18µgm⁻³ (Annual mean)</td>
<td>31/12/2010</td>
<td>01/01/2010</td>
</tr>
</tbody>
</table>

Despite the introduction of the various Euro class engines, pollution levels remained fairly constant as the car numbers and usage continued to grow throughout the EU. Another approach was needed, therefore, to reduce pollutant levels within member states.

Daughter directives of the Ambient Air Quality Assessment and Management Directive 96/62/EC set limits of the ambient target level for air pollutants throughout the European Union [Council of the European Union, 2004]. To date, there have been three daughter directives (99/30/EC, 2000/69/EC and 2002/3/EC) each requiring member states to reduce ambient pollution levels for prescribed pollutants (see Figure 2.1) to below the levels outlined in Table 2.2 by the date shown. As guidance for member states to achieve these targets, the EU has introduced margins of tolerance for intervening years to indicate success or failure by the compliance date.
Chapter 2 – Background

Figure 2.1 Modern European Legislation
The technological improvements required by EU legislation (Euro class engines), and the directives for member states to reduce ambient concentrations, mean that all European cities, with the exception of Athens, are expected to meet the ambient targets by the end of 2009, [Colvile, 2001].

2.2.5 The UK Air Quality Strategy
In 1995, prior to the 1996 European directive on air quality (96/62/EC), the UK Parliament introduced the Environment Act. Whilst Part IV of the act made provision for limits on air quality, it was not until 1997 that the Secretary of State for the Environment published the ‘National Air Quality Strategy’ (NAQS). The NAQS is seen as a response to the EU directive as it took account of the European limits set out within a year earlier alongside advice from the Expert Panel on Air Quality Standards (EPAQS) (Figure 2.2).
The first European daughter directive (99/30/EC) gave European Governments two years with which to respond, and within the UK led to the publication of the main policy document put forward to the United Kingdom Parliament in January 2000. The document entitled "The Air Quality Strategy for England, Scotland, Wales and Northern Ireland - Working Together for Clean Air" defines the main legislative framework for both national and international contexts (Figure 2.2). Commitments to United Nations Resolutions and European legislation are described alongside the national agenda for the reduction of pollutants within the atmosphere [DETR, 2000].

The policy document outlines the legislative targets assigned by the government to which all areas should conform by the set date [DETR, 2000]. The legislative targets are assigned based upon the protection of human health. The objectives are assigned based on medical and scientific evidence according to the specific effect of each pollutant on health, as well as economic efficiency, practicability, technical feasibility and timescales. Advice on the levels at which targets should be set is taken from EPAQS, who advise the Secretary of State. The target
levels for several air pollutants along with the date for achievement for both the EU and UK is shown in Table 2.2.

The second daughter directive published in 2000 changed the objective limits for carbon monoxide and benzene to those outlined in Table 2.2. The UK Government subsequently responded in 2001 by amending the objective levels set out in the main policy document accordingly (see Figure 2.2). The third daughter directive deals with ozone exclusively and as such is not discussed in this thesis.

**Local Authorities**

Within the Environment Act part IV, and the subsequent policy document "Working together for cleaner air", the onus to achieve the targets was placed upon local authorities. The Act and policy document required each local authority to periodically review and assess the current and future air quality within their administrative boundaries. The process consisted of four main stages to establish possible areas that might not meet the AQS objectives (see Figure 2.3).
Stage 1 consisted of local authorities identifying any 'significant' or proposed sources, either within, or outside, their administrative area, that might result in non-compliance. It is important to note that this stage did not require any monitoring or air quality modeling. If a local authority believed that a source was significant enough, they could move to Stage 3.

Within Stage 2, a more detailed review and assessment process was carried out on any areas where there was a likelihood of not achieving the objectives (discerned in stage 1). This included field monitoring and dispersion modeling of pollution levels across the UK. The results from field monitoring within the UK, and around the world, are discussed in Appendix A along with details of the measurement techniques used.

Monitored and modeled areas from Stage 2 that showed high levels of pollution then underwent a detailed assessment of both current and future air quality with more detailed monitoring and modeling in Stage 3. If it was predicted that an area would not meet the objectives, following the detailed investigations, an Air Quality Management Area (AQMA) could be declared to central Government [DETR, 2000].

Within 12 months of an AQMA declaration, the local authority had to create an 'action-plan' for each AQMA on how to reduce pollution to below target levels within that area. After further consultation the action plan had to be in place 12-18 months following the original AQMA declaration; this assessment has become known as Stage 4. The designation of an AQMA may be revoked by the Secretary of State where objectives have been shown, or are likely to be achieved, following a further air quality review.
In tandem with producing their Stage 4 reports, councils have also been asked to revisit Stages 2 and 3 in an 'Updating and Screening Assessment' (USA) to ensure that the conclusions reached continue to apply given new data. This process is, at present, ongoing.

Overall, UK legislation implements Review and Assessment exercises with a view to reducing the levels of air pollution across an area [Beattie¹, 2001; Beattie² et al., 2001]. This has been seen as a positive step that will reduce pollution levels, and a method that should be adopted by other European Governments [Beattie² et al., 2001].

2.2.6 Problems in the Implementation of UK Legislation

Implementation of current legislation has, associated with it, many practical problems:

- Identification of areas likely to exceed guidelines based on local knowledge may omit potential hotspots;
- Monitoring mainly occurs using diffusion tubes, known to have inaccuracies;
- Field monitoring may be sparsely located; and
- Modeling requires skilled users and is often an expensive exercise.

Stage 1 of the review and assessment process required local authorities to identify areas that might result in future non-compliance of legislation. This identification process is often simply determined through the use of local knowledge, and as such, may result in a failure to isolate less obvious locations with elevated air pollution levels.
Field monitoring was generally located in targeted areas often only using diffusion tubes. The diffusion tubes were set out according to guidelines published by the Government to obtain the best possible capture rate [Bush et al., 2003]. In spite of these guidelines it was known that the diffusion tube methodology is inaccurate, and should be used as a guide to how levels change over the long term rather than a definitive measurement method [Bush et al., 2001]. It was, therefore, difficult to attain whether an area was likely to fail the criteria due to inaccuracies inherent in the method. In order to overcome these inaccuracies, a diffusion tube was often co-located with the more accurate real time measurement methods. The variations between the measurement methods were then used to calibrate the other diffusion tubes within the local area. Unfortunately, other studies on the co-location of diffusion tubes have shown that the technique has variations of approximately ±10%-18% [Bush et al., 2001]. This meant that the difference between one or several tubes and a real time unit at one location could not be used for the calibration of other diffusion tubes.

Due to the nature of selection criteria, monitoring sites were often sparsely located across a region. This has meant that information on pollutant levels at monitoring locations was good, however, little was known about other areas in between the sites. Interpolation of data to ascertain air quality between monitoring locations has had limited success. This was most recently highlighted by Lythe et al., where inconsistencies have been observed across political boundaries due to the position of monitoring locations [Lythe et al., 2002].

In order to address some problems associated with monitoring, computer modeling techniques have been used within the latter stages of review and assessment to ascertain air pollution levels across a local area. For many local authorities this has meant outsourcing to technical consultancies as, internally...
they do not have the resources needed for modeling air quality. This outsourcing is a result of modern methods of computer modeling which are generally expensive and require expertise in setting-up and running as they:

- use complex terminology for input values;
- require large amounts of input data (traffic levels, emission rates from point sources, background levels and meteorological data);
- require large amounts of computer processing power and time to resolve complex atmospheric physics calculations describing dispersion; and
- require expertise in Geographic Information Systems (GIS) spatial analysis techniques to gain full advantage of results.

The expertise needed often stems from the number of tools needed to produce results from a dispersion model, and the number of variations of each available tool. The following section discusses the various tools needed to produce results from a dispersion model and a variety of the options available within each tool type. The tools chosen for the production of the advanced screening model – PARADIS are also discussed.

2.3 Tools Used Within Air Quality Modeling

Air quality modeling allows an investigation into ambient pollutant concentrations in any location by combining:

- traffic data;
- emissions inventories; and
- dispersion algorithms that describe atmospheric physics and chemistry.

Support tools such as Geographic Information Systems (GIS) may also be used to display output from models as a pollutant concentration or contour map. In combination, these tools allow local authorities to determine pollutant
concentrations across their administrative area both currently and for future
years.

Modeling allows comparison to, and compliance with, both UK and European
legislation, and allows local authorities to test the effectiveness of proposed
emissions control measures. Modeling has also been used to determine the
impacts of new developments on air quality as part of an Environmental Impact
Assessment (EIA). This section will examine some of the more widely used tools
used by local authorities within review and assessment stage 3 and later, namely
transport models, emission inventories, dispersion models and GIS.

2.3.1 Transport Models
Transport planning is undertaken by the majority of local councils throughout the
UK within their administrative area to assess the impacts on traffic levels from
various transport policies, and the implementation of known future developments.

The output from transport models is a key input in determining air quality as traffic
is a significant source of pollution. The most simplistic approach of obtaining
traffic information is based upon automatic and manual counts, destination
surveys and household surveys undertaken at key locations on the road network.
Often these methods offer a snapshot of the current traffic levels on various
roads at the time of the survey.

Transport models offer the most complete picture of traffic levels, and are based
upon the more simplistic surveys. There are a variety of packages available,
however, they are all based on:

- a representation of the road network;
- socio-economic data; and
• a mathematical formula to distribute trips.

The road network is represented by a series of ‘nodes’ (junctions) and ‘links’ (roads) that connect the nodes. Each link contains information such as:

• link type;
• distance;
• geometrical characteristics;
• flow/delay (speed/flow) relationship (or fixed speed); and
• capacity.

The nodes and links within the study area are described in great detail, often with every A and B-class road included. A buffer zone surrounds the central zone, and includes only major roads. On these roads similar information is included, however a fixed speed is assumed, as delays are not as crucial in understanding the traffic flow within the study area. Beyond the buffer zone only major nationally important roads are identified.

Land use information in the form of socio-economic data is also important as this is a major factor in the number of trips people make. Rates have been determined for the number of trips that generally leave the different land uses, such as shopping or residential areas. Within a traffic model, the various land uses or Traffic Analysis Zones (TAZs) have a special node, known as a ‘centroid’ assigned to designate them.

Mathematical formulas use the link information and socio-economic data to simulate traffic movement within an area. The traffic assignment formulas have been built on three major ideas:

1. areas with job, shops and housing produce and attract more journeys;
2. people are willing to travel further for work than entertainment / shopping, therefore individual zones have an 'attractiveness' value attached; and
3. people usually take the shortest / fastest route, if congestion occurs alternative routes are sought.

After the model has been run, calibration is needed against existing traffic counts. If model flows are found to be incorrect, variations on the emphasis of the importance of road and zones are used to mirror the existing situation.

If there is likely to be little change in the zones within the study area future scenarios may then be tested using documented growth figures. In the case of land use change, the new TAZs may be input in to the model with the agreed traffic level growth factors to determine new flows.

The results from traffic models are key in the understanding of air quality, as they provide patterns of road use and hence patterns of emission levels [Berkshire Planning, 2004].

**Surrey County Transportation Model (SCTM)**

The County of Surrey has developed over many years their own advanced traffic and transportation model based upon the methodologies outlined above. The Surrey County Transportation Model (SCTM) was initially developed to assist with the County's Local Transportation Plan. Throughout the models history, it has undergone many revisions (Table 2.3) to become an extensive model that covers the major motorways, A-roads, B-roads and some minor roads [SCTM, 2004].
Table 2.3 History of the Surrey County Transportation Model adapted from Surrey County Council, 2004

<table>
<thead>
<tr>
<th>Date</th>
<th>Revision</th>
</tr>
</thead>
<tbody>
<tr>
<td>1970s</td>
<td>Model first developed as a ‘four-stage land transportation model’ that assigned traffic in the peak and off peak periods</td>
</tr>
<tr>
<td>1980s</td>
<td>Use of model changed to provide traffic forecasts for highway schemes as a result it became a ‘12-hour capacity restraint model’</td>
</tr>
<tr>
<td>Early 1990s</td>
<td>Model updated to include selected junction modeling and London Area Transport Survey information</td>
</tr>
</tbody>
</table>
| 1996       | Major redevelopment to include data from the old SCTM, the Surrey County Council model and the M25 sub-regional model (developed so show the impact of road widening of the M25 on the County road network). Update also included:  
• an update of the trip matrices from roadside interviews  
• calibration using 92 counts in Surrey and 63 external locations |
| 1995 - 1999| Highway network updated to include all changes for Surrey, the Blackwater Valley route and all M25 improvements |
| 2000 & 2001| Increase of matrices to new base year based on traffic increases recorded by the County Automated Traffic Counts |

The development of the SCTM over time has created one of the most advanced traffic simulation models in use within the United Kingdom. Recently, the model has undergone year on year updates to include a new base year, and the assessment of the model performance against the Local Transportation Plan targets. As a consequence of this investment in a robust transportation model, developed over 30 years, the output in terms of traffic output has been adopted for use as traffic flows within the advanced dispersion model, PARADIS.

Once the level of traffic flow, percentage of heavy goods vehicles and speed of the various links within a traffic model has been determined, it is necessary to understand the emissions from each individual vehicle. This information is held in large databases known as emissions inventories, discussed in the following section.
2.3.2 Emissions Inventories

Poor air quality is the result of the addition of pollutants from multiple sources within the local area. Emissions characteristics for each source may be defined by an emissions rate. The emissions rate for each source is often contained within a database or inventory that may cover a local area or an entire country. For the majority of local authorities, two types of databases are of prime importance:

- a vehicle emissions database; and
- a 'Part A' processes database

as these provide the majority of emissions within administrative areas.

In order to define vehicle emissions, it is important to take into consideration:

- vehicle fleet;
- fuel type;
- year of investigation; and
- speed.

Modern engines are more efficient than their predecessors, as a result of regulations concerning the emissions from engines introduced by the EU [DMRB, 2003]. The regulations have introduced classes of engines defined as Euro groups. The class to which an engine is grouped is dependant upon the year of manufacture and design. A volume of traffic will contain a mix of diesel and petrol engines, each of varying Euro classes. As time progresses, it is expected that the fleet composition will change to include a larger number of modern engines. The rate of change will depend upon the financial health of the general population, and may therefore be linked to the stability of the economy as a whole. In general, it is expected that emissions from individual engines will
decline, whilst traffic volume will continue to increase [DMRB, 2003; SCTM, 2004].

Figure 2.4 Speed emission curves for petrol engine cars, with an engine size between 1.4 and 2 litres for various Euro classes. Reproduced with the kind permission of HMSO Licence number C02W003685 [DMRB, 2003]

The average speed of traffic greatly affects the emissions characteristics of the fleet, as a result of the efficiency. Engines are approximately 32% efficient when the speed of the vehicle is between 75kph and 110kph [Ferreira, 2003]. Outside of these speeds, the engine is less efficient at combustion and more pollution is released in the exhaust gases. Figure 2.4 clearly shows this change in engine efficiency in terms of emissions levels as the speed changes.

Constituents of the vehicle fleet need then to be determined; this may be achieved locally through vehicle counts or nationally through the registration / taxation of vehicles [DMRB, 2003]. Future predictions of the vehicle fleet may then be made using past trends in the registration of new vehicles and projecting the spread of new engine technologies through the fleet [DMRB, 2003].
This information has been contained within an emissions factor database, so that for a given volume of traffic with a defined percentage of HGV, the vehicle fleet is known and emission rates may be calculated using the speed of the road.

Various types of traffic emissions inventories exist. In circumstances where an appropriate inventory is not currently in place they may be constructed locally for a specific region, such as the London Atmospheric Emissions Inventory (LAEI) commissioned by the Greater London Authority. Conversely, often national emissions inventories exist, such as the National Atmospheric Emissions Inventory (NAEI), which comprise information on all emissions to the atmosphere [NAEI, 2003]. From these national databases more specialised databases for traffic may be constructed, such as that contained within the Design Manual for Roads and Bridges [DMRB, 2003].

In order to accurately describe local air quality, other emission sources, such as factories, should also be defined in an emissions database. Information regarding emission rate and the design characteristics of the source should be included. These sources are often part 'A' processes, and as such need a licence from the Environment Agency (EA) for their operation. The EA provides access to the emissions characteristics of part 'A' processes held within their database. Alternatively, local databases, such as the LAEI, often contain information regarding industrial emissions.

**Design Manual for Roads and Bridges (DMRB)**

The emissions inventory contained within the DMRB has been constructed as a national database. Published in 1994, 1999 and 2003 the inventory accounts for variations in, vehicle fleet, fuel type and speed for the years 1996 to 2025.
Vehicle fleet constitution within the DMRB emissions inventory reflects the registration / taxation statistics for the United Kingdom [DMRB, 2003]. The emission factors for each vehicle type within the fleet for a particular year have been described using large scale surveys, of which the latest revision was carried out in 2001 [Barlow et al., 2001]. A combination of these two information sources means that the use of the DMRB emissions inventory assumes that the fleet constitution on a given link reflects the national statistics.

Fuel type is taken into account within the vehicle fleet characteristics. Registration documents contain information on engine types, and therefore, what fuel type is used. Ratios within the vehicle fleet between petrol, diesel and Liquefied Petroleum Gas (LPG), may therefore be determined and the relevant emission rate applied [DMRB, 2003].

As previously discussed, emission rates of engines alter with speed. These changes in emission rates are reflected within DMRB through the emissions curves shown in Figure 2.4.

As discussed past vehicle fleet characteristics have been based on registration and taxation of vehicles. Forecasting fleet composition and emissions for future years is more challenging. To achieve this forecast, past trends in the spread of new technology spread through the vehicle fleet have been taken into account and projected into the future. Knowledge of stricter European legislation such as the Euro IV classification and the potential of future technologies and fuels further reducing emissions also play a part in forecasting future scenarios [DMRB, 2003].
As a prominent traffic emissions inventory for the UK, the DMRB database has been selected for use in the development of the advanced screening model—PARADIS. The use of this database means that emissions for road links within the study area may be calculated for any year from the base year of PARADIS (2002) to 2025.

Total emissions from each road link within the study area may be calculated through the multiplication of the traffic flow, determined with the transportation model, by the results from the emissions inventory. The next section describes the next tool used within air quality modeling, namely dispersion models, needed to determine and predict ambient pollutant concentrations away from source.

2.3.3 Dispersion Models
Dispersion models take information from the output of the transportation models and emissions inventories, described above, and perform calculations to determine ambient concentrations at receptor locations or across a grid. Two model types exist to determine pollutant concentrations at distance from source:

- screening models; and
- advanced dispersion models.

Screening models are often very simplistic in their approach and application. The DMRB screening model is typical of its type. Developed by the Highways Agency, the DMRB model has been recommended for use by local authorities within Governmental technical guidance documents when determining the effect of new road schemes on local air quality [DEFRA, 2003].

In common with other screening models, including the development of PARADIS, dispersion characteristics from the road have been derived from a more
advanced dispersion model. In the case of DMRB, general dispersion characteristics were taken from a model developed by TRL Ltd. [DMRB, 2003]. Essentially, the DMRB model ignores meteorology and assumes that wind direction is constant around the compass meaning that dispersion happens in all directions equally [DMRB, 2003]. The derived Equation 2.2 allows the calculation of quantitative impact of pollutant levels at distance from the road source. As expected, the equation predicts a diminishing impact with distance from the road (Figure 2.5).

**Equation 2.2** Equation used by DMRB to calculate contribution to ambient levels from traffic at distance \(d\) from source

\[
\text{Traffic Contribution} = 0.17887 + 0.00024c - \frac{0.295776}{d} + (0.2596d^2) - 0.042 \ln(d)
\]

![Figure 2.5 Pollutant contribution decays with distance from road within DMRB model. Reproduced with the kind permission of HMSO Licence number C02W0003685 [DMRB, 2003]](image)

Equation 2.2 and Figure 2.5 are used to calculate dispersion of primary pollutants. One chemical reaction is included within DMRB to allow the calculation of NO\(_2\). Attempts have been made to assess and describe empirically how much NO released from source has been oxidised to NO\(_2\) [Derwent and Middleton, 1996; CERC, 2001; Laxen et al., 2002]. The calculation used within the most recent version of the DMRB model is that proposed by Laxen et al., 2002. The technique has similarities to that used by Derwent and Middleton, as it examined the relationship between NO and NO\(_2\) concentrations in measured data. In contrast to previous work, however, measurement locations have been...
separated into categories dependant upon distance from source [DMRB, 2003; Laxen et al., 2002; DEFRA, 2003]. The derived mathematical formula (Equation 2.3), allows the calculation of annual average concentrations of NO\textsubscript{2} from background and road contributions of NO\textsubscript{X}. Results have indicated that this method predicts approximately 85% of measured NO\textsubscript{2}. This method has been adopted for use within Governmental technical guidance papers for local air quality modeling [DMRB, 2003; DEFRA, 2003].

Equation 2.3 Calculation to derive NO\textsubscript{2} from NO\textsubscript{X} [Laxen et al., 2002]

\[
NO_2(\text{road}) = ((-0.068 \times \ln(\text{NO}_X(\text{Total}))) + 0.53) \times \text{NO}_X(\text{road})
\]

Where

\[
\text{NO}_X(\text{Total}) = \text{NO}_X(\text{road}) + \text{NO}_X(\text{background})
\]

To calculate NO\textsubscript{2}(total)

\[
\text{NO}_2(\text{total}) = \text{NO}_2(\text{road}) + \text{NO}_2(\text{background})
\]

The information used to derive the DMRB model has been input into an Excel® spreadsheet. The use of a spreadsheet as an input medium means that its use is open to anyone with the correct information, and is a simplistic way of determining the pollution contribution from road traffic on local sensitive receptors.

Whilst simplistic to use, the DMRB model has many negatives as a screening tool:

- it allows only the calculation of pollutant concentrations at specific sensitive receptors at distance from a road;
- the addition of pollution from a road source to a sensitive receptor may only be assessed one road at a time;
- it does not allow a clear understanding of impacts of all roads within an area on local air quality; and
Chapter 2 – Background

- the single point receptors generated by the model are insufficient for interpolation by a GIS application meaning a spatial understanding of air quality issues by a local authority is not possible.

Advanced dispersion models overcome the problems highlighted for the screening models. Many types of dispersion models exist as applications to be run on desktop computers and include ADMS-Urban, AERMOD and CALINE amongst others.

Dispersion algorithms used by these models are based upon the Gaussian dispersion theory. Originally, Gaussian dispersion theory investigated point source emissions, however in recent times it has been adapted to include linear sources. The theory assumes that the concentration is at a maximum at the point of release, and decays away, in 3-dimensions following a normal or Gaussian distribution (Figure 2.6).

The decay would be equal in all directions were it not for the interaction of meteorology. When wind is considered, it may be understood that in addition to the dispersion, polluted air moves away from source at a given windspeed and in
the given wind direction. Higher windspeeds result in greater dilution and buoyant pollutants are kept nearer their release height due to ‘bending’ [Colls, 1997]. Close to the ground, windspeed is decreased due to friction of the air with the Earth’s surface. The direction in which the wind blows ultimately determines which way pollution is dispersed. Difficulties arise in physically modeling this, as wind direction varies constantly over a range of time scales. Over short time scales, seconds to minutes, changes in wind direction are often due to turbulence within the atmosphere and may consist of either a thermal or mechanical component. Changes in medium time scales, one to several hours, of wind direction are often due to larger scale weather systems resulting in the passage of a front or the cycle of sea breezes in coastal locations. Over much longer time periods, months or years, these multiple changes in wind directions may be recorded to show how often, at what strength and from which direction the wind blows [Colls, 1997].

Perhaps the most important meteorological consideration is atmospheric turbulence, as this may affect both the speed and direction of the wind. Furthermore, whilst wind may cause direction of pollution transport to be determined, turbulence results in the dilution or diffusion of pollutants within the atmosphere.

Atmospheric turbulence exists as either a result of differential solar heating of the Earth’s surface (thermal), or by air passing over a rough surface (mechanical). Thermal and mechanical turbulence are able to dilute emissions by different amounts due to an important physical difference. Dispersion in thermal turbulence is restricted to the height of the top of the boundary layer, whilst for mechanical turbulence, the entire globe is available [Bach, 1972; CERC, 2001].
Thermal turbulence is best described in terms of the Adiabatic Lapse Rate (ALR). As the Earth’s surface is heated, the air close to the ground becomes warmed and less dense. This parcel of air will then begin to rise upward and will be replaced by cooler air, which in turn will become heated. As the parcel of air moves upwards, it will undergo expansion as it is under less atmospheric pressure. The thermal or convective turbulence that is caused by the movement and expansion of the air parcels results in atmospheric mixing, allowing pollutants to disperse more rapidly. Air in this state is termed unstable and results in pollution dispersion.

Usually, temperature decreases with altitude at the rate of 10Kkm\(^{-1}\) within the troposphere up to a height of approximately 10km, this temperature profile is known as the Environmental Lapse Rate (ELR) [Butler, 1979; Colls, 1997]. If a cold air mass ‘moves-in’ above an area of warmer air, the warm air becomes trapped as it cannot rise above the cold air ceiling. This forms a temperature ‘inversion’ with stable, stagnant air under the inversion. Vertical movement is restricted and a build up of pollutants within the trapped air follows.

### Table 2.4 Pasquill stability criteria and meteorological parameters (adapted from Colls, 1997)

<table>
<thead>
<tr>
<th>Surface Wind Speed</th>
<th>Daytime Sun</th>
<th>Night Time</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Strong</td>
<td>Moderate</td>
</tr>
<tr>
<td>&lt;2</td>
<td>Very unstable</td>
<td>Very moderately unstable</td>
</tr>
<tr>
<td>2</td>
<td>Very moderately unstable</td>
<td>Moderately unstable</td>
</tr>
<tr>
<td>4</td>
<td>Moderately unstable</td>
<td>Moderately slightly unstable</td>
</tr>
<tr>
<td>6</td>
<td>Slightly unstable</td>
<td>Slightly unstable neutral</td>
</tr>
<tr>
<td>&gt;6</td>
<td>Slightly unstable</td>
<td>Neutral</td>
</tr>
</tbody>
</table>
The stability in the air was described by Pasquill in terms of 6 stability categories that could be defined by observing solar incidence and surface wind speed (Table 2.4). In essence, the stability criteria define the height of the boundary layer. During the very unstable category, the boundary layer is high enough not to impede vertical movement. During the most stable conditions, however, the boundary layer is close to the Earth's surface to severely restrict vertical movement.

Mechanical or horizontal turbulence is caused by the interaction of the air as it moves over the Earth's surface. This interaction is described by the surface roughness length, which is related to the height of the obstacles over which the air passes. The value of the surface roughness length is in practice the height at which the horizontal air flow is zero. The height at which this occurs varies on the surface over which the air passes. If the ground is very smooth, such as in a sandy desert, then the point at which the air flow equals zero is very small (0.001m). When the surface is very rough, such as a large city with lots of buildings or woodland with tall trees, the height is larger (1m) [CERC, 2001; EPA, 1998].

Although the Pasquill categories were the first method of describing atmospheric stability and have become widely used, it is acknowledged that the categories tend to fail in unstable circumstances [Colls, 1997]. Modern dispersion models calculate the atmospheric stability and boundary layer height using sequential weather data and the Monin-Obukhov length [CERC, 2001 and EPA, 1998].

In unstable conditions, the Monin-Obukhov length is a measure of the height above ground at which convective turbulence becomes more important than mechanical turbulence. In stable conditions the Monin-Obukhov length...
Chapter 2 - Background

represents the height above which vertical turbulent movement is reduced by
stable stratification of the atmosphere [CERC, 2001]. The use of the Monin-
Obukhov length means that the height of the boundary layer may be more
accurately calculated, and dilution due to convective and mechanical turbulence
more accurately predicted.

Equation 2.4 Gaussian dispersion equation including reflection at the boundary
layer and ground

\[ q(x, y, z) = \frac{Q}{2\pi \sigma_x \sigma_y \sigma_z} \exp \left( -\frac{y^2}{2\sigma_y^2} \right) \left\{ \exp \left( -\frac{(z-H)^2}{2\sigma_z^2} \right) + \exp \left( -\frac{(z+H)^2}{2\sigma_z^2} \right) + \right\} \]

\[ \exp \left( -\frac{(z+2H_{bl}-H)^2}{2\sigma_z^2} \right) + \exp \left( -\frac{(z-2H_{bl}+H)^2}{2\sigma_z^2} \right) + \]

\[ \exp \left( -\frac{(z-2H_{bl}-H)^2}{2\sigma_z^2} \right) \}

Where:

<table>
<thead>
<tr>
<th>q</th>
<th>Concentration at receptor</th>
</tr>
</thead>
<tbody>
<tr>
<td>x,y,z</td>
<td>Cartesian coordinates</td>
</tr>
<tr>
<td>Q</td>
<td>Source strength</td>
</tr>
<tr>
<td>u</td>
<td>Wind speed</td>
</tr>
<tr>
<td>\sigma_x, \sigma_y</td>
<td>Standard deviations in x and y directions described by Pasquill stability classes</td>
</tr>
<tr>
<td>H</td>
<td>Release height</td>
</tr>
<tr>
<td>H_{bl}</td>
<td>Height at top of boundary layer</td>
</tr>
</tbody>
</table>

Convective movement is dependent upon atmospheric stability present at the
time of release, described by the Pasquill stability categories and the monin-
obukhov length. When a parcel of air meets the top of the boundary layer it
becomes reflected downwards, and may also be reflected at the ground. This
process may be described mathematically for a continuous release (Equation
2.4).

Gaussian dispersion theory continues to be used within the majority of models to
describe dispersion of gaseous pollutants away from source, despite offering a
Chapter 2 – Background

'crude' description of dispersion behaviour as a result of the simplicity of the equations [CERC, 2001; Colls, 1997].

As an alternative, the mass conservation approach is used as an alternative to Gaussian dispersion theory, and has been assumed by some dispersion models. The mass conservation approach covers two main methodologies:

- the Eulerian (multi-cell); and
- Langrangian (moving-cell),

both time dependant and able to calculate the concentrations of photo-reactive pollutants, such as NO₂ [Lim, 2004].

As opposed to the Gaussian approach used to determine concentrations from point source emissions, the Eulerian method considers emissions distributed over a wide area. The area under investigation is divided in to a number of cells using either a uniform or non-uniform grid. The pollutant flow through each cell is calculated taking account of each pollutant under investigation from all sources and using the principle of mass conservation. This allows a 'snapshot' to be taken of any given moment and the pollutant concentrations achieved through a combination of emissions and meteorology.

**ADMS-Urban**

As discussed several different models exist for the prediction of pollutant concentration over an area. Within the UK, two models are recommended by the Governmental technical guidance, namely AERMOD and ADMS-Urban, for use by local authorities in stage 3, 4 and the Updated Screening Assessment (USA) [DEFRA, 2003].
The input methods for the different models vary, for example two versions of the EPA model AERMOD exist. The first is a freely available version; however, the input is by text file with a series of specific keywords to define:

- traffic emission levels (that need to be pre-calculated);
- source location (start and end coordinates of each straight road section);
- source dimensions (roads are treated as elongated area sources);
- regular grid; and
- output.

The manual input method used by this model means that data input is a laborious task and open to data entry errors. A commercial package of the same software writes the input text files for AERMOD following the selection of various options within a user interface, however, all source information still needs to be entered by hand, again there are likely to be errors in data input.

In order to calculate dispersion, as with other dispersion packages, meteorological data is required. This data needs to be pre-processed, for the specific modeling location, using a program called AERMET [EPA1, 1998]. Similar in use to AERMOD, AERMET needs a run-time file that includes all of the instructions for processing standard American format meteorological data [EPA2, 1998]. Whilst the commercial version provides the facility to write the code for AERMET, the free version requires manual input of the code. Suppliers of meteorological data often supply the data pre-processed for use within AERMOD to avoid the use of AERMET.

Dispersion of non-reactive species such as NOx and PM10 are calculated over a regular grid using Gaussian equations. Calculation of reactive species, such as NO2, need to be undertaken after processing using empirical relationships defined...
within the literature [Derwent & Middleton, 1996; Laxen et al., 2002; DMRB, 2003; DEFRA, 2003].

Background data are not included within the AERMOD at ‘run-time’. This means that the output is restricted to the level of pollutant that is added to the environment from the source following dispersion. To determine ambient concentrations for comparison with statutory regulation, background levels need to be added in post-processing outside of AERMOD.

Another advanced dispersion model, ADMS-urban, overcomes the problems of manual data input by using a GIS interface. This allows the source vertices to be input by using a mouse. Traffic volumes for LGV and HGV are input and the DMRB source apportionment definitions and emission factors applied to the selected speed [CERC, 2001]. Different emissions source databases may also be used, however, this involves complicated manipulation of databases outside of the main ADMS-Urban user interface [CERC, 2001; Lim, 2004].

ADMS-Urban works slightly differently to AERMOD in that meteorological data is processed at run-time as part of the dispersion calculations for each time period. The metrological file needs to be in the correct format; however, inclusion of this file is completed by selecting the file from within a Windows® browser. This is a minor disadvantage of ADMS, in that the meteorological data needs to be processed for each run, slightly increasing run-time for a series of investigations using the same data.

In contrast to AERMOD, ADMS-Urban requires the user to select the surface roughness and the Monin-Obukhov length. These data are used, in addition to the metrological data, to define the boundary layer height and surface turbulence.
to define dispersion within a Gaussian concentration profile [CERC, 2001]. Whilst some ‘online’ assistance is provided in selecting the correct option, an incorrect decision will result in invalid results. Furthermore, the ‘normal’ set-up does not take account of more than one type of surface roughness or Monin-Obukhov length within the area under investigation. Facilities are provided to vary the surface roughness across the area through the use of a ‘surface roughness file’ although this is not recommended as run-time may be increased by 100-times or more [CERC, 2001].

ADMS-Urban allows the user to determine NO₂ concentrations using the Derwent-Middleton correlation or the Generic Reaction Scheme (GRS) [Derwent & Middleton, 1996; CERC, 2001]. Within recent years the Derwent-Middleton correlation has been criticised for using too few data in drawing its empirical relationship between NOₓ and NO₂ [Laxen et al., 2002; DMRB, 2003]. NO₂ concentrations may be calculated after processing, outside of ADMS-Urban using the modern empirical relationships and NOₓ concentrations defined by the model.

Background data may be included, prior to ‘run-time’, within ADMS-Urban meaning that the output at each of the receptor points, and across the grid, is the ambient concentration of each pollutant investigated. Background data may input as either a single value for the entire year, or as a file that has a value for every 15-minute period taken from a nearby background monitoring location. In both cases, the background value is applied to the entire modeled area. This results in the modeled pollutant concentrations appearing to be tied closely to the line of the road. More accurate results may be achieved through the use of the model to calculate additional pollution generated by the various sources and the dispersion due to meteorology. Post-processing of the data may then be used to
add varying background data provided within the national background maps
[DEFRA, 2003, LDA, 2004].

The length of ‘run-time’ for all dispersion models is dependant upon:

- the number of sources;
- the size of the area under investigation;
- the number of receptors; and
- the degree of grid mesh ‘fineness’ calculated.

Whilst the ‘run-time’ for a single road would not be great, when five or more
sources are used, the ‘run-time’ is significantly increased. It is not unusual for the
‘run’ to take over a week when a moderately sized town (approximately 9km$^2$) is
modeled.

Comparison of some of the advanced dispersion models on the market has
shown that ADMS-Urban tended to under predict by approximately 20%, whilst
AERMOD had a tendency to under predict by 40% using the same data sets
[Hanna et al., 2001]. In addition, ADMS has undergone many validation studies
using a variety of techniques [Mensink et al., 1997, Carruthers et al., 1997 and
Carruthers et al, 2000]. The many advantages that ADMS-Urban has over other
similar models, discussed above, contributed to the use of this model in the
construction of the advanced screening model – PARADIS.

Once dispersion calculation have been made using the packages described
above, the results may be interpolated and viewed spatially. Interpolation and
spatial plotting of the results is usually undertaken with the aid of Geographical
Information Systems (GIS) software, described in the next section.
2.3.4 GIS Software

Geographic Information Systems (GIS) software is a computer application that allows the acquisition, plotting, manipulation and representation of spatial data (data with a set of coordinates). This enables cartographic and graphical elements to be displayed simultaneously creating an integrated environment allowing an overview of the geographic context of the data. Further information on the use of GIS applications to produce and display spatial data has been described in detail by Lim [Lim, 2004].

As with the other tools used within the calculation and display of ambient pollutant concentrations, a variety of commercial packages are available. Within the UK, the most popular packages in current use are Mapinfo and ArcMap. Essentially, the two systems work in similar ways and both allow the addition of ‘add-in’ extensions that allow the manipulation of spatial data.

The most useful aspect of GIS software is the ability to ‘interpolate’ between the gridded output from dispersion models to create surface or contoured data. The interpolation algorithms used include:

- Inverse Distance Weighting (IDW);
- Kriging; and
- Spline.

The IDW technique assumes that each point has a local influence that decreases with distance. To predict a value in an unmeasured location, the technique searches for recorded data in the immediate vicinity to determine the missing value [ESRI, 2003].
Kriging uses much the same theory as IDW in that the closest points have the greatest influence. The exact influence each measured point has on the unrecorded location depends not on distance, but a semi-variogram developed through looking at the spatial construction of the data [ESRI, 2003].

The Spline method differs from the other two methods as points in the missing locations are not generated. Conceptually the method is like fitting sheet of rubber to all points with a mathematical function to minimise the curvature of the surface [ESRI, 2003].

During the development of the advanced dispersion model, it was envisaged that following the parametric studies of ADMS-Urban, PARADIS would be programmed as an extension to an existing GIS program. ArcMap uses visual basic, whilst Mapinfo uses its own proprietary software MapBasic as the programming language through which macros may be programmed to build an independent extension. Visual Basic has the advantage over MapBasic of being well supported throughout the IT community, and allows the production of GUIs for the input of additional information and choice selection. As a result of these advantages, ArcMap was selected as the preferred GIS platform through which to deliver PARADIS.

2.4 Summary
In this chapter the background to this research has been detailed. The motivation for on-going air quality investigations is primarily driven by health issues. In particular, the increasing levels of NOx, CO and PM, as a result of elevated traffic levels, have linked with respiratory and heart disease. These health concerns have resulted in legislation, based upon epidemiological studies, at both a European and domestic level, to ensure the reduction in ambient
concentration of these pollutants. Within the UK central Government has defined target levels for a range of vehicle-related pollutants. These are administered at a regional level in which local authorities are required to individually review and assess their air quality. A number of air quality stages have been defined and these are used to identify areas where pollutant concentrations may exceed the statutory targets.

The air quality assessments comprise field measurements and numerical modeling techniques. Field measurements are subject to a number of inaccuracies in particular:

- the ability of Triethanolamine (TEA) to react effectively to NO$_2$ exposure;
- the length of exposure of diffusion tube;
- location of diffusion tube; and
- infrequent manual re-calibration of automated monitors,

in addition field measurements are limited by the sparse distribution of monitoring sites.

Numerical modeling overcomes some of these issues but introduces additional complexities. Four main tools were described namely transportation models, emissions inventories, dispersion models and geographic information systems.

It is the lack of detailed field measurements combined with the complexity of using advanced dispersion models that has provided the motivation for this study.

Current screening spreadsheets such as that proposed within the DMRB methodology only allow concentrations at individual sensitive receptors to be calculated with the source defined as a single road. This method is clearly inaccurate in determining concentrations if more than one road is closely located...
to the source. Moreover, this method does not allow the spatial representation of data within a GIS, and it is not possible to understand how concentrations vary across an urban area.

More complex advanced dispersion programs such as AERMOD and ADMS-urban allow calculation at specific receptors and across a grid taking in to account all sources and metrology to determine concentrations. These models are generally well validated and tested, and are recommended for use with UK Governmental guidelines. In spite of wide usage within air quality work these models also have distinct disadvantages. Most disadvantages are specific to each model, however, some of the more common are:

- data entry by manual input rather than reading from the output of a traffic model;
- complex terminology used during selection criteria for various options relating to dispersion;
- processing of metrological data is either complex or time consuming; and
- long run-times.

This research outlines an alternative approach in developing a screening model. The main objective is to create a fast user-friendly screening model accessed through a GIS interface that may use:

- manual input – clicking along a road and defining the traffic flow; and
- automatic input – reading traffic data from a traffic model output to define pollutant concentrations across a grid. The grid may then be spatially interpolated to understand how concentrations vary throughout the study area. It is envisaged that the parameterisation of an advanced dispersion model is the key to achieving these aims.
Chapter 3 – Study Area

3.1 Introduction

As discussed in chapter 1, the purpose for this research was to produce a numerical model that would have the ease of use, and short ‘run-times’, inherent in screening models, and in addition, the visual output facilities provided with advanced dispersion models. Hence, the main objective was to develop an advanced screening tool that could be used as part of an initial air quality assessment in order to identify potential pollution ‘hot spots’. To achieve this, it was envisaged that an advanced screening model would utilise a local transportation model together with parametrically derived dispersion characteristics in a highly visual GIS environment. The model would, therefore, effectively perform a PARAMetrically derived Dispersion Simulation, hence the name ‘PARADIS’. This would have a distinct advantage over existing advanced dispersion models as:

i. long run times would be eliminated as the model uses look-up tables and exponential equations rather than complex dispersion algorithms;

ii. computational demands would be reduced as algorithms used to calculate pollution levels would be simplified; and

iii. the model would be simple to set-up through the use of automated input and the removal of complex air quality terminology.

iv. specialist training would not be required as the model would use clear easy to follow GUIs.
As a consequence, local councils may not have to outsource modeling to specialist consultancies, and therefore reduce their costs in complying with both EU and UK legislation.

The development of this advanced screening model (PARADIS) was divided into 4 distinct phases, namely:

- study area (selection);
- pollutant dispersion characteristics;
- PARADIS (design, development and implementation); and
- PARADIS (validation) and Case Studies.

The creation of PARADIS, from choice of study area for development, through design, implementation and testing is shown in Figure 3.1. These phases are independent from each other but progress from one another in chronological order.

In this chapter Phase 1, the highlighted section in Figure 3.1, is described; namely, the selection criteria for a study area and the validation of that study area through the use of local monitoring. Whilst the phases are independent of each other this particular phase was carried out first as meteorological data, appropriate to this region, was required in phase 2.
Chapter 3 – Study Area

3.2 Study Area Selection

Whilst PARADIS was designed to be portable to other regions, it was important to select a particular region during the development phase of the model, in order to validate the results. Within any given region there are always a number of local factors, which are only applicable to that area, for example, the parametric studies in the development of PARADIS used statistical weather data to generate

An Advanced Screening Model to Predict Air Quality
the equations and look-up tables used within the model. It was necessary, therefore, to use representative weather data for the study area selected. Hence, PARADIS was developed using data relevant to a particular selected study area. The adaptability of the model to represent other regions is discussed in more detail in Chapter 6.

The choice of study area, however, was more complex as there were also a number of additional factors, which were deemed either necessary or desirable in order to facilitate the validation of the model. In particular, as PARADIS was developed to generate traffic pollution fields it was necessary for the study area to have:

- high levels of traffic throughput; and
- an associated traffic and transport model.

It was also desirable for the chosen area to have:

- accurate field measurements for validation comparison; and
- little traditional industry either within the area or on the borders in order that the field data reflected only traffic related concentrations.

Many areas were excluded from this study as, in general, they either were found to have large industrial ‘Part A’ processes nearby, or the level of traffic on the roads was not sufficiently high to warrant exploration. London was discounted as it has unusually high air pollution levels, associated with the extreme numbers of vehicles and complex dispersion as a result of the many street canyons. Areas to the east of London were considered, however, it was anticipated that the prevailing south-westerly winds crossing London, may unduly influence pollution concentrations.
The County of Surrey was considered as it has:

- a high population density due to its proximity to London;
- an increased level of car ownership in comparison with the rest of the UK due to the affluence of the general population;
- nearly double the national average traffic flow on the county A-roads;
- a sophisticated County Transportation Model (CTM) giving annual average daily traffic (AADT) flows for all major roads within the study area; and
- very few industrial sources located either within the county or close to the county boundaries.

As a consequence, Surrey met the necessary requirements, and most of the desirable requirements in the choice of initial study area. Furthermore, due to the limited industrial plants, and high car usage within Surrey, it was anticipated that the field data available would realistically reflect traffic emissions, as opposed to the cumulative effect of multiple source emissions from both traffic and industrial sources typically experienced in most other regions.

### 3.3 Study Area Validation

Once Surrey had been selected, a number of feasibility checks were performed to test whether the advanced screening model could be developed and tested in this region. These checks were undertaken through the investigation of air quality data from passive diffusion tubes and real-time units collected throughout the county. All of the boroughs with Surrey go beyond the requirements of the Air Quality Strategy, discussed in chapter 2, and maintain several times the requisite number of NO₂ diffusion tubes. In addition, several boroughs have real-time units that measure a variety of pollutants continuously, averaging the results over a 15-minute period (see Figure 3.2 for location).
In particular the following points were investigated to ascertain whether the:

- field data collected from Surrey could primarily be attributed to traffic as opposed to other (commercial) sources;
- major airports adjacent to Surrey influenced the available field data; and
- distribution of the monitored data and its validity were sufficient to be used in testing the new advanced screening model.

### 3.3.1 Field Data

The available field data was initially used to confirm that the emissions being measured could actually be attributed to traffic as hypothesised above. Figures 3.3 and 3.4 show data for CO and NO, two of the primary exhaust pollutants. In each graph, a typical week-day distribution is shown as recorded by one of the real-time monitoring units in Guildford. Guildford is a medium sized urban region in Surrey, with a high traffic throughput, especially during the known ‘rush hour’ periods. The second plot on each graph is barely discernable as it effectively mirrors the ambient background level (nearly the x-axis in the case of CO). These
were also measurements recorded on a week-day, at the same location, but in this case, the date was 25th December, Christmas Day.

![Typical Weekday CO Levels](chart)

Figure 3.3 Average weekday levels of CO in comparison to Christmas Day. The dramatic reduction in pollutant levels on Christmas Day is probably a result of the reduction in traffic.

As there are no major industrial sources surrounding the monitoring unit locations, the only difference between these dates was simply volume of traffic. If other unknown pollutant sources were present then it would be expected that they would be detected even on Christmas Day. The lack of a level above background concentration on Christmas Day indicates that recorded levels may be attributed to traffic. Given that there are so few major industrial sources across the whole of Surrey, it is therefore likely that the field measurements collected across Surrey, and highlighted using the Guildford example do indeed reflect traffic emissions.
The results shown for Guildford are reflected for other monitoring locations across the county including:

- Mole Valley Unit 1 between 1996 and 1998;  
- Mole Valley Unit 2 between 1997 and 2000; and  

### 3.3.2 Airports

As discussed, little traditional industry exists either within or on the borders of Surrey, reflected by pollutant concentrations that indicate that traffic is the dominant source. Two additional pollutant sources, located close to the County Boundaries, need to be considered whilst selecting Surrey as the study area. Heathrow and Gatwick, two major international airports are located just to the north and south of the county boundaries. It is conceivable, therefore, that these.

---

1 Dates are indicative of time when units were active in locations specified in Figure 3.2
airports may have an influence on the background pollution levels within the
boroughs that border them.

Airports are portrayed within the media as responsible for the high levels of
pollutant concentration that surround them [BBC, 2003]. As a result, public
perception is often that aircraft are the main contributors to these elevated
concentrations. In contrast to this, analysis of data from a real-time unit close to
Gatwick Airport in the UK showed little correlation. As the number of flights
significantly increased at Gatwick (to peak values between 7.30am and 8.00pm)
there was no corresponding increase in NO levels. Instead the NO trend was
dominated by the two daily ‘rush’ hour traffic peaks seen in many localities in
Surrey remote from airports. Similar trends were also observed for CO, NO₂ and
PM₁₀. This would suggest that at ground level, vehicles still appear to be the main
pollution sources for these pollutants as opposed to aircraft.

Results from monitoring near to Gatwick were compared with studies surrounding
airports across the USA. Following the shutdown of all airports within the US in
the aftermath of terrorist events on September 11th 2001, Kenney found that
there was little discernable difference in the level of NOₓ, PM₁₀ or CO pollution
[Kenney et al., 2002].

This again supports the premise that the levels of NOₓ, PM₁₀ and CO recorded
across Surrey primarily reflect traffic emissions in the region rather than other
transport or industrial related emissions.
3.3.3 Suitability of Monitoring Data for Model Validation

One of the major tasks in the development of any numerical model is validation of the model. Air quality modeling is far too complex for there to be an exact analytical solution against which to make comparisons. Hence, the alternatives include validation against other numerical models and/or validation against field data. In the case of Surrey, there was a significant history of available field data but the integrity of this data needed to be confirmed. To achieve this, the available field data (both short and long-term data) was analysed to see if it conformed to the expected trends.

A full analysis of these trends within the monitored data may be found in Appendix B, however, a number of general trends are shown here to demonstrate the integrity and validity of the data across the county.

The units in Guildford, Waverley and Mole Valley have been collecting data since 1997, as such they represent the locations with the longest monitoring history, and have been investigated as a representative sample.
Investigation of the real-time data in Surrey demonstrated two diurnal peaks for primary traffic pollutants (Figure 3.6). These peaks coincided with morning and afternoon 'rush' hours, as would be expected as this is the time of highest traffic throughput during day [SCTM, 2004]. The variation in concentration may be attributed to the location of the unit relative to the road source. Whilst the Guildford and Waverley units are classified as kerbside (<5m from the road) the unit in Mole Valley has been designated as background as it is >50m from the road.

Figure 3.6 Average weekday NO and PM$_{10}$ concentration (April 2000 - April 2001) at three monitoring locations throughout the county

Measurements taken over a longer period indicated trends within the data not attributable solely to traffic (Figure 3.7). Peaks were observed for all measured pollutants (in October and January) indicating large scale meteorological factors affect all pollutant concentrations. NO$_2$ concentrations were found to be lower in
summer and higher in winter. This variation was to be expected as a result of increased insolation in summer months resulting in destruction of the NO₂ molecule. These observations were confirmed by other studies in to the long term trends of NO₂ concentrations using diffusion tubes [Lythe et al., 2001; Lythe et al., 2002].

![Graph showing pollution levels recorded at Guildford Unit 1 April 1999 to January 2001](image)

**Figure 3.7** Pollution levels recorded at Guildford Unit 1 April 1999 to January 2001

The results shown in Figure 3.7 have been shown to occur at all other monitoring locations, indicating that these phenomena are a global event within Surrey as a probable result of meteorology.

A comparison of monitoring locations showed that similar patterns were observed at all sites. Comparable patterns at the various measurement locations suggest similar sources and conditions at each site. The terrain in Surrey is fairly flat so little or no topology effects are expected. The weather at various locations across the County is generally much the same and, as a result, the pollution dispersion patterns would be expected to be similar.

The comparable patterns observed within the data, at various locations across the county, indicate that traffic is the dominant source across the whole county,
and therefore this location is suitable for the development of an advanced screening model for traffic related air pollution.

As discussed, the monitoring locations across the county provide discrete positions at which to validate the advanced screening model. In contrast, the geographical spread of these monitoring locations is too sparse to allow interpolation techniques for validation between monitoring locations. The next section discusses this dichotomy, and a methodology that has been developed as a solution.

### 3.3.4 Sparsely Distributed Data Across Surrey

Thus far all the data analysed have been measured at discreet points and hence are only representative of the pollution levels in that immediate vicinity. Surrey has approximately 180 passive diffusion tube measurement sites representing an area of approximately 1663km². The distribution of the diffusion tubes is more heavily weighted to the more urbanized areas in the north and north-west of the County. Real-time units have a very sparse spatial distribution across Surrey with only 8 locations across the area (Figure 3.2) as a direct result of the cost in purchasing and running these instruments.

Whilst there are many more diffusion tubes than real time units, numbers are still insufficient to create anything but a very coarse irregular grid. The position of tubes within each borough is currently designed to meet the needs of the individual borough to determine possible Air Quality Management Areas (AQMAs). As shown by Lythe, this has the effect of high pollution levels stopping at political boundaries when spatial interpolation is undertaken within each borough [Lythe et al. 2002; Lythe et al., 2004]. Furthermore, the location of the tubes within each borough, and across the county at present shows a
geographical bias that is not easily resolved for spatial interpolation. The northwest corner of Surrey is more urbanised than the rest of the county. Governmental target values apply to residential areas, and as a result there are more NO₂ diffusion tubes. A bias in the proportion of site categories in each borough also exists. One borough for example has 70% Kerbside sites and another 60% background sites [Lythe et al., 2001, Lythe et al., 2002].

Whilst comparisons may be drawn between monitoring locations, data usually only applies to the immediate locality in which it was collected. To determine pollutant concentrations between measurement locations spatial interpolation techniques may be employed. For interpolation techniques to give meaningful results collection points need to be

- regularly sited in a grid across the area to understand the general behaviour of pollution levels;
- within an adaptive grid to identify individual features such as roads; and
- have no geographical bias within each borough or across the county.

In practice, the measurement sites are not uniformly distributed, and are far too sparse to make realistic comparisons with a numerical model which may have orders of magnitude more grid points over the same area.

Attempts have been made to reconcile the number of measurement locations available to discern the most appropriate sitting for interpolation purposes, however, results from this work have yet to be implemented [Lythe et al., 2004].
Figure 3.8 Spatially interpolated map of extrapolated data from real-time units with data from NO2 diffusion tubes overlaid

As a result of spatial distribution of the various networks discussed above, validation of the advanced screening model may easily be carried out at discrete points by comparing the model results with measured annual average concentrations. Validation of the advanced screening model between measurement locations is more difficult due to the problems highlighted. Validation has been made possible, however, by the development of a methodology, described in detail in Appendix C. The technique uses:

- the decrease in pollutant concentrations with distance from the road source (observed at real-time monitoring locations within Surrey);
- traffic information from the County Transportation Model;
- Gaussian dispersion equations; and
- interpolation algorithms
to determine pollutant concentrations across the county. The results for NO$_2$ from the methodology (Figure 3.8) have been shown to have good statistical agreement with concentrations recorded with diffusion tubes across the county (appendix C).

3.4 Summary

This chapter has discussed the location of study area in which this investigation has been undertaken. The choice of the Surrey data, prior to the start of the research, was necessary due to the need for weather data during the parametric studies with an advanced dispersion models. As PARADIS was to be designed to reflect pollution levels due to traffic as a source, the chosen study area needed to have a high traffic throughput and very few ‘Part A’ processes.

Monitoring data from real-time units and diffusion tubes within Surrey has shown that:

- the majority of pollution recorded in Surrey may be attributed to traffic;
- there appeared to be no correlation between aircraft movements and ambient concentrations of pollutants levels (NO$_x$, NO$_2$, CO and PM$_{10}$) around airports; and
- there is sufficient data of sufficient quality to validate the advanced screening model.

This confirmed the suitability of Surrey against which to prototype the advanced screening model.

The dichotomy of the availability of data for validation at discrete monitoring locations against the lack of spatial availability of data for validation between monitoring locations has been discussed, and a methodology proposed as a solution. The methodology would allow the use of real-time data to create
'dummy' monitoring locations at all 'nodes' throughout the county with Gaussian dispersion equations used to calculate levels away from road sources. This methodology creates enough 'dummy' monitoring locations to allow spatial interpolation techniques to be applied. The pollution contour maps that result may be used to evaluate the advanced dispersion model in any location throughout the study area.

In the following chapter, phase 2 is described in which inputs such as traffic volume, speed, percentage HGV and road width have been parameterised from a widely used dispersion model. The parameterisation of these inputs has allowed the mathematical description of the pollution fields generated by those inputs, the results of which have been used to develop PARADIS.
Chapter 4 - Model Development

4.1 Introduction

Chapter 4 describes phase 2 of the development process, namely the parametric studies undertaken during the model development of PARADIS, as highlighted in Figure 4.1.

Figure 4.1 Schematic diagram representing developmental process
As discussed in chapter 2, traffic models, and emissions inventories, are readily available and allow the calculation of emissions from road sources. Once emitted from the internal combustion engine pollutants rapidly become diluted and dispersed within the atmosphere. The rate and pattern of this dilution / dispersion is dependant upon several factors, namely:

- wind direction;
- wind speed; and
- surface roughness.

During the dilution / dispersion process complex chemical reactions occur, changing chemical species from one oxidation state to another or transforming them into various compounds. As a result the algorithms used to mathematically describe the physics of the dilution / dispersion process, and chemical reactions, within the atmosphere, are complex.

Also discussed in chapter 2, section 2.3.3, screening and dispersion models that simulate the dilution / dispersion process have different levels of complexity in their use and computational algorithms. These models vary from the spreadsheet form of DMRB, through an intermediate class, such as the use of Gaussian dispersion equations in CALINE4, to the use of complex dispersion algorithms used in ADMS-Urban and AERMOD [DMRB, 2003; CALTRANS, 1989; CERC, 2001; EPA1, 1998].

Algorithms used by the advanced dispersion models describe reflections at the surface and the planetary boundary layer; the height of which is calculated from a variety of meteorological measurements. As a result these calculations are representative of the atmospheric physics and chemistry. Often, however, they...
take large amounts of computation time to process the meteorological data before calculating dispersion.

Production of a contour pollution map, as an output from an advanced dispersion model, is achieved through the calculation of pollution concentration at a number of receptor points within a grid. In order to accurately describe dispersion away from a road source it is necessary to include an ‘adaptive’ grid. The adaptive grid has one general grid spacing over the entire area, and a finer grid within 100m of each road link. This is to ensure that a road link is not missed due to the grid spacing of a regular grid. An adaptive grid often has tens of times the number of receptor locations in comparison to a regular grid; this leads to long processing times, often of several days.

As adaptive grids with closer spacing around roads need to be adopted to resolve fine details of pollution patterns, a method needed to be developed to reduce the computation time required to resolve the pollutant concentration at each point within the grid without loosing the accuracy achieved by the advanced dispersion models. It was envisaged that the most effective method of creating an advanced screening model would be to parameterise results from an existing advanced dispersion model to produce ‘look-up’ tables. The ‘look-up’ tables would be used in place of the complex calculations to describe the pollution field surrounding a road, and hence calculate ambient pollutant concentrations.

The next section describes the process used to parameterise the results from ADMS-Urban for use within a ‘look-up’ table. The process by which any dispersion model could be parameterised would be similar, however ADMS-Urban was chosen as it was recommended for use in review and assessment projects by local authorities by the UK Government, and has been validated in...
several studies [Olesen, 1995; Carruthers et al., 1997; Mensink et al., 1997; Carruthers et al., 2000; CERC, 2001]. ADMS-Urban also links with ArcView 3.x, a GIS, giving ease of input and a visual output.

4.2 Parameterisation

The main aim of the parametric studies was to identify inputs within a dispersion model that had a direct impact of the pollution fields generated by the algorithms used within the model. The results from the parametric studies could then be used either within ‘look-up’ tables, if the results varied due to a change in a second value, or as a factor within the PARADIS program if they were found to remain constant.

As PARADIS has been designed to predict the impact of road traffic pollutants, the parameterisation has been undertaken for each of the main primary road traffic pollutants, NO\textsubscript{x}, PM\textsubscript{10} and CO. For each of these pollutants two main sets of parametric studies were undertaken for each of four road orientations, north-south, east-west, northwest-southeast and northeast-southwest. The main sets of studies were:

- the configuration of the road-links;
  - road configuration;
    - 4 test cases for a varying size of central reservation at 0m, 4m, 8m or 12m; and
    - 2 test cases for a motorway / dual carriageway to decide if this type of road should be considered as one road or two;
  - road width;
    - widths of 8m, 16m, 20m and 24m to describe the various types of road in use within the UK, these were investigated for various speeds and HGV percentages;
Chapter 4 – Model Development

- traffic configuration;
  - vehicle number;
    - 3 test cases at 10kph with 10% HGV and 500, 1000 and 2000 vehicles; and
    - 3 test cases at 20kph with 10% HGV and 500, 1000 and 2000 vehicles;
  - vehicle speed and percentage HGV;
    - 96 test cases from 10kph to 120kph at for 10%, 20% and 30% HGV and road width (not all road widths were investigated for each speed, as it was deemed inappropriate to model a motorway at 10kph).

A full list of runs for each road orientation and pollutant may be found in appendix D. In total there were 1164 studies completed, each run took approximately 10 hours on a 1GHz processor. The processing time was split between two desktop computers running simultaneously in order to reduce the time required.

A set of tools was selected to undertake these parametric studies. These were:
- Dispersion model: ADMS-Urban 1.6;
- GIS: ArcView GIS 3.2; and
- Data storage: Microsoft Excel

4.2.1 Description of the Pollution Field
The 'road-links', used within the studies, were 300m in length and had end effects associated with them (as discussed below). To ensure that the transects, along which mathematical formulas would be derived, were taken in the correct place, it...
was necessary to understand how the chosen dispersion model (ADMS-Urban) treats a road source, and in what way dispersion from them is calculated.

Road sources within ADMS-Urban are considered as a series of point sources along the road [CERC, 2001]. An adaptive grid is used to determine pollutant concentration both across the road and in the surrounding area. Within ADMS-Urban, the concentration of the pollutant is calculated at each individual point for every line of meteorological data, and the average over the time period of the meteorological data is taken [CERC, 2001]. If meteorological data is for one day, and the wind direction is set to the southwest for that day, the resulting pollution plume lies to the north-west, as shown in Figure 4.2. In this instance, the wind direction for an individual day plays a dominant role in the resulting pollution concentrations.

European and British laws require that pollution levels are maintained within limits. These limits are often set as annual average levels, therefore, parameterisation was undertaken to look pollution levels on this timescale.
In order to minimise area dependencies and to investigate annual average concentrations a 10 year statistical meteorological dataset (1987-97) was taken to represent the region. Within the statistical dataset the pollutant concentration is similarly calculated at each point within the grid, and an average taken over the time period of the meteorological data (Figure 4.3).

The result, Figure 4.3, may be unexpected, as it is known there are a larger proportion of southwesterly winds within the dataset (Figure 4.4). However, the southwesterlies, whilst dominant, are not the only influence (as in Figure 4.2) the other wind directions (Figure 4.4) must also be taken into consideration. This means that whilst the dominant wind direction during the year is from the south west (Figure 4.4), the generated pollution field surrounding the road, is not dominated by that wind direction (Figure 4.3).

Further examination of Figure 4.3 shows that towards the end of the road pollutant levels appear to decline. At this location, within the parametric studies, there is less influence from the traffic on the surrounding receptor points due to the road ending. In reality a road does not simply end, therefore, the pollution field may best be described by the concentrations along an orthogonal line across the centre of the road. When the concentrations are taken along four
transepts, at the centre of the road, where end effects are not present, it may be seen that the pollution level does not vary (Figure 4.5). It may be concluded, that only one transept line is needed in order to identify a pollution concentration field. This line of concentration may be repeated along the entire road length to describe the pollution field for that road.

![Figure 4.5 Transepts at various points along the same road](image)

4.2.2 Road Orientation
Within Geographic Information System (GIS) software, vector files, known as 'shapefiles' within ArcMap, may be used to represent the position of almost any geographic feature usually found on a map as points, polylines or polygons. The output from the Surrey County Transportation Model (SCTM) is represented within the GIS as a polyline 'shapefile' with a link defined between two nodes (junctions) where traffic flow changes. The SCTM uses 'polylines' within the shapefile to define the real-world position of the links within the network. Polylines are a collection of straight line segments that constitute a curved feature, such as a road, and are required as a computer is unable to draw a curved line due to its nature as a digital device. The segments are sub-sets of
the polyline and share the same unique feature identification number. This allows each segment to be easily identified with its parent polyline and within the associated database.

The length of each straight line segment is pre-determined during digitisation of the road, for use within a GIS. During digitisation, the number, and length, of segments within each link defines positional accuracy of the road. The more curved a road, more numerous and shorter segments are required to accurately describe the position. This means that the length of an individual segment will vary dependant upon the nature of the road. Typically, however, within the SCTM, a 1km link may contain 20 individual segments, although major roads are likely to be straighter and therefore require fewer segments.

Within the GIS, it is possible to program the system to deconstruct the polyline to define the start and end coordinates of each segment making up the polyline. In the production of PARADIS, it was important to use the start and end points of each individual segment within the polyline rather than the polyline itself to more accurately describe the position of the pollution fields on a curved road. The identification of the multiple straight line segments within an individual polyline allows PARADIS to describe the location of a road when overlaid on an Ordinance Survey map.

There is obviously an infinite number of orientations of individual polyline segments. The development of the methodology for an intermediate model required the road orientations to be set to predefined values. These were selected based upon a balance between optimising the accuracy of the results and minimising computing runtime. Parametric runs of ADMS-Urban to define the exponential curve of pollutant concentrations surrounding a road for an
individual orientation took over 40 days. The optimum number of orientations that would approximate the position of the road with sufficient accuracy was therefore needed.

The SCTM polylines used within the running of PARADIS are based upon a 1:50000 scale Ordnance Survey map. As previously discussed, the majority of segments within the SCTM are 50m or less in length. It was considered, therefore that a low number of orientations would be required to approximate the road position as rotation of lines of length ≤50m at a 1:50,000 scale would be sufficiently accurate in their geographical location.

In the first instance, two orientations were considered:

- north-south; and
- east-west.

It was quickly discerned that a large number of roads lay in the north-east, south-east, south-west and north-west quadrants. When roads in these positions were rotated either to north-south or east-west orientation, the result was a very disjointed pattern of pollution.

The northeast-southwest; and northwest-southeast orientations were therefore additionally considered to create four possibilities for orientation and to remove the disjointed pattern observed. When plotted out, pollution patterns from these orientations closely matched the line of the road at the 1:50,000 scale.

A further investigation considered the additional orientations of:

- north-northwest-South-southwest;
- northeast east – southwest west;
• northwest west-southeast east; and
• north northwest-south southeast.

As expected, pollution patterns again very closely matched the line of the road; however, the variation in plotted concentrations between four orientations and eight orientations was found to be negligible at 1:50,000 scale. Whilst eight orientations would be needed to more accurately describe the position of exceptionally curved/long segmented roads, or when using maps of large scale this was not the case within the study area or the map scale used. It was therefore decided that rotation of the short segments to an orientation divisible by \( \pi/8 \) allowed an effective approximation of the road position with a maximum orientation error of 22.5°. Whilst this degree of accuracy was sufficient for the purpose of demonstrating the usefulness and research implications for an intermediate model, there is possible scope for improvement to the model in this area.

It should be noted that for maps of a larger scale a greater number of orientations would be required due to the greater detail on the map. The intermediate model was designed to look at pollution levels on a town scale and so was restricted to 1:50,000 scale maps.

The effect of wind speed and direction on dispersion with respect to varying road orientation was investigated for the two sets of parametric studies. As discussed, the parameterisation of results from a dispersion model in respect of every possible road orientation would be impractical. To overcome this problem four orientations (N-S, E-W, NE-SW, NW-SE) were considered for the two sets of parametric studies.
As anticipated, a change in road orientation results in adjustment of the pollution field due to a relative modification of wind direction (Figure 4.6). In describing the pollution field for each of the four road orientations it was necessary to examine the change in pollution level along an orthogonal line across the centre of the road. The mathematical description of the orthogonal line was made possible by dividing it in to sections according to distance from road and describe each 'best fit' line as an exponential. An example of this may be seen in Figure 4.7.
A number of curve fitting procedures, available through a spatial analysis package within the GIS environment, was examined to determine the best method of describing the decrease of pollutant concentration with distance from a road. These procedures included a linear, low order polynomials and an exponential best-fit line developed using the least squares method. The least squares method assumes that the best fit line through a set of data will have the minimum sum of the squares of deviations of the data points from the line. Higher order polynomials may be used to 'bend' the best-fit line to the data, however this is often seen as mathematical manipulation rather than discerning trends that may be applied to other scenarios. In each case the least squares method to provide a line of best-fit has been applied only to the data shown on the graphs (Figure 4.8 to Figure 4.11).
In the first instance, the chosen methods were applied to all of the data on each side of the road, however, as can be seen from Figure 4.8, none of the methods accurately described the data. This is especially true of the polynomial and linear best-fit lines which drop below zero ppb of NOx.

![Figure 4.8 NOx concentrations vs. distance from road with curve fitting procedures superimposed - all distances](image)

In order to obtain the closest fit of a trendline to the data, it was necessary to divide the curve into segments as the curve was too complex to describe using one linear, exponential or second order polynomial equation. Clearly, a large number of sections of the line would allow a closer fit of the best-fit line to the data, however this would have meant longer processing time.

The line was split at 10m and 100m from the road in order to define the three segments. These distances were chosen, as in the first instance, pollutant concentrations are often found to be highest and change rapidly over the first 10m due to turbulence caused by passing traffic [CERC, 2001]. At 100m, it has been found that pollutant concentrations attributable to the road source begin to decline less rapidly, as the concentration is much diminished through dispersion and dilution [DMRB, 2003]. This effect may be seen in Figure 4.8 where the
decrease in concentration at distances greater than 100m from the road is much reduced.

When the same curves are applied to the three sections (Figure 4.9 to Figure 4.11), it becomes clear that the linear fit is not suitable in any case. The low order polynomial may be suitable at distances close to the road, however at other locations, the best-fit method for a polynomial results breaks down. This is most notable in Figure 4.11, where the polynomial line of best-fit deviates below the modelled data (between 130m and 100m before the road). The polynomial line of best-fit then begins to increase at distances greater than 1000m from the road.

The exponential best-fit line gives a reasonable approximation of the results from ADMS-Urban at all three defined distances in Figure 4.10. This method is shown to slightly over predict concentrations at distances greater than 15m from the road (Figure 4.10). This provides a worst-case scenario in all results from PARADIS. The exponential best fit line using the least squares method was therefore chosen to represent the data at the 3 distances from the road. The equation for each best-fit line is therefore in the form shown in Equation 4.1.
Chapter 4 – Model Development

Figure 4.10 NOx concentrations vs. distance from road with curve fitting procedures superimposed – 10-100m from the road

Figure 4.11 NOx concentrations vs. distance from road with curve fitting procedures superimposed – >100m from the road

Equation 4.1 Chosen equation form for nest-fit lines for three distance bands

\[ y = c \cdot \exp(mx) \]

where:
- \( y \) – pollutant value
- \( c \) – value of \( y \) at which exponential curve meets the road
- \( m \) – growth/decay factor
- \( x \) – distance from road

The choice of an exponential best-fit line as representing the data is supported by statistical analysis using \( R^2 \) which describes the degree to which the best-fit line represents the data. At an \( R^2 \) value of 1, the trend line passes through each point of the dataset, and values approaching 1 are generally thought representative of the dataset. Table 4.1 shows the \( R^2 \) values obtained from the trend lines fitted to
Chapter 4 – Model Development

the 3 distance datasets for NO\textsubscript{x}, PM and CO using the least squares method. The \(R^2\) values for the selected trend lines all exceed 0.95.

Table 4.1 \(R^2\) values obtained from the trend lines fitted to the 3 distance datasets for NO\textsubscript{x}, PM and CO using the least squares method

<table>
<thead>
<tr>
<th>Pollutant</th>
<th>East, South, South-west or North-west of road dependent on orientation</th>
<th>West, North, North-east or South-east of road dependent on orientation</th>
</tr>
</thead>
<tbody>
<tr>
<td>x &gt;100m</td>
<td>0.9671 0.9655 0.9941</td>
<td>0.9512 0.9686 0.9622</td>
</tr>
<tr>
<td>10m&lt; x &lt;100m</td>
<td>0.9940</td>
<td>0.9501 0.9685 0.9623</td>
</tr>
<tr>
<td>x &lt;10m</td>
<td>0.9672 0.9664 0.9940</td>
<td>0.9504 0.9676 0.9623</td>
</tr>
</tbody>
</table>

The fact that the best-fit of the ADMS-Urban output is an exponential curve is not surprising, although this may be a reflection of a limited number of tested functions. Within a number of air quality models, however, the concentration of a pollutant decreases exponentially with distance from a road source [DMRB, 2003 and Janssen et al., 2003]. This has been based on a number of monitoring studies, replicated within Surrey, which have shown an exponential decrease [DMRB, 2003 and Cowan et al., 2002]. It was therefore decided to use an exponential equation for each distance as this was the best approximation for air quality data. The mathematical description of each road orientation was repeated for the two sets of parametric studies with the results described in detail below.

The growth or decay factor (m) within the equation of the exponential best-fit line (Equation 4.1) is linked both to the distance from, and the width of, the road. In considering the parametric runs of ADMS-Urban for NO\textsubscript{x} along a north-south road (appendix D, table D1.2), it may be seen that the value of \(m\) does not vary for any road width or speed when the distance from the road is >10m. Conversely, when the distance from the road is <10m, variance of the growth/decay factor occurs between the different road widths; whilst each individual road width has the same value of \(m\). A possible explanation for the
variance 'm' with road width at close proximity to the road is due to turbulence caused by the passing traffic on different sized roads. Within ADMS-Urban, (from which the growth/decay factor 'm' has ultimately been derived) turbulence caused by traffic is accounted for in terms of additional lateral turbulence [CERC, 2001].

The results from the parametric runs indicate that as road widths become larger and carry higher volumes of traffic, the induced turbulence increases. This results in greater mixing within 10m of the road and hence a variable value of 'm'. As distance from the road and time, for pollutants to travel, from source to receptor increases, the vehicle induced turbulence becomes less important than the mechanical turbulence. At this point (distance x>10) the growth/decay factor remains constant for all road widths and speeds.

4.2.3 Configuration of 'Road-Links'
The first set of runs were undertaken to investigate the impact of various types of road sources on the output of dispersion models. Within the UK several road types exist and include:

- Single lane with omni-directional traffic (urban and rural);
- Urban dual lane with omni-directional traffic;
- Dual-carriageway (2 lanes in each direction and a central reservation);
- Motorway (3-5 lanes on each carriageway with a central reservation and emergency 'hard-shoulder' lanes on each side).

It was important to investigate dual carriageways and motorways to determine whether they should be modeled as one line source or two. This was done by examining firstly whether the width central reservation had any effect on the pollution field or the pollutant concentration. Secondly, road width was considered to understand the effects on pollutant concentrations.
Road Configuration

The lane configuration of trunk roads and motorways were considered as they have two carriageways each with 2, 3 or 4 lanes. The level of pollution across this type of road may be expected to rise on the first carriageway, fall at the central reservation and rise again at the second carriageway to finally decline away from the road. Figure 4.12 shows that the width between the two carriageways needs to be 8m or more before the double peak is observed. Generally, the width of area used for the crash barrier is equal to that of one lane (approximately 4m). This means that in terms of air quality prediction, the two carriageways act as a single line source rather than two separate sources.

![Figure 4.12 The separation of carriageways by various central reservation widths (legend specifies different widths of central reservation)](image)

To ensure that dual-carriage roads behave as a single line source, further parametric studies were undertaken to explore the difference in pollutant concentration field across a road. Two parametric studies were completed: the first modeled the road as one line source of fixed width, and the second as two line sources equal to the same width. The negligible variation in the results, as shown in Figure 4.13, indicate that there is very little difference between concentrations in considering the road as a whole or the two carriageways separately.
Figure 4.13 The separation of carriageways and the effect on predicted pollution levels

As a consequence of these findings, roads with more than one carriageway have been considered as a single source within PARADIS.

**Road Width**

A second set of parametric runs were completed to identify the impact of road width on pollution dispersion. As discussed above, various road types have different lane numbers and widths. It was decided, therefore to investigate a mixture of road widths for the road types using ADMS-Urban. Various road widths were considered for 12 traffic speeds between 10kph and 120kph.

Table 4.2 shows the road widths that were considered at the various speeds. For each road width and speed the percentage of HGVs was set at 10%, 20% and 30%; this is discussed in detail in section 4.2.4. Not all road widths were considered at all speeds. It was thought unnecessary to investigate some speeds on certain road widths. The effect of traffic at 120kph on an 8m wide road, for
example, as the speed limit on an 8m wide road would never exceed 100 kph in the UK.

### Table 4.2 Parameterised Road widths for varying speeds

<table>
<thead>
<tr>
<th>Speed (m)</th>
<th>Road Width (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>8, 16</td>
</tr>
<tr>
<td>20</td>
<td>8, 16</td>
</tr>
<tr>
<td>30</td>
<td>8, 16</td>
</tr>
<tr>
<td>40</td>
<td>8, 16</td>
</tr>
<tr>
<td>50</td>
<td>8, 16</td>
</tr>
<tr>
<td>60</td>
<td>8, 16</td>
</tr>
<tr>
<td>70</td>
<td>8, 16, 20, 28</td>
</tr>
<tr>
<td>80</td>
<td>8, 16, 20, 28</td>
</tr>
<tr>
<td>90</td>
<td>8, 16, 20, 28</td>
</tr>
<tr>
<td>100</td>
<td>8, 16, 20, 28</td>
</tr>
<tr>
<td>110</td>
<td>20, 28</td>
</tr>
<tr>
<td>120</td>
<td>20, 28</td>
</tr>
</tbody>
</table>

![Graph showing level of NO₂ with varying road widths and speeds](image)

**Figure 4.14** An increase in road width reduces average level of pollution (traffic produced levels only, background has not been included) for a road running north-south. Legend values represent the various road widths.

Figure 4.14 shows the results from one such investigation into the average level of pollution on the central reservation at 70kph with 10% HGV on roads of width 8m, 16m, 20m and 24m. It can clearly be seen that the wider the road the lower the level of pollution, both at the road centre, and on either side. This is a likely result of a wider road aiding dispersion and lowering the 'roughness' level of the...
surface. The results from these studies were included in the ‘look-up’ tables for use within PARADIS.

### 4.2.4 Traffic Configuration

The next set of parametric studies concentrated on the vehicle configuration in use upon each road orientation. A variation in the number of vehicles and percentage HGV was investigated with the exact make-up of the vehicle fleet determined using the DMRB database provided with ADMS-Urban 1.6 for the year 2001. The DMRB database contains historical information concerning percentages of engine size / type for various vehicles based on registrations within the United Kingdom, and predictions of future trends in adoption of new engine technologies within the fleet.

**Vehicle number**

The first parametric studies in the second set were undertaken to understand the relationship between vehicle number and pollutant concentration across a road.

Three runs were undertaken for an 8m wide road for 500, 1000 and 2000 vehicles for each hour within a 24 hour period travelling at 10kph with 10% HGV. The results, Figure 4.15, show the levels of pollution across a road for the various traffic levels. It is clear from Figure 4.15 that a doubling of the traffic level results in a doubling of the concentration of pollutant.
Figure 4.15 NO$_2$ levels across an 8m wide road for varying traffic levels at 10kph with 10% HGV

Obviously, doubling of pollution levels could not continue indefinitely, as there is a finite traffic level that may pass along a road at any given speed. The limiting factors on pollution are, therefore, average speed and road capacity.

The results from these studies allowed a factor to be assigned within the PARADIS program to calculate the concentration dependant on the number of vehicles using the road.

**Vehicle Speed and Percentage HGV**

The final two parameters, vehicle speed and percentage HGV, were investigated simultaneously alongside road width in a suite of 96 runs for each road orientation.
The exact concentration of emissions from an engine is dependant on the speed of the vehicle, with the lowest pollution levels achieved when the vehicle is between 75kph and 100kph [DMRB, 2003]. The variation of pollution emissions with speed produces a speed pollution curve that varies for each pollutant [CERC, 2001]. Figure 4.16 shows the level of pollution at the centre of a road for 500 vehicles at varying speeds.

The speed pollution curves, Figure 4.16, have been taken into consideration when parameterising results from ADMS-Urban. Runs for various traffic mixes and road width have been repeated for 12 speeds from 10kph to 120kph.

For each of the 12 speeds, between 10kph and 120kph, the relevant number of road widths were investigated, as previously discussed in section 4.2.3, and for each road width, three runs were undertaken for 10%, 20% and 30% HGV.

Heavy goods vehicles emit different amounts of traffic related pollutants than lighter vehicles [DMRB, 2003]. A change in the vehicle mix affects a change in the level of pollution. Table 4.3 shows the results from 9 parametric studies to
indicate how concentrations of a pollutant change for 500 vehicles with 10%, 20% and 30% HGV moving at speeds of 10kph, 20kph and 30kph. The results from these studies showed that for a percentage rise in the proportion of HGV there is a constant rise in the level of pollution for each speed. For each distance from the road, the investigations showed that there was also a consistent increase. The relationship between the level of HGV, and pollution concentration, may be used to apply a weighting to percentage levels of HGV within the vehicle mix.

<table>
<thead>
<tr>
<th>% HGV</th>
<th>Speed (kph)</th>
<th>10</th>
<th>20</th>
<th>30</th>
<th>Increase per % HGV</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td></td>
<td>2.4</td>
<td>4.9</td>
<td>7.2</td>
<td>0.24</td>
</tr>
<tr>
<td>20</td>
<td></td>
<td>1.5</td>
<td>2.8</td>
<td>4.3</td>
<td>0.14</td>
</tr>
<tr>
<td>30</td>
<td></td>
<td>1.3</td>
<td>2.6</td>
<td>3.8</td>
<td>0.13</td>
</tr>
</tbody>
</table>

The weighting determined for each speed at various distances from the road was included in the 'look-up' tables for use within the PARADIS program for calculation of pollutant concentration.

4.3 Generation of 'Look-Up' Tables

The results for the 96 runs for each road orientation and pollutant are contained within 12 'look-up' tables (one table for each pollutant and parameterised road orientation) for use by the PARADIS program. Within each table the first two columns define speed of traffic and road width. Following this are an additional 18 columns that are divided in to 6 sets of 3. Each set describes the equation of the exponential line \( y = C \exp^{mx} \) that best fitted the parameterised data for each distance, \( x \), from the road (\( x > 100 \text{m}, 10 \text{m} < x \leq 100 \text{m}, x \leq 10 \text{m} \) for the left and right of the carriageway). The first column, in each set of three, defines the \( y \)-intercept on a graph (\( C \)). The second column contains a multiplier to be used for each percentage of HGV, whilst the final column in each set classifies the...
Chapter 4 - Model Development

growth/decay length scale (m). The format for each ‘look-up’ table may be seen in Table 4.4.

Table 4.4 ‘Look-up’ table format. C and M refer to values obtained from exponential curves to describe the y-intercept and the decay length scale in the equation $y = C \times \exp(mx)$. The three distances are then repeated in reverse each with the same three columns for locations on the other side of the road.

<table>
<thead>
<tr>
<th>Results for each distance from road (m)</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Speed (10kph to 120kph)</th>
<th>Road Width (m)</th>
<th>C</th>
<th>HGV multiplier</th>
<th>M</th>
<th>C</th>
<th>HGV multiplier</th>
<th>M</th>
</tr>
</thead>
<tbody>
<tr>
<td>&gt;100</td>
<td></td>
<td>C</td>
<td></td>
<td>M</td>
<td>C</td>
<td></td>
<td>M</td>
</tr>
<tr>
<td>≤100&gt;10</td>
<td></td>
<td>C</td>
<td></td>
<td>M</td>
<td>C</td>
<td></td>
<td>M</td>
</tr>
<tr>
<td>≤10&gt;0</td>
<td></td>
<td>C</td>
<td></td>
<td>M</td>
<td>C</td>
<td></td>
<td>M</td>
</tr>
</tbody>
</table>

4.4 Grids and resolution

Grid resolution is an important consideration in any model design as it may affect interpolated values and consequently patterns of pollutant concentration over an area. A very fine resolution grid (<10m) (on a scale of 1:50,000) provides a high degree of accuracy when contouring, however the finer the grid, the more calculations are needed and the slower the calculation time. If the grid is too coarse then interpolation algorithms such as Inverse Distance Weighting are inappropriate for modelling rapidly changing pollution fields [Lythe, 2001]. There is, therefore an optimum grid resolution size between calculation time and accuracy. A series of runs of PARADIS was completed varying the coarse output grid starting at 25m with 25m incremental gaps to 300m. It was found that when the coarse grid was greater than 250m the interpolation caused areas of unexpected low concentration points to occur in the middle of high levels. Below 250m grid resolution, the interpolations gave similar results accurate to 2 decimal places. Consequently, 250m was selected as the maximum grid size to sufficiently describe the pollution field.

As a pollutant source, vehicles have an influence on the environment around them. Due to mechanical and convective turbulence, pollutant concentrations become dispersed and diluted so that the proportion of concentration attributable
to the road diminishes with distance from the source and will eventually become negligible. Consequently, it is not necessary to calculate the concentrations across a grid that covers the entire area under investigation. In some models, the distance over which concentrations are calculated is limited by distance [DMRB, 2003]. Within PARADIS, the grid over which a pollutant is output is not defined by distance; instead it is adapted to be dependant upon the pollutant level attributable to a road. Pollutant concentrations lower than 0.001 ppm for CO, 0.01 ppb for NOx or 0.01 mg m⁻³ for PM, were considered negligible. Consequently, these concentrations were not output and did not contribute to final calculations.

4.4.1 Continuity between grids
Each link within the transportation model has unique characteristics such as traffic flow, speed and road width. As previously discussed, the link is a polyline but in order for calculations to be undertaken the segments that make up the polyline need to be treated individually. As previously discussed, concentrations for data points for the entire area under investigation are calculated, however they are only output if the concentration is above certain levels. These levels have been chosen as in the first instance they represent a level below which concentrations from the road may be considered negligible, but secondly to ensure that grids from separate segments overlap. As cars pass from one segment to another, calculations from the overlapped grids ensure that there is continuity between the two datasets.

When the Inverse Distance Weighted (IDW) interpolation technique finds two or more, ‘stacked’ data points in the same location an average concentration is resolved for that location. The IDW interpolation algorithm then uses data from surrounding data to interpolate between the grid spacing. The IDW technique is
best suited to the interpolation of the air quality modelling data as concentrations decrease with distance from the road [Cowan et al., 2001; DMRB, 2003]. It should also be noted that ADMS-Urban uses the IDW routine, by default, to generate pollution contour plots [CERC, 2001]. In areas where the resultant concentration is from two or more sources the concentrations should to be summed rather than averaged, as is the case in this methodology. The results of averaging all 'stacked' data points have proved the methodology used by the IDW routine effective in producing pollutant concentrations. The issues surrounding improving this methodology are discussed as part of future work in chapter 7.

The overlapping grids, and the use of the IDW interpolation algorithm, accounts for the emissions from all segments and polylines. This ensures continuity to give a smooth output across the raster contour map of pollutant concentrations.

4.5 Summary
This chapter has described the need to increase the speed of processing time to resolve air quality without significant loss of resolution or accuracy. To achieve this aim, studies were undertaken with ADMS-Urban. The methodology used could be applied to any advanced dispersion model. The parametric studies were divided in to two sets, namely:

- road configuration; and
- traffic configuration

and were undertaken for four road orientations (N-S, E-W, NE-SW and NW-SE) and three pollutants (NOx, PM10 and CO).

The results from each parametric study have been analysed to determine the equation of an orthogonal line to the orientation under investigation. It was found
that the simplest way to mathematically describe the line was to divide it into 3 distances (x > 100m, 10m < x < 100m and x < 10m) on each side of the road. The line for each distance could then be described as an exponential equation in the form $y = C \exp(mx)$.

The parametric studies for the road configuration determined that roads with more than one carriageway should be treated as one road source and that various road widths affect the pollution field concentrations surrounding a road.

The traffic configuration parametric studies established that:

- a doubling in traffic leads to an approximate doubling in pollutant concentration;
- different traffic speeds result in varying amounts of pollution due to engine efficiency; and
- for each speed there is a constant factor for each percentage of HGV when determining overall pollutant concentrations.

The results from the parametric studies were stored in 12 'look-up' tables that may be used to define a pollutant concentration at any given distance from the source. The 'look-up' tables have been designed for use with the PARADIS program for calculating pollutant concentrations over an area.

Whilst interesting in themselves, the results from the parametric studies are not useful in determining spatial pollutant concentrations, and the interaction of sources, unless they are used to calculate concentrations across adaptive grids. The next chapter describes the development of a calculation program and Graphical User Interfaces (GUIs) that allow manual and automated input into the calculation program. In addition, methods of interpolation are discussed and the
use of further tools, developed to investigate the possible need for AQMAs within an administrative area.
Chapter 5 - Model Implementation

5.1 Introduction
This chapter describes phase 3 of the development process, which involved the creation and coding of the advanced screening model – PARADIS and the Graphical User Interface as highlighted in Figure 5.1.

![Figure 5.1 Schematic diagram representing developmental process](image-url)

An Advanced Screening Model to Predict Air Quality...
As discussed in previous chapters, PARADIS was created as an advanced screening model that local authorities could use quickly and cheaply to identify pollution hotspots within their area. As highlighted in chapter 4, it was felt the most efficient way of achieving this aim was to parameterise the results from an existing dispersion model. The results from the parametric studies have been stored in 12 'look-up' tables, one for each of 4 road orientations and 3 pollutants.

This chapter considers the methods of using the values from transport models with the 'look-up' tables to create a pollutant contour map within a GIS system, as highlighted in Figure 5.1. This has been achieved by separating PARADIS into two separate modules, namely:

- calculation software; and
- Graphical User Interface (GUI) for data input and output manipulation

that work together in a process, outlined in Figure 5.2, to define pollution levels across an area.

![Figure 5.2 Process of running PARADIS](image_url)
The following sections describe, in detail, the design and implementation of the calculation program and GUIs.

5.2 Calculation Software

The calculation software for PARADIS is an integral part of the software system as shown in Figure 5.3. The calculation module has been written separately to the GUI, and was designed to use the results from the parameterisation studies of ADMS-Urban with data from a transportation model to calculate pollutant concentration. The calculation software is written in Fortran95 code, as this language has the advantage over object orientated languages in faster processing speed in running complex calculations.

![Figure 5.3 PARADIS calculation program as an integral part of the system process](image)

5.2.1 Calculation of Primary Pollutants

The input values, Table 5.1, to the calculation programme are stored in an input file by the Graphical User Interface (described in section 5.3). The data within the input file are used to define which ‘look-up’ table and values to use as shown...
in Table 5.1. These values are then utilised to calculate the level of pollution generated by the passing traffic for varying distances away from the road.

### Table 5.1 Input values to PARADIS program and the definitions within the code

<table>
<thead>
<tr>
<th>Input Value</th>
<th>Used to define</th>
</tr>
</thead>
<tbody>
<tr>
<td>Output path</td>
<td>Location in which to store output file</td>
</tr>
<tr>
<td>Road Co-ordinates</td>
<td>Spatial location of road</td>
</tr>
<tr>
<td>Road Orientation</td>
<td>'look-up table'</td>
</tr>
<tr>
<td>Vehicle Number</td>
<td>Value of vehicle factor</td>
</tr>
<tr>
<td>Percentage HGV</td>
<td>Row of 'look-up' Table</td>
</tr>
<tr>
<td>Speed</td>
<td>Row of 'look-up' Table</td>
</tr>
<tr>
<td>Road Width</td>
<td>Row of 'look-up' Table</td>
</tr>
<tr>
<td>Year</td>
<td>Value of Year Factor (see table)</td>
</tr>
<tr>
<td>Pollutant</td>
<td>'look-up' Table</td>
</tr>
<tr>
<td>Background Concentration</td>
<td>Total ambient concentration when added to road source levels</td>
</tr>
<tr>
<td>Spatial Limits of Study Area</td>
<td>The area over which the grid is calculated</td>
</tr>
</tbody>
</table>

Pollutant values are calculated at point ‘receptor’ locations by the program on a grid basis. Two grid meshes are used within the programme, coarse and fine. The coarse grid has 250m X 250m spacing, and is designed to calculate lower levels away from the road. The coarse resolution is not subtle enough to discern sharp changes over a small distance. The fine grid has a 1m X 1m mesh and is used 10m either side of the road in order to resolve small changes typical of these locations.

The spatial location of the receptors allows the calculation of distance to the road and, therefore, the 'look-up' table column to be used. Using this information with the HGV percentage, speed and road width, the equation of the exponential line, defined in the parametric studies, is identified.

Once calculated, the concentrations undergo post processing to determine concentrations in the year selected and, if selected, the concentration of NO₂.
5.2.2 Future Year Predictions

As discussed in Chapter 4 the parametric studies were completed for a base year of 2002. As a result, in the first instance, all concentrations of pollutants are calculated for 2002. Future years are expected to show a general decrease in the level of pollution [DMRB, 2003]. Increased engine efficiency, alongside new technologies and fuels, are predicted to cause this decline in spite of traffic volume levels continuing to rise [DMRB, 2003; SCTM, 2001]. The possibility of predictions for future years has been incorporated with the model calculations by calculating year factors (Table 5.2) from the DMRB emission factors for 2003 to 2025 published in May 2003 [DMRB, 2003].

<table>
<thead>
<tr>
<th>Year</th>
<th>NOx</th>
<th>PM10</th>
<th>CO</th>
</tr>
</thead>
<tbody>
<tr>
<td>2002</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>2003</td>
<td>0.90</td>
<td>0.91</td>
<td>0.83</td>
</tr>
<tr>
<td>2004</td>
<td>0.82</td>
<td>0.83</td>
<td>0.70</td>
</tr>
<tr>
<td>2005</td>
<td>0.76</td>
<td>0.77</td>
<td>0.61</td>
</tr>
<tr>
<td>2006</td>
<td>0.70</td>
<td>0.71</td>
<td>0.54</td>
</tr>
<tr>
<td>2007</td>
<td>0.64</td>
<td>0.64</td>
<td>0.50</td>
</tr>
<tr>
<td>2008</td>
<td>0.60</td>
<td>0.57</td>
<td>0.47</td>
</tr>
<tr>
<td>2009</td>
<td>0.55</td>
<td>0.52</td>
<td>0.46</td>
</tr>
<tr>
<td>2010</td>
<td>0.51</td>
<td>0.48</td>
<td>0.45</td>
</tr>
<tr>
<td>2011</td>
<td>0.48</td>
<td>0.45</td>
<td>0.44</td>
</tr>
<tr>
<td>2012</td>
<td>0.45</td>
<td>0.42</td>
<td>0.43</td>
</tr>
<tr>
<td>2013</td>
<td>0.42</td>
<td>0.40</td>
<td>0.43</td>
</tr>
<tr>
<td>2014</td>
<td>0.40</td>
<td>0.38</td>
<td>0.42</td>
</tr>
<tr>
<td>2015</td>
<td>0.39</td>
<td>0.37</td>
<td>0.42</td>
</tr>
<tr>
<td>2016</td>
<td>0.38</td>
<td>0.36</td>
<td>0.42</td>
</tr>
<tr>
<td>2017</td>
<td>0.37</td>
<td>0.35</td>
<td>0.42</td>
</tr>
<tr>
<td>2018</td>
<td>0.36</td>
<td>0.35</td>
<td>0.42</td>
</tr>
<tr>
<td>2019</td>
<td>0.35</td>
<td>0.34</td>
<td>0.42</td>
</tr>
<tr>
<td>2020</td>
<td>0.35</td>
<td>0.34</td>
<td>0.41</td>
</tr>
<tr>
<td>2021</td>
<td>0.35</td>
<td>0.34</td>
<td>0.41</td>
</tr>
<tr>
<td>2022</td>
<td>0.35</td>
<td>0.34</td>
<td>0.41</td>
</tr>
<tr>
<td>2023</td>
<td>0.34</td>
<td>0.34</td>
<td>0.41</td>
</tr>
<tr>
<td>2024</td>
<td>0.34</td>
<td>0.34</td>
<td>0.41</td>
</tr>
<tr>
<td>2025</td>
<td>0.34</td>
<td>0.34</td>
<td>0.41</td>
</tr>
</tbody>
</table>

The various factors shown within Table 5.2 may are applied to recalculate the results for a specific year.
5.2.3 Nitrogen Dioxide Calculation

Calculation of NO₂ is slightly more complex than for NOₓ, PM₁₀ or CO as it is not emitted directly from the combustion engine in large quantities. As discussed in chapter 2 section 2.1.2 the majority of NO₂ is produced through chemical reactions in the atmosphere. There are several methodologies for calculating the concentration of NO₂. ADMS, for example, offers the choice of Generic Reaction Scheme (GRS) or the Derwent/Middleton correlation.

The GRS consists of the 8 most important reactions that involve nitrogen oxides, Volatile Organic Compounds (VOCs) and ozone that result in the formation or destruction of NO₂. The reactions are used over time periods to determine the overall concentration of NO₂ at a point receptor. Investigations using ADMS-3, a version of ADMS-Urban suited to industrial sources, has found that the GRS can have a significant influence on peak and annual NO₂ concentrations [Air Quality Expert Group, 2003]. As a consequence, it was felt that this method of determining NO₂ was not accurate when comparing results to the AQS objectives.

The Derwent/Middleton correlation is an empirical correlation based upon measurements taken in London. Studies using the correlation in rural and smaller urban areas have found that the methodology gives inconsistent results [CERC, 2001, Laxen et al., 2002 and Stedman et al., 2002]. The Derwent/Middleton correlation was therefore rejected as an option for determining NO₂ concentrations within PARADIS as the correlation does not apply to all areas.

PARADIS uses a new empirical approach proposed by Laxen and Wilson (2002) that has been recommended for use within both the DMRB methodology, and the
UK Government’s technical guidance on Local Air Quality modeling as discussed in Chapter 2 section 2.2.3. The method has been developed in a similar approach to that adopted by Derwent and Middleton. The approach proposed by Laxen has, however, used a wider range of measurements of NOX and NO2 concentrations taken in a variety of settings throughout the UK to derive the empirical relationship [Laxen et al., 2002]. The empirical approach divides the ambient concentration of NO2 into a background constituent derived both locally and from outside the area alongside that from freshly produced NOX. In studying 28 kerbside sites over three years (1999-2001) Laxen and Wilson have determined that NO2(road) may be calculated by use of Equation 5.1 to within ±15% of the true value [Laxen et al., 2002].

\[
NO_{2(road)} = \left( -0.068 \times \ln(NO_{x(total)}) + 0.53 \times (NO_{x(road)}) \right)
\]

\[
NO_{2(total)} = NO_{2(road)} + NO_{2(background)}
\]

Where:

- \( NO_{x(total)} \) = \( NO_{x(road)} + NO_{x(background)} \)
- \( Ln \) is log to the base e
- \( NO_{2(road)} \) is the level of NO2 produced from traffic
- \( NO_{2(background)} \) is the background level of NO2
- \( NO_{2(total)} \) is the total level of NO2
- \( NO_{2(road)} \) is the level of NO2 produced from traffic
- \( NO_{2(background)} \) is the background level of NO2
- \( NO_{2(total)} \) is the total level of NO2

In order to calculate the total NO2 concentration the levels determined for the road need to be added to the background levels (Equation 5.1). Laxen and Wilson suggested that the background levels, needed for the calculations, should come from the national 1X1 km grid of background maps or a local background monitoring site.
The next section describes the development of the Graphical User interface used to input data in to the PARADIS program and process the output in to pollutant concentration maps, and additional tools that may be used to highlight areas of elevated pollutant concentrations.

5.3 PARADIS Graphical User Interfaces
As discussed in the previous section, PARADIS uses a Graphical User Interface (GUI) for the input of data in to the calculation program. In addition, additional GUIs have been developed to assist with the production of pollutant concentrations map and tools used to highlight areas of elevated concentration. As a consequence, the tools are used at both ends of the calculation program described in the previous section, as shown in Figure 5.4.

The GUIs were created as an extension to a Geographical Information System as this provided the added functionality of allowing:

- manual input through a mouse by clicking on the location of the road;

Figure 5.4 PARADIS GUIs surrounding the calculation program
automated input through the use of traffic model shapefiles and associated databases; and
spatial calculations using processed data.

In development possibility terms, ArcGIS by ESRI offered the best prospect for the creation of the additional software needed for input to, and output from, the calculation programme. The ArcObjects model provided with ArcGIS allowed full customisation of all aspects of the GIS package. Customisation may be undertaken using either Visual Basic for Applications (VBA), supplied with ArcGIS, or by creating a DLL file with ActiveX controls through Visual Basic (VB).

5.3.1 Input GUIs
Input to the PARADIS calculation program can be completed using a text file. In order to make the calculation program easier to use, a GUI interface was created that 'writes' the input files for each road 'link'. This form of input was chosen over the use of text files as it:

- is faster; and
- removes the possibility of human error in input file creation.

In terms of data input, two methods of data input were created, namely:

- automated; and
- manual.
Chapter 5 – Model Implementation

The automated version allows the use of traffic databases in the form of polyline shapefiles for direct input, whilst the manual version allows the use of the model by defining road locations with the mouse and inputting relevant information. The two options were provided, as it was noted that whilst the SCTM provided a 'real world' polyline file for the road locations, many traffic model outputs only define traffic volumes at fixed node points with straight line connectors. Use of straight line connectors could result in elevated pollutant concentrations in locations where roads are not actually present. Separate GUIs were required, therefore, for the automated and manual processes. The processes through which input methods are used within PARADIS are shown in Figure 5.5.

Figure 5.5 Flow diagram for manual and automatic input methods and the link to the calculation software
Table 5.3 shows the source and data required for the automated and manual modes. Where the source has been defined as ‘user input’ a GUI has been created, and is discussed below. The processes that use the data are shown in Table 5.3, which represents how the GIS extension functions and links to the calculation programme to produce a pollution map.

Table 5.3 Data required and source for different input types

<table>
<thead>
<tr>
<th>Data</th>
<th>Automated input</th>
<th>Manual input</th>
</tr>
</thead>
<tbody>
<tr>
<td>Folder location</td>
<td>Choose folder from file tree</td>
<td>Choose folder from file tree</td>
</tr>
<tr>
<td>Road coordinates</td>
<td>Shape file coordinates</td>
<td>Input with mouse click</td>
</tr>
<tr>
<td>Road orientation</td>
<td>Determined by internal calculations</td>
<td>Determined by internal calculations</td>
</tr>
<tr>
<td>Traffic count</td>
<td>Transport model</td>
<td>User input</td>
</tr>
<tr>
<td>Road width</td>
<td>Determined from road type taken from transport model</td>
<td>User input</td>
</tr>
<tr>
<td>Speed</td>
<td>Transport model</td>
<td>User input</td>
</tr>
<tr>
<td>Percent HGV</td>
<td>Determined from road type taken from transport model</td>
<td>User input</td>
</tr>
<tr>
<td>Year</td>
<td>User input</td>
<td>User input</td>
</tr>
<tr>
<td>Pollutant</td>
<td>User input</td>
<td>User input</td>
</tr>
<tr>
<td>Background level</td>
<td>Background pollutant map</td>
<td>Background pollutant map</td>
</tr>
<tr>
<td>Output area</td>
<td>Field of view in GIS</td>
<td>Field of View in GIS</td>
</tr>
</tbody>
</table>

As shown in Figure 5.5, both the automated and manual versions of the GIS extension, break the road down into straight lines segments. In both methods these straight lines are then rotated to one of the parameterised positions prior to calculation. Firstly, the orientation of the road is determined by calculating the gradient and from this the angle is resolved. The angle will always be within $\pi/8$ radians of one of the parameterised orientations. The road is then rotated to the nearest orientation using Equation 5.2. The coordinates after rotation are then used by the calculation programme.
Chapter 5 - Model Implementation

Equation 5.2 Formulae for the rotation of roads

\[ X_{Centre} = \frac{(X_1 + X_2)}{2} \]
\[ Y_{Centre} = \frac{(Y_1 + Y_2)}{2} \]
\[ X_{1(new)} = ((X_1 - X_{Centre}) \times \cos(\partial\,Rot)) - (Y_1 - Y_{Centre}) \times \sin(\partial\,Rot) + X_{Centre} \]
\[ X_{2(new)} = ((X_2 - X_{Centre}) \times \cos(\partial\,Rot)) - (Y_2 - Y_{Centre}) \times \sin(\partial\,Rot) + X_{Centre} \]
\[ Y_{1(new)} = ((X_1 - X_{Centre}) \times \sin(\partial\,Rot)) + (Y_1 - Y_{Centre}) \times \cos(\partial\,Rot) + Y_{Centre} \]
\[ Y_{2(new)} = ((X_2 - X_{Centre}) \times \sin(\partial\,Rot)) + (Y_2 - Y_{Centre}) \times \cos(\partial\,Rot) + Y_{Centre} \]

Where:

- \( X_1, X_2, Y_1, \) and \( Y_2 \) are the original coordinates
- \( X_{Centre} \) and \( Y_{Centre} \) are the coordinates of the centre point of the line
- \( X_{1(new)}, X_{2(new)}, Y_{1(new)}, \) and \( Y_{2(new)} \) are the coordinates after rotation
- \( \partial\,Rot \) is the angle through which the road must be rotated

Automated input tool

The automated input tool was designed for use with the Surrey County Transportation Model (SCTM). The SCTM has been developed for use within GIS software as a polyline shapefile that represents the ‘real world’ locations of roads. Information such as road class and index (used to define road width and percentage HGV, see appendix D), traffic flow (as peak or 12 hour flows) and average speed between nodes\(^2\) exists within an associated database. The database is linked to the polyline file through the ‘object ID’. The ‘Object ID’ usually appears in the first column, the remaining format of this database is shown in appendix D. Any transport model that exists as a ‘real world’ shapefile with a similar associated database could be used in place of the SCTM.

\(^2\) Node – Located on road interconnections with traffic flow measured between these points
In stage one, the shape file to be used needs to be identified within the GIS environment in order that the correct database may be accessed. The GUI links to the list of open shapefiles within the GIS system and displays them within a GUI (Figure 5.6).

![Choose Road Shapefile](image)

**Figure 5.6 Screen to choose road shapefile with associated database**

The GIS extension then requests the location to store the output files through the use of a standard Microsoft® drive / directory and file location window.

Another GUI then requests information, not included in the traffic and transport model (Figure 5.7). The year option is located in a pull down list and allows the choice of years from 2002 to 2025. The pollutant option is also a pull down list, and allows the choice of NO$_x$, NO$_2$, CO and PM$_{10}$. The choice of pollutant changes the message next to the list of open raster files informing which background file to select. In the case of NO$_2$ this is NO$_x$, in all other cases the background pollutant should be the same as that under investigation.
Each road section is then taken and split into segments, defined as the straight lines that constitute a polyline section [ESRI, 2003]. These segments are then rotated using Equation 5.2 to the nearest orientation for which parameterisation has been undertaken. All of the data is then used by the calculation programme to determine the level of pollution and the output files are saved in the specified location. The automated process then moves on to the next polyline section and completes the calculations using data extracted from the transportation database and data input.

Manual Input

The manual input allows the definition of road location through the use of a mouse registered\(^3\) map within ArcGIS. At the termination of input of the first road section, a GUI lists the raster files available within the GIS project and allows the

---

\(^3\) Registered – the map used needs to have the ordinance survey coordinates of the corners entered into the GIS software for identification of position
choice of the background file to be used (Figure 5.8). The name of the background file is stored for use within the same session.

![Choose Background Map](image)

Figure 5.8 Choice of background raster maps

A further GUI is then used to gather information concerning traffic flow, percentage of HGV, year and pollutant of interest; this GUI is displayed following the entry of each road link Figure 5.9.

![Manual input window for choices following input of road coordinates using mouse](image)

Figure 5.9 Manual input window for choices following input of road coordinates using mouse

The vehicle number is a pull down menu that has a blank option for user input data, but also suggested are high, medium and low values for motorways, A-roads and B-roads. The suggested values may be used in place of definitive user input if data is not readily available. This allows the use of PARADIS to identify possible pollution 'hot-spots' without the need for exact traffic data.
Chapter 5 – Model Implementation

The second pull down menu defines the level of HGV using the road. Similarly, the pull-down menu appears blank allowing data to be input. Upon clicking the pull-down arrow several percentages for various road types are suggested, these were taken from data issued by the Department for Transport [DfT, 2003].

The third ‘pull-down’ menu allows a choice of speed for the road under investigation from 10kph to 120kph at intervals of 10kph.

The next pull down menu allows a choice of road widths; the list of widths available is dependant upon the speed selected. For speeds of 60kph and below a width of 8m or 16m may be selected. For speeds in the range 70kph to 100kph widths of 8m, 16m, 20m and 28m are available. Speeds above 100kph allow the selection of 20m and 28m widths only. These restrictions were put in place to stop erroneous results from the wrong input. This could result, for example, from the input of very slow average speeds on a motorway, or very fast speeds on a small road. The widths were calculated on a standard lane being approximately 3.75m, as defined within DMRB, with additional width added for pavements or emergency lanes depending on the road type.

In the final two ‘pull-down’ menus, the year (2002 to 2025) and pollutant under investigation (NOx, NO2, CO or PM10) are selected.

The road section is then split in to straight lines that have been used to draw it; each is then rotated and calculated as in the automated process. The next road section is then input and the process is repeated.
5.3.2 Output GUIs
Following the use of either the manual or automated input methods the files created need to be merged in to a single file with comma separated values (CSV) using the combine files tool. The single file may then be loaded in to the GIS software as a list of X, Y points. To produce a pollution map from the point data the values need to be interpolated. Interpolation takes the value of a data point, examines the values of surrounding data points, to calculate levels where there is no data. Several methods exist for interpolation, and include spline, kriging and inverse distance weighting (IDW), all of which are supported by ArcGIS.

Spline
The spline method is best used for values that change gradually, such as water tables or elevations. The method is able to estimate values between data points allowing a minimum of surface curvature, passing through all the existing values. Unfortunately, the method assumes that all points have an influence on the interpolation however distant.

Kriging
Kriging is used where there is a specific directional or spatial bias within the data. The bias type needs to be set before calculations can commence, as each has a specific mathematical function that a number of points, or those within a predetermined radius, are made to fit.

Inverse Distance Weighting (IDW)
The IDW method assumes that each point has a local influence that decreases with distance. Technically, the method estimates the grid cell values by averaging the levels of data points in the vicinity of each cell. The closer a point is
to the centre of the cell being estimated, the more ‘weight’ it has in the averaging process.

It is known both from the parametric studies, and from previous work [Cowan et al., 2001; Cowan et al., 2002] that atmospheric pollution will decrease from source. The IDW method was chosen, therefore, as the best method to represent interpolated values between the known data points. The interpolation results in a concentration map of the chosen pollutant from road sources; the addition of background levels using the spatial calculator within ArcGIS® Spatial Analyst® creates a map of total pollutant concentration.

5.3.3 Additional Tools
Subsequent to the production of pollutant maps it was envisaged that it would be useful to highlight areas with elevated levels of pollution. To achieve this, three similar tools were created within ArcGIS to allow a choice of representations. Upon selection of the tool, the first window allows choice of representation type; ‘Sector’, ‘Bullseye’ or ‘Combination’ (Figure 5.10). This is followed by the selection of pollution map on which to base the representation (Figure 5.11)

![Figure 5.10 Selection of display type](image)
Chapter 5 - Model Implementation

Figure 5.11 Choice of raster map from which to determine levels

Each tool draws an outer circle of diameter equal to the height of the viewable area on the screen. The sector tool divides the circle into eight equal sectors; the bullseye tool creates eight rings of equal area within one another, whilst the combination tool combines the first two methods producing 64 sections. Within all of the methods the average pixel value is calculated, for the selected pollution map, within the relevant area. This then allows colour coding of each section to show which has the highest level of pollution. Each method has advantages and disadvantages, and it is thought that a mixture of the various tools could be used to discard any negative aspects.

Sector Method

The sector method allows an overview of the highest pollution location within an area, and the low number of sectors results in rapid calculations. The sector method does have some minor negative attributes. Firstly, the segments each cover large areas. A highly trafficked road running through one part of the sector may force the average of the whole sector to be high; this may include an area of low pollution. Secondly, the sectors meet at the centre of the circle, and so it is difficult to realise the pollution concentration at this location.
Bullseye Method

The bullseye method also allows an overview of pollutant concentration, and as the number of divisions is the same, the processing time is similar to the sector method. This technique overcomes the main problem of the sector method, as there is no central meeting point of the sectors. One minor disadvantage to this particular method is an area of elevated pollution may exist in one part of the ring. This may result in a high average level for the entire ring which may cover an area of low pollution.

Combination Method

The combination tool allows a more detailed examination of the highest pollution concentrations. The smaller sectors overcome the problems of high values unduly influencing areas of lower values. The larger number of sectors does slightly increase processing time, and the meeting of sectors at the central point poses the same problems as the sector method.

5.4 Summary

In this chapter the program design for the advanced screening model – PARADIS is presented. PARADIS has been divided into a calculation program and GUIs that aid input and process output. These modules work together to produce pollutant concentration maps within a GIS environment.

The PARADIS calculation program uses input values from traffic models, and the 'look-up' tables created from the parametric studies, to calculate pollutant concentrations at receptor locations across an adaptive grid.
Graphical User Interfaces were designed using Visual Basic and the ArcObjects® model for direct interaction with ArcGIS® software. The GUIs allow two input modes, manual and automated.

The automated mode allows the use of 'real-world' polyline shapefiles with an associated traffic database to be used directly. The database is interrogated for traffic data on each link, and additional data such as the year / pollutant under investigation, and background levels are requested in a GUI.

The manual mode allows the definition of each individual link through the use of a mouse. GUIs are then used to define link information such as speed, HGV percentage and road width. The development of the extension was undertaken using VBA and the ArcObject model to enable full control and customisation of ArcGIS features.

The output from the calculation program may then be interpolated to create a pollution map using the Inverse Distance Weighted (IDW) method available within the ArcGIS® Spatial Analyst® extension.

Three additional tools were created within the ArcGIS® environment to highlight areas of high concentration. Each tool draws a circle on the area under investigation of diameter equal to the height of the viewable screen. The first tool divides the area in to 8 segments; the second in to eight circles of equal area; and the third combines these to create 64 segments. Each tool may be used to investigate the study area to identify pollution 'hot-spots' that may require further investigation or the imposition of an AQMA.
The next stage in the development of the PARADIS is to validate the model against existing measured data and use the model to determine pollution patterns within various town configurations. These are discussed in detail in the following chapter.
6.1 Introduction

The parametric studies that led to the development of PARADIS, and the implementation of the results within a calculation program that may be accessed through a GUI integrated with GIS software, have been discussed in Chapters 4 and 5 respectively.

This chapter examines phase 6, the final stage in the development of PARADIS, as highlighted in Figure 6.1. The chapter will discuss:

- the validity of the input data used both for validation and investigations in terms of accuracy and extent;
- validation of PARADIS
  - through the use of the interpolation method (described in chapter 3 and appendix C) if insufficient data is available at discrete locations;
  - against measured data;
- the use of PARADIS in investigating the effects of the built environment on current / future pollutant levels and patterns over urban areas of varying size and type; and
- the use of PARADIS in identifying pollution ‘hot-spots’ and areas that require further investigation of monitoring and / or modeling and possible designation as AQMAs.
Chapter 6 - Validation & Case Studies

6.2 **Input Data Used for Validation and Investigations**

Traffic data (including flow, speed and percentage HGV) and background concentrations are required in order to run PARADIS. In both validation and case study work, PARADIS was run using the automated process (described in Chapter 5 section 5.3.1) with traffic data from the Surrey County Traffic and Transport Model (SCTM). Within validation and investigations into pollution in urban areas, the 2002 model output of the SCTM was used. For future prediction...
the relevant increases, suggested by the transportation group at Surrey County Council, were applied for the different road types to achieve flows for the years under investigation [Fanstone, 2002].

The background data required to run the advanced screening model was taken from the 'UK Background Concentration Maps' available through AEAT [Stedman et al., 2002]. The maps are accepted by the UK Government for the annual reporting of 'Local Air quality Modeling' [Stedman et al., 2002]. The background maps are a point data file on 1kmX1km grid spacing. The grid may either be filled out to 500m with the same value from each point or interpolated using the appropriate scheme. Applying the point value to the surrounding area gave a block style output. It was decided, therefore, to use an IDW scheme to interpolate between the regular grid for two reasons. Firstly, the spacing made good interpolation using IDW possible and secondly, the variation in values between one point and those surrounding it within the grid was small. This meant that the results achieved for background values using an IDW interpolation differed at around the third decimal place from applying the value around the point, rendering the variation between the two techniques negligible.

6.2.1 Input Data Accuracy
Prior to model validation, the accuracy of the input data was examined to ascertain the performance:

- of the SCTM in reflecting 'real world' traffic levels; and
- the background concentration maps against measured data.

**Surrey County Transportation Model**
During parametric studies it was found that the traffic flow levels have a substantial effect on the generated pollution field (see 4.2.3). It was known that
the SCTM, from which the flow rates were taken, performed well when compared with traffic counts, although the values were not always correct [Lim, 2004].

PARADIS was run three times to investigate how variation between modeled and actual traffic values might affect PARADIS output. The first run used traffic data given in the SCTM to determine NO\textsubscript{2} concentrations in Woking for 2002. The second and third runs altered traffic values within the SCTM by ±10%. This provided evidence as to whether a performance difference of this order between the transport model and traffic counts would make a significant change to the level of pollution predicted. The results (Table 6.1) showed that there is little change (0.21 ppb) over the range ±10% of given traffic model flows.

| Table 6.1 Average level of NO\textsubscript{2} across Woking for 2002 at given and ±10% traffic flows from SCTM |
|-----------------------------------------------|-----------------|
| +10%                  | 16.60           |
| Given flow            | 16.39           |
| -10%                  | 16.18           |

Given the excellent performance of the transportation model in relation to traffic counts, and the minimal effect of a 10% divergence from modeled flows, the predicted traffic volumes were accepted for validation and case study work.

**Background data**

Background concentration maps were chosen for use with PARADIS as they indicate the variation of background data over an area rather than a static value that may be obtained from a background monitoring location. When compared to the national network of background monitoring stations, only 11% of results from the maps are outside the data quality objectives [Stedman et al., 2002]. The background concentration maps have, therefore, been validated as being accurate and are recommended for use by local authorities when undertaking modeling exercises [DEFRA, 2003]. The background concentration maps were
therefore accepted as accurate for use with PARADIS in validation and case study work.

6.3 **PARADIS Validation**

Validation of a model is usually completed by comparison with monitored data or against another pre-validated model using the same input values. The PARADIS model output was compared to measured data taken from both 'real-time' units and diffusion tubes. Whilst diffusion tubes are known to be inaccurate, they were used for validation purposes, in addition to the 'real-time' units, to utilise as many data points as possible [Bush et al., 2001].

The validation of PARADIS by comparison with monitored data within Surrey may be restricted in specific areas due to the location of the majority of monitoring equipment in the vicinity of residential settings [Lythe et al., 2002]. As a result, validation of the model would not be possible in all case study locations. Where a limited number of monitoring locations are available within a specific study area the methodology to create dummy data points, discussed in Chapter 3, and described in detail in appendix C, may be applied.

Overall, the number of data points available across Surrey proved sufficient for validation purposes. If PARADIS had needed to be validated in a single location where no data had been available the interpolation method described in appendix C would have been used.

The following sections discuss validation of the model against diffusion tubes and 'real-time' monitoring data.
6.3.1 Validation Against NO\textsubscript{2} Diffusion Tubes

Several towns across Surrey were modeled for NO\textsubscript{2} in 2002 using PARADIS, see section 6.4. Where monitoring data had been collected within these areas using diffusion tubes during 2002, comparisons were made. This allowed validation of PARADIS against 32 diffusion tube measurements, Figure 6.2 shows the results of this evaluation.

![Figure 6.2: Diffusion tube data compared to modeled output.](image)

The mismatch of data between modeled and monitored, shown by Figure 6.2, may be explained in two ways. Firstly, the inaccuracy of the diffusion tubes (±18% for an annual average [Bush et al., 2001]) is likely to account for some disparity between the values. Secondly, every dispersion model has an element of uncertainty, and as such, the model parameterised is quoted as being accurate to within ±10% with an over prediction of 0%-12% [Colvile et al., 2002]. As PARADIS is derived from ADMS-Urban it is likely to have a similar accuracy. When these are taken into account (error bars in Figure 6.2), it becomes clear that PARADIS shows excellent correlation with diffusion tube data.
Diffusion tubes are generally within Surrey used for measuring NO$_2$, as a consequence they may only be used for validation of PARADIS for this pollutant. The next section discusses validation against 'real-time' units that allow validation of PARADIS against all pollutants predicted by the advanced screening model.

6.3.2 Validation Against 'Real-Time' Units

Problems with the inaccuracy and limitation of the diffusion tube measurement method may be overcome by validation against 'real-time' units. The chemical methods used in 'real-time' analysis are more accurate than diffusion tubes, and allow the comparison of multiple pollutants [Horiba, 2004]. Unfortunately, due to the expense of this method, and the difficulties faced when locating a 'real-time' unit, those available for evaluation of the model output within Surrey were limited.

The annual averaged data from four "real-time" units, across Surrey, were compared to the results from PARADIS. A favourable comparison, predominantly within the model precision of ADMS-Urban [Colvile et al., 2002], was achieved between the modeled and measured data (Figure 6.3).

PM$_{10}$ were the exception, and were underestimated by PARADIS at each 'real-time' unit location. A likely explanation for this is the method by which the parameterised model deals with particulate matter. ADMS-Urban calculates the emission and dispersion of 'new' particulates from motor vehicle sources, including the deposition of particulates according to size fraction. The resuspension of particulates, either by wind or passing vehicles, is not accounted for by ADMS-Urban [CERC, 2001]. Yet, resuspended particles account for approximately 50% of particulates within the lower troposphere [Harrison et al., 2001], which is approximately the level of under-estimation of particulate concentration by PARADIS. The addition of the resuspended particles would
effect a doubling of the concentration. Study of Figure 6.3, shows that doubling the concentration of PM$_{10}$ would lead to a near perfect correlation of the PARADIS with monitored data.

In Farnham and unit 2 in Guildford, the level of NO$_x$ has been over estimated by PARADIS. The over estimation of NO$_x$ may be attributable to factors that allow rapid dispersion at these locations that were not foreseen during parameterisation nor accounted for within ADMS-Urban. The predictions of NO$_2$ levels, at the same location, were found to be within the precision of the parameterised model. This apparent paradox may be due to the correlation equation (described in chapter 5 section 5.2.3) that uses a logarithmic approach, meaning that very high values for NO$_x$ will be calculated to represent more realistic 'lower' levels of NO$_2$.

The next section discusses the 6 sets of case studies that investigated the effect of various urban configurations on air pollutant concentrations and patterns of pollution.
Figure 6.3 PARADIS comparison with monitored data. Error bars for PARADIS represent the model precision of ADMS-Urban on which the parameter studies were based.
6.4 Case studies

Successful validation of PARADIS was followed by investigations into:

1) the relationship between town size and pollution levels;
2) the effect of town size on pollutant patterns;
3) the impact of motorways near urban areas on local air quality;
4) air quality within conurbations;
5) future air quality; and
6) the use of the additional tools in defining potential AQMAs.

Examination of pollution levels was extended to the full range of pollutants that PARADIS is able to model. For clarity and continuity, the results for NO$_2$ have been provided and discussed within this chapter.

6.4.1 The Relationship between Town Size & Pollutant Concentration

The quality of air within small, medium and large towns within Surrey was investigated to discover whether larger towns have greater problems with air quality. It was postulated that large towns with a high population would have more roads per km$^2$ and a greater number of vehicles on the roads creating additional pollution.

Figure 6.4 shows population density for various towns from the 2001 census in comparison to the average level of pollution for the same area modeled by PARADIS. The average level of pollution, across the area modeled, was determined by obtaining the value of each pixel within the generated raster map, and the average calculated using a script written for ArcGIS® using the ArcObjects® model.
The results showed that in a location without a motorway or trunk road the level of all pollutants rose in a linear fashion with the population density. In areas where motorways or trunk roads were close to urban areas (shown in Figure 6.4 as TNM) the average level of pollution across the area was increased. The percentage increase due to the presence of a motorway / trunk road was found to be dependant upon the pollutant (Figure 6.4). NO\textsubscript{x} showed the highest percentage increase when a motorway / trunk road is present, this was probably due to the combination of NO and NO\textsubscript{2} within NO\textsubscript{x}, and the chemical reactions that occur.

![Figure 6.4 The mean level of various pollutants across modelled areas against population density](image)

The towns near motorways or trunk roads (TNM) are shown but not included in the equation for the 'best fit' line

Analysis of the effect of town size on pollutant concentrations has shown that the density of population, and hence the number of vehicles, within an area results in an increased level of pollution averaged over the same area.

6.4.2 The Effect of Town Size on Pollutant Patterns
This section considers the effect of town size on pollutant patterns by looking at NO\textsubscript{2} concentrations in:
Large towns with a population of approximately 60,000;

medium sized towns with a population of approximately 20,000 to 30,000; and

small sized towns with a population of less than 10,000

within the County of Surrey.

**Large Towns**

Guildford and Woking were selected as large towns to investigate. Both have a population of over 60,000 and a road system radial to the town centre. The road layout of a large urban area is often as a result of its historical growth.

Guildford grew as a market town from the centre outwards and as such has a circular shape. The road system is radial to the centre with 7 major roads accessing the central area from all surrounding areas. Guildford has, in addition, a trunk road running through part of the urban area.

Figure 6.5 shows the annual average NO₂ levels for Guildford in 2002, as calculated by PARADIS. As expected, the largest influence in Guildford was found to be the A3 trunk road. It is interesting to note, that PARADIS predicts an unexpected reduction in the level of pollution in the highlighted area 1. This is a likely result of the exit slip roads from the A3 for Guildford town centre that exist either side of area 1. Area 2 also showed a lower level of NO₂ than the rest of the A3. This may be due to the lower speed limit of 80kph, imposed along the stretch of road encompassed by area 1 and 2, which would encourage engine efficiency [DMRB, 2003].
Figure 6.5 Annual average NO$_2$ pollution levels for 2002 in Guildford, calculated by PARADIS.\(^4\)

As would be expected, the most heavily polluted roads, aside from the A3, connect the town centre to the trunk road. It should be noted that areas that contain few roads, such as the south-east corner of Figure 6.5, exhibit background levels of pollution.

Woking offers a different aspect of large town development from Guildford, the pattern of pollution observed, however is similar. Developed as a commuter town with the arrival of the railway, Woking has a clearly pronounced linear shape that follows the railway and the main access routes. The main road network within Woking is also radial to the town centre with 5 access routes.

\(^4\) Reproduced from Ordnance Survey map with the permission of the Controller of Her Majesty’s Stationery Office. © Crown Copyright NC/03/21947
Figure 6.6 shows the annual average NO₂ levels for Woking in 2002, as calculated by PARADIS. As expected, the most heavily trafficked roads show the highest concentrations pollution. Within a commuter town, such as Woking, these are observed to be the radial routes leading from the town centre to the highly residential areas, and the roads linking the town to major transitory routes such as the M25.

The results of the investigation into the pollution patterns generated by large towns indicate that concentrations of pollutants are located along the access routes. Within large towns in Surrey, the access routes are radial to the centre, this has the effect of linear areas of elevated pollution stretching out from the town centre.

Medium Sized Towns
With a population between 20000 and 30000 Godalming and Horley were ideal for investigating the patterns and levels of pollution in a medium sized town. Medium sized towns often exist close to transitory routes such as trunk roads and

---

An Advanced Screening Model to Predict Air Quality

.................................................. 132
motorways. These transitory routes may have helped to facilitate the growth of the urban areas as commuter towns. It was expected, therefore, that a heavily trafficked transitory route, close to a town of this size would exhibit the highest values of pollution within the area.

The centre of a medium sized town may also be expected to show elevated levels of pollution in comparison with the surrounding area. Similarly to larger towns, a medium sized town centre provides shopping, financial and leisure facilities for the population. This attracts the population in to the centre from surrounding areas. Higher traffic volumes at lower speeds would be likely which would result in increased pollution levels.

Godalming is a medium sized town situated to the south of Guildford. As such Godalming is a commuter town as it has good access links to Guildford and to London via the railway and A3.

![Diagram showing high NO2 levels on trunk road and elevated NO2 levels in town centre](image)

**Figure 6.7 Annual average NO2 pollution in Godalming for 2002 calculated by PARADIS4**
Modeling of the Godalming area using PARADIS showed, as expected, the highest levels of pollution were located around the A3 trunk road that passes to the west of the urban area (Figure 6.7). Elevated levels of NO$_2$ were also predicted by PARADIS in Godalming town centre, however, the majority of pollution across the modeled area remains at background level. Other elevated levels occur within the modeled area to the north-east of Godalming; these are possibly due to other urbanized areas or roads connecting Godalming to Guildford.

In spite of similar population sizes, Horley represents a vastly different situation to that of Godalming. Located on the northern boundary of London’s Gatwick Airport pollutant concentrations in Horley may be expected to be elevated due to emissions from both aircraft and traffic accessing the airport. The background pollution maps, used in the calculation of total pollution, include all area emissions, such as those from airports [Stedman et al., 2002]. Indeed, the background maps delineate a clear ‘ring’ of pollutants radiating out from the airport, which may also be seen in Figure 6.8.

![Figure 6.8 Annual average NO$_2$ pollutant levels in Horley for 2002, calculated using PARADIS$^4$.](image)
The heightened background pollutant level masks the expected elevated levels in the town centre and exacerbates the problems associated with pollution from motorways shown clearly by the level of NO₂ along the M23 in Figure 6.8. In addition elevated traffic levels accessing Gatwick may have caused the increase in pollutant levels seen on all approach roads.

Medium sized towns often act as commuter towns with increased levels of pollution on the road links to the larger urban areas. The centres of medium sized towns often show elevated concentrations of pollutants as they have enough facilities to attract people resulting in an increase in traffic related pollutants.

Medium sized towns located near to areas with elevated background pollutant concentrations, such as airports, often have the traits of medium sized towns masked by background concentrations.

**Small Towns**

Dorking and Haslemere with populations of approximately 10,000, are representative of small towns within Surrey. Small towns do not generally attract large volumes of traffic. It was expected, that investigations in to pollution levels in small towns would have shown that the highest pollutant concentrations would be restricted the main roads and any transitory routes located nearby.

Dorking is a small town located in the heart of Surrey. The town centre is unusually busy for a town of this size as it serves as a small shopping area for the surrounding villages and the main non-motorway east-west route across Surrey.

The results from Dorking (Figure 6.9) showed that, as expected, the roads in towns of this size exhibited elevated pollution levels along the major routes in the
area. The highest pollutant levels were found on the trunk road that runs north-south and the High Street. The elevated pollutant levels on the trunk road are probably as a result of the high volume of traffic. The increased pollution levels along the High Street (Figure 6.9) may, in part, be due to the lower speeds that vehicles travel at along this road (30kph-40kph) in comparison with other roads of similar type in the area [SCTM, 1999].

![Map of Dorking showing pollution levels](image)

**Figure 6.9 Annual average NO₂ pollution for 2002 in Dorking, calculated by PARADIS³**

The location of Dorking may also have an impact on the patterns of pollution that are found. Dorking is located at the intersection of a north-south and east-west route across the county of Surrey. There are few main east-west routes across the county that avoid the heavily congested M25 (situated to the north). This cross-road at Dorking provides access to this east-west route, which may explain the almost cross shaped pattern of elevated pollution levels found at this location. Investigations in Haslemere, located on the county boundary, showed a similar pollution pattern to that of Dorking (Figure 6.10). The high levels of pollution were again restricted to the major roads within the area, with the highest concentration...
found along the trunk road to the north-west of the area. As in the case of Dorking, roads running to the town centre have higher than background levels of pollution.

In contrast to Dorking, however, the major routes through the town centre do not show an increase in pollution over and above those present on other parts of the same route. This is probably due to the maintenance of speed, at 50kph, along the entire length of road through the central area [SCTM, 1999].

![Diagram of NO2 pollution distribution in Haslemere](image)

**Figure 6.10 Annual average NO2 pollution in Haslemere for 2002, calculated by PARADIS**

The results from the investigation into small towns indicate that in these areas elevated pollutant concentrations are located along nearby trunk roads and the main feeder routes in to the town centre. Where town centre speeds are considerably lower than the rest of the route in the same area, increased pollutant concentration are observed.
Analysis of individual locations and town sizes showed that pollution patterns, and where precisely elevated pollutant levels are found, is often a result of both location and role of the town. In addition, it was clear that the air quality of relatively small towns may be greatly influenced by developments such as airports, both in terms of the pollution coming from the airport, and the access roads.

The results shown in Figure 6.8 clearly illustrated that a motorway has an impact on local air quality of the region through which it passes. The next section discusses the impact of motorways on urban air quality.

### 6.4.3 The Impact of Motorways on Urban Air Quality

![Figure 6.11 Annual average NO\textsubscript{2} levels for Camberley in 2002 using PARADIS\textsuperscript{a,b}](image)

Each motorway within the County of Surrey regularly carries in excess of 100,000 vehicles a day at speeds around 110kph. It was expected that such a high

\footnote{H represents areas where levels are higher than would normally be expected possibly due to the presence of the motorway}
volume of traffic passing through urbanised areas would result in pollution levels above the threshold limits set by both British and European Parliaments for residential areas.

Camberley and Leatherhead were investigated using PARADIS, to determine the levels of pollution within an urban area near to a motorway. The results from modeling using PARADIS show that the levels of pollution along the motorway 'corridor' are far higher than found at other urban locations around the county (see Figure 6.5 to Figure 6.10). The outcome of investigations in Surrey, using PARADIS, suggests that a heavily trafficked (non-motorway) road within a 'large' urban area usually has an annual average NO₂ of approximately 25ppb at the central reservation. The elevated levels of NO₂ will dissipate to background levels in the region of 150m, and are often below the target value within 100m.

In contrast, the results from PARADIS for both Camberley and Leatherhead indicate that at the centre of a motorway the annual average levels of NO₂ for 2002 were around 50ppb. Figure 6.11 and Figure 6.12 clearly show that the

---

Chapter 6 - Validation & Case Studies

Figure 6.12 Annual average NO₂ levels for Leatherhead in 2002 using PARADIS

An Advanced Screening Model to Predict Air Quality
areas at distance from the road elevated levels of pollution are maintained (indicated by H1), possibly due to the presence of the motorway. The dissipation of levels found at the centre of the motorway to the 'elevated' levels across the urban area did not occur until approximately 500m from the motorway. More importantly, the modeled values of annual average NO2 for 2002 did not fall below the target value of 21ppb (2005) until at least 300m from the central reservation of the motorway. The implications of these results for urban areas mean that all residential areas within 300m of a motorway should be modeled for future years to determine whether it is likely to be in breach of British and European law.

6.4.4 Air Quality within Conurbations
Following the observation that the centre of an urban area often shows elevated levels of pollution, locations with two town centres linked by urbanisation were investigated to discern whether the same phenomenon occurs. Several different types of conurbation exist within Surrey, and may have resulted from the growth of a nearby urban area that encompasses the two towns, the growth and merging of each town, or the joining of two urban areas for political / planning reasons.

This section therefore considers 3 types of urban areas with double centres that are due to:
- urban sprawl;
- ribbon development; and
- regional transport hubs.

Urban Sprawl
In the north of Surrey town centres have often been linked by urbanisation, as London has 'sprawled' outward joining individual towns. This section considers two conurbations within Surrey, formed as London has grown. These are:
- Weybridge and Walton-on-Thames; and
Epsom and Ewell.

The conurbation of Weybridge and Walton-on-Thames grew along the main London to Portsmouth railway line, and today may be considered part of the urban sprawl of London.

![Image of pollution map]

**Figure 6.13** Annual average NO$_2$ levels for Weybridge & Walton on Thames in 2002 using PARADIS.

Whilst cartographically the two urban town centres are not distinct, Figure 6.13 shows that the two town centres may be discerned when looking at pollution concentrations as the NO$_2$ concentration is higher in the town centre. Figure 6.13 also shows that the road network that connects, and is radial to, each town centre also show elevated levels of NO$_2$. In terms of pollutant concentration each town centre is behaving independently of each other as if it were a separate town.
Within a conurbation, background levels are generally expected to be elevated as a result of the increased density in population and vehicles on the road network. In the case of Weybridge and Walton-on-Thames this increased background level is not observed. This urban area is on the fringes of London and has large reservoirs that cover this area to the north of the town centres, and open spaces of the 'Green Belt' to the south of the conurbation. The density of population that would be expected in the surrounding area does not exist, and as a result the background concentrations are suppressed.

Figure 6.14 Annual average NO₂ levels for Epsom & Ewell in 2002 using PARADIS

Epsom and Ewell is another conurbation located in the north of Surrey created as London has grown. Modeling using PARADIS clearly defines the two town centres in terms of increased NO₂ (Figure 6.14). In addition, and in common with similar conurbations, the connecting road system also showed increased pollution levels.
Whilst the two town centres are indeed distinct, background concentrations with the conurbation are generally elevated in comparison to the suburbs of larger towns. This is due to the higher density of urbanisation and hence more vehicles per km².

Town centres that have been joined together by urbanisation, through the expansion of another large urban area, continue to exhibit high pollution levels within each individual town centre. The roads, which are radial to each town centre, also continue to exhibit higher pollution concentrations. Each town within the conurbation may therefore be thought of as a separate entity when considering air quality.

Background concentrations in a conurbation were generally found to be higher than the fringes of larger urban areas within Surrey; this was a likely result of the increased density of population and vehicles that results in an elevated background level.

The next section discusses conurbations that have formed as each individual urban area has spread outward. These areas have often grown as commuter towns and are separated from Greater London by the 'Green Belt'; an area preserved from building to halt the spread of large urban areas.

**Conurbations from Ribbon Development**
A further conurbation within Surrey is slightly different to those discussed above. Reigate and Redhill are separated from the urban sprawl of London and are located south of the M25 motorway. As such, this conurbation did not occur as a result of the growth of a larger urban environment. Instead, this is a ribbon development that follows a railway line.
In spite of these differences, the pollution patterns observed from modeling with PARADIS were very similar to those in other conurbations nearer Greater London (Figure 6.15). The centres of both towns, and the road network radial to them, were shown to display higher than background concentration of pollution. In addition, the general level of pollution between road sources is higher than might be expected. This may be due to the proximity of both the M25 and M23 that line two sides of this conurbation resulting in an elevation of background levels.

Urban areas that have grown together through the extension of each individual town continue to exhibit pollution concentrations typical of a single urban area. Each town centre, and the road network radial to each town, continues to demonstrate elevated pollutant concentrations.
Regional transportation hubs

Separate towns may be defined as one urban area for 'geo-political' reasons in spite of there being no urban link. One example of 'geo-political' conurbations is Regional Transportation Hubs (RTH). Defined by the regional transport strategy, a RTH may be either an individual town or two towns close together where there are large quantities of both local and intra-regional transport links [Government Office for the Southeast, 2004].

The regional transport strategy for the southeast has defined Guildford and Woking as being one urban area in terms of a transportation hub [Southeast Regional Transport Strategy, 2003]. This 'geo-political' conurbation has been created in spite of the two urban areas being physically distinct.

![Figure 6.16 Annual average NO2 levels for Guildford & Woking (defined as one urban area as a transportation hub) in 2002 using PARADIS4](image)

Figure 6.16 Annual average NO2 levels for Guildford & Woking (defined as one urban area as a transportation hub) in 2002 using PARADIS4
From an air quality perspective it may clearly be seen from Figure 6.16 that these areas show some similarities to conurbations. The two town centres, and a main road connecting the two, all show elevated levels of pollution. In contrast to other conurbations, however, it is possible to distinguish between the two areas of elevated pollutant levels associated with each urban area. Each location may, therefore, be modeled as individual locations. The separation of the urban areas in terms of air quality is likely to be due to the 'green area' between the two towns. An area of non-urbanisation consists of fewer roads per km² than an urban area, and may also allow greater dispersion of pollutants.

In cases where the double centres were due to urbanisation between the two, both town centres were shown to have higher than background levels of pollution. As expected the highly trafficked road connecting the two centres also showed an increased level of pollution. Interestingly, conurbations showed an overall elevated level of pollution across the area. Locations of this type must, therefore, be modeled as one area when determining air quality.

Locations that are deemed to be double centred for 'geo-political' reasons do not follow the same patterns. Investigations using PARADIS have shown that whilst there may be elevated levels of pollution, both along a linking road and in town centres, the two locations have a decreased area of pollution between them, and therefore may be modeled separately.
6.4.5 Future Air Quality
Traffic levels within Surrey are predicted to increase by an average of approximately 4% per year until 2016 [SCTM, 2003]. If emission levels remained static during this period, it may be expected that pollution levels would escalate at a similar rate in future years. Emission levels are, however, expected to decrease due to the introduction of more efficient and cleaner engines in to the vehicle fleet as a result of European Legislation.

Figure 6.17 shows the percentage change in NO\textsubscript{2} levels for various locations modeled for 2002, 2005 (UK regulatory compliance date) and 2010 (EU regulatory compliance date). The results indicate that in every area, the NO\textsubscript{2} levels are predicted to decline substantially by 2010. These reductions are based on a forecast decrease in emission levels from the DMRB, and traffic increases as

![Figure 6.17 Percentage reduction of NO\textsubscript{2} in various town sizes for 2002, 2005 and 2010](image-url)
Future emission factors are dependant on the predicted vehicle fleet composition as this plays an important role in determining the emission characteristics of traffic at varying speeds. The vehicle fleet may be split into several emission classes described as Euro groups. The Euro group into which an engine is placed is defined by the year of manufacture and the pollution reducing technologies used in the design.

A vehicle fleet model was compiled for the National Atmospheric Emissions Inventory (NAEI) by NETCEN [DMRB, 2003]. The fleet model predicts composition with regard to annual mileage over the period 1996 to 2025. The survival rates of older Euro group engines, and annual mileages as a function of age, were derived from DETR statistics and included in the fleet model [DMRB 2003]. In short, the make-up of the UK fleet was described by the proportion of distance travelled per year by vehicles in each of the Euro emission groups. Within the fleet model a number of key assumptions were made that may affect the composition predictions.

1) 20% of new car sales would be diesel;
2) 5% annual catalyst failure rate (of which 98% would be rectified at the MOT);
3) an early introduction of the Euro IV engine in the petrol class; and
4) fitting of particulate traps to some diesel LGV.

These assumptions were based on UK policy and the most likely events at the time of publication in 2003 [DMRB, 2003].

It is possible that due to a change in outside influences, such as economics or delays in the introduction of new engines, the assumptions made during the
prediction of fleet composition may not prove to be true. This may result in a higher emissions rate for future years than currently predicted by the DMRB.

Using PARADIS, two runs were completed for Guildford for 2005 (the UK regulatory compliance date). The first run used the published DMRB emission factors. The second run included an 80% reduction in expected emissions, as shown in the comparison between plots (a) and (b) in Figure 6.18.

Figure 6.18 Predicted annual average concentration of NO₂ in Guildford for 2005 (a) using the DMRB emission factors & (b) 80% of the expected emissions improvement included in plot (a)
factors, whilst the second run set the predicted improvements of emission factors from DMRB at 80% of their given value (Figure 6.18).

Figure 6.17 showed there will be very little reduction in NO$_2$ levels in various town sizes by 2005. As expected, therefore, the results (shown in Figure 6.18 and described in Table 6.2) illustrated that there was no discernable difference across the modeled area for 2005 when the emission factors were increased by 20%.

Table 6.2  Annual average levels for the areas modeled around Guildford for 2005 and 2010 using DMRB predicted emission factors and a 20% increase.

<table>
<thead>
<tr>
<th>Year</th>
<th>DMRB Emission Factors</th>
<th>20% increased emission factors</th>
</tr>
</thead>
<tbody>
<tr>
<td>2005</td>
<td>16.21</td>
<td>16.26</td>
</tr>
<tr>
<td>2010</td>
<td>13.44</td>
<td>13.93</td>
</tr>
</tbody>
</table>

Larger reductions in NO$_2$ concentrations were observed for 2010 (Figure 6.17). It was expected, therefore, that as the emission factors were predicted to be much lower, a 20% increase in this emission factor would have a considerable impact due to a negative bias.

Two runs were therefore completed for Guildford for 2010 (the European regulatory date). Again, the first run used the DMRB emission factors whilst the second run set the predicted improvements of emission factors from DMRB at 80% of their given value.

The results (Figure 6.19) indicated that typically a 20% increase in emissions, from the currently predicted level, causes an expansion in the field of pollution surrounding roads (highlighted areas 1 and 2). Also shown in the results were the extension of higher level pollution fields surrounding roads also led to a general increase in the average concentration over the whole area (Table 6.2). Such a
general increase in pollutant levels over an area may indicate some possible non-compliance with EU law in 2010 if the predicted reduction in emission rates fails to materialise.

Figure 6.19 Predicted annual average concentration of NO2 in Guildford for 2010 (a) using the DMRB emission factors & (b) 80% improvement
6.4.6 The Use of Additional Tools in Defining Potential AQMAs

As discussed in chapter 2 section 2.2.5, the definition of an AQMA has, in the past, initially resulted from local knowledge of an area rather than purely scientific results in Stage 1 of the review and assessment process. In Stage 2, the use of local knowledge has led to selective monitoring in areas expected to show elevated air pollutant concentrations. In Stage 3, the modeling of only those areas that were expected, and shown to exhibit high levels of monitored pollution, may have given a false impression that pollution levels were elevated across the entire area. This sequence of events has often been a consequence of a deficiency in finance and computing resources to model the locality for air quality at the outset of the review and assessment process.

Spelthorne was one such borough that followed this approach (located between the M25, Heathrow airport and the edge of Greater London); the level of background pollution is elevated and the level of traffic throughput is high. It might be expected therefore, due to the proximity of these sources to the borough, that the whole area would not meet the AQS objectives by 2005. Selective monitoring and subsequent modeling in the northern half of the borough and the highly trafficked roads in the south of the area, reinforced this view. At Stage 3, the borough declared the entire borough an AQMA in respect of NO₂.

This section shows how through the use of the additional tools provided with PARADIS it may be clearly seen that the entire borough of Spelthorne does not need to be declared an AQMA. Resources may then be focussed on failing locations to meet the 2005 AQS objectives.
It was clear from the modeling of annual average NO₂ levels for 2005 in Spelthorne, that large residential areas may have a level of NO₂ in exceedance of 21 ppb (Figure 6.20).

The additional tools, described in Chapter 6 section 6.3.3, were applied to the borough to determine locations that may require further monitoring, detailed modeling and ultimately AQMA status.

The position of the areas of elevated concentration meant that the sector tool was inappropriate as there are high concentrations within each sector; meaning that this tool would show an exceedance across the whole area.

Similarly, the ‘Bullseye’ tool was rejected as the only location where elevated concentrations were not observed was the central area. The ‘Bullseye’ tool would
indicate that everywhere, but the central area, would exceed to the 2005 NO$_2$
AQS objective.

In the case of Spelthorne, it was decided to use the 'combination tool' due to the
fractured nature of areas with predicted levels greater than 21 ppb for 2005. The
small segment divisions provided by the combination tool allowed a clear
understanding of where possible problem areas were located. Areas for concern
(shown in dark blue in Figure 6.21) were found to be the north-west corner of the
borough and to the south-west of the central region. In this instance, it would
therefore be suggested there is possibly a need for AQMAs in these areas, and
further monitoring and modeling should be initiated to determine whether this is
the case.

Figure 6.21 'Combination tool' used to define possible AQMAs by showing areas with
a predicted annual average concentration greater than 21 ppb in 2005.
Chapter 6 - Validation & Case Studies

The additional tools developed for PARADIS provide local authorities with a clear picture of where monitoring and modeling should be concentrated. The additional tools developed for use with PARADIS may be used with any raster map, meaning that the results from other dispersion models may also be interrogated in this manner.

6.5 Summary

This chapter has described the process of validation against NO₂ diffusion tubes and 'real-time' data at various locations across the County of Surrey. The comparison of results has shown that PARADIS performs within the accuracy range of ADMS-Urban when compared to diffusion tubes and 'real-time' data. This accuracy indicates that PARADIS may be used as a screening tool within local air quality studies.

The chapter then considered case studies concerning town size, the effect of motorways of urban areas, urban areas with double town centres, and regional transport hubs.

It was found that large urban areas had higher amounts of pollution than smaller towns and various patterns could be discerned for differing town shapes and sizes. Furthermore, the use of PARADIS enabled a direct correlation to be drawn between population density and average pollution concentration across the area. It was noted that a nearby motorway raised the average concentration, but a similar trend with population density against pollution concentration continued.

Urban areas with nearby motorways were found to have levels of pollution in excess of statutory guidelines along a 1km wide corridor (500m from the central reservation) of the motorway. The results have indicated that in these areas...
further investigation should be undertaken to determine whether an AQMA is required.

Towns with double centres were investigated to understand the nature of pollution in these environments. It was clear from the results that in terms of air quality the two town centres retain their individuality in spite of being joined by the suburbs. Each town centre, and the roads that link them, exhibit a higher level of pollution than the surrounding areas.

The use of additional tools to define AQMAs was also used in the case of Spelthorne that has declared the entire borough an AQMA. Results from PARADIS indicate that whilst the northern half of the borough should be declared as an AQMA, only corridors along busy roads in the southern half of the borough need this status.

In summary, the results from PARADIS are within the error margins quoted for ADMS-Urban; a dispersion model recommended for use by local authorities. PARADIS is an effective tool in determining absolute concentrations, examining patterns of pollution within varying environments, and has several useful additional tools for determining possible locations for the designation of AQMAs. The process of determining these locations for an entire borough, from selection of the traffic information through to use of the additional tools, may be completed with PARADIS within a few hours.
7.1 Introduction
In this chapter the main conclusions from this research project are presented.

This is followed by a discussion on:

- future research for modelling air pollution;
- the future of PARADIS; including,
  - enhancements;
- integration and acceptance for review and assessment; and
- advantages of PARADIS for use by the scientific community and local authorities.

7.2 Concluding Remarks
The quality of urban air has caused concern throughout the world due to its direct impact on human health. Emissions such as NOx, CO and PM$_{10}$, from the internal combustion engine, are the main source of air pollution in UK urban areas. As a consequence of European directives and UK law, local authorities within the UK are required to improve air quality within their area through a review and assessment process.

The first stage of the review and assessment process saw the identification of pollution ‘hot-spots’ through the use of local knowledge. These areas were then monitored and modeled in depth to identify possible exceedences of the AQS
objectives. This process may have missed less obvious locations of elevated pollutant concentrations.

During the later stage of the review and assessment process, modeling was used to predict future air quality. At present, different tools such as transport and dispersion models are needed to predict air quality over an area. These tools often require specialist knowledge of dispersion theory to set-up and run. In addition, the complex algorithms used to describe the atmospheric physics of dispersion may often take days to complete using a standard desktop computer. This process consumes vital computing resources within a local authority. Modeling is often contracted out to consultancies as the process may be time consuming, and consequently expensive.

The aim of this thesis was to investigate the dispersion of traffic related pollutants in the local environment. This was achieved through the development and application of an intermediate screening model. The intermediate model would retain the spatial resolution and visual output inherent in advanced dispersion models, whilst keeping the method of input, terminology used, and speed of processing at a level used within screening models. This allowed additional research into the field of modelling air pollution. Several aspects important in both screening and advanced models were examined including:

- vehicle flow;
- speed;
- percentage of Heavy Goods Vehicles (HGV);
- road width;
- meteorology;
- grid size; and

Chapter 7 - Conclusion
Chapter 7 – Conclusion

• interpolation techniques.

A detailed literature review examined the current methodologies of emissions determination, measurement and modelling dispersion, and included the review of existing screening and advanced dispersion models.

This led to the development of a prototype intermediate model designed to meet the aims of the thesis. During development, parametric studies were undertaken of an existing dispersion model to determine how important aspects, such as those described above, affect the pollution fields of NOx, CO and PM10 surrounding a road link. An orthogonal line to that of the road link was taken and the mathematical equation of the line calculated in respect of pollution concentration. The results from these parametric studies allowed the calculation of any pollutant concentration at a given distance from the road source. The identified equations were stored in 12 'look-up' tables, one for each pollutant and each of the 4 road orientations.

To facilitate use of the calculation program, and to allow the post processing of data, input and output Graphical User Interfaces (GUIs) were created as an extension to ArcGIS® through the use of the ArcObjects® model. The input function allowed both manual and automated input providing the facility to either:

• enter the road vertices using a mouse and entering data through a GUI form; or

• through the direct import of a transport model database with an associated road shapefile.

The pollutant concentration was calculated across an adaptive grid, of general spacing 250mX250m, and a finer spacing of 1mX1m around the road. Inputs to the model, such as road orientation, pollutant, road width, speed and distance
from road are then used to define both the look-up table and the equation to be used.

The output GUIs facilitated the post-processing of data to a format that could be used by the ESRI Spatial Analyst® extension to interpolate the adaptive grid and create a pollution map.

Additional tools were created that divided the area into eight segments, eight circles of equal area or a combination of these creating 64 equal area segments. These additional tools allow visual identification of areas with high pollution levels, facilitating the concentration of resources to those areas based on scientific judgement rather than local knowledge.

Validation of the system was undertaken through comparison of modeled areas with 2002 data from NO₂ diffusion tubes and real-time monitoring units. Results from the validation exercise indicated the model compared well with monitored data.

The prototype model was used in several case studies across Surrey to investigate:

- the effect of town size on pollutant concentration and patterns;
- the impact of motorways on local air quality in urban areas;
- air quality in conurbations;
- the future of air quality; and
- the use of additional tools in defining AQMAs.

A linear correlation between town size and average pollutant concentration across the area was observed, with motorways further raising the average
concentration of each pollutant. Elevated pollutant concentrations in large towns were found to be concentrated along the access routes to, and within, the town centre. Medium sized towns were found to act as commuter towns as they are often located near to trunk roads or motorways. The town centres of medium sized towns were shown to have elevated pollutant concentrations, this is a likely result of the towns having sufficient facilities to attract people. Small towns were found to have high concentrations of pollution along nearby trunk roads and feeder routes in to the town centre.

Conurbations were found to behave as individual towns in terms of air quality, each having elevated pollutant concentrations in the individual town centres and on the radial routes.

The results from the investigation into future air quality indicated that if the predicted improvement in emissions standards are not realised, then the pollution field surrounding the roads are likely to increase in area as well as concentration. This may result in the failure of specific locations to comply with EU regulations that have currently been assessed as being within guidance values. Finally, the additional tools were successfully used to refine the area of an AQMA, in a region that had declared the entire borough.

An intermediate model was found to be particularly advantageous in the reduction of the runtime for air quality predictions, when compared to existing dispersion and screening programs. Each investigation was completed in 2-3 hours using the automated input method. This was a distinct advantage over existing screening models that need many hours of data input to create an entire road network, and the advanced dispersion models that may take up to a week to complete calculations for an area the size of Guildford [Lim, 2004]. The quick
'run-times' and the additional tools have many advantages to both the scientific community and local authorities. In spite of the encouraging results, future research is needed for both intermediate and advanced dispersion models in order to improve resolution and aid the decision making process.

7.3 Future research for modelling air pollution
This section will consider two important issues concerning the future development of intermediate models, namely:

- gridding; and
- personal exposure mapping.

7.3.1 Gridding
Gridding, or grid size selection, is an important issue for any model that delivers output in a form suitable for interpolation. Within currently available screening models, there are no options to output results as a grid, although future development of the DMRB screening model as a GIS application is likely to include this feature [Highways Agency, 2004].

Within advanced dispersion models grid sizes are dependant on the model chosen. Aermod, for example, leaves the final grid size up to the user; however it does not allow intelligent gridding around roads and a very fine grid is therefore required to resolve these features within the output. Other models such as ADMS-Urban use a large grid spacing across the general region, and finer intelligent grid spacing around roads. This allows an overall regular grid to be used and yet the finer detail surrounding the road continues to be defined, thus reducing the number of calculations needed. Within ADMS-Urban, the grid spacing is chosen by the model with the regular grid of size 67m X 133m and an intelligent grid of size 12m X 16m either side of the defined road width. Currently within PARADIS, the grid system defines a grid of general resolution 250m X
250m with a finer grid of 1m X 1m around the road segment in order to pick out subtle changes close to the road.

The factors which influence and ultimately determine appropriate grid sizes for modelling and monitoring of air pollution are complex, and often under review [Chock et al., 2002; Lythe et al, 2002 and Lythe et al, 2004]. Ideal or optimum grid sizes may be entirely dependent on each individual scenario being modelled. Hence the selection of a ‘fixed’ or pre-determined grid system applicable to all scenarios may not be appropriate. The determination of suitable grid sizes would be an interesting area for future research. This could investigate a range of intelligent gridding systems, optimised for individual scenarios. Ultimately this could be incorporated into the models themselves either automatically or through user-defined grid-size options within the GUI.

7.3.2 Personal Exposure Modelling
Personal exposure modelling may be used to precisely determine concentrations in locations where human health may be affected. These locations are specified in European and British legislation as locations where a person may spend a significant portion of the averaging period, or where there are susceptible people [DETR, 2000]. Such locations are termed sensitive receptors, and include:

- houses;
- hotels/motels;
- nursing homes;
- hospitals; and
- schools.

The regulations for these sensitive receptors apply at the building façade rather than inside were other emissions from cooking, for example, may affect pollutant concentrations.
Within current screening models, personal exposure modelling is undertaken by defining the distance of individual sensitive receptors to one or more road links with supplied traffic information. Background concentrations are added and an annual average concentration to which the receptor is exposed is determined [DMRB, 2003]. Concentrations at each sensitive receptor need to be calculated individually in order to create an exposure map. Consequently, this process is time consuming in areas with large numbers of sensitive receptors. The screening model methodology therefore suggests targeting areas with sensitive receptors in 'likely' areas of high concentrations, making the process subjective rather than analytical. The screening model is then used only in these selected areas to determine personal exposure [DMRB, 2003]. Additionally, screening models take no account of the height of the receptor above ground. This can be an important factor, at flats above shops for example, in determining whether a sensitive receptor is exposed to levels exceeding the objectives.

Advanced dispersion models use the geographical positions of sensitive receptors to calculate concentrations for each hour of metrological data at these specific locations. This allows the calculation of both the annual mean and percentiles for comparison with legislation [CERC, 2001]. Additionally, advanced dispersion models allow height information to be provided for each receptor, meaning that sensitive receptors above street level may be taken into account. Within ADMS-Urban, 50 specific sensitive receptors may be identified in any particular 'run'. In high risk areas, this may mean that several runs are needed to build up an exposure map.

The limitations of both screening and advanced dispersion models in personal exposure mapping could be overcome using the output from the developed
intermediate model. The Ordinance Survey 'AddressPoint' database contains information concerning the location of all buildings with a postcode. Also included in this database is the ability to discriminate between building usage. Within a GIS, an additional query tool could be developed to identify pollutant concentrations at sensitive receptors such as housing, schools or hotels within areas that are above the objective limit. The tool would allow a user to determine changes in air quality at identified sensitive receptors that may occur due to alterations in the traffic network flow patterns or over time.

This new tool would allow output of concentrations at all addresses within a local authority's administrative area rather than the limited number allowed by some advanced dispersion models. All areas where personal exposure is above the UK objectives could be quickly identified, output to an Excel file, and steps initiated to address issues in those areas.

Further research could be initiated to investigate, through additional literature reviews and runs of ADMS-Urban, how concentrations vary with height. This information would be invaluable to both local councils and the scientific community in allowing the factoring of measurements, and modelled concentrations, to levels at a variety of heights. The findings of this research would also allow the GIS tool to be further enhanced to calculate concentrations at a variety of heights.

7.4 The future of PARADIS
PARADIS has performed well against existing monitoring data, although several enhancements to the model are likely improve its performance in terms of runtime efficiency and user interface. Validation of PARADIS within other regions of
the UK would then allow the model to be accepted for use by local authorities within the review and assessment process.

### 7.4.1 Model Enhancements
PARADIS requires some cosmetic enhancements in terms of usability, improvements in run-time performance and additional features to enable councils a full suite of tools to assess air quality within an administrative area. These enhancements include:

- operations with manual input data;
- inclusion of industrial sources;
- improved gridding;
- calculation of percentile for direct comparison with legislation; and
- demonstration of accuracy relative to other methods.

Two further enhancements, namely a:

- link to a transport model; and a
- link to a public information system,

would increase the usefulness of the model in finding a solution to air quality issues and delivering the results to the public.

**Operations with manual data input**
The manual input method could be further developed to allow input to be saved and displayed. This could be achieved by using a ‘shapefile’ that is ‘opened for editing’ whilst inputting data, and ‘closed to editing’ in order to save the information. As each individual link is created, a polyline within the ‘shapefile’ would be defined. At the end of each road link, information such as link traffic volume, percentage HGV and speed should be requested using the existing GUIs. The information for a link could then be added to the database associated with the ‘shapefile’. As each road ‘link’ is defined, an update button, such as that used within ADMS-Urban, would enable display of newly entered data. This
would allow data entry to be undertaken in stages, building up the model gradually, rather than in one go as is presently the case. Once all of the manual input has been completed, the result should represent a similar 'shapefile' as that provided by the SCTM. The tool currently used for automated input could then be used to process the manual input.

**Industrial Sources**

As discussed in Chapter 3, PARADIS has been developed for an area where traffic emissions are the major source of pollution. The model would not, therefore, be suitable in its current form for an area that was dominated or at least had a significant minority of emissions from industrial sources.

Further parametric studies would allow critical inputs for industrial sources to be determined. These additional sources could take the form of point sources for chimneys, area sources for larger areas of industrial development, and grid sources for multiple sources over a wide area. Additional algorithms could then be included within the calculation code to determine pollutant concentration as a result of all sources across the adaptive grid. This would provide a more complete dispersion simulation model that could be used in more industrialised areas.

**Gridding**

Within the current design of PARADIS, all individual grids are written to separate files at the time of execution, and then amalgamated in to one file at the end. This file is then loaded in to the GIS and interpolated. This method has worked well within the prototype however a minor enhancement to the methodology would allow a faster and more accurate interpolation process.
Within air quality models, emissions for any given link are calculated over the entire link length in the form g km\(^{-1}\) s\(^{-1}\). The breakdown of the link to the constituent segments and the use of grids around these segments with PARADIS results in 'stacked' grid points. The IDW interpolation algorithm in ArcMap Spatial Analyst averages 'stacked' points prior to interpolation, which may result in long processing times (>2 hours). Whilst the IDW algorithm is appropriate for air quality data, the averaging of 'stacked' grid points means that influence on overall pollutant concentrations at a particular receptor may be given to more than one part of the same link.

Optimisation of the grid system at the time of calculation to remove this stacking would improve the time taken for interpolation, and remove control from the algorithm. Where stacking occurs due to segments of the same polyline, the highest concentration should be used as this would avoid double counting of emissions from the same link. Where stacking is due to a different links, the resulting concentration for that point should be the sum of the stacked points. This would allow the impact from all roads links to be accounted for and represented on a map. The non-linear "sausage" shape observed in some results presently due to the grid-field 'stacking' and cross-roads would then be eliminated.

As discussed, the present methodology writes the grid results of individual polyline segments to separate files at the time of calculation. At the end of all calculations, the individual files are combined and all temporary files are deleted. One potential area of research would be to incorporate the use of dynamic arrays to store the grid calculations from individual polylines. This may enhance the methodology by improving processing time, but may require large quantities of memory. Thought needs to be given as to whether this should be a 2-
dimentional or 3-dimentional array (with each 'layer' within a 3-dimentional array containing results for the grids of individual polyline segments). At the end of calculating the grids for all segments within one road link, a sorting of the array would allow all points with the same spatial co-ordinates to be identified. As concentrations in this case would be due to the same road link, the highest concentration of the stacked points should be selected and written to either a separate array or an output file. If it is found that arrays use too much memory for average desktop PCs then file swapping (writing, amalgamating and deleting) could be used as an alternative approach.

At the end of processing all links, either the array or file containing all grids points from the different links should be post-processed. Theoretically, concentrations from different road links should be summed; however this may lead to double counting at locations close to the road junctions. The research should investigate how this may be resolved, possibly using a similar methodology as that proposed for the DMRB methodology for roads that are linked [DMRB, 2003].

**Calculation of percentile for direct comparison with legislation**
The AQS objectives define pollutant concentrations not only in terms of their annual mean, but also in terms of a daily, and in some cases, hourly averages. Exceedences of this short-term concentration limit are allowed on a given number of occasions per year to account for pollution episodes. A percentile calculation is often used of all hourly or daily average concentrations to determine whether the short-term limit has been exceeded. In order to achieve this, a dispersion model needs to undertake calculations for each period of every day. It would be useful if PARADIS were able to undertake these short-term percentile calculations; however, in model development, parametric investigations were limited to long-term concentrations in this version. Recent research in to
monitored data has shown that there is a relationship between annual means and percentile levels [DEFRA, 1998, DEFRA, 2003]. An additional tool, such as the algorithm used within DMRB that converts annual average to relevant percentiles would be useful for comparison with AQS objectives.

**Accuracy relative to other methods**

When using any model in a new area it is important to validate the model for the particular location. Currently available screening and advanced dispersion models do not allow this to be done automatically and values given by the monitored data and the output from numerical modelling need to be manually compared. There is, therefore, a need for an additional tool that completes validation automatically. The additional tool could obtain data from a pre-prepared point layer that contains information on field monitoring locations and data. Pollutant concentrations could be compared by obtaining the calculated concentration from the interpolated grid. The tool could:

- prepare graphs and tables for a simple comparison;
- perform additional statistical analysis, such as
  - the normalised mean;
  - bias;
  - fractional bias; and
  - Pearson's Correlation.

This information could then be exported to an excel spreadsheet for ease of access and use in report writing.

**Link to a transport model**

The output from PARADIS, and the use of the additional tools, allows the identification of roads and areas that exhibit high concentrations of pollution. Currently, the model allows the manual manipulation of data within the Transport Model database to try various scenarios to reduce pollutant concentrations on
those road links. A further extension of the PARADIS model would be to include various scenarios that automatically updated the traffic database. These scenarios could include the removal of HGVs, a reduction in overall flow, the re-routing of some vehicles through less polluted areas or a change in traffic speeds along the affected roads.

Each of these scenarios would impact on the road with elevated pollution and surrounding routes as drivers either find, or are directed to, alternative routes. Cooperation and further research with traffic modellers could lead to the development of an additional function within PARADIS that directly allows the reading and writing of traffic model files for a variety of popular traffic models. Such research would establish a circular link between PARADIS and traffic models that does not currently exist in other air quality models. This circular link would allow the air quality impact of new traffic schemes to be investigated through one integrated model.

**Link to public information system**

European legislation requires member states to make information concerning air quality available to the public [Council of the European Union, 2004]. As discussed, the current methodology calculates annual average concentrations based on the results from parametric studies using statistical meteorological period that provided a 'normal case' analysis of pollution concentration. PARADIS could be adapted to provide short-term concentration maps if further parametric studies were undertaken to determine air quality patterns across a road link in various meteorological conditions. Once completed, these may be integrated in to PARADIS to allow pollution forecasting. The short 'run-time' of PARADIS is ideal for this type of forecasting on an hour by hour or day by day basis. This information could then be used by a local authority and publicised on
a website, in newspapers, on television or on the radio to allow sensitive groups
to take precautions against air pollution episodes. The publication of this
information on a regular basis may also encourage people to take a more active
role in improving local air quality.

7.5 Integration and acceptance for review and assessment

The intermediate model, PARADIS, was developed as a research tool, however
in practical terms it already meets many of the necessary requirements for work
by local councils in the review and assessment process. The technical guidance
published by the UK Government for local authorities suggests some models that
may be used (ADMS-Urban, AERMOD, DMRB and AAcquire) [DEFRA, 2003].
The technical guidance also makes it clear that the list of models given within the
document is not exhaustive and any reference to a particular model is not a
recommendation [DEFRA, 2003]. Provided, therefore, that a further enhanced
PARADIS model is fully validated, there would be no reason why this new
approach could not be employed in the review and assessment process by local
authorities and accepted as an 'approved' method by DEFRA.

Validation of PARADIS could be achieved in two ways, namely through
comparison of modelled results with:

- monitoring data across the UK; and
- existing methodologies.

7.5.1 Comparison of modelled results with monitoring data
across the UK

Validation against monitored data could be achieved through comparison with
data from the Automatic Urban and Rural Network (AURN) that collects real-time
data at many locations throughout the UK. Failure of model validation in any
region may be due to the meteorological data on which the intermediate model, PARADIS, is currently based. PARADIS was not designed for use countrywide, as it was developed to investigate the dispersion of traffic related pollutants in the local environment within a specific study area. The weather data, used to develop PARADIS has, therefore, been taken from Heathrow Airport. If further validation were to determine difficulties in applying PARADIS to other locations throughout the UK, the 'look-up' tables could be updated for new regions through additional parametric studies using different meteorological data. Further parametric studies for the calculation short-term objectives would not be required. As previously discussed, correlation algorithms between the annual average and short-term objectives may be used to convert the calculated annual averages, provided by PARADIS, to determine compliance with the short-term objectives [DEFRA, 1998, DEFRA, 2003].

PARADIS has been tested against all currently available field measurements within the County of Surrey. The results indicated that the methodology has a similar degree of accuracy as other methods. It should be noted that in order to calculate future years, the methodology relies on published data that indicate an improvement in air quality with time, as engine technology advances [DEFRA, 2003]. Field measurements are continuously ongoing, and consequently, PARADIS should be re-tested against future data to ensure agreement with the published data.

7.5.2 Comparison of modelled results against existing methodologies
Validation against existing methodologies would provide further data concerning the accuracy of PARADIS. Concentrations should be calculated using DMRB, PARADIS, ADMS-Urban and AERMOD and comparisons made between all results. Comparisons between the models should consider time taken for data
entry, run-time of the model and time taken for interpolation within the GIS environment.

7.6 Advantages of PARADIS to the Scientific Community and local authorities

The use of PARADIS, as an intermediate model, has many advantages to the scientific community and local authorities. Input through the automated tool within PARADIS removes the need for the manual input of road vertices, reducing the time needed to set up the model. Additionally, the 'run-time' of each study is shortened to a few hours rather than the days taken by more traditional dispersion models. The significant decrease in setup and run time means that more investigations may be undertaken, improving the likelihood that a solution may be found to improve local air quality.

Controls, icons and pull-down menus used within GUIs PARADIS are standardised to a Windows® format meaning that the interface presents a familiar working environment. This allows users with some GIS experience but little knowledge on air quality to produce air quality concentration maps. The use of Windows controls also means that time needed for familiarisation of the model interface is reduced, allowing the user more time for air quality investigations.

The manual input method PARADIS enables the local council to obtain 'ball-park' pollution concentration map from approximate traffic concentration data. The use of PARADIS in identifying possible areas of high pollution concentration would allow resources to be targeted at addressing any identified problems.

Councils have a duty under their charters to publish work undertaken on behalf of the public, and paid for through local taxes. The public often understand maps showing areas of high, medium and low concentrations of pollutants more easily.
than through the publication of data in either ppb or μg/m³ [Bailey, 1999]. Through a GIS environment, PARADIS allows the division of the pollutant concentrations shown on the maps into the high, medium and low concentration bands published by DEFRA. These maps may then be published and understood by the public.

Local authorities are more likely to adopt this methodology as the ease of input, facilitated by an intermediate model, means that work may be undertaken by Environmental Health Officers (EHOs) rather than outsourcing the work. This would vastly reduce the cost currently incurred by local authorities in meeting their requirements under the 1995 Environment Act.

The addition of a circular link with transportation models would further appeal to councils completing air quality action plans for their areas. EHOs would be able to try a variety of traffic management scenarios, re-running the traffic model and using the new output directly within the model. This would ensure that the correct measures are put in place, and that the removal of an AQMA in one area does not lead to the creation of an alternative AQMA in another location. As all of this work could be carried out ‘in house’, this will further reduce time and costs involved in this process, delivering better value for money than current practices.

7.7 And Finally...
Future legislation and improvements in engine technology will only contribute to better air quality to a certain degree. In order to achieve significant progress in reducing urban air pollution people will need to change their travel habits, using private vehicles only when absolutely necessary. The uptake of new engine technologies such as bio-fuels and dual fuel engines will need to be actively encouraged both in terms of taxation and within the media. The understanding of
air quality issues may be furthered by research, however cleaner air is the responsibility of and benefit to everyone.
References


An Advanced Screening Model to Predict Air Quality


Laxen, & Wilson (2002). *A New Approach to Deriving NO2 from NOx for Air Quality Assessments of Roads United Kingdom: DEFRA.*


References


*Clean Air Act, 1956*. United Kingdom: HMSO


Monitoring Techniques within the United Kingdom

A1.1 Introduction

Monitoring is the only definitive method of determining the level of pollution in any one location. Several methods exist for determining air pollutant levels; these include passive diffusion tubes and various chemical techniques.

Diffusion tube measurements provide good spatial coverage; unfortunately, there is doubt on the accuracy of these instruments, with some studies suggesting that any one reading could be ±24%-38% [Bush et al., 2001]. These inaccuracies have led to many monitoring studies to be conducted using real time units [Kutler et al., 1999; Borrego et al., 2000 and Vautard et al., 2000]. As the name suggests, these instruments collect data in real time giving readings every 15 minutes. The results are far more accurate with possible drifts of less than 1% occurring throughout a day followed by automatic recalibration [Horiba, 2003].

Generally, chemical techniques are favoured, as these provide very accurate real-time results. Measurements of air pollution are only applicable in the immediate vicinity, and do not, therefore, provide any indication of pollution levels across a town or borough area.

Further to a brief discussion of monitoring within Surrey in Chapter 2, the next section investigates the diffusion tube methodology and the measurement of
three traffic related pollutants (NO\textsubscript{x}/NO\textsubscript{2}, CO and PM) by real time unit. Each measurement technique is discussed in terms of:

- chemistry of the measurement method;
- technique accuracy; and
- results from the UK.

### A1.1.1 Nitrogen dioxide diffusion tube measurement

The diffusion tube is most extensively used by local authorities within the United Kingdom. This is in contrast to the majority of Europe, and the rest of the world who often prefer the more accurate real-time methods. Diffusion tube measurement is used within the UK, in spite of the inaccuracies, as they are relatively cheap, and easy to maintain [Bush et al., 2001]. Diffusion tubes are occasionally used elsewhere in the world in small local studies to gauge the long-term trends of nitrogen dioxide (NO\textsubscript{2}).

The UK Government requires each borough to maintain at least four diffusion tubes and report the monthly readings to the network co-ordinator, AEAT [AEA, 2000]. This has resulted in reports on NO\textsubscript{2} levels within the United Kingdom from the diffusion tube network [Loader et al., 2001 and Loader et al., 2002].

**Chemistry of measurement method**

The diffusion tube sampler consists of a plastic tube, open at one end with a disk impregnated in triethanolamine (TEA) at the other (see Figure A 1.1). The tube is exposed for a period of time; often this is a minimum of four weeks. During exposure, air enters the tube at the open end and diffuses along its length according to Fick's law [Colls, 1997]. Upon contact with the disk soaked in TEA, any NO\textsubscript{2} causes a reaction with the TEA to produce nitrite, triethanolamine nitrite or triethanolamine nitrate [Levaggi et al., 1972 and Gold 1977]. Following the
exposure period, the ratio of TEA to the reaction species is measured to determine the concentration of NO₂ pollution at the measurement location.

Figure A 1.1 – NO₂ diffusion tube

Diffusion tube accuracy

The accuracy of the diffusion tube method has been subject to much debate [Bush et al., 2001, Expert Air Quality Group, 2004]. A recent review of the available literature on diffusion tube accuracy by the United Kingdom Expert Air Quality Group stated that the following factors:

- the laboratory preparing and analysing the tubes;
- the exposure interval – weekly, 2-weekly or monthly;
- the time of year;
- the exposure setting – sheltered or exposed;
- the exposure location – roadside or background;
- the tube preparation method; and
- the exposure concentration and NO₂/NO could lead to an over-estimation of concentration by as much as 28% for an individual tube, although this varied for each location [Expert Panel on Air Quality, 2004].
**Diffusion tube results from the UK**

NO$_2$ diffusion tubes have been used occasionally outside the UK for small studies on the long term trends of NO$_2$ [Glasius, 1999]. In contrast, diffusion tubes have been used within the UK on a much larger scale to determine compliance with both EU and British legislation. The extensive use of passive samplers within the UK led to the creation of the nitrogen dioxide diffusion tube network in 1993. The network was formed as a means to consider the levels of NO$_2$ both locally and nationally. Due to the doubt in the accuracy of the diffusion tubes, the data from the network may only be used to determine general trends in the data both spatially and temporally [Bush et al., 2001]. In spite of the problems of accuracy associated with the diffusion tube, it remains the most cost effective method of determining levels of NO$_2$.

<table>
<thead>
<tr>
<th>Table A 1.1 — Diffusion tube categories</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Category</strong></td>
</tr>
<tr>
<td>Roadside</td>
</tr>
<tr>
<td>Intermediate</td>
</tr>
<tr>
<td>Background</td>
</tr>
</tbody>
</table>

The survey is primarily concerned with population exposure, and therefore, levels within towns and cities are measured. Before 2001, the network consisted of three categories of diffusion tube in relation to distance from road (Table A 1.1). The intermediate category was discontinued in December 2000, as the data was found to show little additional information [Loader et al., 2002]. The diffusion tubes formally used for intermediate locations have been relocated to roadside positions [Loader et al., 2002]. Additional restrictions have been implemented on the location of diffusion tubes, to ensure that the data collected is of good quality and to mitigate against some of the accuracy problems. These limitations are shown in Table A 1.2 [Bush et al., 2003].
Appendix A – Monitoring Techniques within the United Kingdom

Table A 1.2 - Guidance on location of NO₂ diffusion tube. Adapted from Bush et al., 2003

<table>
<thead>
<tr>
<th>Location</th>
<th>Guidance</th>
</tr>
</thead>
<tbody>
<tr>
<td>Building</td>
<td>• 0.5m-1.0m from face of building</td>
</tr>
<tr>
<td></td>
<td>• Not in recess</td>
</tr>
<tr>
<td></td>
<td>• Not on corner</td>
</tr>
<tr>
<td>Street furniture</td>
<td>• &gt;1m from kerb</td>
</tr>
<tr>
<td></td>
<td>• 2m-5m from ground</td>
</tr>
<tr>
<td></td>
<td>• &gt;0.05m from lamp post / road sign using ‘spacer’</td>
</tr>
<tr>
<td>Locations to Avoid</td>
<td>Within 10m of:</td>
</tr>
<tr>
<td></td>
<td>• Heater flues</td>
</tr>
<tr>
<td></td>
<td>• Trees</td>
</tr>
<tr>
<td></td>
<td>• Air conditioning outlets</td>
</tr>
<tr>
<td></td>
<td>• Extractor vents</td>
</tr>
<tr>
<td></td>
<td>• Underground ventilation shafts</td>
</tr>
</tbody>
</table>

Throughout the measurement period (1993-present) the roadside level of NO₂ measured by the diffusion tube network has decreased. This reduction can be shown by measurement sites with an annual average level of NO₂ of less than 38µgm⁻³ (20ppb). The proportion of these locations has increased from 30% in the mid 1990s to 53% in 2001 [Loader et al., 2002].

The interpolation of intermediate and background measurements throughout the UK has, in the past, shown that areas of high levels of NO₂ correlate well with highly urbanised regions and are, therefore, more representative of these locations [Loader et al., 2001]. This level of correlation was most obviously identified by annual average measurements greater than 38µgm⁻³ [Loader et al., 2002]. It was found that over the period 1993-1997 that these areas decreased in size until 1998, when they disappeared from the interpolated maps for intermediate and background measurements [Loader et al., 2002]. This is further supported by the frequency distributions of intermediate and background measurements.
locations that show a general downward trend in pollutant levels between the mid-1990s and 2001 [Loader et al., 2002].

Results from the diffusion tube network have also shown variation in pollutant levels throughout the year. Generally, levels during the winter months (October to March) have been shown, on average, to be higher than those during the summer months (April-September). Such results may be explained by the major chemical reactions for the creation and destruction of the NO₂ molecule. The oxidation of NO to NO₂ may occur by the addition of an oxygen radical to an NO molecule [Bridgman, 1994]. The destruction of the NO₂ molecule requires light at wavelength <415nm [Colls, 1997 and Bridgman, 1994]. A reduction in insolation values, due to greater cloud cover, shorter day length and low solar elevation, may result in less photo-disassociation of NO₂, and thus higher concentrations.

The aim of the diffusion tube network, aside from showing both spatial and temporal patterns on NO₂, is to determine whether the UK will be broadly in compliance with both the UK Air Quality Strategy (AQS) and the EU daughter directive 1999/30/EC. Based on modelling and emissions inventory projections, it is estimated that approximately 26% of all roadside locations and 0.3% of urban background sites will fail to meet the AQS targets by 2005 [Loader et al., 2001]. In respect of the EU legislation, the projections for 2010 estimate that 9% of roadside locations and no urban background locations will be in breach of the daughter directive [Loader et al., 2001].

A1.1.2 Real time measurement
Measurement by real-time unit is used by major industrial plants, airports and a minority of local unitary authorities. As a method of determining air pollution, this process has greater scientific validity as the chemistry used to ascertain the level
of pollutant is more accurate [Bush, 2001]. Real-time units are not generally used by local authorities within the UK due to the cost and difficulty in sighting the equipment.

Chemistry of measurement methods

The method of measurement within a real time unit varies depending on the pollutant measured. Each technique is dependant on a chemical or physical property of the pollutant to determine a level. A variety of methodologies exist for determining ambient pollutant concentrations in real-time, those discussed in this section are standard UK methods.

This section considers the measurement methods of 3 traffic related pollutants, namely:

- NOx/NO2
- CO
- PM

NOx/NO2

NO2 measurement often uses chemiluminscent analysis which relies on the equation \( NO + O_3 \rightarrow NO_2^* + O_2 \) and is measured as part of NOx. Ozone (O3) is added to a sample and the above reaction occurs to form an excited NO2 molecule and O2. As the excited NO2 returns to ground state, light is emitted in the region \( \lambda 600-3000 \)nm. The intensity of the light is in proportion to the concentration of NO within the sample. Firstly, the level of NOx in a sample is measured by passing a portion of the sample through a deoxydation chamber, to convert all of the NO2 to NO. The NO concentration is then obtained by measuring without passing the sample through the deoxydation chamber. The NO2 concentration is achieved by subtracting the level of NO from NOx [Horiba].
The measurement of CO relies on its physical property of light absorption. It is known that CO absorbs infra-red (IR) light of λ4.7μm. Reference and sample gases are injected alternately into the sampler. Each is exposed to IR light, and the intensity is measured by an IR detector after it has passed through the sample. The level of IR light measured by the detector is inversely proportional to the concentration of CO in the sample [Horiba].

**PM**

Real-time measurement of PM$_{10}^1$ and PM$_{2.5}^2$ is performed by two methods, namely:

- β-ray adsorption
- Tapering Element Oscillating Microbalance (TEOM)

β-ray adsorption relies on adsorption of β-rays by particulate matter. The air sample is passed through the measurement chamber and any particulate matter is captured on a tape. The mesh width of the tape is dependant on the diameter of particles that are to be measured. β-rays are then passed through the tape, and their intensity measured by either a plastic scintillator or a Geiger-Muller counter. The exposure of a blank section of the tape to β-rays is then carried out as a control. In this method, the number of scintillations recorded is inversely proportional to the level of particulate matter [Horiba].

The tapering element oscillating microbalance (TEOM) method allows the measurement of mass rate, mass concentration and total mass accumulation. This measurement method works on the principal that particles may be continuously collected on an interchangeable filter cartridge. The cartridge is

---

$^1$ PM$_{10}$ – Particulate matter of less than 10μm in aerodynamic diameter.

$^2$ PM$_{2.5}$ – Particulate matter of less than 2.5μm in aerodynamic diameter.
mounted at the tip of a hollow tapered glass tube that oscillates in an applied electric field. During operation, a flow controller pulls sample air through an inlet filter. The inlet filter has a mesh diameter dependant on the size of the particles to be measured. At this point the sample is heated to 50°C to drive off any water. The hollow tube is vibrated at its resonance frequency, and as mass accumulates on the filter the resonance frequency of the glass tube changes. The internal microcomputer then calculates the mass rate and mass concentration in real time based on the relationship between mass and frequency [EPA, 1999].

**Method accuracy**

The measurement of pollutants by chemical and physical means is known to be more accurate than the diffusion tube method [Bush et al., 2001]. Each measurement method has a lower detectable limit (LDL), and over time, drift in the results may occur (Table A 1.3). The measurement methods for particulate matter are known to have particular accuracy problems [CEPA, 1999 and DEFRA, 2003]. The presence of water in the β-ray adsorption method is known to cause errors in the results [CEPA, 1999], whilst heating during the TEOM process has the net result of driving off volatile species resulting in a low measurement of particulate matter [DEFRA, 2003]. The errors in both measurement methods have been shown to under-record by approximately 30% in comparison with the gravimetric criteria set out in the legislation [DEFRA, 2003].

<table>
<thead>
<tr>
<th>Pollutant</th>
<th>LDL</th>
<th>Drift/Accuracy</th>
</tr>
</thead>
<tbody>
<tr>
<td>NO₂</td>
<td>0.5ppb</td>
<td>±1.0ppb/day ±2.0ppb/week</td>
</tr>
<tr>
<td>CO</td>
<td>0.05ppm</td>
<td>±0.1ppb/day ±0.2ppb/week</td>
</tr>
<tr>
<td>PM</td>
<td>-</td>
<td>±10μg/m³ or ±10% of reading</td>
</tr>
</tbody>
</table>

An Advanced Screening Model for Air Quality

---

Appendix A – Monitoring Techniques within the United Kingdom
**Real-time unit results**

Real-time units are used in a variety of situations, such as measuring pollution from factories, airports or roads. Due to this, the results achieved from real-time units are only applicable in that locality. In spite of this limitation, real-time units have allowed a general understanding of short term air pollution chemistry [Brimblecome, 1986], and the effects of local sources on air pollution [Cowan et al., 2001 and Cowan et al., 2002].

The diurnal measurement of traffic-related primary and secondary pollutants, by real-time units in an urban background location, has been most clearly demonstrated in Los Angeles [Brimblecome, 1986; Bridgman, 1994]. Further investigations in other locations have confirmed these results [Cowan et al., 2001 and Vautard et al., 2000]. In general, it has been found that there is a peak in NO levels at around 6am and, as a primary pollutant, is likely to be associated with rush hour traffic [Bridgman, 1994]. Night levels of ozone (O₃) are found to persist throughout the morning. This low O₃ is probably due to the reaction with NO, resulting in the disassociation of O₃, and the formation of NO₂ which has been found to peak in several studies between 8am and 9am [Brimblecome, 1986; Cowan et al., 2001 and Kuttler et al., 1999]. As the morning progresses, higher levels of non-methane hydrocarbons and methyl species accumulate from motor vehicles exhaust, resulting in the formation of hydroxyl and peroxy radicals [Bridgman, 1994]. These radicals react with NO to produce complex molecules reducing the overall level of NO within the atmosphere. This results in an increase in O₃ from late morning, peaking around 2pm [Brimblecome, 1986].
The general results have given way to more detailed studies in which real-time measurements have been taken closer to sources. Investigations by Cowan et al. in Surrey, for example, have shown that the primary and secondary pollutant (NOx, NO2, CO and PM10) levels follow traffic patterns. The urban background pattern, described above, remains within the data, but is enhanced by road-traffic pollution sources close to the monitoring location [Cowan et al. 2001]. These results show two daily peaks in traffic related pollutants; one occurring 7am to 8am and the second between 5pm and 8pm. The two peaks are likely to be a result higher traffic volumes that normally occur at these times of day [Cowan et al., 2001]. In respect of NO and NO2, the morning peak is generally found to show a higher concentration of pollutant than the afternoon peak, probably as a result of the diurnal chemistry described above. Results from both CO and PM10 also show two daily peaks, occurring in the same time periods. Levels of these pollutants are often similar during both the morning and afternoon peaks. The increase in pollutant levels is again likely to be caused by higher traffic flow. The absence of a higher peak in the morning, like that of NO and NO2, is probably due to an absence of chemistry resulting in constant background values.

A1.2 Summary
This appendix has discussed the various methods used to measure ambient pollutant concentrations within the UK. These approaches have been examined in relation to

- the way in which a pollutant is measured
- accuracy
- results from use within the UK.

Measurements taken with diffusion tubes have been found to be accurate to within ±18% for an annual average or ±28% for any one individual location. Real
time units use chemilluminescent methods of analysis and have been found to drift by less than 1% over the course of a day. Furthermore, these units often auto recalibrate at the start of each day.

The extensive use of diffusion tubes within the UK has yielded some general observations:

- elevated NO\textsubscript{2} concentrations are usually closely associated with urban areas.
- levels of NO\textsubscript{2} are generally higher during the winter months than in the summer
- NO\textsubscript{2} concentrations have decreased in recent years.

Real-time units have been used to define short-term trends in air quality due to the change in traffic patterns and atmospheric chemistry. It has been observed in many studies that the changes in daily patterns of vehicle use are reflected in pollutant concentrations. This increase in concentration as a result of increased traffic has often been characterised by a double diurnal peak coinciding with local rush hour times.
B1.1 Introduction
This appendix further describes details of patterns and trends observed within recorded data from real-time monitoring units (Figure B 1.1) across the county of Surrey that have been briefly discussed in Chapter 3. The appendix has been divided into:

- daily trends
- monthly trends
- long term trends.

Figure B 1.1 – Location of real time monitoring units in Surrey

The appendix describes data from three real-time monitoring locations within the County of Surrey. The appendix then compares each of the monitoring locations and draws similarities between them.
B1.1.1 Daily trends
Data collected every 15 minutes by the real time units allowed observations on the daily variation in ambient pollution levels at several locations. Figure B 1.2 shows the average weekday trend for April 2000 to April 2001 at three locations across the Surrey.

Diurnal peaks observed within the day coincide with the traffic 'rush' hours that take place at the beginning and end of the working day. Between 8am-9am, a distinct peak was noted that coincides with the morning 'rush' hour when there is the greatest throughput of traffic [Surrey County Council Transportation Model] (Figure B 1.2). The afternoon peak was observed to be more extended (Figure B 1.2) which may be attributed to an earlier school collection time (between 3pm-4pm) followed by the return trip for daily commuters that extends until after 9pm.

![Figure B 1.2 - Average weekday NO levels (April 2000 - April 2001)](image)

During a normal working week, the morning rise in pollution from overnight levels was observed at approximately 5am (GMT), October to March and 4am(GMT) (5am BST) April to September. The relative time shift for the increase in pollution levels is likely to be associated with daylight saving and the traffic-related movement of people.
Appendix B – Analysis of Monitoring Data within Surrey

During the autumn months, the daily reduction of NO, after the morning peak, was found to be greater than during the summer months. A possible explanation is that there are higher levels of pollutants experienced at this time of year due to people returning to school and work following the summer vacation. Similar results were observed for CO, NO$_2$ and PM$_{10}$.

**B1.1.2 Monthly trends**
Monthly and annual trends were assessed for measured data using a monthly average (a single value for each month) (Figure 1.6). The measuring period used was from April 1999 to January 2001 as this was the longest period of available data from one unit in one location.

The patterns observed indicate that the primary pollutants CO and NO have a strong correlation. This strong relationship is most clearly shown during September to October 1999 when the average level of NO and CO rose from 26.5ppb to 48ppb and 0.8ppm to 1.0ppm respectively (Figure B 1.3). Whilst less distinct than the correlations between the primary pollutants NO and its secondary counterpart NO$_2$ also showed coinciding increases and decreases in their levels (Figure B 1.3).

The magnitude of increases and decreases in the level of PM$_{10}$ was less pronounced than that of NO or CO. The patterns observed remained similar however with peaks and troughs occurring at comparable times. The presence of coinciding variations in the levels of CO, NO, NO$_2$ and PM$_{10}$ indicate that the source of each pollutant is the same. The sharp increases for each pollutant, relative to the average level, in October 1999 and January 2000 also indicate that the impact of meteorological changes throughout the year is similar for each pollutant.
B1.1.3 Long term trends

NO$_2$ is created through many chemical reactions; however, the largest proportion is formed through an oxidation reaction with tropospheric ozone (Equation B 1.1). This reaction scheme (Equation B 1.1) suggests that when more light is available, NO$_2$ is easily destroyed, and as a result of the oxygen radical created ozone is formed.

Equation B 1.1- Production / destruction of NO$_2$ cycle

\[
\begin{align*}
NO + O_3 & \rightarrow NO_2 + O_2 \\
NO_2 + Light & \rightarrow NO + O^* \\
O_2 + O^* & \rightarrow O_3
\end{align*}
\]

Where:
- NO is nitric oxide
- NO$_2$ is nitrogen dioxide
- O$_2$ is oxygen
- O$_3$ is ozone
- O$^*$ is an oxygen radical

Within the UK the greatest amount of insolation is received in the summer months, signifying that at this time NO$_2$ levels would be at their lowest. Data recorded over longer time periods have shown that there are higher levels of NO and NO$_2$ during the winter months, with an increase in O$_3$ during the summer.
This change in levels throughout the year is demonstrated in Figure B 1.4 with data from 1999. The results shown in Figure B 1.4 were also confirmed in a review of dispersion tube data across Surrey [Lythe et al., 2001]. The study concluded that winter levels of NO$_2$ were on average higher than those in the summer, peaking in December. Furthermore, the observed trends were found to be most obvious within the intermediate and background data, but less clear at kerbside sites. Lythe et al., noted therefore, that any high levels of pollution ‘camouflage’ the effect of changes in insolation values on pollutant levels throughout the year [Lythe et al., 2001].

![Figure B 1.4 – NO, NO$_2$ and O$_3$ levels April to December 1999](image)

**B1.1.4 Location comparison**

The data from the Guildford real-time unit were compared with those from the Waverley and Mole Valley units. These units were selected as they were collecting data concurrently, whilst other units were not online at this time. It is clear from the results for NO, shown in Figure B 1.5, that as expected, the overall trends were repeated at all three locations. The distance of the units from the nearest major road varies in each case (Table B 1.1); however, the units are all
located near to a road with a similar volume of traffic. It is clear from the results in Figure B 1.5, that the distance from the road is clearly reflected in the levels of pollution recorded, but that the overall pattern remains the same. This conclusion is corroborated by Lythe et al., who developed a method for projecting forward intermediate and background NO\textsubscript{2} diffusion tube measurements due to the linear decrease observed [Lythe et al., 2001].

Table B 1.1- Designation of sites by distance from the main carriageway as defined by DEFRA, 1998

<table>
<thead>
<tr>
<th>Location</th>
<th>Distance from main road</th>
<th>Designation according to DEFRA</th>
</tr>
</thead>
<tbody>
<tr>
<td>Guildford</td>
<td>=3m</td>
<td>Kerbside</td>
</tr>
<tr>
<td>Waverley</td>
<td>&lt;1m</td>
<td>Kerbside</td>
</tr>
<tr>
<td>Mole Valley</td>
<td>&gt;50m</td>
<td>Background</td>
</tr>
</tbody>
</table>

As expected, night time values at all locations were similar. This suggests that once the traffic volume has been reduced, the pollutants were quickly dispersed and background levels were attained.

The diurnal patterns observed for NO were repeated with the measurement PM\textsubscript{10}, across the three units (Figure B 1.6). This repetition of a similar pattern, comparable to that given by traffic levels, suggests that traffic is the major source of pollution within Surrey.
A greater variation between the magnitudes of the PM$_{10}$ levels in comparison to those of NO was observed at the three locations. This was possibly a result of the higher density of PM$_{10}$ in contrast to that of the gaseous pollutant NO, leading to a lower transportation distance. In short, this would mean that the results of PM$_{10}$ are far more sensitive to the proximity of the unit to the road source than the NO value. The results achieved are supported by work in Kraków, Poland by Wróbel et al., who found that PM from road sources declined dramatically with distance [Wróbel et al., 2000].

**Appendix B - Analysis of Monitoring Data within Surrey**

B1.2 Summary
This appendix has further investigated pollution trends at three real-time monitoring units located across the county of Surrey.

Each of the monitoring units have been found to show two daily peaks in NO and PM$_{10}$ levels. The first rise in pollution was detected at 5am at all times of the year (4am GMT during the summer months). The morning peak was found to be more pronounced, whilst the afternoon peak was generally lower and more extended.

Figure B 1.6 – Averaged daily levels of PM$_{10}$ at three real time monitoring units
Appendix B – Analysis of Monitoring Data within Surrey

The distance of the monitoring location from source was found to have a direct impact on the concentration measured. During the night, however, pollutant concentrations were found to fall to similar levels at all locations indicating that once traffic levels are reduced background concentrations are quickly attained.
SPATIAL ANALYSIS OF REAL-TIME DATA

C1.1 Introduction

As discussed in chapter 3, a method of projecting sparse real-time data over a large area was needed in order that PARADIS could be validated at any location. In the chosen study area for validation and case studies, Surrey, the very low number of measurement points meant that traditional spatial interpolation algorithms were not applicable, due to the large distance between each data point.

This appendix describes a new methodology which was developed to obtain a more realistic pollution map over an area the size of a borough or county given a sparse number of data values. The technique combines real-time data with a local transportation model, to create ‘dummy’ or ‘virtual’ measurement points across a large study area. These points may then be spatially interpolated and presented using a Geographic Information System (GIS). Whilst the methodology was developed for Surrey, provided that some pollution monitoring and traffic flow data is available then the method may be used in any location. The method does not rely on any meteorological data, rather it is similar to the DMRB model, and assumes an equal distribution of wind direction and strength. The technique was designed to be used over large areas (borough or county) rather than in depth small scale studies. Whilst the case study used within this chapter is for NO₂, the technique could be used for any monitored pollutant.
C1.2 Methodology

Figure C 1.1 shows the new methodology developed for obtaining a spatial map of air quality of a large area from measured data and traffic flow information. The process consists of 6 stages, namely:

- data collection
- data projection
- concentration calculations at kerbside
- concentration calculations at distance from source
- spatial interpolation of ‘dummy’ points
- presentation using a GIS system.

![Flowchart of method used to produce spatially interpolated pollutant maps](image)

Figure C 1.1– Flowchart of method used to produce spatially interpolated pollutant maps
These stages are described in detail in the following sections.

1.2.1.0. **Collection of data (Stage 1)**
Data to produce 'dummy' points may be obtained from any real time unit within the area of interest. At least 3 units are required to ensure compatibility of the data. Each unit chosen needs to have a similar volume of traffic on an adjacent significant road source, with at least one unit in a kerbside location. It is recommended that the same entire year of data from each unit is used to enable comparisons of results to the Air Quality Strategy guidelines. Once obtained the data needs to be converted to a uniform format for ease of use. The exact format used is left to the individual to discern, but it is suggested that there is one line of data for each day of the year.

C1.2.2 **Projection of monitoring points (Stage 2)**
Monitoring units may not be positioned at the kerbside, as the local authority might be interested in understanding how pollution levels are affected by distance from the source. Comparison between the datasets can still be achieved by projecting the results to a kerbside position. Projection can be undertaken using an adapted version of the technique presented by Lythe et al. [Lythe et al., 2001]. The projection technique relies on weightings for measurements away from kerbside. Traffic volumes along the nearest roads need to be considered, and in the case of any differences, the monitoring units at distance from the road should be factored to have the same traffic volume as the monitor nearest the kerb. A comparison of distance from road source with the annual average of the pollutant of interest then allows a linear trend line to be drawn. The gradient of the trend line may then be used to project the unfactored annual average of the monitoring units to a kerbside position.

C1.2.3 **Calculation of pollution at all kerbside nodes (Stage 3)**
Traffic throughput within the study area is needed to determine the contribution of each vehicle to ambient pollution levels. Over large areas traffic throughput is
often defined by the production of a validated traffic and transportation model. Usually, the traffic model is defined by a series of 'nodes', located at road junctions. The model provides the levels of traffic between the nodes in each direction of flow for roads within the study area. A comparison between the projected annual averages and the traffic flow then allows an average concentration per vehicle passing to be determined. This calculation may then be applied to as many nodes as are available across the study area.

C1.2.4 Calculation of concentration away from kerbside (Stage 4)
The dummy points may then be expanded to allow for atmospheric dispersion away from road source. This may be achieved using Gaussian equations (Equation C 1.1) that describe a normal distribution (Figure C 1.2) to calculate dispersion away from road source in the predominant wind direction (Figure C 1.3).

![The standard Gaussian (normal) distribution](image)

Figure C 1.2 – The standard Gaussian (normal) distribution
Appendix C – Spatial Analysis of Real-Time Data

Equation C 1.1 – Gaussian dispersion equation including reflection at the ground (adapted from Colls, 1997)

\[ q(x, y, z) = \frac{Q}{2\pi \sigma_x \sigma_y \sigma_z} \exp \left\{ \frac{-y^2}{2\sigma_y^2} \left[ \exp \left( -\frac{(z-H)^2}{2\sigma_z^2} \right) + \exp \left( -\frac{(z+H)^2}{2\sigma_z^2} \right) \right] \right\} \]

Where:
- \( q(x, y, z) \) Concentration at receptor
- \( x, y, z \) Cartesian coordinates
- \( Q \) Source strength
- \( \bar{u} \) Wind speed
- \( \sigma_x, \sigma_y, \sigma_z \) Standard deviations in x and y directions described by Pasquill stability classes
- \( H \) Release height

Figure C 1.3 – Wind rose for statistical data

The Gaussian equation uses Pasquill stability categories for the calculation of \( \sigma_y \) and \( \sigma_z \) Table C 1.1 and Table C 1.2. The stability categories are valid in the range 0.1 km ≤ 100 km, as the equations were empirically derived and designed for medium distance scales (Colls, 1997).

Table C 1.1 – Pasquill stability classes and their occurrence in the UK (Colls, 1997)

<table>
<thead>
<tr>
<th>Stability Class</th>
<th>% Incidence in UK</th>
<th>Weather</th>
</tr>
</thead>
<tbody>
<tr>
<td>Very unstable</td>
<td>1</td>
<td>Very sunny</td>
</tr>
<tr>
<td>Moderately unstable</td>
<td>5</td>
<td>Sunny</td>
</tr>
<tr>
<td>Slightly unstable</td>
<td>15</td>
<td>Part cloud (day)</td>
</tr>
<tr>
<td>Neutral</td>
<td>65</td>
<td>Overcast</td>
</tr>
<tr>
<td>Stable</td>
<td>6</td>
<td>Part cloud (night)</td>
</tr>
<tr>
<td>Very stable</td>
<td>6</td>
<td>Clear night</td>
</tr>
<tr>
<td>Even more stable</td>
<td>2</td>
<td>Very clear night</td>
</tr>
</tbody>
</table>

An Advanced Screening Model for Air Quality.......................... C5
### Table C.1.2 - Definitions of $\sigma_y$ and $\sigma_z$ with reference to stability classes (Colls, 1997)

<table>
<thead>
<tr>
<th>Stability Class</th>
<th>$\sigma_y$</th>
<th>$\sigma_z$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Open Country</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Very unstable</td>
<td>$0.22x(1 + 0.0001x)^{-0.5}$</td>
<td>$0.20x$</td>
</tr>
<tr>
<td>Moderately unstable</td>
<td>$0.16x(1 + 0.0001x)^{-0.5}$</td>
<td>$0.12x$</td>
</tr>
<tr>
<td>Slightly unstable</td>
<td>$0.11x(1 + 0.0001x)^{-0.5}$</td>
<td>$0.08x(1 + 0.0002x)^{-0.5}$</td>
</tr>
<tr>
<td>Neutral</td>
<td>$0.08x(1 + 0.0001x)^{-0.5}$</td>
<td>$0.06x(1 + 0.0015x)^{-0.5}$</td>
</tr>
<tr>
<td>Stable</td>
<td>$0.06x(1 + 0.0001x)^{-0.5}$</td>
<td>$0.03x(1 + 0.0003x)^{-1}$</td>
</tr>
<tr>
<td>Very Stable</td>
<td>$0.04x(1 + 0.0001x)^{-0.5}$</td>
<td>$0.016x(1 + 0.0003x)^{-1}$</td>
</tr>
<tr>
<td>Urban</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Very unstable –</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Moderately unstable</td>
<td>$0.32x(1 + 0.0004x)^{-0.5}$</td>
<td>$0.024x(1 + 0.001x)^{0.5}$</td>
</tr>
<tr>
<td>Slightly unstable</td>
<td>$0.22x(1 + 0.0004x)^{-0.5}$</td>
<td>$0.20x$</td>
</tr>
<tr>
<td>Neutral</td>
<td>$0.16x(1 + 0.0004x)^{-0.5}$</td>
<td>$0.14x(1 + 0.0003x)^{0.5}$</td>
</tr>
<tr>
<td>Stable – Very Stable</td>
<td>$0.11x(1 + 0.0004x)^{-0.5}$</td>
<td>$0.08x(1 + 0.0015x)^{0.5}$</td>
</tr>
</tbody>
</table>

Whilst accuracy would dictate that receptors should be calculated as close together as possible, and for an infinite distance, limitations need to be included for ease of use. Background levels are achieved after 150m to 200m from roadside (Figure C 1.4), there is little point, therefore, calculating concentrations further than 200m from roadside as they will always remain a constant background [DMRB, 2003].

![Figure C 1.4](image-url)  
Figure C 1.4 – The contribution of traffic to pollution at various distances from the road centre. Reproduced with the kind permission of HMSO Licence number C02W0003685 [DMRB, 2003].
A separation of 25m between receptors was found to have little effect on the output from interpolation techniques. It is recommended, therefore, that for this technique, that 4 additional dummy points are created per node for distances of increment of 25m from 100m to 175m from source.

C1.2.5 Interpolation (stage 5)
Interpolation fits a mathematical function to a specified number of points, or all of the points within a radius, to determine a concentration at points within a very fine regular grid. Points of equal value are then joined together to create contours and a spatial map of pollution is created. Several interpolation techniques exist for different types of data, and these are often available as part of or ‘add-ons’ to GIS packages.

In the case of pollution from traffic, it is known that concentrations decrease away from source and therefore have a distinct directional bias. Furthermore, it has often been observed, that the dispersion rate is often non-uniform and that pollution levels change rapidly over short distances [Wröbel et al., 2000 and Colls, 1997]. It is suggested, therefore, that Kriging (Equation C 1.2) is selected as the interpolation technique as it has been shown to be appropriate if there is directional bias within the data [ESRI, 1996].

\[
\hat{Z}(S_0) = \sum_{i=1}^{N} \lambda_i Z(S_i)
\]

Where
- \(Z(S_i)\) is the Measured value at the \(n^{th}\) location
- \(\lambda_i\) is the Unknown weight for \(n^{th}\) location
- \(S_0\) is the Prediction location
- \(N\) is the Number of measured values

Equation C 1.2 – Equation for Kriging

An Advanced Screening Model for Air Quality
An additional ‘linear with sill’ algorithm should be used within the Kriging technique to take account of the decrease of pollution concentration away from each point (linear) to a continuous background (sill).

The Kriging package determines the size of the grid mesh needed based on the extent of the study area and the position of the input data, although this may also be manually input. The weighting \( (\lambda_i) \) within Equation C 1.2 is also determined by the Kriging package, for information purposes, this number is based upon the distance between the input data and the prediction location for which the computer is calculating a concentration, along with the overall spatial arrangement of the input data.

**C1.2.6 Presentation of spatial air quality map (stage 6)**
The output of the Kriging process is a concentration map of pollutants across the study area. This map may then be interrogated, using tools within the GIS system, to determine ambient annual average pollutant concentration at any location. The majority of GIS systems also allow the export of this map to many formats for presentation purposes.

**C1.3 Case study**
The described method was used to determine annual average pollutant levels of \( \text{NO}_2 \) across the County of Surrey. \( \text{NO}_2 \) was chosen as the pollutant to investigate, as measurements from diffusion tubes were available for validation purposes.

**C1.3.1 Collection of data (stage 1)**
The data to produce ‘dummy’ points were obtained from three real time monitoring units that collected data in 1999 (Figure C 1.5). The units were specifically chosen as they were located adjacent to major road sources that each carried similar volumes of traffic (Figure C 1.6) [Surrey County Transportation Model].
Appendix C – Spatial Analysis of Real-Time Data

Figure C 1.5 – Location of real-time units within Surrey

Figure C 1.6 – Location of units from which data was used relative to the nearest major road Reproduced from Ordnance Survey map with the permission of the Controller of Her Majesty's Stationery Office, © Crown Copyright NC/03/21947

The data files were accessed from the relevant council offices, and were downloaded either on site or remotely. Once obtained, it was found that each data file had been stored in a different format. All of the data files were therefore converted into a uniform format through the use of a short visual basic script so that one line of data represented one day of the year.
C1.3.2 Projection of monitoring points (Stage 2)
Table C 1.3 shows the differences between the monitoring points and the annual average level of NO₂ for 2000. In order to obtain an ambient level of pollution per vehicle passing an adaptation of a projection technique presented by Lythe et al. was undertaken [Lythe et al., 2001].

Table C 1.3 - Information on the three real-time monitoring units

<table>
<thead>
<tr>
<th>Unit</th>
<th>Distance from main road source (m)</th>
<th>DEFRA classification</th>
<th>Vehicle Volume</th>
<th>Annual Average NO₂ 2000 (ppb)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Waverley</td>
<td>0</td>
<td>Kerbside</td>
<td>25375</td>
<td>18.99</td>
</tr>
<tr>
<td>Guildford</td>
<td>5</td>
<td>Kerbside</td>
<td>23610</td>
<td>17.80</td>
</tr>
<tr>
<td>Mole Valley</td>
<td>190</td>
<td>Background</td>
<td>24982</td>
<td>13.69</td>
</tr>
</tbody>
</table>

For the Guildford and Mole Valley units, a factor was calculated from the vehicle volumes for use with the annual averages to show what the levels would be if the traffic volumes were the same, the results are shown in Figure C 1.7.

Figure C 1.7 – Pollution levels at monitoring units after adjustment for varying traffic levels. Linear trend line and equation show decrease of ambient levels from roadside to background.

The resulting equation from the linear trend line (Figure C 1.7) was used to project the original annual average concentration from their varying positions to a kerbside location.
C1.3.3 Calculation of pollution at all kerbside nodes (stage 3)
The annual average level of pollution for each projected unit was compared to
the annual average daily total (AADT) traffic levels. This provided a factor of
7.4x10^4 ppb for each passing vehicle. The factor was applied to each node within
the Surrey County Traffic and Transportation Model, creating 3188 dummy data
points of estimated pollution levels at the Kerbside of roads across the county.

C1.3.4 Calculation of concentration away from kerbside
(Stage 4)
The expansion of these nodes away from roadside to account for atmospheric
dispersion from source was calculated through the use of a Gaussian dispersion
equation that includes one reflection at ground level discussed in C1.2.4. Four
additional dummy points at each node (100m, 125m, 150m and 175m from each
node) on a line in the predominant wind were created. σ_y and σ_z were calculated
using both 'Urban' and 'Open-country' equations dependent on the location of the
node. In all cases the Pasquill stability category D was selected as neutral
conditions occur 65% of the time in the UK. These calculations allowed a total of
12752 dummy points to be available for interpolation.

C1.3.5 Interpolation (stage 5)
Interpolation was used to determine concentrations in locations where dummy
data points did not exist. Kriging using a 'linear with sill' algorithm was selected
as the interpolation technique for the reasons outlined in C1.2.5. The
interpolation was undertaken in 'ArcView', a commercially available GIS software
with the 'Spatial Analyst' add-on and a free script 'Kriging Interpolation for Spatial
Analyst' available for download from the ESRI website (www.esri.com).

C1.3.6 Presentation of spatial air quality map (stage 6)
The GIS software allows the presentation of the spatially interpolated data in a
variety of forms. The spatial calculator provided with 'Spatial-Analyst' allowed the
cropping of the interpolated map to the county boundary and data such as the positions of roads overlain to determine spatial relationships.

C1.3.7 Results

NO₂ concentrations were calculated for the County of Surrey using the Surrey County Transportation model for traffic data; the results are shown in Figure C 1.8.

Higher concentrations of NO₂ clearly follow the major roads across the county. Pollution 'hot spots' were also visible within the results, which coincided with junctions and towns with high traffic throughput. These are discussed in the following sections.

Junction hotspots

Hotspots at junctions were most clearly visible where the M25 meets other major motorways and A-class roads. This is most visibly seen in highlighted areas 1 and 2 in Figure C 1.8 where the M25 meets the M3 and M23 respectively. These hotspots are likely to be due to the high volumes of traffic that interchange between the motorways at these locations. High levels of NO₂ are indicated along the M25 corridor from the area where it enters Surrey in the north-west of the county to the junction with the A24. This part of the M25 is known as the Surrey section and carries more traffic per day than any other section of the M25 [Highways Agency, 2004].
Appendix C - Spatial Analysis of Real-Time Data

Figure C 1.8 - Spatially interpolated map of extrapolated data from real-time units with data from NO\textsubscript{2} diffusion tubes overlaid (all units in ppb)

**Town hotspots**

Towns with high traffic throughput may also be identified in Figure C 1.8. This is most clearly seen in Guildford (highlighted area 3). As the county town, Guildford has high residential and visiting traffic flows due to work opportunities and available shopping facilities. The proximity of the A3 to the town centre provides both easy access and high transient vehicle volumes. The high traffic volumes moving within the town and past on the A3 allow the formation of high NO\textsubscript{2} concentrations.

**C1.3.8 Validation**

Validation of the interpolated data consisted of a comparison of values with existing diffusion tube data. Across the study area 148 NO\textsubscript{2} diffusion tubes have collected monthly data since 1993 (with further NO\textsubscript{2} tubes available from varying
The data for each individual tube have been averaged for 1999. The results for kerbside locations are represented as varying sized dots on Figure C 1.8. Diffusion tubes have often been placed in areas of high population density, to ascertain the level of residential exposure. The north of the county is more urbanised, and has resulted in a disproportionate amount of NO₂ diffusion tubes in this region.

The mean values of all diffusion tube data and for the spatially interpolated map at the same location were then compared across the county. The average concentration determined by all diffusion tubes across the county was approximately 18ppb, whilst the interpolation technique provided an average level of 16ppb.

A further more detailed comparison using individual annual mean values from the diffusion tubes for 1999 was also undertaken. The results were divided in to the classifications of Kerbside and Background for distance from the roadside as designated by DEFRA (Figure C 1.9).

The results showed reasonable agreement in the Background category, with slightly more variations between the measured and predicted values at Kerbside locations.
Appendix C - Spatial Analysis of Real-Time Data

Figure C 1.9 - Comparison of NO₂ values from diffusion tubes and interpolation process.

Further validation of the data presented in Figure C 1.9 was undertaken with the use of a standard Pearson's correlation. Pearson's correlation is a dimensionless index ranging from -1.0 (perfect negative) to +1.0 (perfect positive) and defines the extent of a linear relationship between two data sets. The results for the correlation coefficient 'r' are displayed in Table C 1.4. The basic assumption of the interpolation method, that there is a one to one correlation between traffic volume and pollution within the study area, the results achieved (Table C 1.4) are extremely good when it is understood that:

1. the basic assumption may not be true in all cases
2. the interpolation method assumes that street canyons do not exist
3. the interpolation method assumes a flat topography with no buildings to ‘mask’ areas
4. the diffusion tubes may represent an area that has been ‘masked’ from true pollution by buildings
Table C.1.4 - Pearson’s correlation of diffusion tube values against spatially interpolated data

<table>
<thead>
<tr>
<th></th>
<th>Background</th>
<th>Kerbside</th>
</tr>
</thead>
<tbody>
<tr>
<td>r-value</td>
<td>0.7</td>
<td>0.6</td>
</tr>
</tbody>
</table>

C1.3.9 Discussion
As shown in Figure C.1.9 and Table C.1.4, background locations showed the closest agreement between the annual average monitored values, and the interpolated maps. This is likely to be the result of the local environment surrounding a background site. Background sites are generally located remote from urban areas, or within the suburban regions, there are often fewer buildings within a background area, and the resulting dispersion is often Gaussian in nature (Figure C.1.10).

Figure C.1.10 - Gaussian dispersion often occurs in a background location
Conversely, Kerbside locations often show more variability in the correlation of results (Figure C.1.9 and Table C.1.4). Local borough councils often placed Kerbside positions within urban areas, therefore, buildings and street canyons, were likely to affect the build-up and dispersion of pollutants (Figure C.1.11). The interpolation method was found to be less effective in urban areas as the Gaussian equations used were less applicable, resulting in an under prediction of the pollutant concentrations.
Appendix C – Spatial Analysis of Real-Time Data

Mean wind direction

Figure C 1.11 – Canyon effect when the wind is perpendicular to the road direction

C1.4 Summary
Spatially, the collection of accurate monitoring of pollution levels across large areas is not sufficient with the UK to allow interpolation. For the use of simpler interpolation algorithms, and to improve computation time in determining pollution levels across a large area, more data points are needed.

This method allows the creation of ‘dummy’ points, based on real time data, at traffic model node locations. The generation of 4 additional ‘dummy’ points associated with each node in the predominant wind direction are also produced using Gaussian dispersion equations. Kriging interpolation techniques with a ‘linear with sill’ algorithm may then be used to determine pollutant concentrations over a large area.

The initial results from the interpolation technique were encouraging, and offer a low cost preliminary assessment of traffic related air quality over a large area. The results indicate that this technique may be employed to determine areas where pollutant concentrations may exceed target values for the purposes of placement of diffusion tubes.
The results showed that the assumption of a near one-to-one relationship between traffic and pollution for this region was correct, as a Pearson correlation between measured data and the interpolated values showed strong linear agreement.

The technique was most effective in rural areas where Gaussian dispersion can occur freely. In urban areas, good correlation between measured and interpolated data still occurs, however, the results indicate that dispersion in these regions is more complex and as such needs more rigorous methods to describe it accurately.

The method of using the Surrey County Traffic and Transportation model data as the basis for a screening model therefore needs to be further developed to

1. Include speed in correlation between traffic and pollution
2. Increase number of receptor points both along the road and away from source
3. Take in to account wind direction throughout the year
4. Take in to account the boundary layer
5. Take in to account more complex dispersion in urban areas
6. Remove the need for monitored data to determine concentrations in other locations.
Appendix D – Supplementary Information

SUPPLEMENTARY INFORMATION

D1.1 Parametric Studies undertaken

Table D 1.1 shows the parametric runs that were undertaken for each of the pollutants (NOx, CO and PM$_{10}$) and for each road orientation (N-S, E-W, NE-SW, NW-SE). The influence of road width and vehicle number is discussed in detail in Chapter 4.

<table>
<thead>
<tr>
<th>Run No</th>
<th>Road Width</th>
<th>Vehicle No</th>
<th>kph</th>
<th>Vehicle Mix</th>
<th>Run No</th>
<th>Road Width</th>
<th>Vehicles</th>
<th>Speed</th>
<th>Vehicle Mix</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>8</td>
<td>500</td>
<td>10</td>
<td>90:10</td>
<td>24</td>
<td>16</td>
<td>500</td>
<td>40</td>
<td>70:30</td>
</tr>
<tr>
<td>2</td>
<td>16</td>
<td>500</td>
<td>10</td>
<td>90:10</td>
<td>25</td>
<td>8</td>
<td>500</td>
<td>50</td>
<td>90:10</td>
</tr>
<tr>
<td>3</td>
<td>8</td>
<td>500</td>
<td>10</td>
<td>80:20</td>
<td>26</td>
<td>16</td>
<td>500</td>
<td>50</td>
<td>90:10</td>
</tr>
<tr>
<td>4</td>
<td>16</td>
<td>500</td>
<td>10</td>
<td>80:20</td>
<td>27</td>
<td>8</td>
<td>500</td>
<td>50</td>
<td>80:20</td>
</tr>
<tr>
<td>5</td>
<td>8</td>
<td>500</td>
<td>10</td>
<td>70:30</td>
<td>28</td>
<td>16</td>
<td>500</td>
<td>50</td>
<td>80:20</td>
</tr>
<tr>
<td>6</td>
<td>16</td>
<td>500</td>
<td>10</td>
<td>70:30</td>
<td>29</td>
<td>8</td>
<td>500</td>
<td>50</td>
<td>70:30</td>
</tr>
<tr>
<td>7</td>
<td>8</td>
<td>500</td>
<td>20</td>
<td>90:10</td>
<td>30</td>
<td>16</td>
<td>500</td>
<td>50</td>
<td>70:30</td>
</tr>
<tr>
<td>8</td>
<td>16</td>
<td>500</td>
<td>20</td>
<td>90:10</td>
<td>31</td>
<td>8</td>
<td>500</td>
<td>60</td>
<td>90:10</td>
</tr>
<tr>
<td>9</td>
<td>8</td>
<td>500</td>
<td>20</td>
<td>80:20</td>
<td>32</td>
<td>16</td>
<td>500</td>
<td>60</td>
<td>90:10</td>
</tr>
<tr>
<td>10</td>
<td>16</td>
<td>500</td>
<td>20</td>
<td>80:20</td>
<td>33</td>
<td>8</td>
<td>500</td>
<td>60</td>
<td>90:20</td>
</tr>
<tr>
<td>11</td>
<td>8</td>
<td>500</td>
<td>20</td>
<td>70:30</td>
<td>34</td>
<td>16</td>
<td>500</td>
<td>60</td>
<td>90:20</td>
</tr>
<tr>
<td>12</td>
<td>16</td>
<td>500</td>
<td>20</td>
<td>70:30</td>
<td>35</td>
<td>8</td>
<td>500</td>
<td>60</td>
<td>70:30</td>
</tr>
<tr>
<td>13</td>
<td>8</td>
<td>500</td>
<td>30</td>
<td>90:10</td>
<td>36</td>
<td>16</td>
<td>500</td>
<td>60</td>
<td>70:30</td>
</tr>
<tr>
<td>14</td>
<td>16</td>
<td>500</td>
<td>30</td>
<td>90:10</td>
<td>37</td>
<td>8</td>
<td>500</td>
<td>70</td>
<td>90:10</td>
</tr>
<tr>
<td>15</td>
<td>8</td>
<td>500</td>
<td>30</td>
<td>80:20</td>
<td>38</td>
<td>16</td>
<td>500</td>
<td>70</td>
<td>90:10</td>
</tr>
<tr>
<td>16</td>
<td>16</td>
<td>500</td>
<td>30</td>
<td>80:20</td>
<td>39</td>
<td>20</td>
<td>500</td>
<td>70</td>
<td>90:10</td>
</tr>
<tr>
<td>17</td>
<td>8</td>
<td>500</td>
<td>30</td>
<td>70:30</td>
<td>40</td>
<td>28</td>
<td>500</td>
<td>70</td>
<td>90:10</td>
</tr>
<tr>
<td>18</td>
<td>16</td>
<td>500</td>
<td>30</td>
<td>70:30</td>
<td>41</td>
<td>8</td>
<td>500</td>
<td>70</td>
<td>80:20</td>
</tr>
<tr>
<td>19</td>
<td>8</td>
<td>500</td>
<td>40</td>
<td>90:10</td>
<td>42</td>
<td>16</td>
<td>500</td>
<td>70</td>
<td>80:20</td>
</tr>
<tr>
<td>20</td>
<td>16</td>
<td>500</td>
<td>40</td>
<td>90:10</td>
<td>43</td>
<td>20</td>
<td>500</td>
<td>70</td>
<td>80:20</td>
</tr>
<tr>
<td>21</td>
<td>8</td>
<td>500</td>
<td>40</td>
<td>80:20</td>
<td>44</td>
<td>28</td>
<td>500</td>
<td>70</td>
<td>80:20</td>
</tr>
<tr>
<td>22</td>
<td>16</td>
<td>500</td>
<td>40</td>
<td>80:20</td>
<td>45</td>
<td>8</td>
<td>500</td>
<td>70</td>
<td>70:30</td>
</tr>
<tr>
<td>23</td>
<td>8</td>
<td>500</td>
<td>40</td>
<td>70:30</td>
<td>46</td>
<td>16</td>
<td>500</td>
<td>70</td>
<td>70:30</td>
</tr>
</tbody>
</table>
### Table D 1.1 Continued

<table>
<thead>
<tr>
<th>Run No</th>
<th>Road Width</th>
<th>Vehicle no</th>
<th>kph</th>
<th>Vehicle Mix</th>
</tr>
</thead>
<tbody>
<tr>
<td>47</td>
<td>20</td>
<td>500</td>
<td>70</td>
<td>70:30</td>
</tr>
<tr>
<td>48</td>
<td>28</td>
<td>500</td>
<td>70</td>
<td>70:30</td>
</tr>
<tr>
<td>49</td>
<td>8</td>
<td>500</td>
<td>80</td>
<td>90:10</td>
</tr>
<tr>
<td>50</td>
<td>16</td>
<td>500</td>
<td>80</td>
<td>90:10</td>
</tr>
<tr>
<td>51</td>
<td>20</td>
<td>500</td>
<td>80</td>
<td>90:10</td>
</tr>
<tr>
<td>52</td>
<td>28</td>
<td>500</td>
<td>80</td>
<td>90:10</td>
</tr>
<tr>
<td>53</td>
<td>8</td>
<td>500</td>
<td>80</td>
<td>80:20</td>
</tr>
<tr>
<td>54</td>
<td>16</td>
<td>500</td>
<td>80</td>
<td>80:20</td>
</tr>
<tr>
<td>55</td>
<td>20</td>
<td>500</td>
<td>80</td>
<td>80:20</td>
</tr>
<tr>
<td>56</td>
<td>28</td>
<td>500</td>
<td>80</td>
<td>80:20</td>
</tr>
<tr>
<td>57</td>
<td>8</td>
<td>500</td>
<td>80</td>
<td>70:30</td>
</tr>
<tr>
<td>58</td>
<td>16</td>
<td>500</td>
<td>80</td>
<td>70:30</td>
</tr>
<tr>
<td>59</td>
<td>20</td>
<td>500</td>
<td>80</td>
<td>70:30</td>
</tr>
<tr>
<td>60</td>
<td>28</td>
<td>500</td>
<td>80</td>
<td>70:30</td>
</tr>
<tr>
<td>61</td>
<td>8</td>
<td>500</td>
<td>90</td>
<td>90:10</td>
</tr>
<tr>
<td>62</td>
<td>16</td>
<td>500</td>
<td>90</td>
<td>90:10</td>
</tr>
<tr>
<td>63</td>
<td>20</td>
<td>500</td>
<td>90</td>
<td>90:10</td>
</tr>
<tr>
<td>64</td>
<td>28</td>
<td>500</td>
<td>90</td>
<td>90:10</td>
</tr>
<tr>
<td>65</td>
<td>8</td>
<td>500</td>
<td>90</td>
<td>80:20</td>
</tr>
<tr>
<td>66</td>
<td>16</td>
<td>500</td>
<td>90</td>
<td>80:20</td>
</tr>
<tr>
<td>67</td>
<td>20</td>
<td>500</td>
<td>90</td>
<td>80:20</td>
</tr>
<tr>
<td>68</td>
<td>28</td>
<td>500</td>
<td>90</td>
<td>80:20</td>
</tr>
<tr>
<td>69</td>
<td>8</td>
<td>500</td>
<td>90</td>
<td>70:30</td>
</tr>
<tr>
<td>70</td>
<td>16</td>
<td>500</td>
<td>90</td>
<td>70:30</td>
</tr>
<tr>
<td>71</td>
<td>20</td>
<td>500</td>
<td>90</td>
<td>70:30</td>
</tr>
<tr>
<td>72</td>
<td>28</td>
<td>500</td>
<td>90</td>
<td>70:30</td>
</tr>
<tr>
<td>73</td>
<td>8</td>
<td>500</td>
<td>100</td>
<td>90:10</td>
</tr>
<tr>
<td>74</td>
<td>16</td>
<td>500</td>
<td>100</td>
<td>90:10</td>
</tr>
<tr>
<td>75</td>
<td>20</td>
<td>500</td>
<td>100</td>
<td>90:10</td>
</tr>
<tr>
<td>76</td>
<td>28</td>
<td>500</td>
<td>100</td>
<td>90:10</td>
</tr>
<tr>
<td>77</td>
<td>8</td>
<td>500</td>
<td>100</td>
<td>80:20</td>
</tr>
<tr>
<td>78</td>
<td>16</td>
<td>500</td>
<td>100</td>
<td>80:20</td>
</tr>
<tr>
<td>79</td>
<td>20</td>
<td>500</td>
<td>100</td>
<td>80:20</td>
</tr>
<tr>
<td>80</td>
<td>28</td>
<td>500</td>
<td>100</td>
<td>80:20</td>
</tr>
<tr>
<td>81</td>
<td>8</td>
<td>500</td>
<td>100</td>
<td>70:30</td>
</tr>
<tr>
<td>82</td>
<td>16</td>
<td>500</td>
<td>100</td>
<td>70:30</td>
</tr>
<tr>
<td>83</td>
<td>20</td>
<td>500</td>
<td>100</td>
<td>70:30</td>
</tr>
<tr>
<td>84</td>
<td>28</td>
<td>500</td>
<td>100</td>
<td>70:30</td>
</tr>
<tr>
<td>85</td>
<td>20</td>
<td>500</td>
<td>110</td>
<td>90:10</td>
</tr>
<tr>
<td>86</td>
<td>28</td>
<td>500</td>
<td>110</td>
<td>90:10</td>
</tr>
<tr>
<td>87</td>
<td>20</td>
<td>500</td>
<td>110</td>
<td>80:20</td>
</tr>
<tr>
<td>88</td>
<td>28</td>
<td>500</td>
<td>110</td>
<td>80:20</td>
</tr>
<tr>
<td>89</td>
<td>20</td>
<td>500</td>
<td>110</td>
<td>70:30</td>
</tr>
<tr>
<td>90</td>
<td>28</td>
<td>500</td>
<td>110</td>
<td>70:30</td>
</tr>
<tr>
<td>91</td>
<td>20</td>
<td>500</td>
<td>120</td>
<td>90:10</td>
</tr>
<tr>
<td>92</td>
<td>28</td>
<td>500</td>
<td>120</td>
<td>90:10</td>
</tr>
<tr>
<td>93</td>
<td>20</td>
<td>500</td>
<td>120</td>
<td>80:20</td>
</tr>
<tr>
<td>94</td>
<td>28</td>
<td>500</td>
<td>120</td>
<td>80:20</td>
</tr>
<tr>
<td>95</td>
<td>20</td>
<td>500</td>
<td>120</td>
<td>70:30</td>
</tr>
<tr>
<td>96</td>
<td>28</td>
<td>500</td>
<td>120</td>
<td>70:30</td>
</tr>
</tbody>
</table>
### D1.2 ‘Look-up’ Tables

#### D1.2.1 Example ‘Look-up’ table

Table D 1.2 – Example of a lookup table used by PARADIS. This example is for the NS option for calculating NOx.

<table>
<thead>
<tr>
<th>Match</th>
<th>West of Road</th>
<th>East of Road</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>&gt;100m from Road</td>
<td>&gt;100&gt;10m from Road</td>
</tr>
<tr>
<td></td>
<td>C</td>
<td>Factor for % HGV</td>
</tr>
<tr>
<td>0</td>
<td>10</td>
<td>0.34</td>
</tr>
<tr>
<td>16</td>
<td>10</td>
<td>0.34</td>
</tr>
<tr>
<td>8</td>
<td>20</td>
<td>0.35</td>
</tr>
<tr>
<td>16</td>
<td>20</td>
<td>0.35</td>
</tr>
<tr>
<td>8</td>
<td>30</td>
<td>0.38</td>
</tr>
<tr>
<td>16</td>
<td>30</td>
<td>0.38</td>
</tr>
<tr>
<td>8</td>
<td>40</td>
<td>0.37</td>
</tr>
<tr>
<td>16</td>
<td>40</td>
<td>0.37</td>
</tr>
<tr>
<td>8</td>
<td>50</td>
<td>0.38</td>
</tr>
<tr>
<td>16</td>
<td>50</td>
<td>0.38</td>
</tr>
<tr>
<td>8</td>
<td>60</td>
<td>0.36</td>
</tr>
<tr>
<td>16</td>
<td>60</td>
<td>0.36</td>
</tr>
<tr>
<td>8</td>
<td>70</td>
<td>0.4</td>
</tr>
<tr>
<td>16</td>
<td>70</td>
<td>0.4</td>
</tr>
<tr>
<td>20</td>
<td>70</td>
<td>0.4</td>
</tr>
<tr>
<td>28</td>
<td>70</td>
<td>0.4</td>
</tr>
<tr>
<td>8</td>
<td>80</td>
<td>0.51</td>
</tr>
<tr>
<td>16</td>
<td>80</td>
<td>0.41</td>
</tr>
</tbody>
</table>
### Appendix D – Supplementary Information

**Table D 1.2 Continued**

<table>
<thead>
<tr>
<th>Match</th>
<th>Left hand side of Road</th>
<th>Right hand side of Road</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>&gt;100m from Road</td>
<td>≤100m&gt;10m from Road</td>
</tr>
<tr>
<td>Road Width (m)</td>
<td>Speed (kph)</td>
<td>C</td>
</tr>
<tr>
<td>20</td>
<td>80</td>
<td>0.41</td>
</tr>
<tr>
<td>28</td>
<td>80</td>
<td>0.41</td>
</tr>
<tr>
<td>8</td>
<td>90</td>
<td>0.49</td>
</tr>
<tr>
<td>16</td>
<td>90</td>
<td>0.49</td>
</tr>
<tr>
<td>20</td>
<td>90</td>
<td>0.49</td>
</tr>
<tr>
<td>28</td>
<td>90</td>
<td>0.49</td>
</tr>
<tr>
<td>8</td>
<td>100</td>
<td>0.55</td>
</tr>
<tr>
<td>16</td>
<td>100</td>
<td>0.55</td>
</tr>
<tr>
<td>20</td>
<td>100</td>
<td>0.55</td>
</tr>
<tr>
<td>28</td>
<td>100</td>
<td>0.55</td>
</tr>
<tr>
<td>20</td>
<td>110</td>
<td>0.67</td>
</tr>
<tr>
<td>28</td>
<td>110</td>
<td>0.67</td>
</tr>
<tr>
<td>20</td>
<td>120</td>
<td>0.77</td>
</tr>
<tr>
<td>28</td>
<td>120</td>
<td>0.77</td>
</tr>
</tbody>
</table>

The Parameterisation of Air quality Dispersion Models for Traffic Related Pollutants.
### D1.3 Class / Index of Road Links used by SCTM

Table D 1.3 Class/Index in the Surrey CTM and Associated Road Width used by PARADIS

<table>
<thead>
<tr>
<th>Class</th>
<th>Index</th>
<th>Description</th>
<th>PARADIS Road Width (m)</th>
<th>% HGV</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>1 Lane</td>
<td>4</td>
<td>13</td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td>6 Lane</td>
<td>28</td>
<td>13</td>
</tr>
<tr>
<td>1</td>
<td>3</td>
<td>2 lane rural</td>
<td>8</td>
<td>13</td>
</tr>
<tr>
<td>1</td>
<td>4</td>
<td>2 lane urban</td>
<td>8</td>
<td>13</td>
</tr>
<tr>
<td>1</td>
<td>5</td>
<td>3 lane</td>
<td>16</td>
<td>13</td>
</tr>
<tr>
<td>1</td>
<td>8</td>
<td>4 lane</td>
<td>20</td>
<td>13</td>
</tr>
<tr>
<td>1</td>
<td>7</td>
<td>5 lane</td>
<td>28</td>
<td>13</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>2 lane suburban</td>
<td>8</td>
<td>10</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>3 lane suburban</td>
<td>8</td>
<td>10</td>
</tr>
<tr>
<td>2</td>
<td>3</td>
<td>Dual 2 lane urban</td>
<td>20</td>
<td>10</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
<td>Dual 3 lane urban</td>
<td>20</td>
<td>10</td>
</tr>
<tr>
<td>2</td>
<td>5</td>
<td>2 lane 10m rural</td>
<td>8</td>
<td>10</td>
</tr>
<tr>
<td>2</td>
<td>6</td>
<td>Dual 2 lane rural</td>
<td>20</td>
<td>10</td>
</tr>
<tr>
<td>2</td>
<td>7</td>
<td>Dual 3 lane rural</td>
<td>28</td>
<td>10</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>2 lane non-central urban</td>
<td>8</td>
<td>4</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>2 lane suburban</td>
<td>8</td>
<td>4</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>3 lane suburban</td>
<td>16</td>
<td>4</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>Dual 2 lane urban</td>
<td>20</td>
<td>4</td>
</tr>
<tr>
<td>3</td>
<td>4</td>
<td>2 lane rural 7.3m</td>
<td>8</td>
<td>8</td>
</tr>
<tr>
<td>3</td>
<td>5</td>
<td>2 lane 10m rural</td>
<td>8</td>
<td>8</td>
</tr>
<tr>
<td>3</td>
<td>6</td>
<td>Dual 2 lane rural</td>
<td>20</td>
<td>8</td>
</tr>
<tr>
<td>4</td>
<td>0</td>
<td>2 lane non-central urban</td>
<td>8</td>
<td>8</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>2 lane suburban</td>
<td>8</td>
<td>8</td>
</tr>
<tr>
<td>4</td>
<td>2</td>
<td>3 lane suburban</td>
<td>16</td>
<td>8</td>
</tr>
<tr>
<td>4</td>
<td>3</td>
<td>Dual 2 lane urban</td>
<td>20</td>
<td>8</td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>2 lane rural 7.3m</td>
<td>8</td>
<td>4</td>
</tr>
<tr>
<td>4</td>
<td>5</td>
<td>2 lane 10m rural</td>
<td>8</td>
<td>4</td>
</tr>
<tr>
<td>4</td>
<td>6</td>
<td>Dual 2 lane rural</td>
<td>20</td>
<td>4</td>
</tr>
<tr>
<td>5</td>
<td>0</td>
<td>2 lane central urban</td>
<td>8</td>
<td>2</td>
</tr>
<tr>
<td>5</td>
<td>1</td>
<td>2 lane urban suburban</td>
<td>8</td>
<td>2</td>
</tr>
<tr>
<td>5</td>
<td>2</td>
<td>Wide 2 lane urban suburban</td>
<td>16</td>
<td>2</td>
</tr>
<tr>
<td>5</td>
<td>3</td>
<td>Dual 2 lane urban suburban</td>
<td>16</td>
<td>2</td>
</tr>
<tr>
<td>5</td>
<td>4</td>
<td>2 lane 7.3m rural</td>
<td>8</td>
<td>2</td>
</tr>
<tr>
<td>5</td>
<td>5</td>
<td>2 lane 10m rural</td>
<td>8</td>
<td>2</td>
</tr>
<tr>
<td>5</td>
<td>6</td>
<td>2 lane rural poor standard</td>
<td>8</td>
<td>2</td>
</tr>
<tr>
<td>6</td>
<td>0</td>
<td>2 lane urban</td>
<td>8</td>
<td>2</td>
</tr>
<tr>
<td>6</td>
<td>1</td>
<td>2 lane BCC</td>
<td>8</td>
<td>2</td>
</tr>
<tr>
<td>6</td>
<td>2</td>
<td>Dual 2 lane urban suburban</td>
<td>8</td>
<td>2</td>
</tr>
<tr>
<td>6</td>
<td>3</td>
<td>2 lane BCC</td>
<td>8</td>
<td>2</td>
</tr>
<tr>
<td>6</td>
<td>4</td>
<td>2 lane 7.3m rural</td>
<td>8</td>
<td>2</td>
</tr>
<tr>
<td>6</td>
<td>5</td>
<td>2 lane BCC</td>
<td>8</td>
<td>2</td>
</tr>
<tr>
<td>6</td>
<td>6</td>
<td>2 lane BCC</td>
<td>8</td>
<td>2</td>
</tr>
</tbody>
</table>
### D1.4 Database associated with SCTM Polyline File

Table D1.4 – Example of part of the SCTM database table used by PARADIS

<table>
<thead>
<tr>
<th>OBJECTID*</th>
<th>ANODE</th>
<th>BNODE</th>
<th>LINKID</th>
<th>PARID</th>
<th>CLASS</th>
<th>INDEX</th>
<th>ANODEX</th>
<th>ANODEY</th>
<th>BNODEX</th>
<th>BNODEY</th>
<th>GRID_NAME</th>
<th>SPEED</th>
<th>TRAFFIC</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>802</td>
<td>5382</td>
<td>80255382</td>
<td>29609128</td>
<td>5</td>
<td>1</td>
<td>523000</td>
<td>155500</td>
<td>523900</td>
<td>156100</td>
<td>Road Clip 1</td>
<td>40</td>
<td>11229</td>
</tr>
<tr>
<td>2</td>
<td>806</td>
<td>5381</td>
<td>80655381</td>
<td>29604797</td>
<td>3</td>
<td>3</td>
<td>524100</td>
<td>155700</td>
<td>524000</td>
<td>156100</td>
<td>Road Clip 1</td>
<td>80</td>
<td>39042</td>
</tr>
<tr>
<td>3</td>
<td>807</td>
<td>5380</td>
<td>80755380</td>
<td>29595649</td>
<td>3</td>
<td>7</td>
<td>524100</td>
<td>156300</td>
<td>524100</td>
<td>156300</td>
<td>Road Clip 1</td>
<td>40</td>
<td>34464</td>
</tr>
<tr>
<td>4</td>
<td>810</td>
<td>3893</td>
<td>8103893</td>
<td>15811549</td>
<td>5</td>
<td>1</td>
<td>524800</td>
<td>159200</td>
<td>525300</td>
<td>159400</td>
<td>Road Clip 1</td>
<td>40</td>
<td>21951</td>
</tr>
<tr>
<td>5</td>
<td>810</td>
<td>5337</td>
<td>8105337</td>
<td>29139669</td>
<td>3</td>
<td>3</td>
<td>524800</td>
<td>159200</td>
<td>524800</td>
<td>159800</td>
<td>Road Clip 1</td>
<td>50</td>
<td>28443</td>
</tr>
<tr>
<td>6</td>
<td>811</td>
<td>3894</td>
<td>8113894</td>
<td>15820957</td>
<td>4</td>
<td>1</td>
<td>524800</td>
<td>160300</td>
<td>524600</td>
<td>160300</td>
<td>Road Clip 1</td>
<td>50</td>
<td>28810</td>
</tr>
<tr>
<td>7</td>
<td>811</td>
<td>3895</td>
<td>8113895</td>
<td>15828746</td>
<td>4</td>
<td>1</td>
<td>524800</td>
<td>160300</td>
<td>525000</td>
<td>160300</td>
<td>Road Clip 1</td>
<td>40</td>
<td>23692</td>
</tr>
<tr>
<td>8</td>
<td>811</td>
<td>5337</td>
<td>8115337</td>
<td>29141290</td>
<td>3</td>
<td>3</td>
<td>524800</td>
<td>160300</td>
<td>524800</td>
<td>159800</td>
<td>Road Clip 1</td>
<td>50</td>
<td>35373</td>
</tr>
<tr>
<td>9</td>
<td>813</td>
<td>3895</td>
<td>8133895</td>
<td>15831994</td>
<td>4</td>
<td>1</td>
<td>525900</td>
<td>160200</td>
<td>525000</td>
<td>160300</td>
<td>Road Clip 1</td>
<td>30</td>
<td>25652</td>
</tr>
<tr>
<td>10</td>
<td>813</td>
<td>5236</td>
<td>8135236</td>
<td>28076665</td>
<td>4</td>
<td>4</td>
<td>525900</td>
<td>160200</td>
<td>527300</td>
<td>161000</td>
<td>Road Clip 1</td>
<td>60</td>
<td>50721</td>
</tr>
<tr>
<td>11</td>
<td>815</td>
<td>3892</td>
<td>8153892</td>
<td>15811889</td>
<td>5</td>
<td>1</td>
<td>525200</td>
<td>159600</td>
<td>525500</td>
<td>159700</td>
<td>Road Clip 1</td>
<td>40</td>
<td>17471</td>
</tr>
<tr>
<td>12</td>
<td>815</td>
<td>3893</td>
<td>8153893</td>
<td>15816764</td>
<td>5</td>
<td>1</td>
<td>525200</td>
<td>159600</td>
<td>525300</td>
<td>159400</td>
<td>Road Clip 1</td>
<td>40</td>
<td>20036</td>
</tr>
<tr>
<td>13</td>
<td>815</td>
<td>3895</td>
<td>8153895</td>
<td>15832550</td>
<td>5</td>
<td>1</td>
<td>525200</td>
<td>159600</td>
<td>525300</td>
<td>159400</td>
<td>Road Clip 1</td>
<td>40</td>
<td>16304</td>
</tr>
<tr>
<td>14</td>
<td>816</td>
<td>3893</td>
<td>8163893</td>
<td>15821305</td>
<td>5</td>
<td>1</td>
<td>525800</td>
<td>158700</td>
<td>525300</td>
<td>159400</td>
<td>Road Clip 1</td>
<td>50</td>
<td>2677</td>
</tr>
<tr>
<td>15</td>
<td>818</td>
<td>5324</td>
<td>8185324</td>
<td>29014100</td>
<td>5</td>
<td>1</td>
<td>527500</td>
<td>158300</td>
<td>527500</td>
<td>158100</td>
<td>Road Clip 1</td>
<td>40</td>
<td>15971</td>
</tr>
<tr>
<td>16</td>
<td>819</td>
<td>3892</td>
<td>8193892</td>
<td>15818425</td>
<td>5</td>
<td>1</td>
<td>525900</td>
<td>159900</td>
<td>525500</td>
<td>159700</td>
<td>Road Clip 1</td>
<td>40</td>
<td>18527</td>
</tr>
<tr>
<td>17</td>
<td>824</td>
<td>5380</td>
<td>8245380</td>
<td>29623376</td>
<td>5</td>
<td>1</td>
<td>524800</td>
<td>156600</td>
<td>524100</td>
<td>156200</td>
<td>Road Clip 1</td>
<td>40</td>
<td>20299</td>
</tr>
<tr>
<td>18</td>
<td>832</td>
<td>3848</td>
<td>8323848</td>
<td>15499328</td>
<td>2</td>
<td>5</td>
<td>528700</td>
<td>156000</td>
<td>528900</td>
<td>155500</td>
<td>Road Clip 1</td>
<td>70</td>
<td>23179</td>
</tr>
<tr>
<td>19</td>
<td>835</td>
<td>5265</td>
<td>8355265</td>
<td>28417450</td>
<td>6</td>
<td>7</td>
<td>533400</td>
<td>156200</td>
<td>533500</td>
<td>156300</td>
<td>Road Clip 1</td>
<td>40</td>
<td>8160</td>
</tr>
<tr>
<td>20</td>
<td>838</td>
<td>5265</td>
<td>8385265</td>
<td>28424689</td>
<td>6</td>
<td>1</td>
<td>533000</td>
<td>155300</td>
<td>533500</td>
<td>156300</td>
<td>Road Clip 1</td>
<td>40</td>
<td>4213</td>
</tr>
<tr>
<td>21</td>
<td>946</td>
<td>5265</td>
<td>8465265</td>
<td>28435941</td>
<td>6</td>
<td>1</td>
<td>534800</td>
<td>157200</td>
<td>533500</td>
<td>156300</td>
<td>Road Clip 1</td>
<td>50</td>
<td>601</td>
</tr>
<tr>
<td>22</td>
<td>948</td>
<td>5265</td>
<td>8485265</td>
<td>28439329</td>
<td>6</td>
<td>1</td>
<td>534000</td>
<td>158600</td>
<td>533500</td>
<td>156300</td>
<td>Road Clip 1</td>
<td>50</td>
<td>6737</td>
</tr>
<tr>
<td>23</td>
<td>879</td>
<td>5264</td>
<td>8795264</td>
<td>28482337</td>
<td>6</td>
<td>7</td>
<td>526200</td>
<td>152400</td>
<td>528300</td>
<td>152500</td>
<td>Road Clip 1</td>
<td>30</td>
<td>8883</td>
</tr>
</tbody>
</table>

*aside from the object ID the exact order to the columns is not important as PARADIS has been designed to search for column 'Headers'"