



## APPENDIX AVAILABLE ON REQUEST

### Research Report 155

## The Impact of the Congestion Charging Scheme on Air Quality in London

### Part 1. Emissions Modeling and Analysis of Air Pollution Measurements

Frank Kelly et al.

#### Appendix E. Air Pollution Modeling Methods

Note: Appendices Available on the Web may appear in a different order than in the original Investigators' Report, and some remnants of their original names may appear in Table and Figure numbers. HEI has not changed the content of these documents, only the letter identifier.

Appendix E was originally Appendix B.

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Correspondence may be addressed to Dr. Frank Kelly, Professor of Environmental Health, Environmental Research Group, MRC-HPA Centre for Environment & Health, School of Biomedical Sciences, King's College London, 150 Stamford Street, London SE1 9NH, U.K.  
Tel ++44 20 7848 4004 Fax ++44 20 7848 3891 frank.kelly@kcl.ac.uk.

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# APPENDIX E

## Air Pollution Modelling Methods

### Dispersion modelling in London

The Environmental Research Group (ERG) at King's College London predicts London's air pollution using a combined modelling-measurement approach. It uses a kernel modelling technique to describe the initial dispersion. The kernel model relates to a set of model concentration fields that were produced using an emissions source of unity: either  $1 \text{ g s}^{-1}$  (point sources),  $1 \text{ g m}^{-3} \text{ s}^{-1}$  (volume sources) or  $1 \text{ g km}^{-1} \text{ s}^{-1}$  (road sources). The assumption in this case is that one can calculate the contribution of any source to total air pollution concentrations by applying the model concentration field and adjusting for the source strength, so long as each source exhibits similar emissions characteristics. Each kernel was created using hourly met. data but was applied to the emissions sources as an annual mean. As such details of individual hours performance is implicit within the model but cannot be readily created to compare with measurements. This approach has a number of limitations especially in assessing the hourly model performance and the models ability to recreate daily concentration profiles. However the modelling method was chosen as a reasonable goal given the limitations of a number of key inputs, as well as enabling more detailed spatial information and computational efficiency. As such the modelling system reflects a consistent approach with the LAEI emissions which are only expressed as annual average values, as well as the limitations of meteorological data in London, which is confined to a single location, the Heathrow met. station. Finally, whilst the hourly performance of the model would be desirable in understanding the assessment of the road traffic impact of the CCS this too is published as a change in annual mean vehicle km (during charging hours) with no additional temporal information provided. As a consequence the changes associated with the CCS are applied as an average value (AADT) over the entire CCZ region with much of the inevitable detailed changes at a road by road level being unavailable. As such the model results should only be considered as a guide to the possible impacts of the scheme and in support of the measurement analysis undertaken elsewhere in the report.

Elsewhere comparisons have been reported between the results of the LAQN measurements and the ADMS model predicting hourly values of  $\text{NO}_x$ ,  $\text{NO}_2$  and  $\text{PM}_{10}$  in London, using the LAEI and Heathrow met. data (DfT 2006, CERC 2003b). They provide useful information regarding the likely model performance in London. The report for Heathrow (DfT, 2006) suggests that the 70 % of the hourly  $\text{NO}_x$  results were within a factor of 2. Other work using ADMS in York has shown that 77 % of hourly  $\text{NO}_x$  results are within a factor of 2 from measurements (Westmoreland et al. 2007)

### Meteorological measurements

All model years considered (2001 to 2004) used hourly average meteorological data, which is summarised into  $10^\circ$  wind sectors and recorded at a height of 10 metres at the UK Meteorological Offices site at Heathrow Airport. The parameters measured included temperature, wind speed, wind direction, precipitation, relative humidity and cloud cover. The assumptions used in the kernel model included a surface roughness of one metre and a minimum Monin-Obukov length of 100 metres.

The model assumed two principal source types: the road network close to measurement sites, and the combined road traffic emissions from more distant locations plus the effects of all other source types. This approach recognises the dominance of road traffic sources at most locations, where a very detailed treatment was required. Other sources and more distant road traffic sources were then modelled as shallow volume sources of varying dimension. The contribution of each source was then calculated through multiple regression as described below. The following paragraphs describe how the approach was developed and summarise how the approach was applied.

The road network around each monitoring site in London (all site types) was modelled in a detailed way. Each road link is split into 10 m lengths based on geographically accurate Ordnance Survey road centreline data. This approach allowed the roads to be represented in a geographically accurate way, see example in Figure E1. This is very important for sites close to roads where strong concentration gradients exist. For dual carriageways, each side of the road was modelled separately, to reflect the important separation of two or more lanes of traffic and the varying separation distance between carriageways. This approach essentially recognises a larger degree of pre-mixing for wider roads. Roads were modelled in this way to 500m from each monitoring site, thus covering a 1km<sup>2</sup> area around the site. The ADMS roads model was used for this purpose (CERC 2003) plus the OSPM model v5.0.64 where street canyons exist (Berkowicz 2000, Berkowicz 2002).

The dispersion kernels held within the model were created using hourly met. data and a unit emissions source. However to reflect the change in emissions during both weekdays and weekends an average emissions profile was applied to the model. This was based upon the average emissions calculated for all major roads in London and reflects not only the hourly weekday profiles but also the relative change between weekday and weekends, especially Sunday, where large reductions in HGV's occur (see Figure E2).

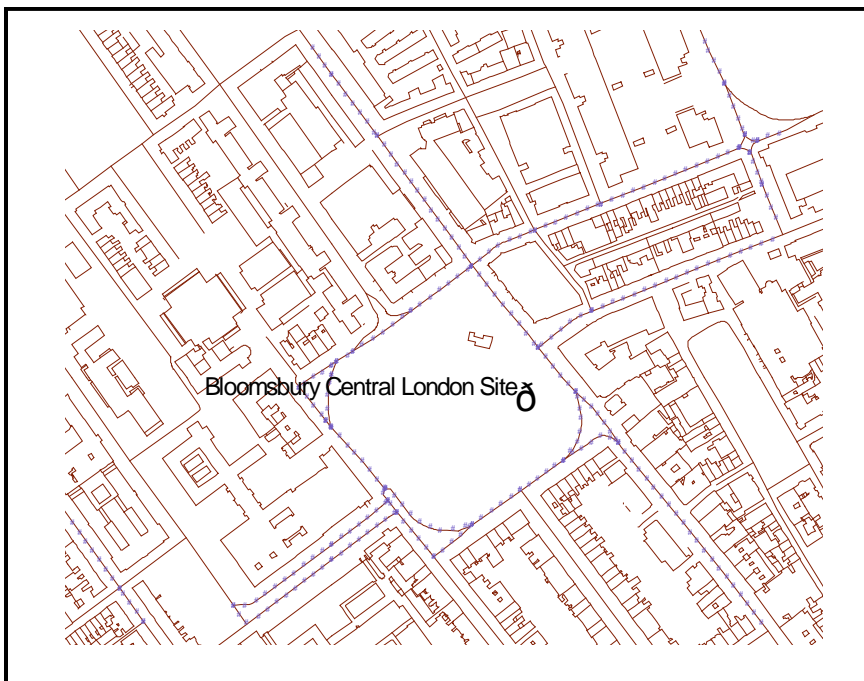


Figure E1. Map showing the 10 m road sections close to the Bloomsbury monitoring site

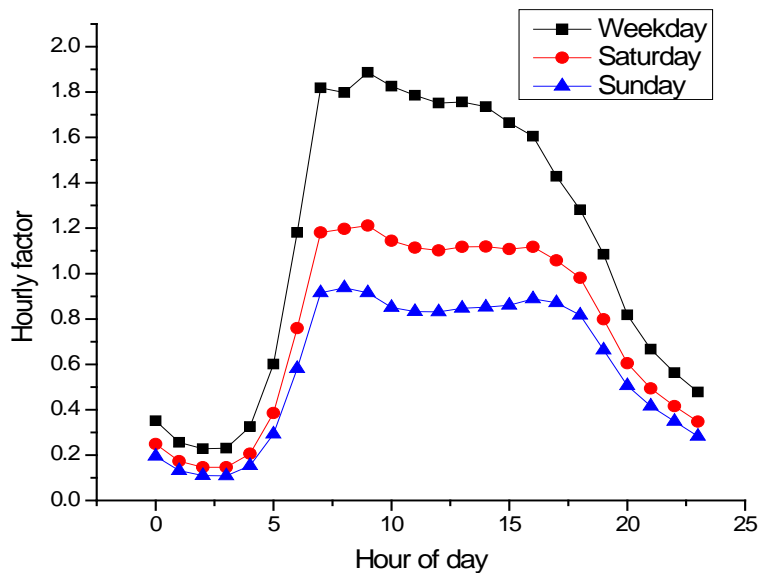


Figure E2. Example of the hourly emissions profiles applied to the ADMS road model

Emissions from train sources were also treated explicitly in the same way as the example given for roads. For the most part trains in London are electric and hence the rail network does not provide significant emissions of oxides of nitrogen ( $\text{NO}_x$ ) and particles with an aerodynamic diameter of  $10 \mu\text{m}$  or smaller ( $\text{PM}_{10}$ ). However this is not the case for some lines, the most notable of which is the line running west from Paddington station. Many of the intercity trains on this line are ageing diesel trains and represent a significant source of both  $\text{NO}_x$  and  $\text{PM}_{10}$ . There was a paucity of specific details relating to these trains and as an initial assumption they were modelled in the same way as for road traffic except the release height assumption was taken to be 5m.

Other sources and road emissions from further than 500 m from each site were modelled as shallow volume sources using the ADMS 3 (CERC 2004) model. Different volume heights were assumed, depending on the characteristics of each source type. It was assumed that road transport emissions were released into a volume 2 m deep and all other sources were released into a 50 m deep volume, apart from the emissions from large (Part A) industrial processes, for which specific emissions data were available. It should be noted however that Part A sources give a very small contribution to annual mean  $\text{NO}_x$  and  $\text{PM}_{10}$ .

A list of the major non-vehicle related emissions sources in London are given below:

- Part A Processes (i.e., large regulated industrial processes)
- Part B Processes (i.e., smaller regulated industrial processes)
- Boilers (i.e., large boiler plants)
- Gas (domestic, industrial-commercial and gas leakage)
- Oil (domestic and commercial oil fuel combustion)
- Coal (domestic and commercial combustion)

- Agriculture-Nature (agricultural and natural)
- Rail
- Ships (marine vessels)
- Airports

For each location the model makes predictions based upon:

- The local road/rail sources, split into 10m sections for the 500m x 500m around the site (including major and minor roads);
- All the other sources outside this area (2466 km<sup>2</sup>), estimated using shallow volume sources (2 m volume height for roads or 50 m volume height for other sources);
- A constant value (intercept C), which represents the contribution from outside London.

A multiple regression was then undertaken in the form:

$$C_M = A.E_{ROAD} + B.E_{OTHER} + C$$

Where A, B are constants to be derived through multiple regression, C was assumed to be the rural contribution of NO<sub>x</sub> taken from measurements, E<sub>ROAD</sub> was the contribution made from the nearby road network, E<sub>OTHER</sub> the contribution from other sources and roads further than 500 m from each site (see Table E1). C<sub>M</sub> was the annual mean NO<sub>x</sub> concentration at a monitoring site. Once the analysis was complete predictions are made for receptor locations, other than at monitoring sites, so long as the values E<sub>ROAD</sub> and E<sub>OTHER</sub> can be calculated.

It should be noted that approximately 30 monitoring sites throughout London were used in the multiple regression. Subsequently a further model evaluation was undertaken using approximately 50 - 60 NO<sub>x</sub> sites and 40 PM<sub>10</sub> sites. This gives some confidence that the model works well at all sites in London and not just at those that were part of its development. The comparison of measurements and model results at those sites not used in the multiple regressions are given in the left hand column of Figure E4.

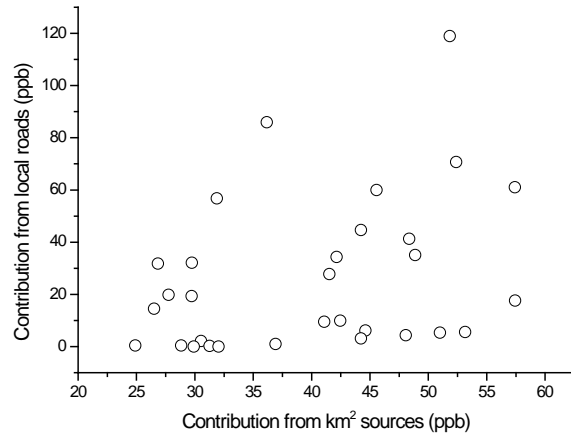
Table E1. Multiple regression coefficients used for model scaling

Year	Factor A	Factor B	P value (A,B)	C (ppb)
2001	0.97	0.63	1.8e <sup>-10</sup> , 3.3e <sup>-7</sup>	14.3
2002	1.72	0.94	9.1e <sup>-13</sup> , 3.9e <sup>-6</sup>	12
2003	1.64	1.42	5.3e <sup>-11</sup> , 4.9e <sup>-7</sup>	13.3
2004	1.59	1.09	1.9e <sup>-9</sup> , 5.3e <sup>-6</sup>	11.4

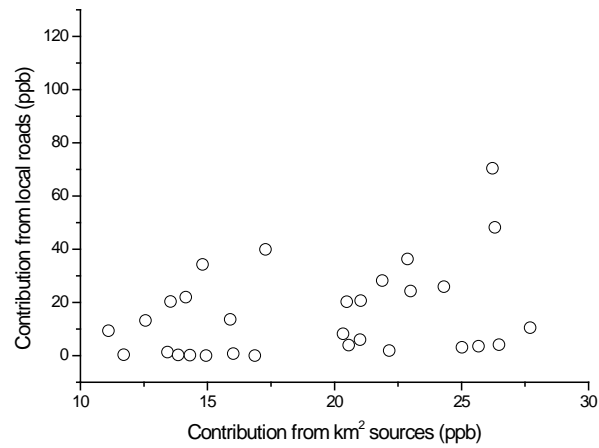
To have confidence in the multiple regressions, it was necessary for several criteria to be fulfilled. First, the variables must be independent of one another. Plotting one against the other can check whether a relationship exists. This check is shown Figure E3, where for all years there is little correlation between the contribution from the local road network and the other emissions.

Year  
2001

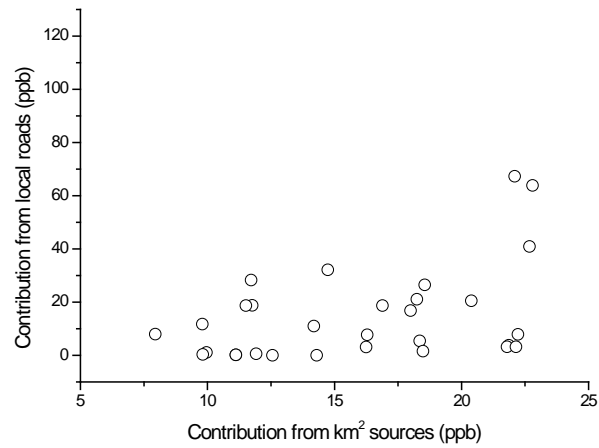
Relationship between nearby road sources and other emissions in  
London 2001 – 2004



2002



2003



2004

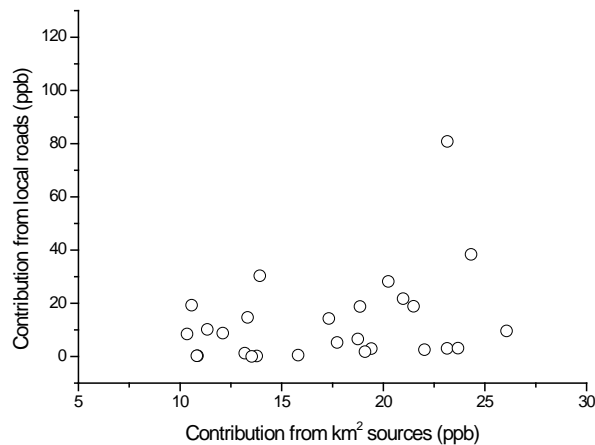


Figure E3. The relationship between nearby road sources and other sources in London in 2001 – 2004

### **Model performance throughout the evaluation process** (see Table E1 and Figure E4)

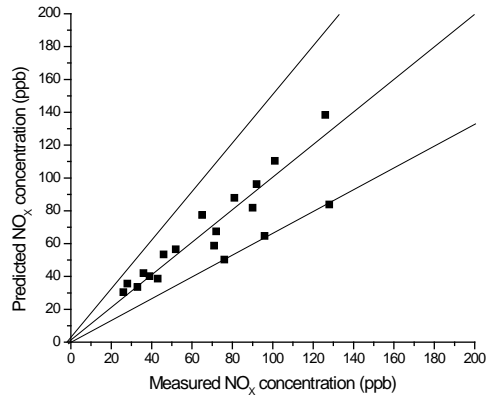
The factors (A and B) applied to the model provide a good indicator of the model performance prior to any correction being applied. For example the factor A was reasonably consistent for the years 2002 to 2004 and suggested a combination of model and/or emissions inventory under prediction. In contrast the factor A for 2001 provided almost no correction at all, 0.97, suggesting that the model predicted higher concentrations for the same emission rate. This was surprising and suggested the met. data as a possible concern. For the 2001 factor B a similar argument would apply.

For the remaining years the model performance at background was closer to real measurements than for the roadside concentrations. This was not surprising and as a consequence the corrections for 2002 and 2004 were relatively small. However 2003 also stands out and in this case and one possible reason may be the model's ability to predict concentrations during such an exceptional met. year with a long summer and high temperatures. However, more work would be required to substantiate these conclusions.

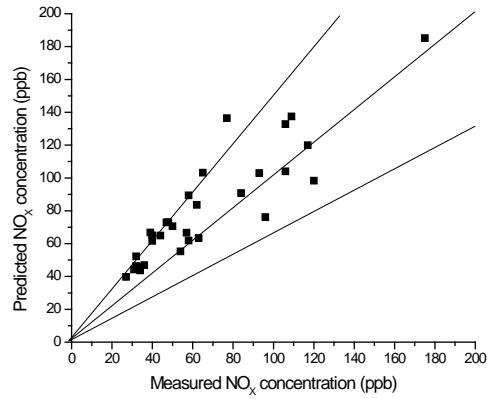
The 'before correction' results can be seen on the graphs in the right hand column of Figure E4 and other than 2001, which is a special case due to met. data issues it is evident that for the most part the model performs reasonably well at background locations but that at roadside there is a large under prediction. Roadside locations are difficult to predict for many reasons, given the complexity of the monitoring locations, the steep concentration gradients and emissions inventory limitations.

Year  
2001

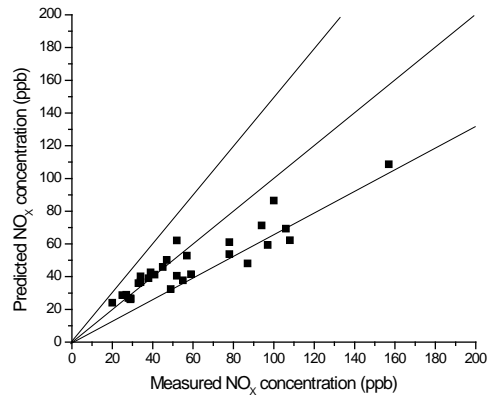
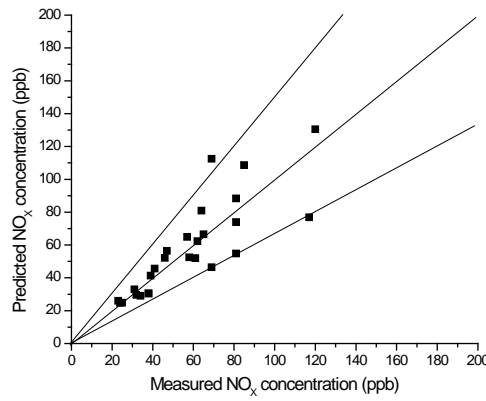
Model v measured NO<sub>x</sub> concentrations for non-calibration sites



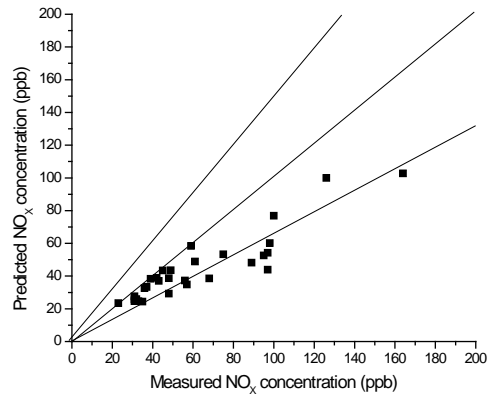
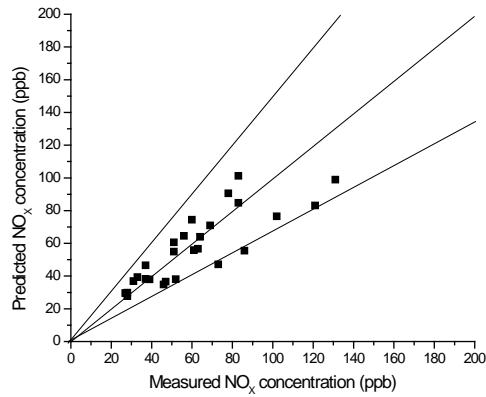
Model v measured NO<sub>x</sub> concentrations without model correction



2002



2003





2004

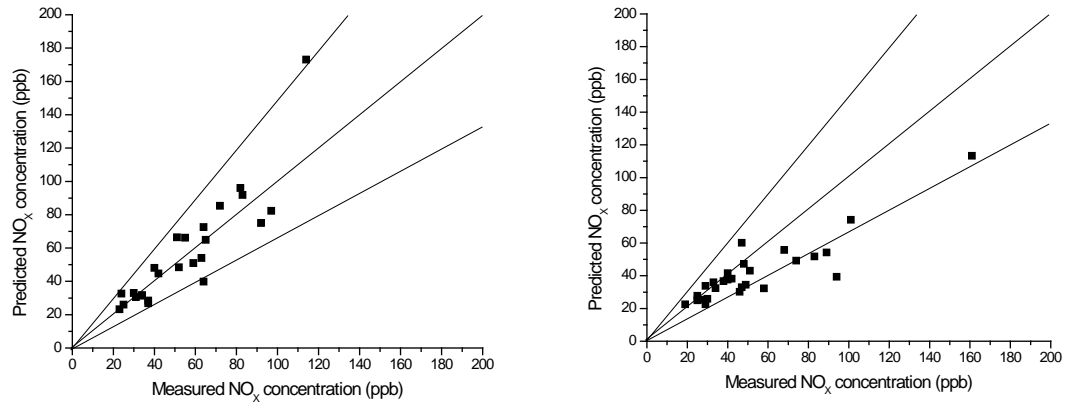


Figure E4. The relationship between nearby road sources and other sources in London in 2001 - 2004

### Conversion from NO<sub>x</sub> to NO<sub>2</sub>

The toolkit model uses specially derived relationships for the conversion of annual average NO<sub>x</sub> to NO<sub>2</sub> (Carslaw et al, 2001). These curves were created by combining the NO<sub>x</sub> frequency distribution and the relationship between hourly average NO<sub>2</sub> and NO<sub>x</sub> for any measurement site and for any year. An example of these data is given in Figure E5. The method used all the hourly measurements of NO<sub>x</sub> and NO<sub>2</sub> for each curve and hence reflects the different regimes in which nitric oxide (NO) is converted to NO<sub>2</sub>. In the first part of the curve in Figure E6 and Figure E5a (between 0 and approximately 100 ppb NO<sub>x</sub>) a steep NO<sub>2</sub> gradient exists and this is the region in which there is generally enough ozone (O<sub>3</sub>) present to convert NO to NO<sub>2</sub>, i.e. a NO<sub>x</sub>-limited regime. As the NO<sub>x</sub> concentration increases further, the gradient of the curve decreases markedly, corresponding to conditions where little O<sub>3</sub> remains due to titration by NO. Under these conditions, little conversion from NO to NO<sub>2</sub> occurs, i.e. it is an O<sub>3</sub>-limited regime. A similar shape of NO<sub>2</sub> vs. NO<sub>x</sub> curves was seen at all monitoring sites and for all years, however, the precise relationship was always both year and site-dependent.

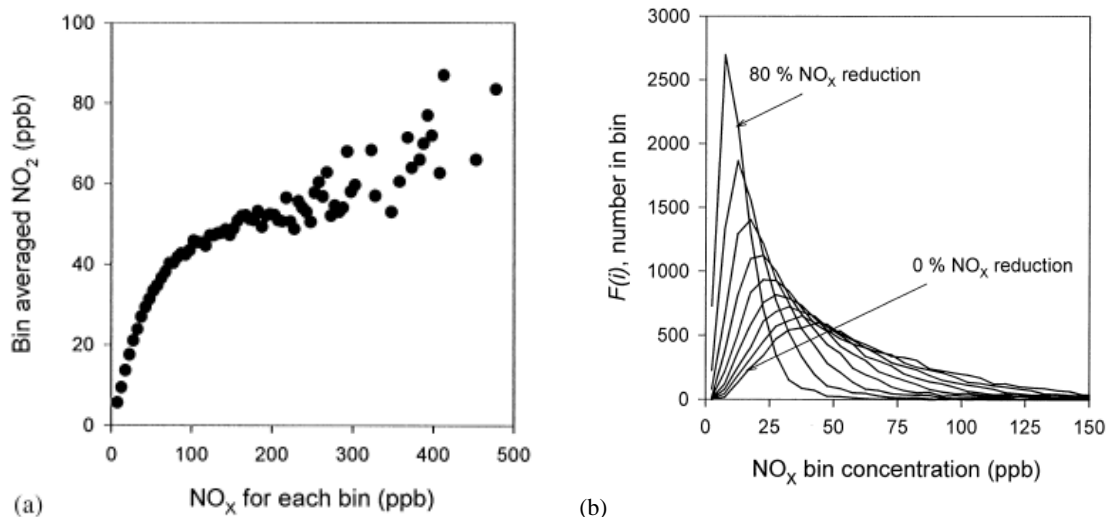


Figure E5. Annual average NO<sub>x</sub> vs. NO<sub>2</sub> relationships in 2002 (Carslaw et al 2001)

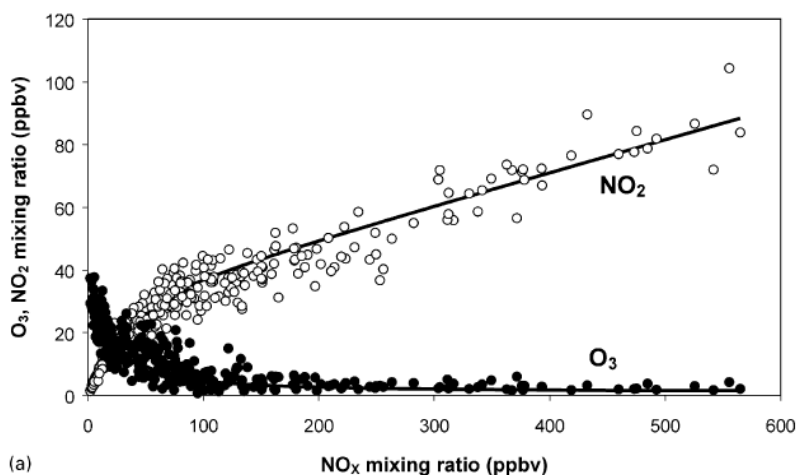


Figure E6. 2002 annual average  $\text{NO}_x$  vs  $\text{NO}_2$  relationships (Clapp and Jenkin 2001)

The second set of curves in Figure E5b summarizes the frequency of hourly  $\text{NO}_x$  concentrations in different  $\text{NO}_x$  bins. The first curve (0%  $\text{NO}_x$  reduction) was the actual frequency distribution for the site and year being processed. Multiplying this curve and the curve in Figure E5a together gave the measured annual average at that site. Reducing the  $\text{NO}_x$  concentrations towards the 80%  $\text{NO}_x$  reduction curve reflects both a reduction in emissions and also the increased number of hours in the year that exist within the  $\text{NO}_x$ -limited regime. The consequence of this is that more  $\text{O}_3$  exists and over time this will result in an upward trend in  $\text{O}_3$ . This can be clearly seen in Figure E7, taken from a number of measurements made in London.

The method used to create the annual average  $\text{NO}_2$  vs  $\text{NO}_x$  concentrations therefore implicitly account for changes in future emissions and also for the change in  $\text{NO}_x$  and  $\text{NO}_2$  regime described above.

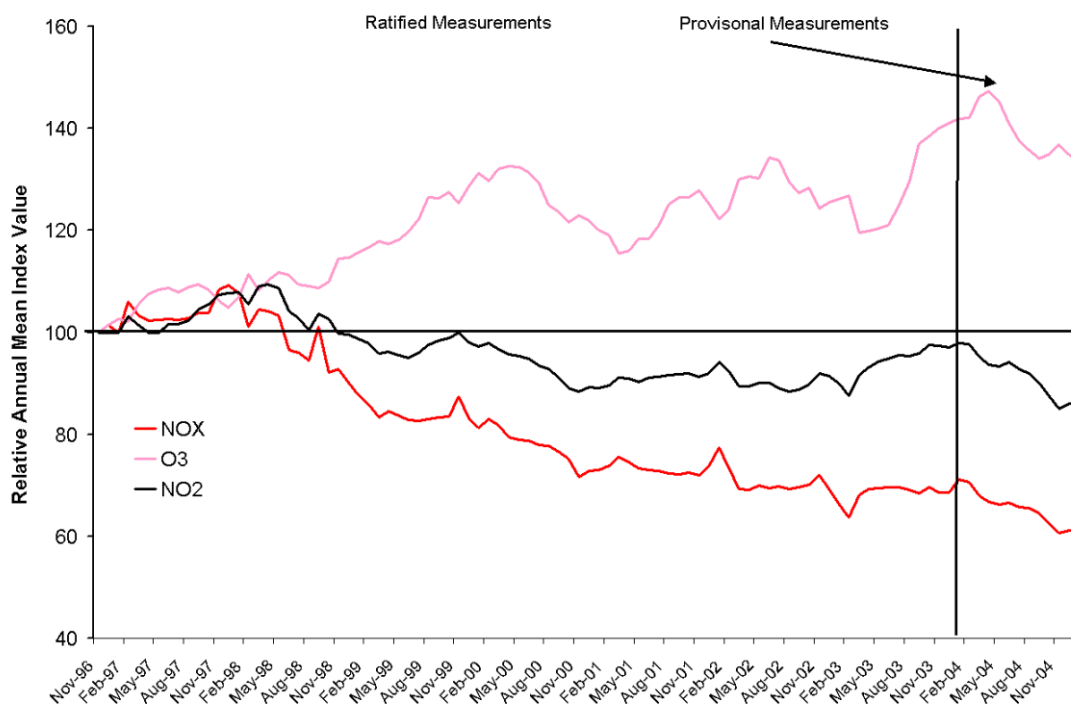


Figure E7. Trends in  $\text{NO}_x$ ,  $\text{NO}_2$  and  $\text{O}_3$  in London

Future concentrations of NO<sub>2</sub> also depend on emissions of vehicle primary NO<sub>2</sub>, which are increasing rapidly. To include this effect a new NO<sub>x</sub>-NO<sub>2</sub> relationship has been derived based on the NO<sub>x</sub> increment above a background site (see Figure E8).

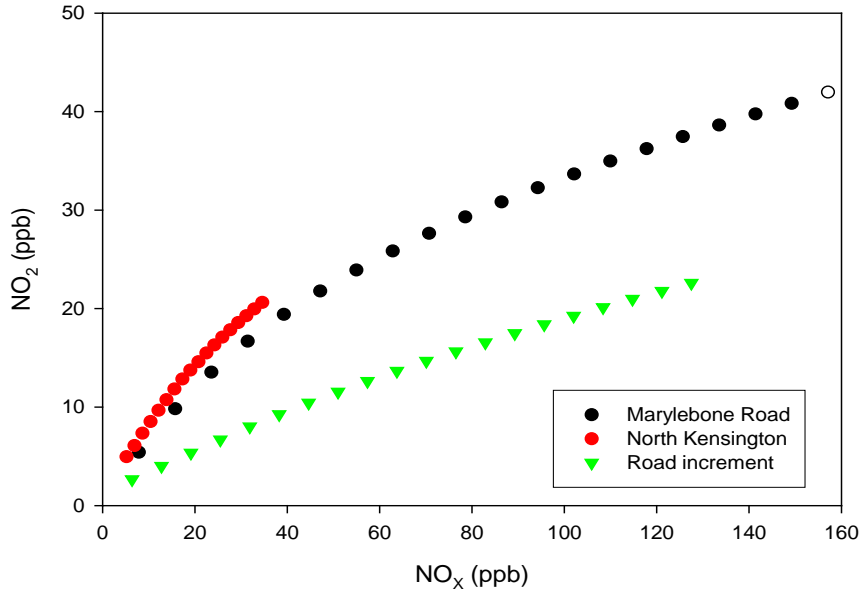


Figure E8. Annual average NO<sub>x</sub> vs NO<sub>2</sub> relationships in 2002

The NO<sub>x</sub>-NO<sub>2</sub> curve for the increment above background takes the form:

$$NO_2 = y_0 + A_1*(1 - \exp(-NO_X / t_1)) + A_2*(1 - \exp(-NO_X / t_2)) \quad [7]$$

where  $y_0$ ,  $A_1$ ,  $t_1$ ,  $A_2$  and  $t_2$  are constants. The equation above was based on an analysis of Marylebone Road where the mean primary NO<sub>2</sub> emissions fraction was estimated to be 9.5 % of NO<sub>x</sub> (Carslaw and Beevers, 2005a). From this a more general case, where the primary NO<sub>2</sub> % by volume (primary nitrogen dioxide [NO<sub>2</sub>(p)]) is known, the equation above can be re-written:

$$NO_2 = [NO_2(p)/100 - 0.095] + y_0 + A_1*(1 - \exp(-NO_X / t_1)) + A_2*(1 - \exp(-NO_X / t_2)) \quad [8]$$

Tests have been undertaken for London roadside sites using the background and incremental NO<sub>x</sub> and NO<sub>2</sub> equations plus knowledge of the primary NO<sub>2</sub> % by volume. The estimated primary NO<sub>2</sub> % by volume was taken from Carslaw and Beevers (2005a) and varied by site across the range 3.9 % (Hillingdon) to 23.4 % (Redbridge). The results are summarised in Figure E9 and have an R<sup>2</sup> value of 0.98. The conclusion reached is therefore that using this approach a very good annual mean NO<sub>2</sub> concentration can be predicted at roadside locations if the model produces good estimates of NO<sub>x</sub> and there is some knowledge of the primary NO<sub>2</sub> value.

However, questions still remain as to whether this relationship works for site types at different locations in London and for different years. To attempt to answer these questions, first, an analysis of the NO<sub>x</sub> vs NO<sub>2</sub> relationship at background locations was undertaken. This focused on Kensington and Chelsea (KC1), a central London

background site. Using the method described above a background  $\text{NO}_x$  to  $\text{NO}_2$  curve was created for each year. From Figure E10 it can be seen that each curve was very similar for all years despite the recent changes in primary  $\text{NO}_2$  and one of the years, 2003, having exceptional meteorology and a long photochemical season.

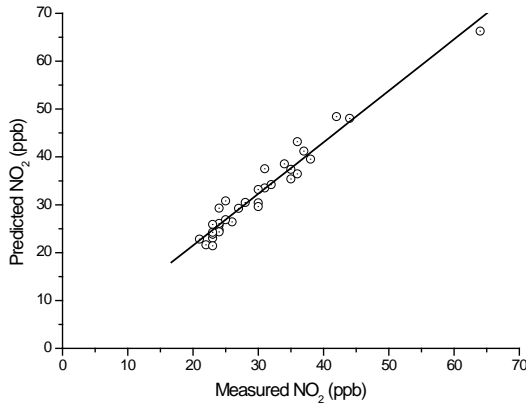


Figure E9. Comparison between annual mean measured and modelled  $\text{NO}_2$  with a wide range % vol direct  $\text{NO}_2$  (2002)

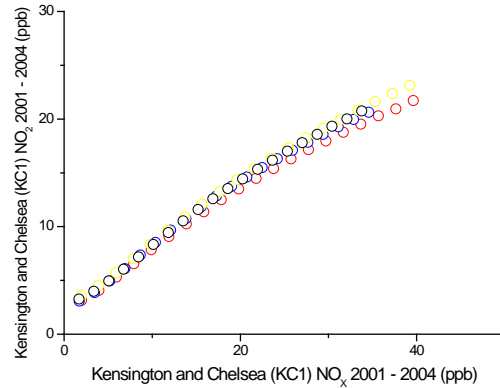


Figure E10. Annual average  $\text{NO}_x$  vs  $\text{NO}_2$  relationships at Kensington and Chelsea (2001 – 2004) Red – 2001, Blue – 2002, Yellow – 2003, Black - 2004

Second, a similar analysis of the  $\text{NO}_x$  –  $\text{NO}_2$  relationship at Marylebone road was undertaken for 2001 to 2004 (Figure E11). Here the curves created change significantly between 2001/02 and 2003/04 and within the model it is assumed that this change is largely associated with increases in locally generated primary  $\text{NO}_2$ . To test whether this change in relationship can be replicated using the generalised roadside increment method within the model, use was made of a time series of estimated primary  $\text{NO}_2$ , created for Marylebone road using the method described in Carslaw et al, 2007 (see Figure E12). From these data the average  $\text{NO}_{2p}$  value at the site was incorporated into the generalised roadside increment equation and this compared with the actual measured roadside increment for each of the years. The results are given in Figure E13 showing that the measured roadside increment (open triangles) and modelled roadside increment (solid squares) lie very close to each other for all years. This again supports the conclusion that a very good mean  $\text{NO}_2$  concentration can be predicted at roadside locations so long as the model predicts annual mean  $\text{NO}_x$  well and there is a good estimate of primary  $\text{NO}_2$ .

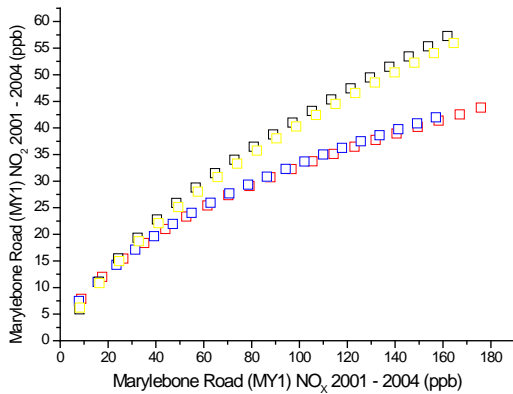


Figure E11. Annual average  $\text{NO}_x$  vs  $\text{NO}_2$  relationships at Marylebone Road (2001 – 2004) Red – 2001, Blue – 2002, Yellow – 2003, Black - 2004

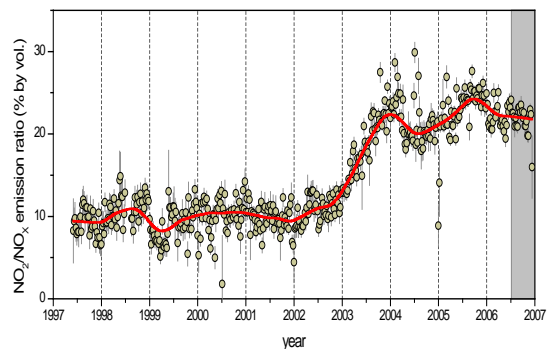


Figure E12. Estimated time series of  $\text{NO}_2$  :  $\text{NO}_x$  ratio ( $\text{NO}_{2p}$ ) at Marylebone Road (Carslaw – personal communication)

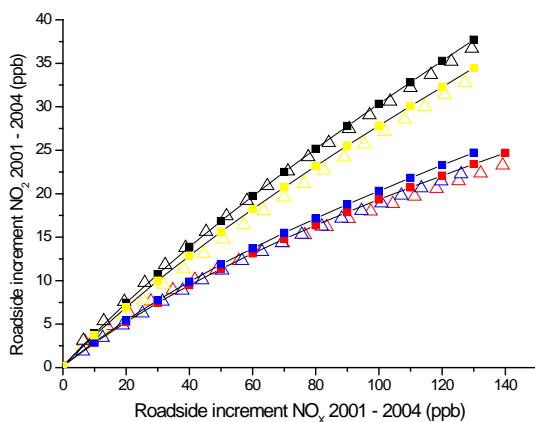


Figure E13. Roadside increment  $\text{NO}_x$  vs  $\text{NO}_2$  concentrations incorporating primary  $\text{NO}_2$   
 Red – 2001, Blue – 2002, Yellow – 2003, Black - 2004

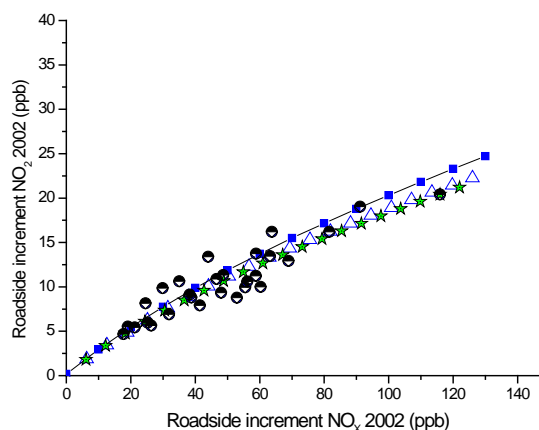


Figure E14. Results of the roadside increment relationships in 2002

One further test was undertaken to understand how well the roadside increment method compares with a simple constrained chemistry scheme of the kind described in (Carslaw and Beevers, 2005a) and whether using this scheme with 28 other roadside sites in London and assuming the same  $\text{NO}_2\text{p}$  value (9.5 %) they fall onto the same curve. The test of the chemistry scheme at Marylebone road (gold stars) was undertaken for each hour of 2002 whilst reducing the roadside  $\text{NO}_x$  increment from 95 % to 5 % of the measured hourly values in steps of 5. The resulting curve provides good agreement with the actual measured roadside increment (blue triangles). Furthermore, the test at different London roadside sites using the assumption that  $\text{NO}_2\text{p} = 9.5\%$  also confirmed that for the majority of sites (blue/black circles) the curve created within the Air Pollution Toolkit (APT) (blue squares), the measured roadside increment (blue triangles) and the curve derived from the simple chemistry scheme (gold stars) were all in reasonable agreement. The conclusion was therefore that the method used to convert  $\text{NO}_x$  to  $\text{NO}_2$  in the model reflects the measurements in London whilst incorporating changes to primary  $\text{NO}_2$ . There are however about 7 sites which lie farthest from the line, both above and below, for which further investigation is required.

### PM<sub>10</sub> Model Description

Unlike  $\text{NO}_x$  and  $\text{NO}_2$ , the composition of  $\text{PM}_{10}$  and the wide variety of sources makes it difficult to construct models to describe urban concentrations. Many of the processes that lead to  $\text{PM}_{10}$  in the atmosphere are difficult to describe in a deterministic way e.g. wind-blown dusts. Furthermore, a significant proportion of measured  $\text{PM}_{10}$  concentrations are derived from the oxidation of species in the atmosphere such as  $\text{NO}_x$  and sulphur dioxide. These processes can take place over hundreds to thousands of kilometres and therefore involve other UK and European sources. A detailed treatment of the secondary component of  $\text{PM}_{10}$  therefore requires the use of sophisticated models e.g. Eulerian models such as CMAQ. However, the emissions of  $\text{PM}_{10}$  from road traffic and many other “local” sources can be treated in much the same way as the modelling approach used for  $\text{NO}_x$ . For these reasons, alternative approaches based on receptor modelling techniques e.g. describing observed concentrations have proved to be very effective e.g. Stedman *et al.*, 2001, Fuller *et al.* 2002, Kukkonen *et al.*, 2001, Fuller and Green, 2006.

In London, where there is good availability of PM<sub>10</sub> and particles with an aerodynamic diameter of 2.5 µm or smaller (PM<sub>2.5</sub>) measurements a PM<sub>10</sub> model has been developed (Fuller et al., 2002) utilising the comprehensive PM<sub>10</sub>, PM<sub>2.5</sub> and NO<sub>x</sub> measurements.

Regression analysis of NO<sub>x</sub> with PM<sub>10</sub> has been used by Deacon et al. (1997), by APEG (1999) and by Stedman et al. (2001) to determine the amount of PM<sub>10</sub> from combustion sources, reasoning that these combustion sources are both sources of PM<sub>10</sub> and NO<sub>x</sub>. In the APT this approach has been extended to PM<sub>2.5</sub> and thus allows the division of PM<sub>10</sub> into four source components:

- *PM<sub>2.5</sub> that is related to NO<sub>x</sub>:*  $PM_{2.5} f(NO_x)$
- *PM<sub>2.5</sub> that is not related to NO<sub>x</sub>:*  $PM_{2.5} \langle \rangle f(NO_x)$
- *PM<sub>C</sub> that is related to NO<sub>x</sub>:*  $PM_C f(NO_x)$
- *PM<sub>C</sub> is not related to NO<sub>x</sub>:*  $PM_C \langle \rangle f(NO_x)$

Where  $PM_C$  refers to  $PM_{10}-PM_{2.5}$ .

And  $PM_{10}f(NO_x) = PM_{2.5}f(NO_x) + PM_Cf(NO_x)$   
 $PM_{10}\langle \rangle f(NO_x) = PM_{2.5}\langle \rangle f(NO_x) + PM_C\langle \rangle f(NO_x)$

From this the total PM<sub>10</sub> can be calculated:

$$PM_{10} = PM_{10}f(NO_x) + PM_{2.5}\langle \rangle f(NO_x) + PM_C\langle \rangle f(NO_x)$$

In the formulation above it was assumed that the particle fractions that were related to NO<sub>x</sub> were primary emissions. This would include both tail-pipe and non tail-pipe PM<sub>10</sub> emissions from road transport and also emissions from stationary combustion sources that are also sources of NO<sub>x</sub>. The particle fraction definitions also include a coarse component that can be related to concentrations of NO<sub>x</sub>, which includes tyre, brake and mechanical wear and possibly a resuspension component.

PM<sub>2.5</sub>, which cannot be related to NO<sub>x</sub>, were assumed to comprise secondary aerosol. PM<sub>C</sub> that was not related to NO<sub>x</sub> might be expected to consist of secondary particulate matter (PM), wind-blown dusts and other natural particles. It is an initial assumption of the model that PM<sub>10</sub> from these sources is regional and that the concentration of PM<sub>10</sub> from these sources is equal across the modelled area.

Rolling annual mean concentrations of NO<sub>x</sub>, PM<sub>10</sub> and PM<sub>2.5</sub> were calculated at monthly intervals for sites with co-located measurements. Rolling annual means were chosen to eliminate the effects of seasonality and a minimum 75% data capture was required to ensure that the measurements were representative of the year. Relationships between annual mean NO<sub>x</sub> and PM<sub>10</sub>, and between NO<sub>x</sub> and PM<sub>2.5</sub> were established, using linear regression. Each monthly analysis used annual mean measurements from all site types including kerbside, roadside, urban background, suburban and rural locations. A maximum of 66 sites were used for the PM<sub>10</sub> analysis by 2005 and a maximum of 5 sites for PM<sub>2.5</sub>.

Linear regressions were derived of the form:

$$PM_{10} (\mu\text{g m}^{-3}) = A NO_x (\text{ppb}) + B (\mu\text{g m}^{-3})$$

$$PM_{2.5} (\mu\text{g m}^{-3}) = C NO_x (\text{ppb}) + D (\mu\text{g m}^{-3})$$

The gradient (A and C) enabled the calculation of the  $PM_{10}$  and  $PM_{2.5}$  that was related to  $NO_x$ . The intercept (B and D) gives the annual mean of the  $PM_{10}$  and  $PM_{2.5}$  that was not related to  $NO_x$ . From these relationships a yearly estimate has been made of the non-primary  $PM_{10}$  component in London which when added to the explicitly modelled  $PM_{10}$  emissions give a total annual average  $PM_{10}$  concentration.

The explicitly modelled  $PM_{10}$  emission sources were treated in the same way as emissions of  $NO_x$  and the model does not undergo any additional model calibration. The reasons for this were based upon the expectation that the  $NO_x$  emissions are the most reliable estimate within the LAEI as well as being the most reliable measurements within the LAQN. Given the problems associated with the measurements of  $PM_{10}$  alone would be reason not to undertake additional model calibration using these results. Furthermore, primary PM emissions are likely to be predominantly in the fine fraction and given that resuspension in the UK is a relatively small component of primary PM (see below) deposition velocities are likely to have a negligible effect over distances of the order of 100m –1-2 km. Whilst this may not be true for the secondary and long range components of  $PM_{10}$  entering London, these were calculated using the method described above and as such are implicit in the calculations. Therefore it does not seem an unreasonable assumption to treat primary PM and  $NO_x$  in the same way.

$PM_{10}$  predictions also use the detailed road network in combination with other  $PM_{10}$  sources, represented as volume sources of varying dimension. Using this approach the annual average  $PM_{10}$  predictions were shown to be in good agreement with measurements.

Two components that were not included in the PM model were road wear and resuspension. This may be a weakness as non-exhaust emissions of PM such as resuspension are often considered to be a highly significant source.

However, these were excluded for a number of reasons. First, in the UK the Air Quality Expert Group (AQEG, 2004) identified the estimation of non-exhaust primary PM as a priority area but one which has a high degree of uncertainty. Second, emissions estimates from the published literature may not be directly applicable to UK conditions. Third, of the measurements made in the UK, resuspension and road wear have not been identified as large contributors to the roadside increment of PM mass (Harrison et al, 2004, Abbott, 2007). Finally, comparisons between the ratio of primary PM (exhaust + tyre wear + brake wear) emissions and those of  $NO_x$  from road transport closely agree with the equivalent linear relationship between  $NO_x$  and  $PM_{10}$  measurements from 32 roadside and kerbside sites in the LAQN. This provides confidence that in the LAEI estimates of emissions of  $NO_x$  and  $PM_{10}$  are in a similar ratio to that of the LAQN measurements. However it is unlikely that PM resuspension and road wear are not a negligible source of primary PM and therefore it is an area where further model development is required.

## Model Caveats

The APT model gives estimates of typical air pollution concentrations throughout London. As such there are many factors that cannot be adequately described using the techniques described above. These factors include:

- The effect of street canyons and other local dispersion issues are only reflected by enhancing the concentration in areas where street canyons exist. The model does not explicitly account for different building heights in complex areas where different building types exist. In addition, the representation of different sources, whose emissions are released at height (e.g. commercial gas combustion) are presently represented using volume sources rather than using specific release characteristics;
- Also the local variation of emissions was not adequately represented, for example, emissions close to queuing traffic or those vehicles that are undergoing high levels of acceleration;
- Emissions were calculated using vehicle stock which was applied London wide, and whilst this works well for London as a whole there is evidence that vehicle stock changes throughout London;
- The effect of direct NO<sub>2</sub> was important for model predictions. At present, use was made of a NO<sub>2</sub> emissions inventory on which these estimates were based. As this is a developing area of research however the uncertainty associated with these predictions is unknown;
- The comparison between pre and post congestion charge scheme periods has highlighted the variability of road traffic counts and perhaps speed. This is likely to be as a consequence of the base LAEI data being a periodic sample of each road rather than a continuous count. Improvements in the treatment of traffic data are therefore required to minimise the noise of the traffic count signal within the LAEI;
- Non-exhaust road traffic emissions are very uncertain and whilst the model includes brake and tyre wear, there are no specific road wear or resuspension components;
- Atmospheric chemistry is highly complex. The effects on PM<sub>10</sub> concentrations of atmospheric chemistry across London are not treated explicitly and those of NO<sub>x</sub>/NO<sub>2</sub> are represented empirically. This simplistic approach is another area of uncertainty within the model;
- Finally, whilst the APT model has been compared with measured data a model uncertainty estimate has not been provided. Work on this issue is currently underway at ERG.



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## Abbreviations

APT	Environmental Research Group, Air Pollution Toolkit
ERG	Environmental Research Group
LAEI	London Atmospheric Emissions Inventory
LAQN	London Air Quality Network
NO	nitric oxide
NO <sub>2</sub>	nitrogen dioxide
NO <sub>2p</sub>	primary nitrogen dioxide
NO <sub>x</sub>	oxides of nitrogen

OX	oxidant
O <sub>3</sub>	ozone
PM	particulate matter
PM <sub>2.5</sub>	particles with an aerodynamic diameter of 2.5 µm or smaller
PM <sub>10</sub>	particles with an aerodynamic diameter of 10 µm or smaller
SO <sub>2</sub>	sulphur dioxide