A3.1. Summary

Note: This appendix contains extracts of a report written on behalf of the Department of Environment, Transport and the Regions (DETR), entitled: ***Estimating the Uncertainty of Model Predictions using a Monte Carlo Simulation*** **[1].**

A3.1.1. Predictions of the concentration of NO_2 at roadsides throughout London[2,3] have shown a high sensitivity to the pass/fail statistic of 21 ppb. These predictions are crucial to the development of air pollution control, through local authority action plans, and it is therefore essential to completely understand the uncertainty associated with them. Only then will the strengths and weaknesses of the predictive process be understood enough for decision-makers to make informed policy judgements. It is the uncertainties associated with these predictions which are the subject of this appendix.

A3.1.2. Monte Carlo modelling techniques have been used to calculate the uncertainties associated with roadside NO_2 predictions. It also includes a full sensitivity analysis to determine the most important input variables to the model. Specific tests include the uncertainties associated with flows and emissions from LGVs, HGVs and buses, vehicle speed, the dispersion model, and the pollution climate mapping technique, used for calculating background concentrations.

A3.1.3. In *Monte Carlo* analysis, the input variables are varied simultaneously and independently of each other, and the effect on important outputs, assessed. The model uncertainty, relating to the input parameters, is calculated by treating them as random variables. By studying the resulting probability distribution of the output (i.e. the concentration or emission estimate), information is obtained regarding the model uncertainty.

A3.1.4. The original study has focused on Marylebone Road for a base year of 1997 for meteorology and atmospheric chemistry and uses the LTS traffic model. Further uncertainty assessments have also been undertaken for an 'average road' in central and outer London, as well as a 'Motorway' in outer London.

A3.1.5. The sensitivity analysis revealed that roadside NO_X predictions are mostly sensitive to the assumptions regarding HGV emissions and flows and the dispersion model used to predict roadside concentrations. For the prediction of NO_2, the NO_X-NO_2 relationship used is the most important factor. Table A3.1 below shows how each input data or modelling method affects the final concentration, for the Marylebone road example.

Table A3.1 The Relative Importance of Model Parameters in Predicting NO_2 at Marylebone Road

Model Parameter	Relative Importance 2005 (% of mean at 2σ)	Relative Importance 1997 (% of mean at 2σ)
NO_X-NO_2 relationship	13.9	11.9
HGV emissions	7.9	8.1
Dispersion model	7.3	6.8
HGV flow	5.5	5.5
LGV emissions	4.2	4.7
LGV flow	4.2	4.7
Vehicle speed	3.6	2.1
Background mapping	1.8	1.7
Bus emissions	1.2	0.9
Bus flow	0.6	0.4

A3.1.6. For 1997, NO_X was predicted to be 258 +/- 83 ppb and NO_2 47 +/- 10 ppb, at two standard deviations – equivalent to the 95 % confidence interval. These statistics assume that the resultant distribution is normal.

A3.1.7. The overall uncertainty of NO_2, which corresponds to 22 % is less than that for NO_X (32 %). This feature is a result of the non-linear NO_2 relationship, which is quite insensitive to NO_X concentrations, implying that a stated NO_X uncertainty is a better indication of the quality of a prediction.

A3.1.8. Measurements for the Marylebone Road site for NO_X and NO_2 are within the uncertainty limits calculated here. NO_X was between 213 and 229 ppb and NO_2 between 44 and 48 ppb for 1997. The range reflects the two different monitoring techniques used at the Marylebone site.

A3.1.9. Similarly, for 2005, NO_X is estimated to be 117 +/- 35 ppb and NO_2 33 +/- 7 ppb, at two standard deviations – equivalent to the 95 % confidence interval. It can therefore be concluded that with a probability of 95 % the true value lies within the ranges given above. This would indicate that, despite the calculation of uncertainty associated with the 2005 predictions the NO_2 concentration always exceeds 21 ppb and therefore Marylebone Road will exceed the NAQS objective. This may not always be the case however and with a prediction whose range straddles 21 ppb, a decision must be made concerning the approach to be taken. For example, a prediction of 20 +/- 2 ppb could be considered a pass or a fail.

A3.1.10. It is further concluded that the prediction of NO_2 concentrations in London depend most on the NO_X-NO_2 relationship used and the traffic data for HGVs. It is flows of, and emissions from, HGVs and buses that become more important in the future, as emissions from these vehicles will make up a greater proportion of the total.

A3.1.11. The results from the analysis of a further three roads is given in Table A3.2. These represent an average road at a central and outer location and an average motorway in outer London. The flow and percent HGV for the average road was derived from all 10,000 roads in the LTS 91 network.

Table A3.2 NO_2 Uncertainty Estimates for Typical Roads in London in 2005

Road Type/Location	Total vehicle flow	Percent HGV	Uncertainty (% of mean at 2σ)
Average road (central London)	17,000	9	16
Average road (outer London)	17,000	9	18
Motorway (outer London)	80,000	9	21

Our best estimate of the uncertainty in annual mean NO_2 predictions is therefore +/- 16-21 % at two standard deviations.

A3.1.12. It has not been possible to quantify the uncertainty of PM10 predictions in the same way as NO_2. This is because the uncertainty of the measurement techniques themselves and the sources and sinks of particles has not been well established. ***However, it is reasonable to expect that the uncertainty in PM10 predictions is larger than NO_2.***

References

1. Carslaw D, Beevers S (1999) ***Estimating the Uncertainty of Model Predictions using a Monte Carlo Simulation*****,** Department of the Environment, Transport and the Regions, April 99.

2. Beevers S, Carslaw D (1999) ***Evaluation of Local Transport Measures in Tackling National Air Quality Strategy (NAQS) Objectives***, Department of the Environment, Transport and the Regions, January 99.

3. Beevers S, Carslaw D (1999) ***Side by Side Analysis of Predictions of Roadside NO2 by AEAT and SEIPH***, Department of the Environment, Transport and the Regions, January 99.

4. ***Comparison of ATC Data from London Core Sites with LTS 91 Flows***, Working Note 3, Government Office for London, February 99.

5. Eerens *et al.* (1993) The CAR Model: ***The Dutch Method to Determine City Street Air Quality***, *Atmospheric Environment* Vol. 27B, No. 4, pp 389-399.

6. London Transport Studies, ***Technical Note 256***, Department of Transport, October 94.

7. London Transport Studies, ***Technical Note 25***, Government Office for London, June 98.

8. T. Murrells – Personal Communication.

9. Press W H et al. (1989) ***Numerical Recipes*** (FORTRAN version), Cambridge University Press.

Acknowledgements

SEIPH gratefully acknowledge the support of the DETR for funding this research.