

Appendix E

1 Model Uncertainty Assessment

1.1 Introduction

This appendix describes the application of Bayesian Monte Carlo (BMC) analysis to the ERG model developed to predict present and future concentrations of annual average NO₂ in London. Model uncertainties arise because of limited scientific knowledge, limited ability to assess the uncertainty of model inputs, for example, emissions from vehicles, poor understanding of the interaction between model and/or emissions inventory parameters, sampling and measurement error associated with NO_x and PM10 sites in London and whether the model itself completely describes all the necessary atmospheric processes. The application of the BMC technique here results in the reduction in uncertainties predicted through the additional information provided by the measurements themselves.

1.2 Uncertainty Assumption in Model Input Parameters

Selection of the uncertainty of input variables are obtained through access to published literature, the opinions of experts in the field, and through the assessment of relationships used within the model. A summary of the assumptions made for the model are given in the table below:

Table 1 Uncertainty Assumptions (1 σ) use for the Uncertainty Predictions

	(%)
Road Traffic Emissions	30
Other Emissions	50
London + Rural NO _x Contribution	10
Pollution Climate Mapping (NO _x)	11
NO _x -NO ₂ Relationship	10
Roadside Dispersion	20

1.3 Bayesian Monte Carlo Analysis

In Monte Carlo analysis, the model is run with the input variables varied simultaneously and independently of each other and a resulting probability distribution of the output information, obtained. Bayes' theorem is then applied to derive a final uncertainty estimate, by assigning a high probability to those predictions that agree with the measurements and a low or zero probability to those, which do not. The application of probabilities to the model prediction uses the likelihood function (Equation 1) and results in the best estimate of overall model uncertainty.

$$L(Y_k | O) = \frac{1}{\sqrt{2\pi}\sigma_e} \exp\left(-\frac{1}{2}\left[\frac{O - Y_k}{\sigma_e}\right]^2\right) \quad (1)$$

A mathematical summary of BMC is given below. From Bayes’ theorem the final probability of model output is defined by equation 2 as

$$p(Y_k | O) = \frac{L(Y_k | O)p(Y_k)}{\sum_{j=1}^N L(Y_j | O)p(Y_j)} \quad (2)$$

1.4 Results at Background

A BMC uncertainty analysis was carried out for annual average NO₂ concentration throughout London.

The prior and posterior distributions for an average of the measurement sites in London are included in Table 2. The application of BMC analysis reduces the final uncertainty giving a standard deviations in this case are 2.0 ppb (8.5 %).

The BMC analysis was then applied for 5 sites individually and the results summarised in Table 3. Again BMC analysis results in a significant reduction in σ providing a reduction in uncertainty. The average σ for the 5 sites was 1.8 ppb.

Table 2 Final uncertainty and measured annual mean NO₂ concentrations (ppb) at all sites in London for 1998

Average Model Prediction (ppb)	σ (ppb)	Uncertainty %	Measured Result (ppb)
23.6	2.0	8.5	23.2

Table 3 Final uncertainty and measured annual mean NO₂ Concentrations for separate Sites in London for 1998

Site Location	Final Model Prediction (ppb)	σ (ppb)	Uncertainty %	Measured Results (ppb)
Bridge Place	30.6	2.2	7.2	30.2
Bexley 2	19.1	1.5	7.8	18
Tower Hamlets 1	24.1	1.8	7.5	24.6
West London	26.8	2.0	7.5	26.8
Sutton 2	18.6	1.4	7.5	19.8

1.5 Results at Roadside

Predictions of the concentration of NO₂ at roadsides throughout London have shown a high sensitivity to the pass/fail standard 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.

Monte Carlo modelling techniques have been used to calculate the uncertainties associated with roadside NO₂ 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.

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.

The original study has focused on Marylebone Road for a base year of 1997 for meteorology and atmospheric chemistry and uses the London Transportation Studies (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.

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 NO₂, the NO_x-NO₂ relationship used is the most important factor. Table 4 below shows how each input data or modelling method affects the final concentration, for the Marylebone road example.

Table 4 The Relative Importance of Model Parameters in Predicting NO₂ 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

For 1997, NO_x was predicted to be 258 +/- 83 ppb and NO₂ 47 +/- 10 ppb, at two standard deviations – equivalent to the 95 % confidence interval. These statistics assume that the resultant distribution is normal.

The overall uncertainty of NO₂, which corresponds to 22 %, is less than that for NO_x (32 %). This feature is a result of the non-linear NO₂ 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.

Measurements for the Marylebone Road site for NO_x and NO₂ are within the uncertainty limits calculated here. NO_x was between 213 and 229 ppb and NO₂ between 44 and 48 ppb for 1997. The range reflects the two different monitoring techniques used at the Marylebone site.

Similarly, for 2005, NO_x is estimated to be 117 +/- 35 ppb and NO₂ 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 NO₂ concentration always exceeds 21 ppb and therefore Marylebone Road will exceed the AQS 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.

It is further concluded that the prediction of NO₂ concentrations in London depend most on the NO_x-NO₂ 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.

The results from the analysis of a further three roads is given in Table 5. 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 5 NO₂ 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 NO₂ predictions is therefore +/- 16-21 % at two standard deviations.

It has not been possible to quantify the uncertainty of PM10 predictions in the same way as NO₂. 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 NO₂.*