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THE PERFORMANCE OF DISPERSION MODELLING FOR THE PREDICTION OF NITROGEN DIOXIDE IN THE UK REVIEW AND ASSESSMENT PROCESS*Michael A Bull*

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Abstract: This paper investigates the performance of dispersion modelling for nitrogen oxides in the UK review and assessment process. Most detailed assessment reports prepared for this purpose include a model verification exercise that compares the predicted and the modelled pollutant concentrations. These verification results have been used to compile nearly 500 data points that allow an analysis of the performance of dispersion modelling. The results demonstrate that the underlying performance of the modelling used in review and assessment shows a general under prediction of nitrogen dioxide concentrations but also that there is a considerable degree of uncertainty in the final modelling result. The results have been further analysed to demonstrate a risk based interpretation of the modelling results that can be used to assess the probability of an exceedance of the annual mean nitrogen dioxide objective and limit value. This approach takes into account the inevitable uncertainty in dispersion modelling and allows policy makers to choose what level of risk would be appropriate for individual situations.

Keywords: *Dispersion modelling, Local Air Quality Management, Verification.*

INTRODUCTION

Dispersion modelling is known to contain inherent uncertainties and hence where it is used to assess compliance with air quality standards and/or objectives these should be acknowledged. The potential uncertainties both in the input data used and the model itself were considered in a detailed study (NRPB, 1986). This report demonstrated that that predicted could be in error by $\pm 100\%$ as a result of model input error (for instance the wind speed) and summarising other reported validation results noted that predicted annual average concentrations could be $\pm 100\%$ of the observed values and that the predicted short term concentrations could be up to 10 times higher or lower than those observed. Where modelling is used to assess compliance with regulatory standards appropriate techniques must be applied to take into account this inherent uncertainty.

There are several previous studies that have examined the performance of dispersion models although several of these have examined the performance of models for point sources such as ADMS and AERMOD (USEPA, 2003, CERC 2007) and there are fewer studies examining model performance where the predominant emission sources are motor vehicles although this is reported by model developers (CERC, 2003). However, in the UK, a formal process of air quality review assessment has operated for several years that now allows a detailed assessment of model performance to be carried out where the major emission sources are road sources.

In the UK, Part IV of the Environment Act 1995 introduced the process of Review and Assessment of air quality into the UK. This is part of the overall approach to improve air quality and to meet statutory air quality standards. Local authorities are required to undertake a review of air quality and identify if there is a risk that air quality objectives may be exceeded. The process has been carried out in stages, starting with screening assessments and then moving onto more detailed assessments where a risk of an air quality problem was identified. If the detailed assessment identifies that there is a risk that the air quality objectives may be exceeded then an Air Quality Management Area (AQMA) must be declared. Local authorities are provided with Technical Guidance regarding the approach that can be used to assess air quality, most assessments have been carried out in accordance with guidance published in 2003 (DEFRA, 2003) although this guidance has been recently updated (DEFRA 2009). The guidance is not prescriptive in terms of the methods used and local authorities can choose to use modelling or monitoring methods to assess air quality. If a modelling approach is selected the guidance does not require particular models to be applied although it does provide an overall framework under which the assessment should be carried out. The Review and Assessment procedures are intended to determine whether there is a risk that air quality objectives might be exceeded. As such, the assessments should take into account all the available evidence on pollutant concentrations in the study area to determine the risk of an exceedance.

Many of these assessments carried out by local authorities have moved onto detailed studies using dispersion modelling used to calculate pollutant concentrations. Where dispersion modelling has been used, the government guidance (DEFRA 2003, 2009) suggests that a model verification exercise is carried out where the model results are compared with measured values. This exercise is intended to assess how the modelling compares with measured values and the guidance suggests an approach for adjusting the model results so that the final modelled value compares better with the measured concentrations. This adjustment process simply factors the results of the dispersion modelling to match the observed values. This is a simplistic process and it makes an overall assumption that the differences between the modelled and observed concentrations have a linear relationship and the relationship is constant across the modelling domain. Given the many factors that can contribute to a model error this assumption is very unlikely to be valid, for instance, the difference between the wind speed used for modelling and the actual wind speed around the model domain will not be a constant. However, an alternative approach would be to examine the output of several modelling studies where comparisons had been made between the modelled and measured values and assess the overall performance of the modelling process. By examining predicted and actual observed concentrations from several air quality studies it is possible to obtain the probability of exceeding an air quality standard based on the predicted concentration.

As a result of the UK Review and Assessment process, there are well over one hundred detailed review and assessment studies have been carried out that include a comparison of modelled with observed concentrations. These studies therefore

provide a valuable resource to assess the performance of the modelling process that can add to our understanding of the performance of dispersion models. This study has therefore collated the information reported by local authorities on model validation. It has examined these results to assess the reliability of the modelling in the prediction of an exceedance of the UK annual mean nitrogen dioxide objective and proposes a risk based approach to air quality modelling where the aim is to assess compliance with an air quality standard.

APPROACH

This study was concentrated on those local authorities that have identified a risk of an exceedance of the air quality objective for nitrogen dioxide and have declared an Air Quality Management Area. These authorities were identified from the UK Government's air quality website www.airquality.co.uk and the air quality assessments were obtained from the relevant local authority websites. This study concentrated on the 3rd Stage Review and Assessment and the Detailed Assessment reports as these generally report model validation results. The reports were reviewed to obtain reported model validation for both nitrogen oxides and nitrogen dioxide although the majority of reported results were for the latter pollutant. In total, results were obtained from 59 local authorities with 623 and 349 results for nitrogen dioxide and nitrogen oxides respectively. The results were analysed as follows. Firstly, a simple comparison of predicted concentrations with measured values for both NO_x and NO₂ with a statistical analysis using the BOOT Software Package (Chang, J. C. and S. R. Hanna, 2005), this provides basic details of the overall performance of the air quality modelling with the standard statistical parameters frequently used for model evaluation. The results were further analysed by sorting the modelling results into concentration ranges or "bins". Thus the results were sorted into 5µg/m³ bins of predicted concentrations (i.e. 15-20µg/m³, 20-25µg/m³ etc). Within each of the bins of predicted values, the associated observed concentrations were used to derive probability density functions and basic statistical information. Based on the results of the above the probability of an exceedance of the annual mean nitrogen dioxide objective has been calculated as a function of the predicted nitrogen dioxide concentration.

RESULTS

Because the technical guidance is not prescriptive local authorities can carry out their air quality studies using any suitable approach. However, the final reports are reviewed by DEFRA to ensure that the report has followed general guidelines and that the conclusions are robust. As a result, a range of modelling approaches have been applied in the UK for Review and Assessment, however, the main models used are ADMS (Roads and Urban versions), AIRVIRO, Caline and some bespoke approaches developed by individual consultancies. However, the intention of this study is not to determine the performance of any individual model, rather, it is intended to assess the performance of the modelling used in the UK Review and Assessment process. Any differences between modelled and measured values will result from model error but also from errors in the model input data and the latter will be common to whatever modelling approach is used. Table 1 provides further information on the models used in the studies.

Table 1. Models used in the air quality assessment

Model Name	Number of Studies
AAQUIRE	7
ADMS (version not specified)	2
ADMS -Roads	22
ADMS-Urban	12
Airviro	3
Caline	6
Kings College ERG Model	3
AEA Model LADS	10

The measured nitrogen dioxide concentrations were almost always obtained using diffusion tubes although some results were obtained from continuous monitoring. The use of diffusion tubes clearly is associated with some measurement error, but given the large database of results the general trends in model error should be robust. Figure 1 plots the predicted and measured NO₂ concentrations.

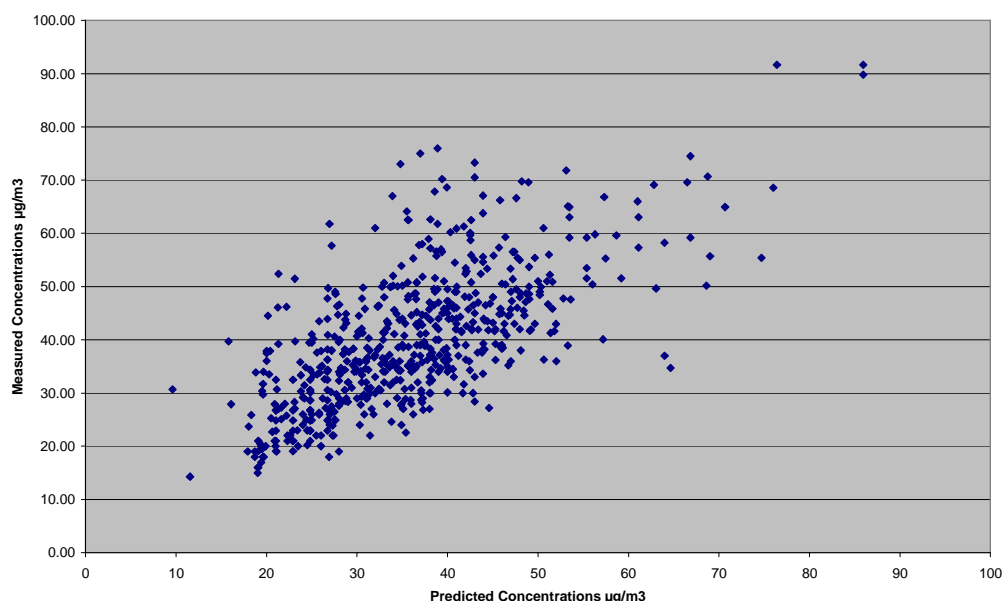


Figure 1: Comparison of Predicted and Measured Nitrogen Dioxide Concentrations

Examination of Figure 1 shows that there is a general tendency for the model to under predict nitrogen dioxide concentrations. 67% of the modelled results were lower than the measured values. There is a reasonable visual similarity between predicted and measured values but it is evident that there is a substantial spread in results. Even assuming that the model used was perfect, errors would be expected as a result of input data errors and the errors in the monitored results used for comparison. Input data used for modelling is obtained from various sources but the principal sources are traffic modelling and surveys, emission databases and meteorological monitoring together with errors in the monitoring used. Most models also are based on the prediction of nitrogen dioxide concentrations which are subsequently converted to nitrogen dioxide concentrations using various correlations. This conversion and the input data all have inherent uncertainty and this is reflected in the results obtained. It is acknowledged that even models that are considered to be performing well will have an associated uncertainty of at least 50%. Processing the results using the BOOT software provided the following basic statistics detailed in Table 2.

Table 2. Results of BOOT software analysis

Data	Mean	Standard Deviation	Bias	Corr	Fractional Bias
Measured	39.95	12.59	NA	NA	NA
Predicted	35.84	11.00	4.11	0.688	0.108

The BOOT results reflect the observation that the modelled concentrations are more frequently under predicted whilst the spread of observed data can be seen by the standard deviation which is approximately 30% of the mean value. To examine this uncertainty within the modelled values the predicted concentrations have been “binned” into 5µg/m³ ranges. The median and standard deviation of the measured concentrations within each of the bins has been calculated, the results are shown in Figure 2.

As can be seen from Figure 3, the median of the measured values in each concentration bin compare relatively well although the tendency for an under prediction is evident in the results, on average, the median measured value is 4.5 µg/m³ higher than the mean value in each predicted concentration bin. The standard deviation of the measured values within each concentration bin is also shown in Figure 2, these are typically 25% of the median value. To examine the spread in measured values within the concentration bins further, a frequency analysis of the measured values has been carried out. An example is shown in Figure 3 (compared with a normal distribution (red bars))

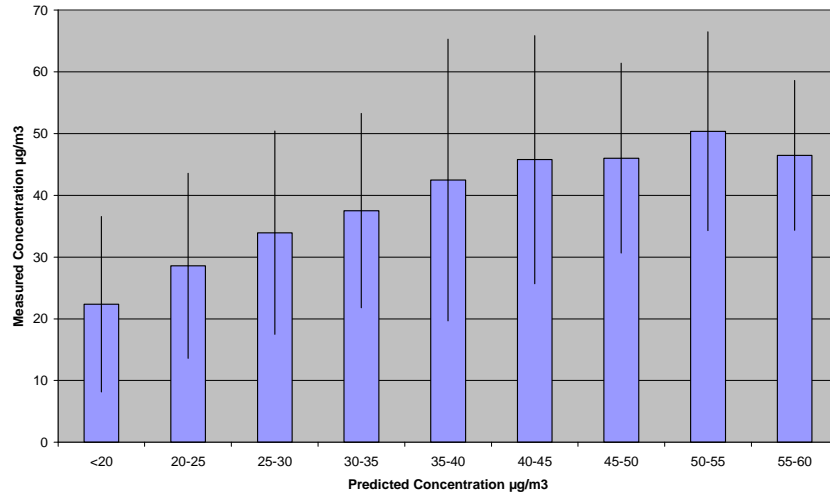


Figure 2. Measured median and standard deviation NO2 concentrations within 5µg/m³ predicted concentration ranges.

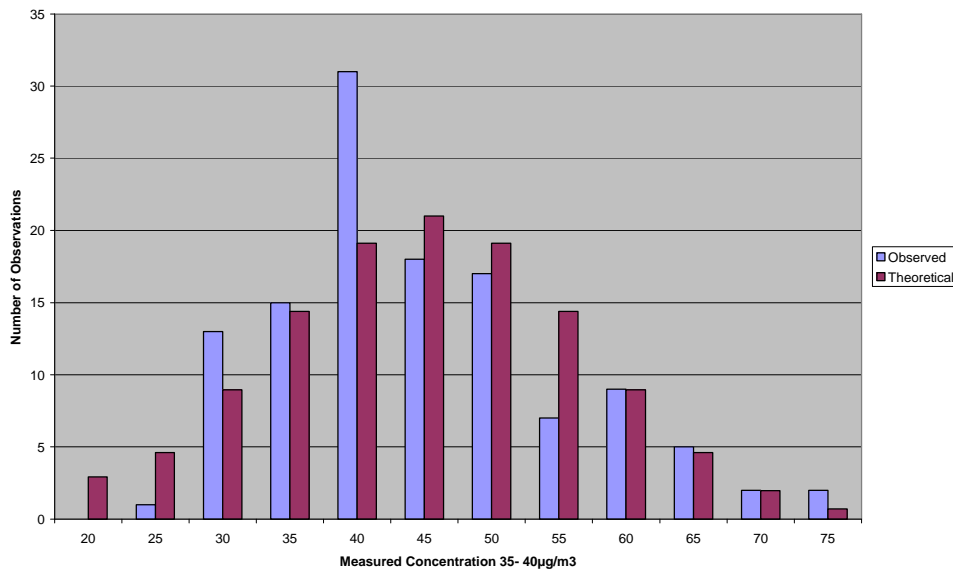


Figure 3. Frequency of occurrence of observed NO2 concentrations where predicted concentrations are in the range 35-40µg/m³

The results illustrate the substantial variation in measured values within a 5µg/m³ range of predicted values. When compared with a normal distribution (within the same median and standard deviation) there is a reasonable visual fit. If the assumption is made that the data are normally distributed, the probability of an exceedance of the 40µg/m³ objective can then be derived for each of the concentration ranges. Therefore, the cumulative frequency distributions for each of the concentration ranges has been calculated, assuming a normal distribution and the observed median and standard deviation. The probability of an exceedance of the 40µg/m³ annual mean nitrogen dioxide concentration has been obtained from the frequency distributions, the results are shown in Figure 4. As expected, the probability of an exceedance increases as the predicted concentration increases, however, it is interesting to note a number of points. Firstly, even when predicted nitrogen dioxide concentrations are below 30µg/m³ there is a 20% probability that the measured value exceeds the 40µg/m³ objective. Secondly, where the predicted concentrations are above 40µg/m³ there is a 30% probability that the actual measured values are below the objective level. This suggests that modelling results would be far better interpreted in terms of the probability of an exceedance rather than as definitive predictions of concentrations. Some review and assessment reports do acknowledge this uncertainty but generally much greater emphasis is placed on a comparison of the predicted value with the appropriate standard.

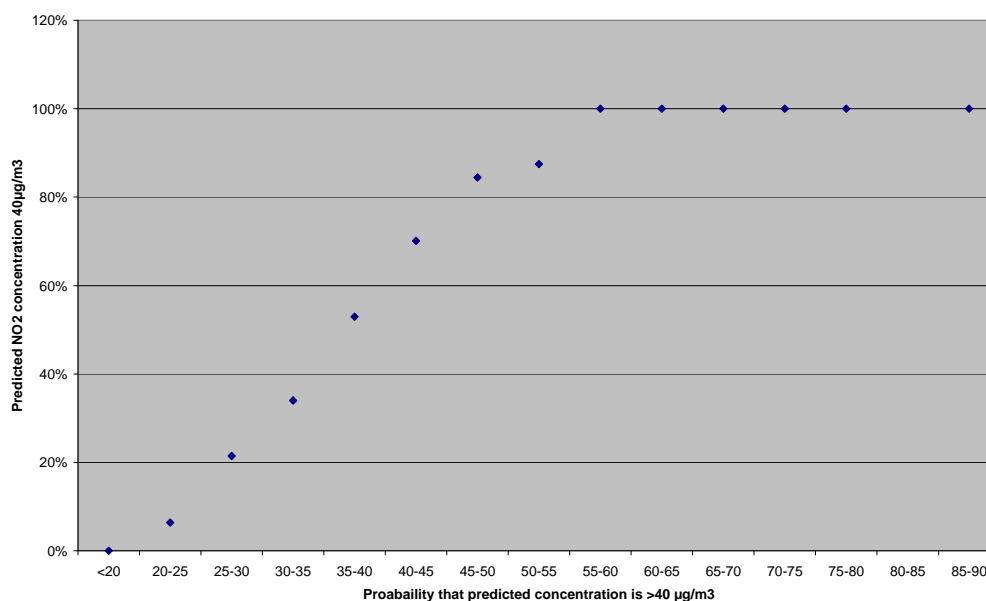


Figure 4. Probability of an exceedance of the $40\mu\text{g}/\text{m}^3$ nitrogen dioxide objective based on predicted concentration ranges

These results would also allow the use of a probabilistic approach to assess significance in air quality assessment. Typically significance assessment has been carried out by comparing the predicted concentration with the relevant air quality standard and also by examining the change in concentrations predicted. However, this approach clearly has some shortcomings given the inaccuracy found in the modelling process. An alternative approach would be to assess the change in probability of an exceedance of a standard. These results are based on a wide range of modelling approaches and there is therefore the potential that different risks profiles will exist for each method. However, in the absence of further information, the information presented in this paper can be used to determine the probability of an exceedance of the UK annual mean nitrogen dioxide objective.

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