Appendix 10-E Model Calibration

10-E.1 Introduction

10-E.1.1 The dispersion model (ADMSRoads) was set up to incorporate all road links comprising the baseline scenario for 2004 (see Appendix 10-C for link data), together with receptors located at the monitoring sites described in Appendix 10-B. Pollutant emissions per link, derived from traffic flow and speed data and emissions factors, were entered into the model and the model was run to derive resultant NO_x concentrations at each receptor location.

10-E.1 Conversion of NO_x to NO_2

10-E.1.2 NO_x concentrations were converted to NO_2 using the method described by Laxen (2002):

i) NO_2 (road) = ((-0.068 x Ln(NO_x (total))) + 0.53) x NO_x (road)

ii) where NO_x (total) = NO_x (background) + NO_x (road) , and Ln is log to the base e

iii) Add the NO_2 (road) to the NO_2 (background) to derive the NO_2 total at the location of interest.

10-E.1 Model Calibration

10-E.1.3 The predicted NO_2 concentrations were compared to the monitored values by constructing a scatter plot and calculating the correlation coefficient (R^2). The model was then calibrated and further statistical analysis undertaken with reference to a series of statistical tests and comparing the results with 'perfect' and 'imperfect' datasets. This approach reduces the potential for error in interpretation which may arise from over reliance on a single statistical test. The 'perfect' dataset was generated from a series of randomised x values between 0 and 50 with the y values equal to the paired x values. The 'imperfect' dataset was generated by repeatedly randomising the y values until the lowest correlation coefficient was reached. This method provides suitable boundaries for evaluating individual statistical test data.

10-E.1.4 Figure 10-E.1 compares modelled and monitored annual mean NO_2 concentrations. The trendline and R^2 value (0.7951) indicate a good correlation between the two sets of results but a necessity for calibration of model results; the model underestimates NO_2 concentrations.

10-E.1.5 Both raw and calibrated results are presented in Figure 10-E.2 with the linear regression forced to the origin. The model was calibrated by applying a factor of 2.5 to the modelled NO_x concentration. Note that this factor is applied to the raw modelled NO_x results rather than the subsequent NO_2 concentrations after adding the background components and allowing for atmospheric oxidation as per the Laxen (2002) method.

10-E.1.6 The AQEG Report (2003) suggests that emissions factors, as employed in calculation of emissions in this assessment, are derived assuming a cyclical journey of virtually continuous motion once the vehicle is in motion. In cases where vehicle travel is slow or vehicles are idling, emissions will be greater. This explains the model's under-

prediction. The Report states the emissions may be up to ten times greater than those modelled, greater than the factor of 2.5 necessarily applied to NO_2 results here.

10-E.1.7 The linear relationship is very close to unity with little change in the R^2 value (reduced to 0.7836) All the data are within a factor of two of x = y, represented by the dashed red lines. The linear trend, represented by the black line, indicates the model under predicts consistently by approximately 4 %.

10-E.1 Model Verification

10-E.1.8 The results of statistically comparing the calibrated model results with monitored data are presented in Table 10-E.2. The Normalised Mean Deviation, providing a simple measure of uncertainty. This is supported by the subsequent statistical measures of correlation and spatial accuracy, all of which are close to the 'perfect' test boundary. All of the modelled data are within a factor of two of the monitored data, providing further evidence the model is robust. The Root Mean Square Difference in Concentrations provides a measure of the systematic error, or bias, of the model and can be used for calibration purposes. However, as the model does not generate the 'final' value (i.e. does not include for background contributions and conversion from NO_x to NO_2) this test is included for completeness only.

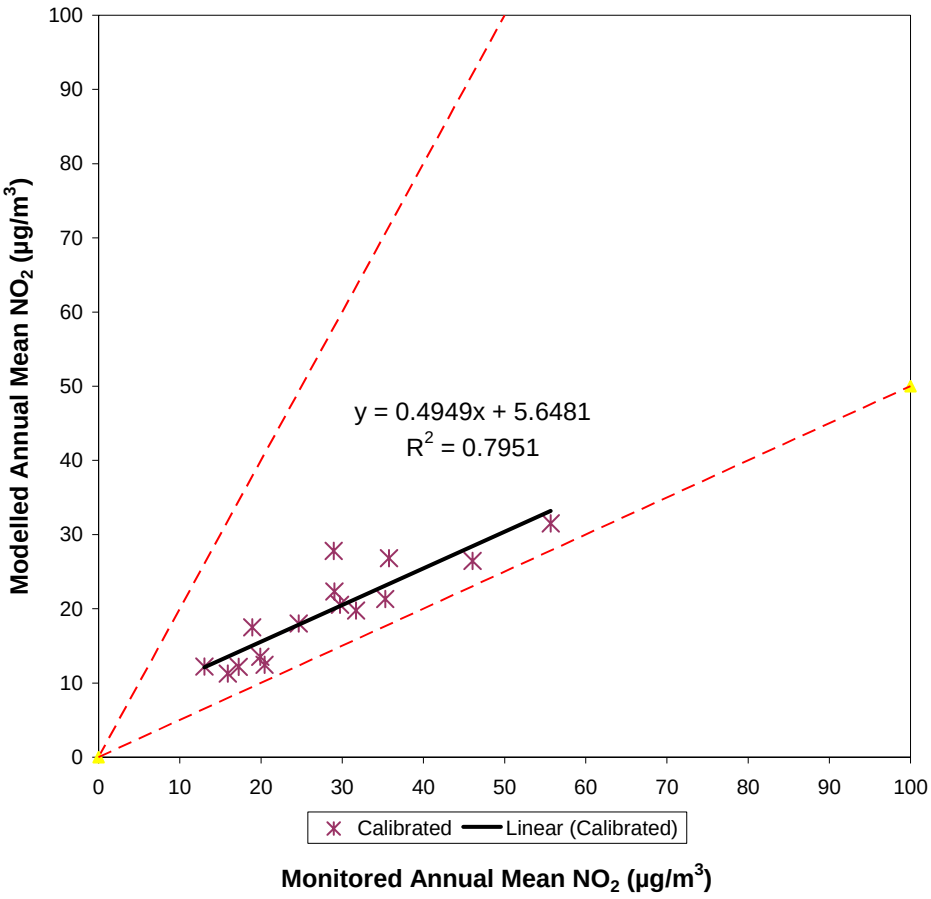

Figure 10-E.1 Scatterplot of Raw Modelled versus Monitored Annual Mean NO_2

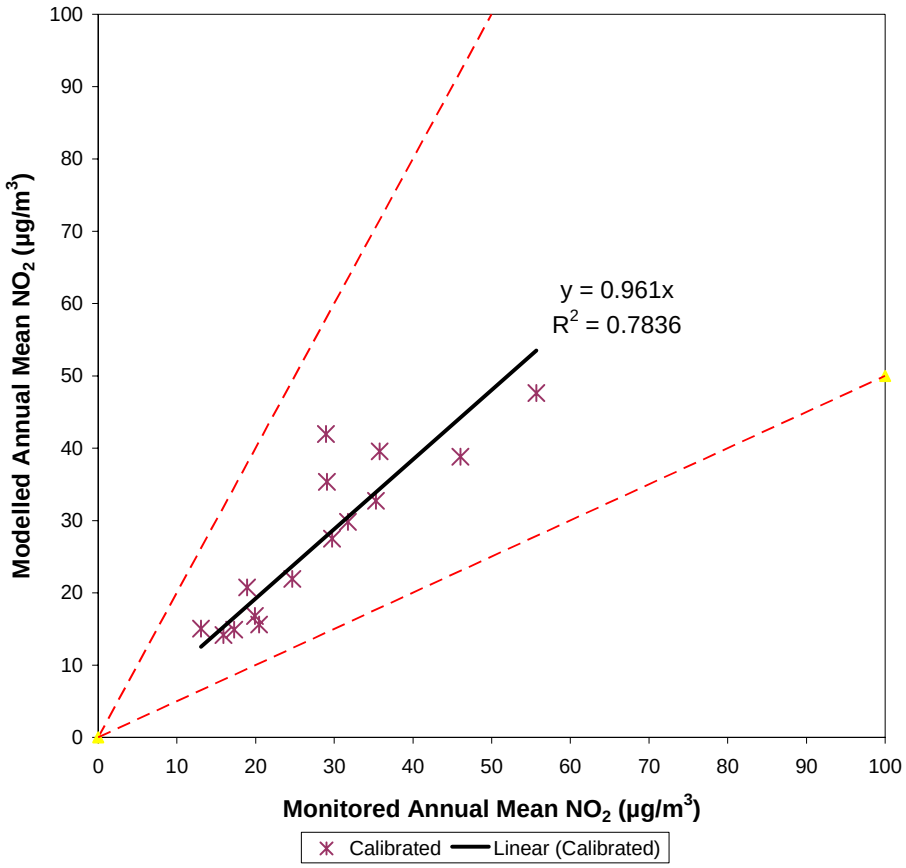

Figure 10-E.2 Scatterplot of Calibrated Modelled versus Monitored Annual Mean NO_2

Table 10-E.1: Model Verification

Statistical Test	Description	Test Boundaries		Results for this Study
		Perfect	Imperfect	
Normalised Mean Distribution	Measure of uncertainty	0	±5.4	0.39
Index of Agreement	Measure of correlation, indication of spatial accuracy	1	-7.4	-0.84
Normalised Mean Square Error	Measure of correlation, indication of spatial accuracy	0	2.2	0.23
R^2	Measure of correlation, indication of spatial accuracy	1	0.2	0.74
Fa2	Fraction of data within a factor of two, a measure of data scatter	0	0.9	0
Root Mean Square Difference in Concentrations	Systematic error (bias) which can be quantified and used to calibrate models	0	15.8	10.13
Normalised RMSE	An indication of spatial accuracy	0	1.9	0.25

Notes:

The test boundaries for these tests were derived by generating two dummy data sets based on the x values randomised between 0 and 50. For the 'perfect' dummy dataset, the subsequent y values were made equal to the x values. The 'imperfect' dummy data set was compiled using randomised data for the y values as well, repeating the randomisation until the lowest R^2 value was achieved