Annex 4 Technical Annex to Chapter 5

439. This is a technical annex to the report of the Air Quality Expert Group (AQEG) on Ozone in the United Kingdom. It provides more detailed information on the modelling of urban ozone decrements in the UK to support the response to Chapter 5 on *What are the likely future trends in urban ozone concentrations, over the next two decades and what is driving them?*

440. Various analyses presented in the AQEG report confirm the view that ozone can be represented by a regional component and an urban ozone decrement (see also Clapp and Jenkin, 2001; Jenkin, 2004). In this paper, the urban ozone decrement is taken to be the difference between the values of the ozone concentration or metric at the urban location and the corresponding quantity at a surrounding rural site (taken to be representative of the regional component).

441. Urban decrements in ozone concentrations are explored for a range of metrics using two UK process-based models (the Ozone Source-Receptor Model (OSRM) (Hayman *et al.*, 2008a,b) and ADMS-Urban models (Williams *et al.*, 2006)) and an empirical approach based on monitoring data (Pollution Climate Model, PCM (Kent *et al.,* 2006)). The relationships between the urban decrements and local NO_x concentrations have been examined and the results of the analysis indicate that the empirical approach to estimating urban ozone decrements currently used in mapping studies (as presented in the supporting evidence to Chapter 2) is in reasonably good agreement with process based models.

A4.1 Modelling of Urban Ozone Decrements

A4.1.1 A comparison of estimated urban decrements for a range of metrics at sites in the national monitoring network

442. OSRM runs were undertaken to 41 receptor sites - representing the locations of 20 rural, 10 London and 11 other urban background O_3 monitoring sites - for each hour of 2003 using year-specific emission inventories and meteorology. The model runs were initialised using daily concentrations fields derived from the STOCHEM model and modified for ozone to take account of the trend in baseline concentrations (see Section 4.4 of Hayman *et al*., 2006). All other model parameters were set to those used in the ozone modelling runs undertaken for the Review of the Air Quality Strategy (Hayman *et al*., 2006).

443. The hourly ozone concentrations were processed to derive the ozone metrics of interest. The output OSRM hourly concentrations are taken to represent mid boundary-layer concentrations and an algorithm can be used during the post-processing phase to take account of the vertical gradient in ozone concentrations arising from losses (i) to the surface by deposition and (ii) by titration in areas of high NO_x emissions. In this analysis, the urban ozone decrement is taken to be difference between the 'unconverted' and 'converted' outputs. As there are still local NO_x emissions, albeit small, at the rural sites, this, together with any deposition, explains why there is a decrement at the rural sites.

444. Panel (a) of Figure A4.1 shows the dependence of the modelled percentage decrement in annual mean ozone in 2003 on the modelled local NO_x annual mean concentration within the surface conversion algorithm of the OSRM model. The decrement in annual mean ozone due to the local titration effects is almost linearly related to the modelled annual mean NO_x concentration, as would be expected. The annual mean NO_x concentration has been calculated by applying a dispersion kernel to the 1km NO_x inventory. Of more interest is that the model also predicts that the relationship between the annual ozone

decrement and annual mean NO_x is approximately linear for all of the health based metrics and the number of days with 8-hour mean ozone concentrations greater than 100 µg m^{-3} and 120 µg m^{-3} (as shown in panels (b)-(f) of Figure A4.1)

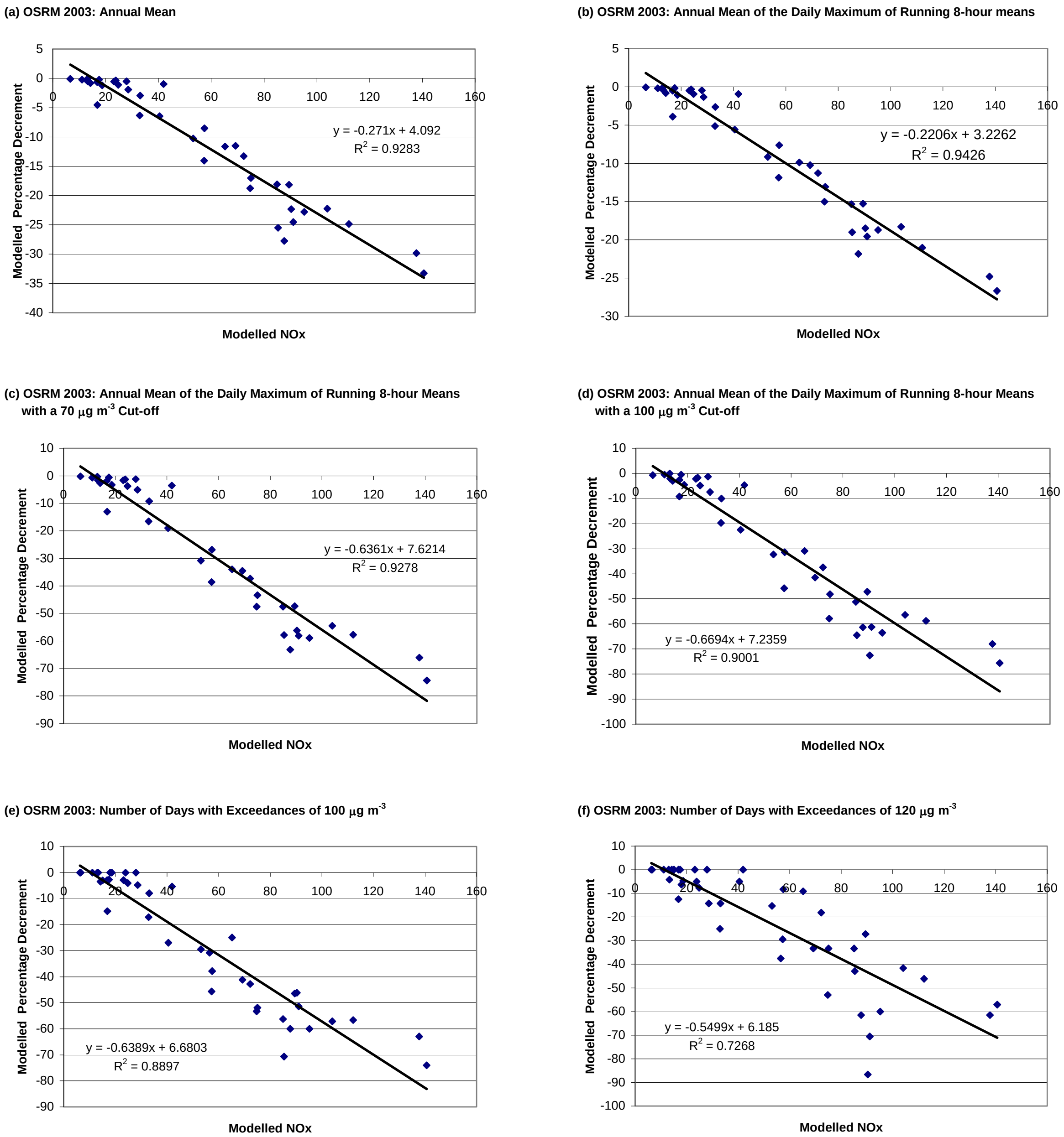

Figure A4.1 Ozone decrements calculated for 41 UK ozone monitoring sites in 2003 using the Ozone Source Receptor Model as a function of the modelled NO_x concentration (µg m^{-3}, as NO_2).

445. Figure A4.1 shows the corresponding dependences of the urban ozone decrements derived using the empirical Pollution Climate Modelling approach on the modelled annual mean NO_x concentrations. In this instance, the PCM decrement has been calculated by subtracting a regional value for the ozone metric estimated by interpolating rural monitoring sites from the measured value of the ozone metric at the monitoring site location. An altitude correction has been applied for the regional annual means, as described by Coyle *et al.* (2002) and Kent *et al.* (2006). The modelled annual mean NO_x concentrations have been derived using the PCM model (Stedman *et al.*, 2005). The contribution of point sources is modelled explicitly while area sources are modelled using a dispersion kernal approach (similar to that used in the OSRM). These are then combined with a regional rural NO_x background concentration.

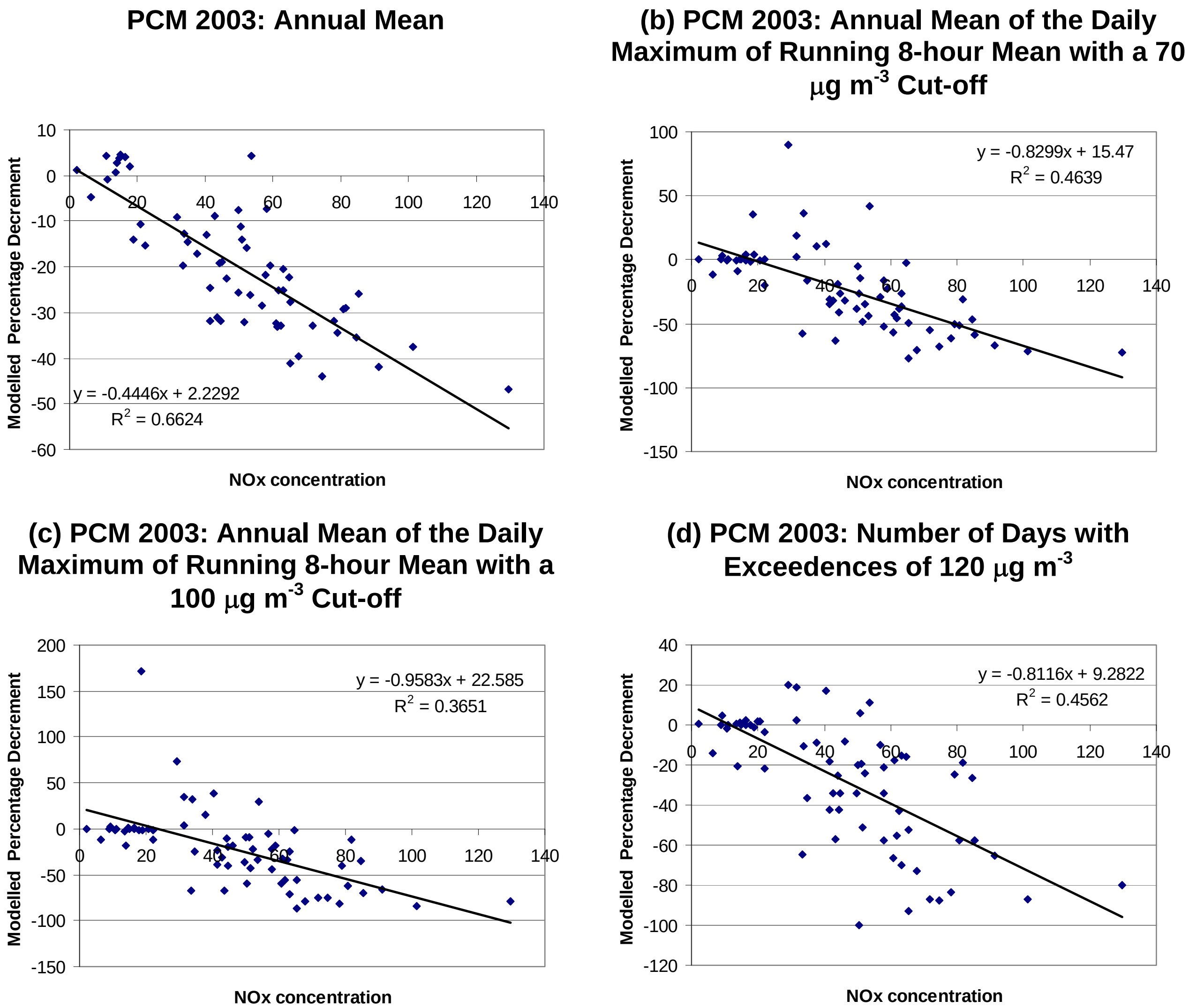

Figure A4.2 Ozone decrements calculated for UK ozone monitoring sites in 2003 using the Pollution Climate Model, as a function of the modelled NO_x concentration (µg m^{-3}, as NO_2).

446. The results presented in Figure A4.1 and Figure A4.2 support the assumption in the empirical modelling approach that the urban decrement in ozone concentration varies approximately linearly with annual mean NO_x concentration (the regression lines are shown here for illustrative purposes only). There is however considerable scatter in these plots. This is to be expected since the regional ozone field will incorporate uncertainties associated with the interpolation procedure and very local effects may affect the measured ozone concentrations. The positive outliers are due to measured urban ozone metrics exceeding the values measured at rural sites in the same region. Extreme positive outliers are generally caused by the percentage difference between two small numbers.

447. Figure A4.3 shows a comparison of the modelled NO_x concentrations from the OSRM and PCM models and Figure A4.4 shows a comparison of the decrements for the ozone metrics derived by both the PCM and OSRM, with the 1:1 lines shown in red. To recap, the OSRM decrement has been calculated by estimating the impact of local NO_x emissions on an hourly basis on the modelled regional ozone concentration and the PCM decrement has been calculated by subtracting an interpolated rural field from the measured value for the metric.

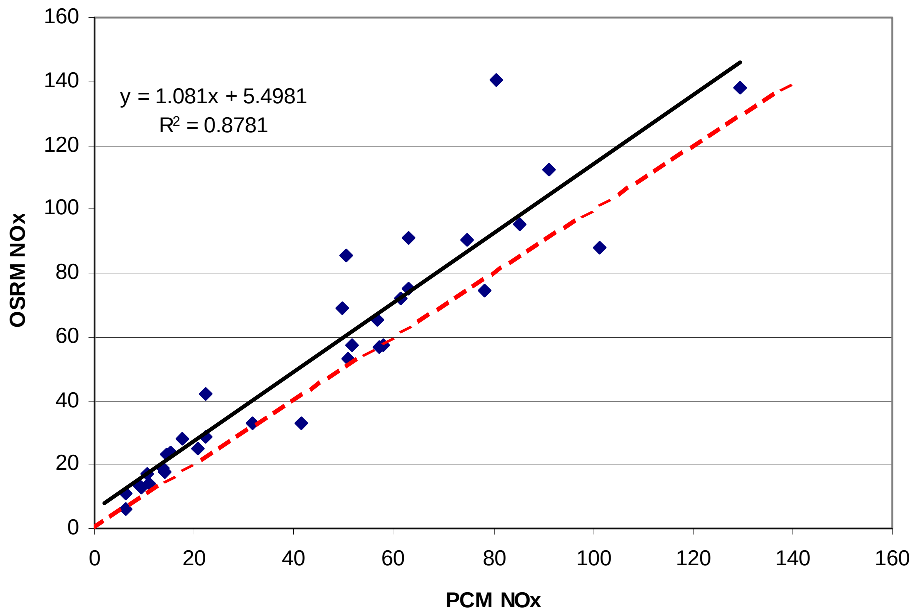

Figure A4.3 Comparison of the 2003 annual mean NO_x concentrations (µg m^{-3}, as NO_2), calculated using the PCM and OSRM.

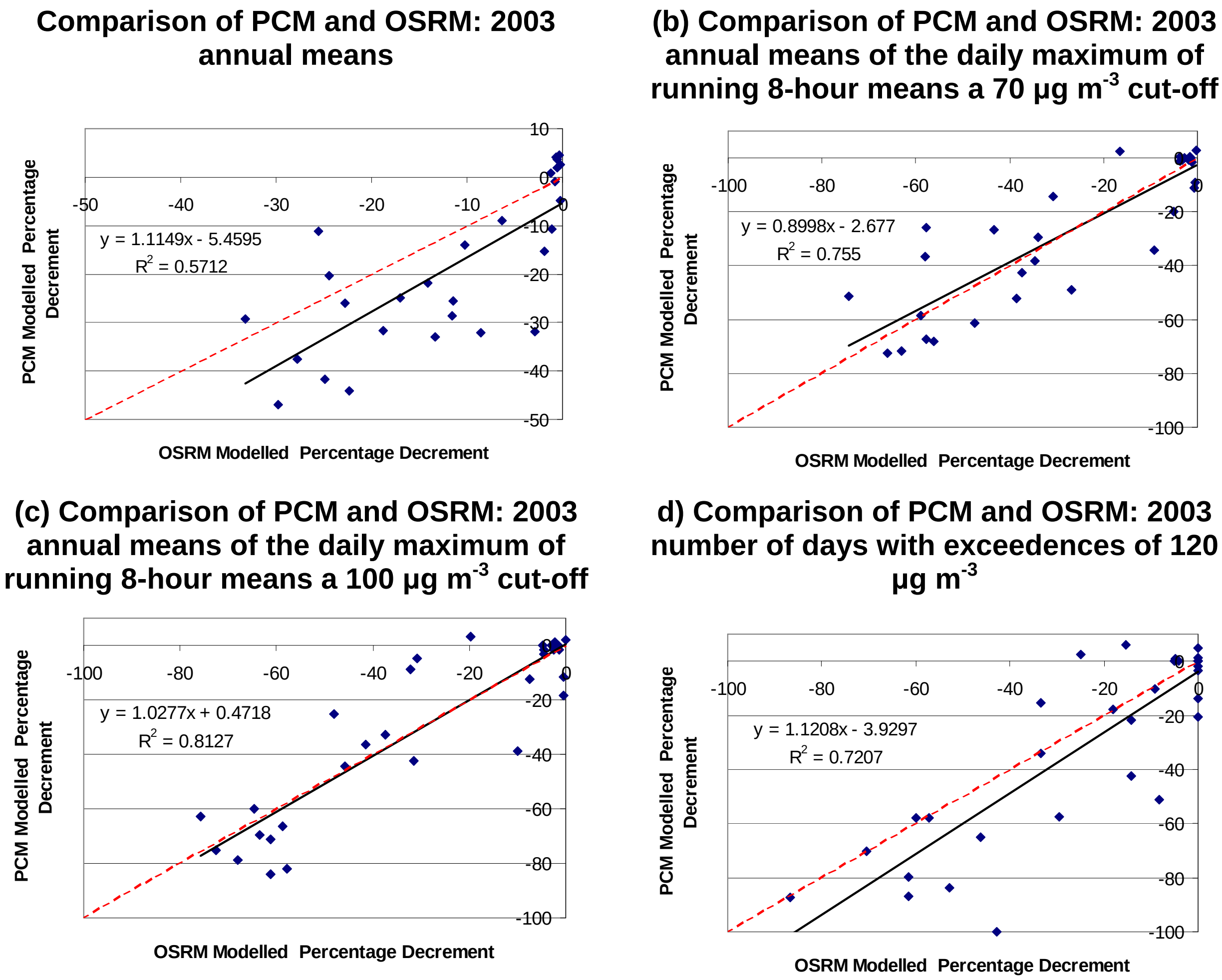

Figure A4.4 Comparison of the ozone decrements in 2003 calculated using the PCM and OSRM for four ozone metrics used to assess impacts on human health.

448. As expected, the graphs show considerable scatter but the gradients of all of the graphs are close to unity. This comparison of the two approaches suggests that the urban

decrement in these ozone metrics can be assumed to be approximately linearly related to local annual mean NO_x, concentrations, and hence NO_x emissions. Thus the OSRM modelling supports the use of linear relationships with NO_x for various ozone metrics applied within the PCM models (Coyle *et al.*, 2002, Bush *et al.*, 2005, Kent *et al.*, 2006).

A4.1.2 A comparison of estimated urban decrements for a range of metrics at sites in London

449. Urban ozone decrements have also been calculated for monitoring site locations in London for various metrics using ADMS-Urban. Figure A4.5 shows a comparison of the percentage decrements plotted against the modelled NO_x concentration, calculated using the OSRM, ADMS-Urban and from ambient monitoring data using the empirical PCM approach. This analysis suggests that all three approaches estimate a similar magnitude of annual mean ozone decrement at similar NOx concentrations at urban background locations. The decrements calculated for other metrics are also quite similar in magnitude for the different approaches. This provides additional evidence that process-based models are now available which can provide a good description of how the decrement in ozone varies spatially across urban areas. The OSRM model seems to generally predict a lesser decrement for the ozone metrics than ADMS-Urban. The PCM derived values are based on ambient monitoring data and also incorporate additional uncertainties associated with spatial interpolation of data from rural monitoring sites and therefore show greater scatter than the process model based estimates.

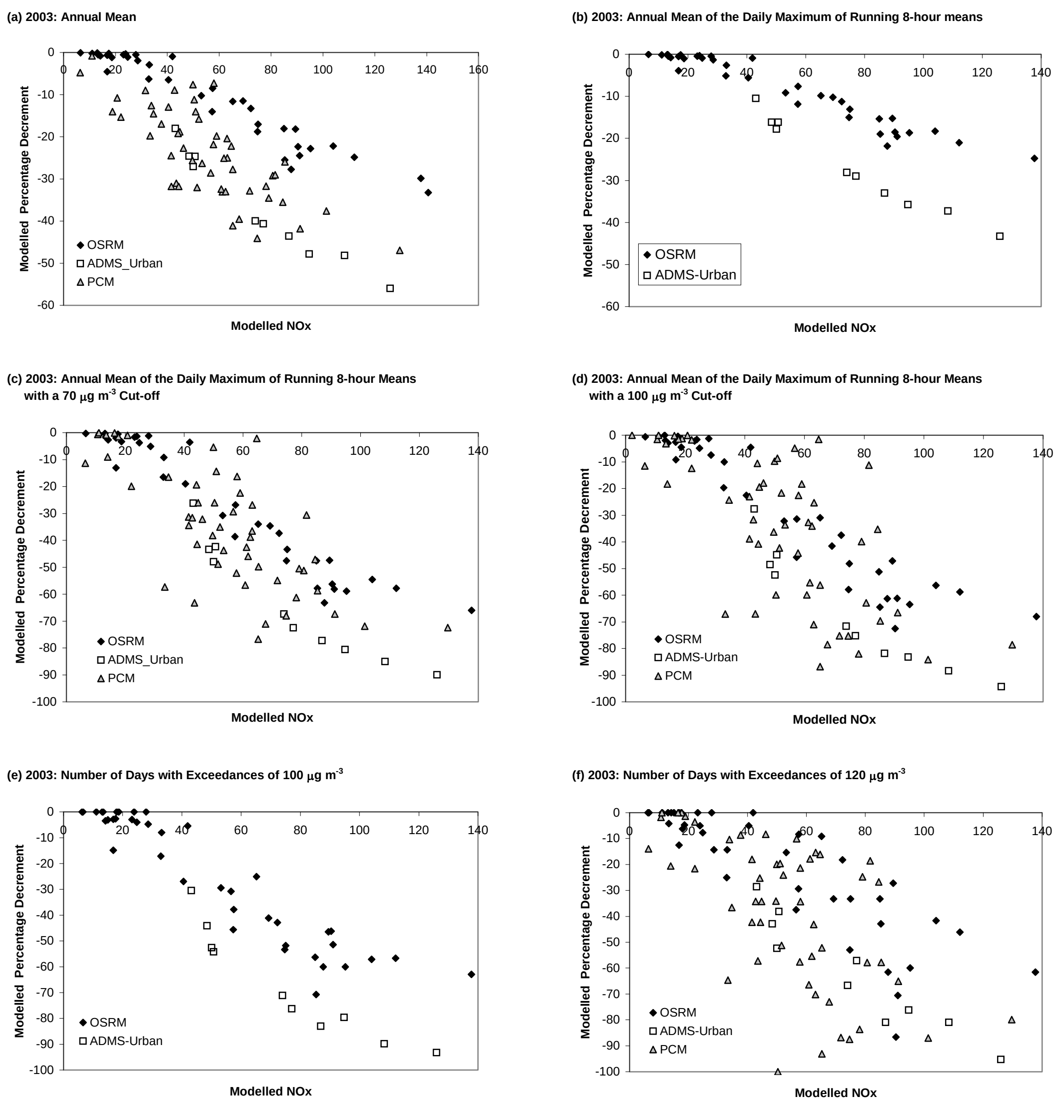

Figure A4.5 Comparison of the percentage decrements plotted against the modelled NO_x concentration, calculated using the OSRM and ADMS-Urban, and from ambient monitoring data using the empirical PCM approach for the following ozone metrics: (a) annual mean concentration; (b) annual average of the daily maximum running 8-hour concentration; (c) annual average of the daily maximum running 8-hour concentration with at cut off of 70 μg m^{-3}; (d) annual average of the daily maximum running 8-hour concentration with at cut off of 100 μg m^{-3}; (e) days above 100 μg m^{-3}; (f) days above 120 μg m^{-3}.

450. Table A4-1 shows a comparison of the absolute decrements (in μg m^{-3} or days) for metrics and sites for which estimates are available from all three methods. Once again there is reasonably good agreement between the different methods, with the OSRM model tending to predict smaller absolute decrements. The lower absolute decrements derived by the OSRM appear to arise from the lower rural values used to derive the decrements. While the rural values given for the ADMS and Pollution Climate models are based on measured values of the metrics (actual or interpolated), the values for the OSRM are those calculated by the model and these were generally lower than the observed values particularly for sites in the southern part of the UK.

Table A4-1 A comparison of the absolute decrements for metrics and sites for which estimates have been calculated using the OSRM and ADMS-Urban, and from ambient monitoring data using the empirical PCM approach.

	annual mean µg m^{-3}	mean >70 µg m^{-3} µg m^{-3}	mean >100 µg m^{-3} µg m^{-3}	days >120 µg m^{-3} days
Absolute Ozone Decrements: ADMS				
Rural Value of Metric	59.2	14.3	3.5	21.0
London Bloomsbury	-33.1	-12.9	-3.3	-20.0
London Teddington	-10.7	-3.7	-1.0	-6.0
London Brent	-14.6	-6.1	-1.6	-8.0
London Eltham	-16.0	-6.9	-1.9	-11.0
London Bexley	-14.6	-6.2	-1.7	-9.0
Absolute Ozone Decrements: PCM				
Rural Value of Metric	56.5	14.7	4.1	24.8
London Bloomsbury	-26.5	-10.6	-3.2	-19.8
London Teddington	-8.2	-2.2	-0.4	1.7
London Brent	-16.8	-4.3	-0.2	-2.6
London Eltham	-18.4	-7.2	-1.8	-12.6
London Bexley	-14.1	-5.5	-1.4	-7.8
Absolute Ozone Decrements: OSRM				
Rural Value of Metric	50.4	10.5	2.2	13.0
London Bloomsbury	-14.0	-5.6	-1.2	-8.0
London Teddington	-5.2	-3.2	-0.7	-2.0
London Brent	-5.7	-3.2	-0.6	-1.0
London Eltham	-4.1	-2.7	-0.7	-1.0
London Bexley	-5.4	-3.4	-1.0	-5.0