Pilot Scottish Air Quality Mapping Exercise

Produced by **netcen** on behalf of the Scottish Executive
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1.0 Introduction

This pilot mapping exercise undertaken on behalf of the Scottish Executive is intended to provide a comparison of the results of a national air quality modelling method in 2004 with results from Scottish air quality monitoring data and to examine possible improvements to the model in representing Scottish concentrations.

Each year **Netcen** performs detailed modelling exercises on behalf of Defra and the Devolved Administrations (DAs) to produce up-to-date maps and projections for the future (2010, 2015 and 2020) in order to supplement data from the national monitoring networks to satisfy the UK's Daughter Directive reporting requirements. The outputs are maps of background air pollutant concentrations on a 1 x 1 km grid and roadside air pollutant concentrations for urban road links. The models are calibrated using data from the national networks (chiefly the Automatic Urban and Rural Network, AURN) and are verified using independent monitoring data from local authorities and ad-hoc monitoring campaigns that have been quality assured to the same standard as the AURN. Because the modelling employs a single set of calibration coefficients to represent the whole of the UK, there are some regions that might be better represented by a more specific calibration relationship. Scotland, as a result of its wide rural expanses, is such a region that may not conform as well as other areas to the general calibration performed for the UK as a whole.

The exercise will consist of two parts:

- **Task 1** – an assessment of the model performance against Scottish air quality monitoring data
- **Task 2** – attempting to improve the model by tailoring components to Scotland.

Task 1 is a detailed examination of the national model's current performance for Scotland in 2004. This includes plotting the model results against Scottish monitoring data as verification charts. Associated tables summarising this verification are also provided and include the average modelled values, average measured values, coefficient of variation (R^2), the number of sites used and the percentage of these that fall within the EC data quality objectives (DQOs) for modelled data for each pollutant. The national output maps (1 x 1 km background maps and roadside maps for urban road links) are presented for Scotland.

Task 2 has attempted to improve the model results by tailoring model components to Scotland. This has involved remodelling of several pollutants (deemed appropriate for improvement for Scotland) and an assessment of these results to examine the degree to which the model represents the monitoring data. The two methods of model improvement that were been identified were:

- Use of Scottish meteorological data – the ADMS modelling was performed using meteorological data from Edinburgh Airport. A new dispersion kernel was derived using this met data.
- Calibration of the model using only monitoring data from Scottish monitoring sites.

The pollutants examined in this analysis are limited to those pollutants and metrics covered by the EU air quality objectives and UK Air Quality Strategy that are routinely mapped by **Netcen** on behalf of Defra and the DAs. A further restriction on the pollutants and metrics examined here are the presence of adequate monitoring in Scotland to allow the analysis. The period under examination, 2004, was selected as the most recent year for which **Netcen**'s national scale models had been developed. This meant that monitoring data from Scotland was limited to relatively few sites and as a result ozone, benzene, 1,3 butadiene or $PM_{2.5}$ are not presented. Table 2.1, presents a summary of the national

network sites that were used in the recalibration and verification of the national models for Scotland.

The pollutants and metrics routinely mapped for Defra and the DAs and covered by this analysis include:

- CO annual average concentration (mg m^{-3})
- CO maximum 8 hourly concentration (mg m^{-3})
- NO_x annual mean concentration ($\mu g\ m^{-3}$)
- NO_2 annual mean concentration ($\mu g\ m^{-3}$)
- PM_{10} (TEOM) annual mean concentration ($\mu g\ m^{-3}$)
- PM_{10} (gravimetric) annual mean concentration ($\mu g\ m^{-3}$)
- SO_2 annual mean concentration ($\mu g\ m^{-3}$)
- SO_2 99.9th percentile of 15 minute means ($\mu g\ m^{-3}$)
- SO_2 99.73rd percentile of hourly means ($\mu g\ m^{-3}$)
- SO_2 99.18th percentile of daily means ($\mu g\ m^{-3}$)

The particulate matter modelling has been performed in both TEOM and gravimetric units. Gravimetric mapping was performed using Partisol data from the national networks, other instruments were omitted.

The small number of Scottish sites measuring some pollutants makes it very hard to achieve a meaningful verification of the model performance and is a significant limitation on the recalibration of the models for Scotland. It should be noted that due to the limited availability of monitoring data in 2004, all of the sites used in the verification of the models were also used in the calibration of the national models and so do not provide an independent quality check. In Task 2 it should be noted that there were cases where an inadequate number of monitoring sites were available to make a recalibration of the model possible. This was the case for background and roadside gravimetric PM_{10} models and the roadside TEOM PM_{10} model. A more detailed explanation is provided in the PM_{10} section (section 5.0).

This report first provides an overview of the methodology used in this comparison and then examines each pollutant in turn and describes the changes made the to the model, presents the new calibration plot, presents the new verification plot to compare the national model results and the Scottish model results with the monitoring data.
Background and roadside maps from the national models and the new Scottish models are also presented for comparison.

It is not the intention of this report to document the complete methodology of the modelling process – this can be found in Stedman et al (2006). This report focuses on changes made to the models to try and improve the results for Scotland and covers both tasks of the pilot study.

2.0 Methodology

The modelled maps are calculated from National Atmospheric Emissions Inventory (NAEI) data using a dispersion modelling approach which is calibrated using monitored data from the national networks (AURN). Each of the Scottish monitoring stations used in this analysis is in the national networks and this fully ratified and quality assured data have been included in the calibration relationship used in the national modelling. The modelled maps are then verified against independent monitoring data held by **Netcen** (local authority sites within the **Netcen** 'Calibration Club', ad-hoc monitoring campaigns run by **Netcen** and other publicly available data from networks). Complete versions of these maps or the whole of the UK and detailed explanations of the modelling methodology and verification are presented in Stedman et al (2006).

The locations of each of the Scottish air quality monitoring sites were plotted with GIS on the modelled pollution maps and the corresponding modelled background concentration for the relevant 1 x 1 km grid square extracted. A 75% data capture threshold was applied to the monitoring data for this analysis - any site with data capture below this was omitted. At roadside sites, the corresponding modelled road link (where available) was used to ascertain a modelled roadside value rather than the modelled background concentration.

SO_2 is not modelled at roadside locations because roadside values are not significantly different from background values. As a result, modelled background concentrations were used for comparison with the monitored data at roadside sites instead.

The modelled information was directly compared with the corresponding monitored metric from each site and plotted in a scatterplot. Lines at 30% or 50% are shown on the scatterplots – these are the data quality objectives (DQOs) specified in the 1st and 2nd Daughter Directives. Lines at 50% for the 99.9th percentile of 15-minute SO_2 concentration and annual mean CO concentration and 30% for annual mean NO_x concentration have been included for illustrative purposes although there are no formal DQOs for these metrics. These scatterplots are presented below with tabulated statistics (Tables 2 to 10) including the number of sites included in the analysis for each metric, the R^2 of the relationship between monitored and modelled data, the average of the modelled and monitored data for all sites and the number of sites within the data quality objectives. The analysis was performed separately for background (non-roadside) and roadside sites.

All the monitoring sites included in this analysis are part of the AURN and have therefore been included in the calibration of the national model and examined in the UK scale study. Comparing the national model results for Scotland with data already used in the calibration offers no fully independent check but simply serves to illustrate the extent to which the model represents a single particular region.

A Scottish dispersion kernel was used to model all area sources in this work. This kernel was created in ADMS using Edinburgh Airport meteorological data for 2004. This provided a grid representing the proportional contribution of the central square to each surrounding squares. The matrix was then inverted to represent the contribution from the surrounding squares to the central square. This was the completed dispersion kernel.

The 2004 data from the national network sites has been fully ratified by **Netcen**.

Table 2.1 Complete list of Scottish sites used in analysis

Site name	Easting	Northing	Site type	NO_x/NO_2	O_3	CO	PM_{10}	SO_2	Hydrocarbons *
Bush Estate	324626	663880	RURAL	✓	✓				
Eskdalemuir	323500	602800	RURAL	✓	✓				
Glasgow City Chambers	259528	665308	URBAN BACKGROUND	✓		✓			
Strath Vaich	234829	874785	REMOTE	✓	✓			✓	
Glasgow Centre	258902	665028	URBAN CENTRE	✓	✓	✓	†	✓	
Aberdeen	394416	807408	URBAN BACKGROUND	✓	✓	✓	†	✓	
Grangemouth	293840	681032	URBAN INDUSTRIAL	✓		✓	†	✓	
Edinburgh St Leonards	326250	673132	URBAN BACKGROUND	✓	✓	✓	†	✓	
Glasgow Kerbside	258708	665200	KERBSIDE	✓		✓	†		✓
Dumfries	297012	576278	ROADSIDE	✓		✓	‡		
Inverness	265720	845680	ROADSIDE	✓		✓	‡		

* Benzene and 1,3 Butadiene
† TEOM instrument
‡ Gravimetric Instrument

3.0 CO

There were 5 Scottish background monitoring sites available to recalibrate the CO models. These were Glasgow City Chambers, Glasgow Centre, Aberdeen, Grangemouth and Edinburgh St. Leonards. The calibration plots for the background models are shown in Figure 3.1 and 3.2 and the roadside calibration of the two metrics are presented in Figures 3.3 and 3.4. The national modelling process established two background relationships – one for large conurbations (such as London and Birmingham) and the another relationship for all other areas. Scotland contains no areas identified as large conurbations and so the models use only one relationship. Figure 3.1 shows the calibration relationship for the annual mean model. This is derived from a comparison of the annual mean measured concentrations, corrected for contributions from Part A processes and uncalibrated area source component derived from summing the scaled source emission grids from the NAEI together and applying the new Scottish dispersion kernel. The maximum 8-hour model is calibrated by defining a relationship between the measured annual mean and the measured 8-hour mean at Scottish sites and this coefficient is then applied to the annual mean map to obtain modelled maximum 8-hour concentrations.

The roadside model is calibrated by comparing for each modelled road link the calculated roadside increment (difference between the measured concentration at roadside sites and the background modelled concentration) and the traffic flow adjusted emissions for that road link. The maximum 8-hour model again uses the relationship between measured annual mean and measured maximum 8-hour concentration in the same way as the background map was calculated. Although Table 2.1 shows that there are 3 roadside sites in Scotland, Glasgow Kerbside is not located on one of the built up urban road links that is modelled and so there was no specific road link emissions data available. Therefore, this site was removed from the calibration and verification. It is recognised that 2 sites is not really enough for a robust calibration but despite this the modelling has been undertaken in order to provide illustrative results and demonstrate the method.

Figures 3.5 and 3.6 show the verification results for the annual mean and maximum 8-hour models. All sites fell within the +/- 50% range for both the recalibrated Scottish model and the national model for both annual mean and maximum 8-hour models. The summary statistics for the verification process are shown in Tables 3.1 and 3.2. The average of the annual mean modelled values compares extremely favourably with the measured values for the Scottish model. For the national model the average annual mean modelled concentrations were slightly lower than the average measured concentrations, indicating a slight underestimation. The R^2 value of 0.82 was a good fit for the Scottish annual mean model but was slightly higher at 0.84 for the national model. No R^2 could be calculated for the roadside annual mean model because this included only 2 points (Glasgow Kerbside having been excluded). Despite the higher R^2 value for the national model results, the Scottish annual mean model results show a better fit around the 1:1 line than the national model results, especially when the background and roadside data are taken into account together.

There is more variability around the 1:1 line for the maximum 8-hour mean models for both the Scottish and national models. Average Scottish model concentrations compared more favourably with the measured concentrations than the national model results which marginally overestimated the background concentrations and more significantly underestimated the roadside concentrations. The R^2 values were very similar between the models with the national model value being slightly higher again. No roadside R^2 was calculable as described above.

Figures 3.7 and 3.8 show the output annual mean background maps from both the Scottish model and the national model. Both maps identify the large urban areas of Edinburgh and particularly Glasgow as the areas of the highest annual mean CO concentrations. The Scottish model highlights Glasgow more than the national model and also picks out the motorways running into Glasgow more prominently than the national model. Maps of the maximum 8-hour concentration are in Figures 3.9 and 3.10. The Scottish model illustrates higher concentrations more restricted to the urban areas than in the national model results in which these are more widespread around the urban areas. Figures 3.11 to 3.14 show the roadside maps. The Scottish model results in higher

modelled roadside concentrations than the national model in Glasgow, Edinburgh and Aberdeen.

Figure 3.1 Calibration of Scottish background CO annual mean 2004 model (mg m^{-3})

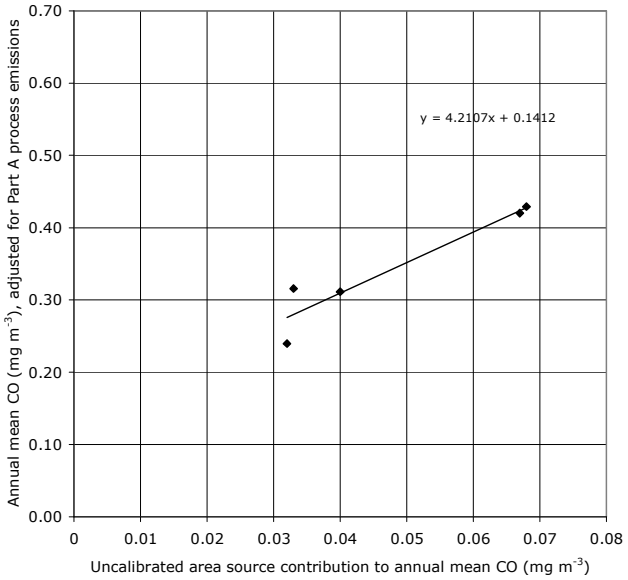


Figure 3.2 Calibration of Scottish background CO maximum 8-hour 2004 model (mg m^{-3})

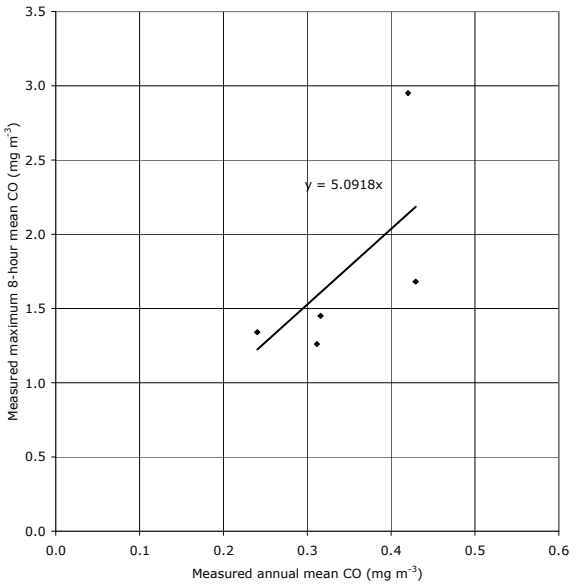


Figure 3.3 Calibration of Scottish roadside CO annual mean 2004 model (mg m^{-3})

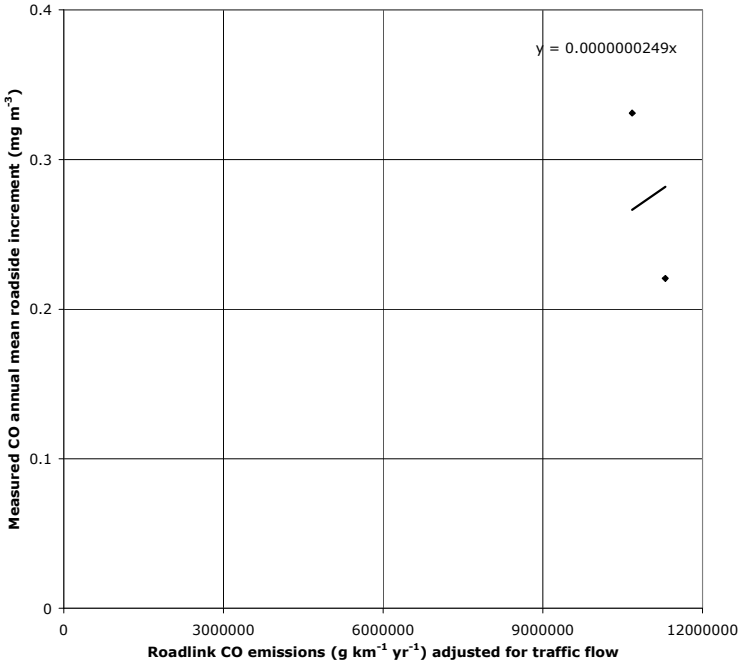


Figure 3.4 Calibration of Scottish roadside CO maximum 8-hour 2004 model (mg m^{-3})

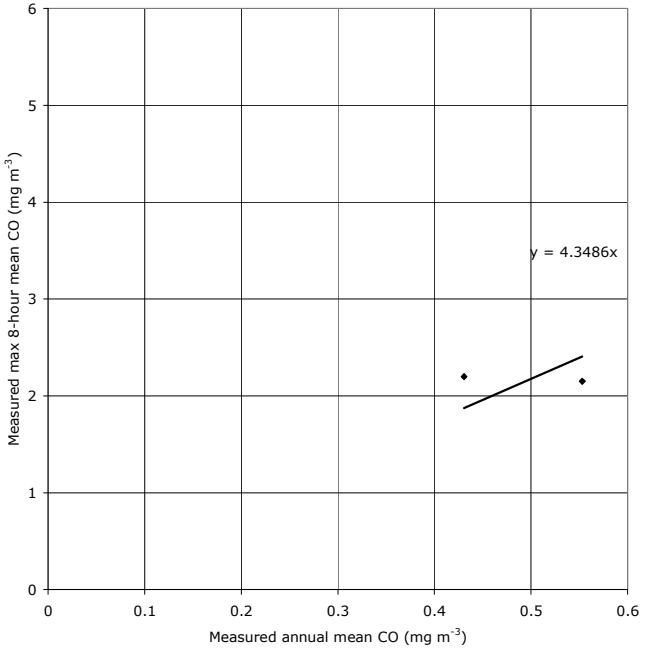


Figure 3.5 Verification of Scottish CO background and roadside annual mean 2004 models (mg m^{-3})

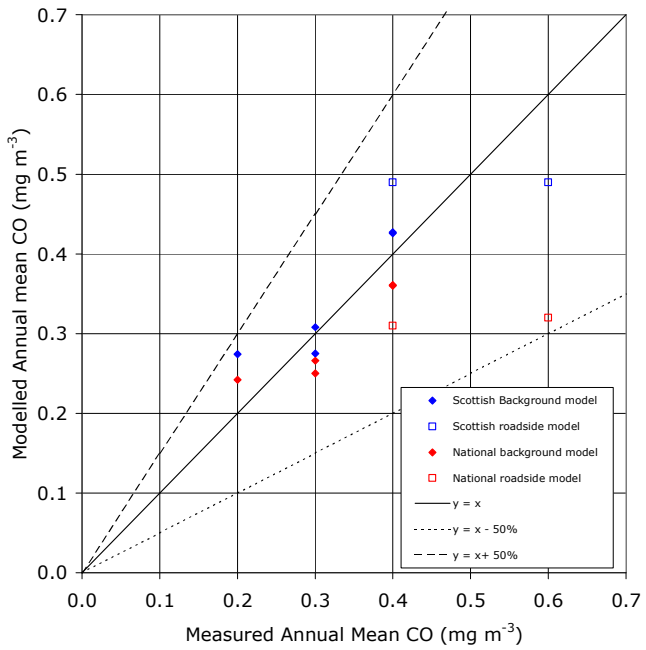


Figure 3.6 Verification of Scottish CO background and roadside maximum 8-hour 2004 models (mg m^{-3})

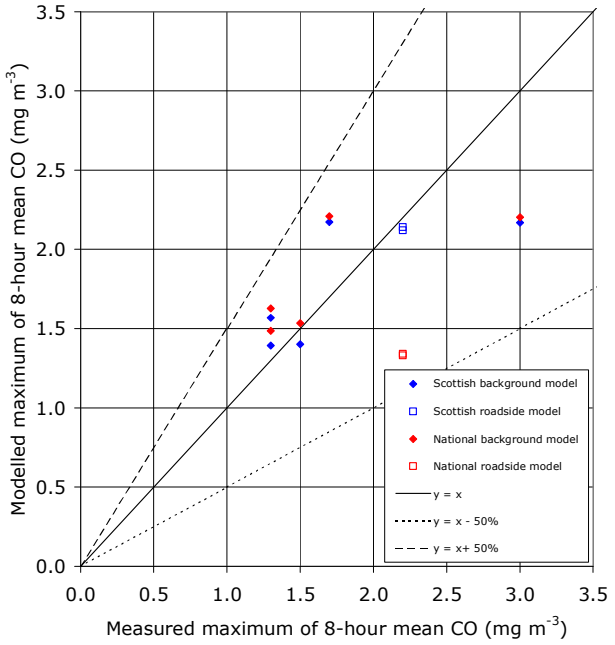


Table 3.1 CO annual mean 2004 verification summary (mg m^{-3})

a) Scottish model results

	Average modelled	Average monitored	R^2	Number sites used	Number sites within range	% sites within range
Background	0.34	0.34	0.82	5	5	100
Roadside	0.49	0.49	-----	2	2	100

b) National model results

	Average modelled	Average monitored	R^2	Number sites used	Number sites within range	% sites within range
Background	0.30	0.34	0.84	5	5	100
Roadside	0.32	0.49	-----	2	2	100

Table 3.2 CO maximum 8-hour 2004 verification summary (mg m^{-3})

a) Scottish model results

	Average modelled	Average monitored	R^2	Number sites used	Number sites within range	% sites within range
Background	1.74	1.74	0.54	5	5	100
Roadside	2.13	2.18	-----	2	2	100

b) National model results

	Average modelled	Average monitored	R^2	Number sites used	Number sites within range	% sites within range
Background	1.81	1.74	0.55	5	5	100
Roadside	1.34	2.18	-----	2	2	100

Figure 3.7 Scottish model CO background annual mean 2004 map (mg m^{-3})

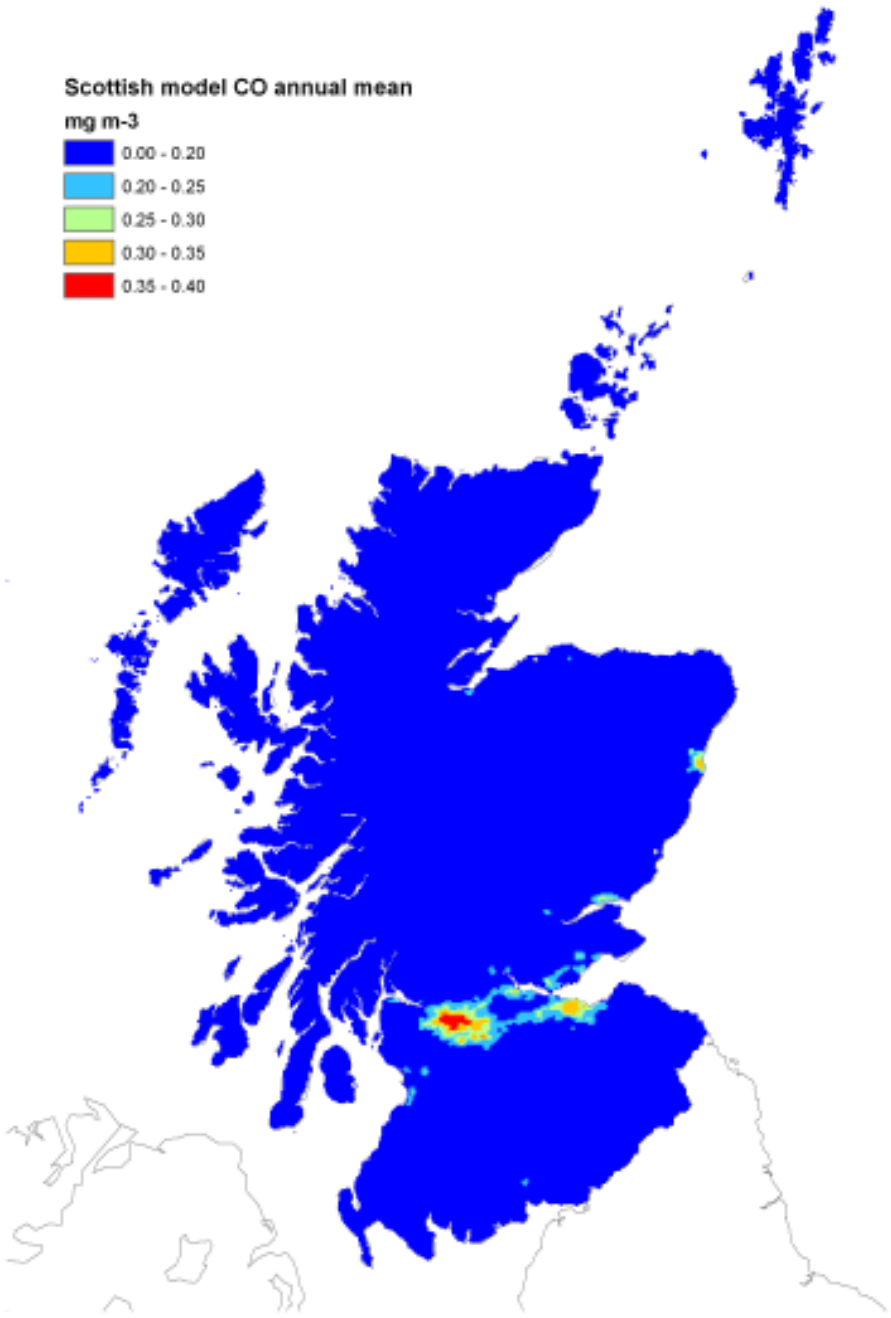


Figure 3.8 National model CO background annual mean 2004 map for Scotland (mg m^{-3})

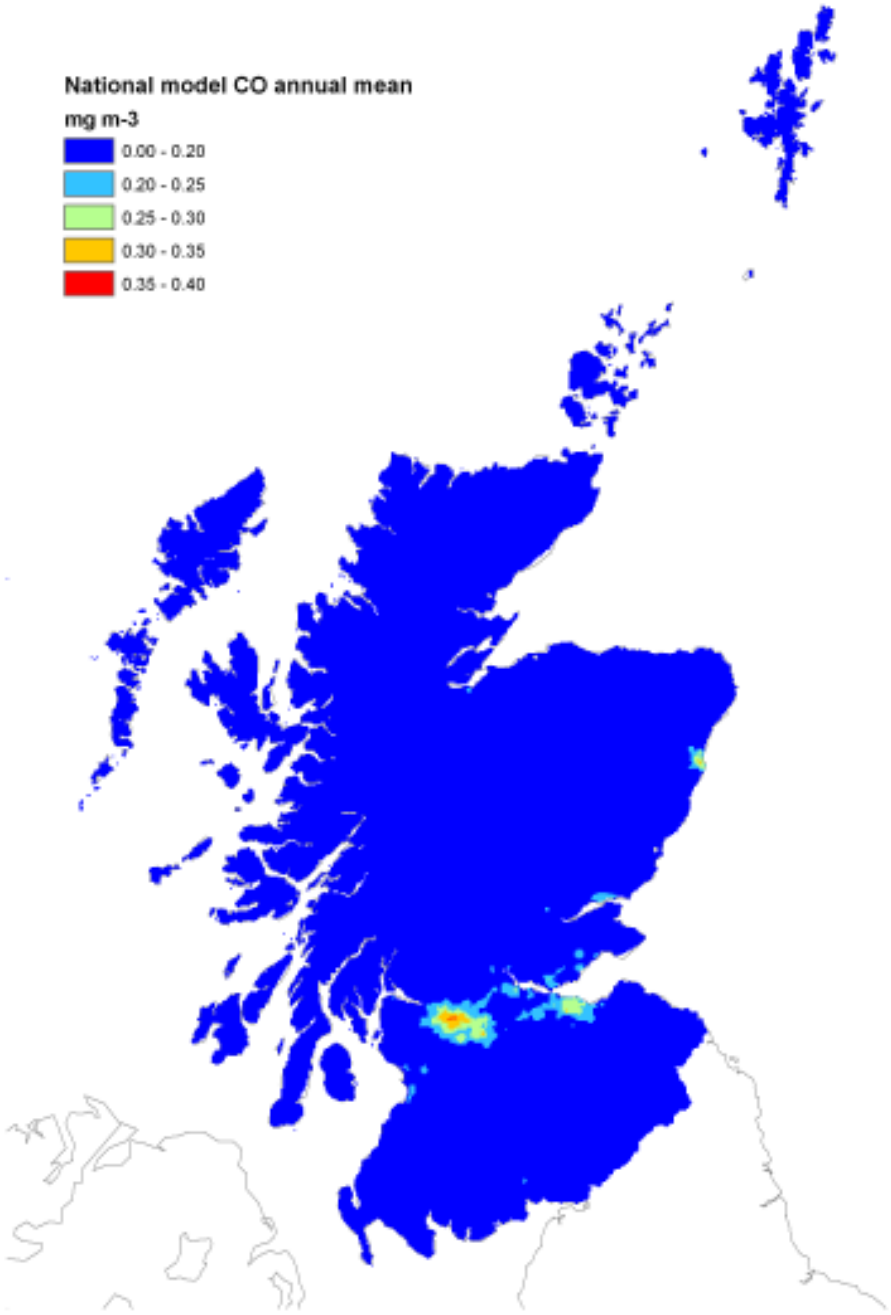


Figure 3.9 Scottish model CO background maximum 8-hour 2004 map (mg m^{-3})

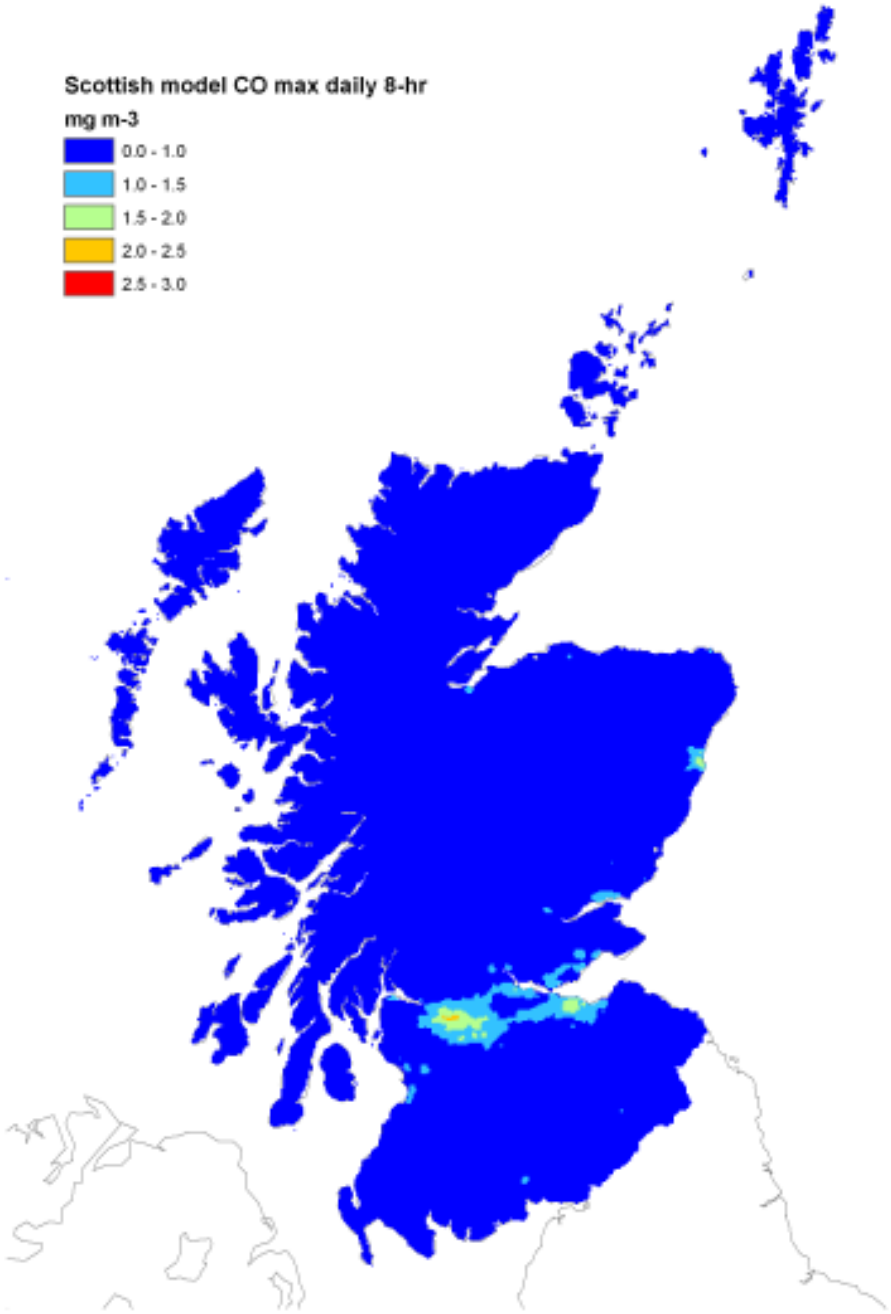


Figure 3.10 National model CO background maximum 8-hour 2004 map for Scotland (mg m^{-3})

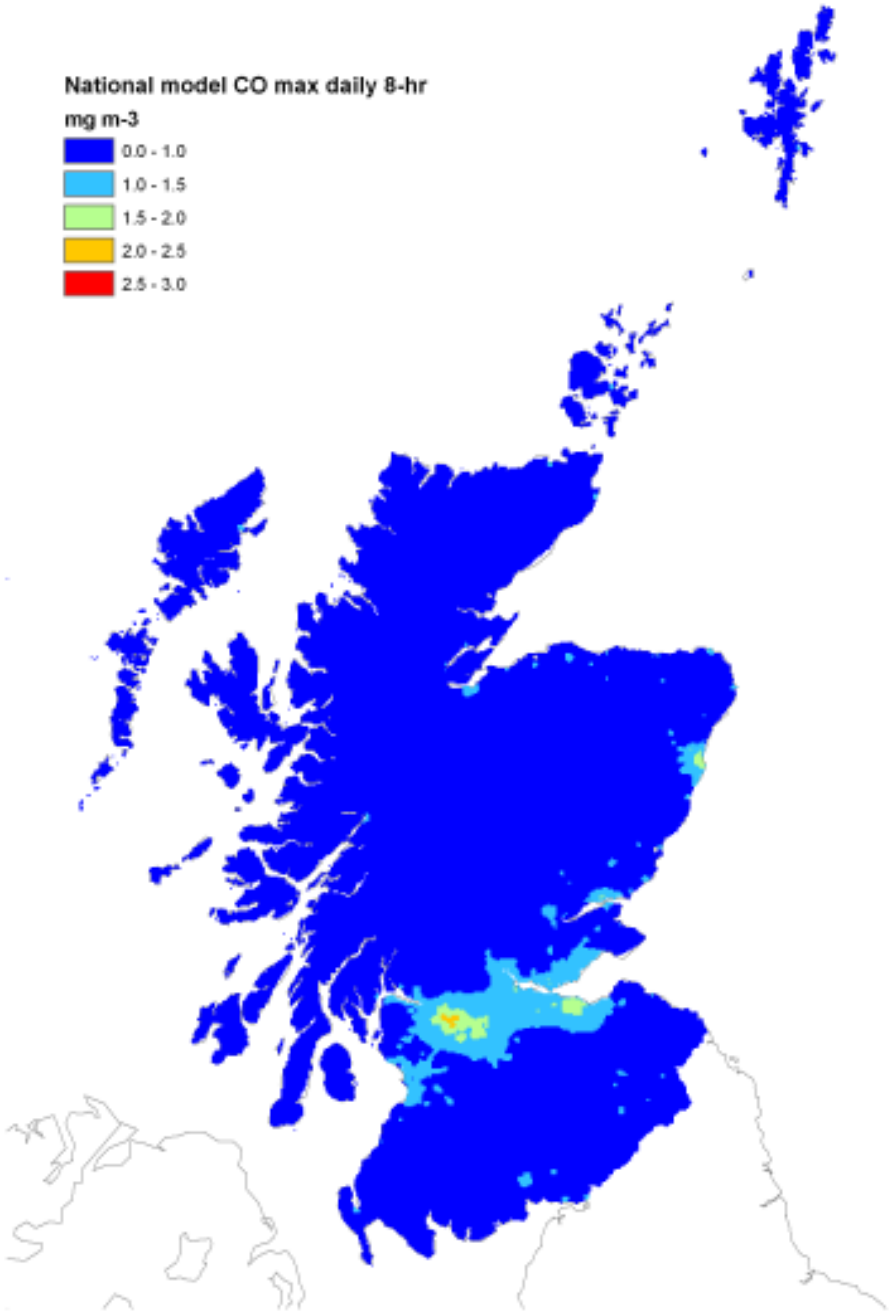


Figure 3.11 Scottish model CO roadside annual mean 2004 map (mg m^{-3})

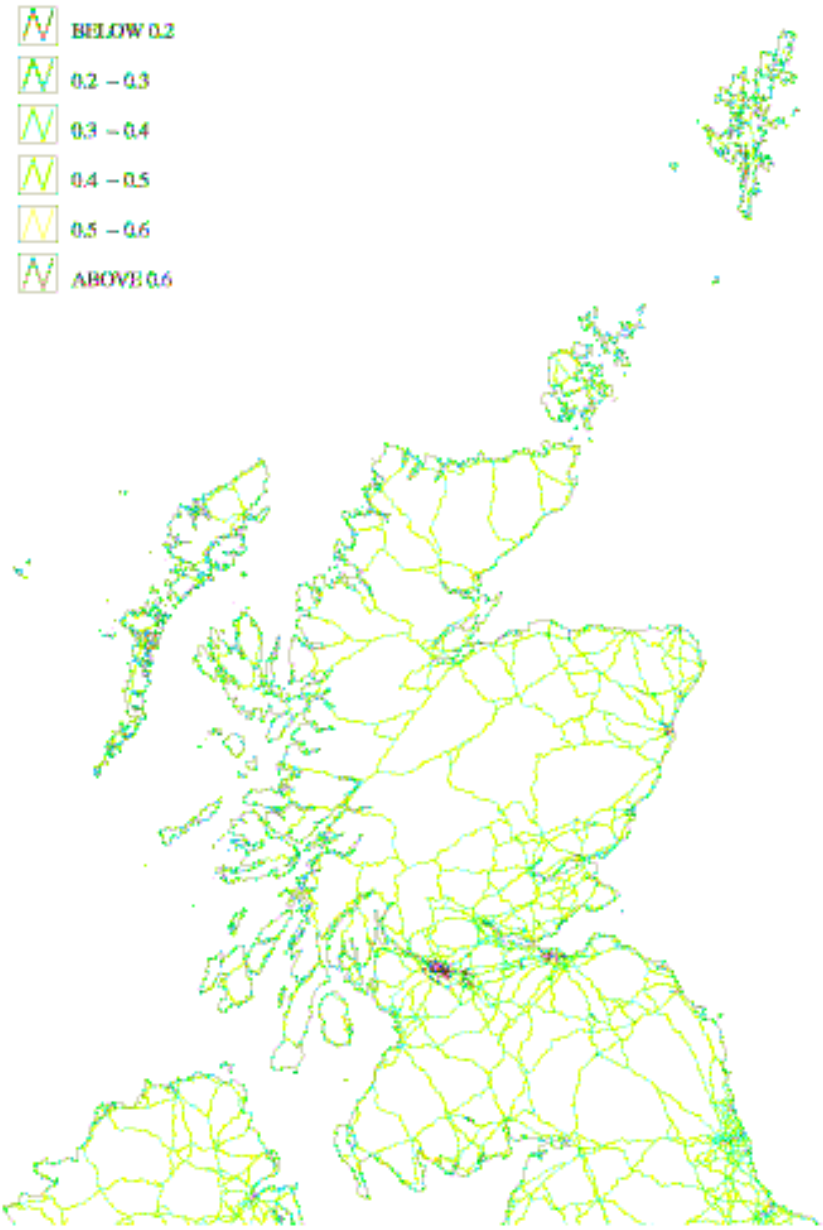


Figure 3.12 National model CO roadside annual mean 2004 map for Scotland (mg m^{-3})

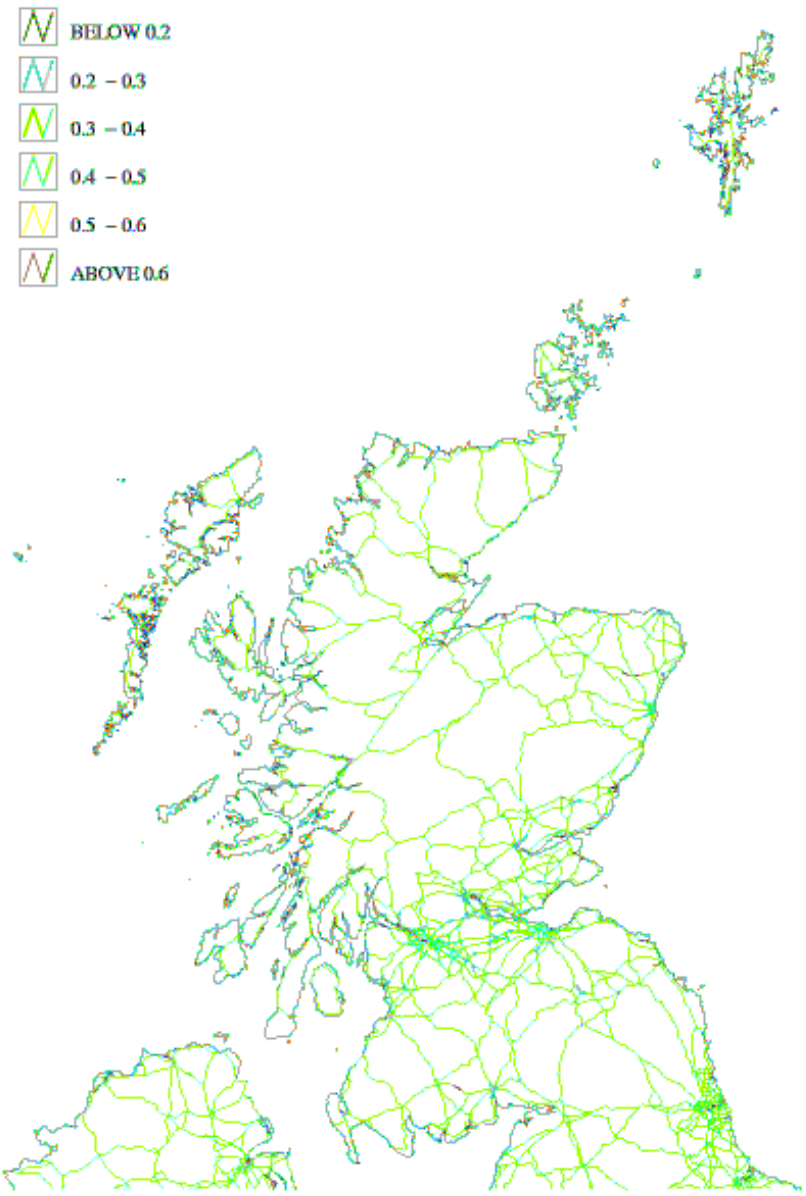


Figure 3.13 Scottish model CO roadside maximum 8-hour 2004 map (mg m^{-3})

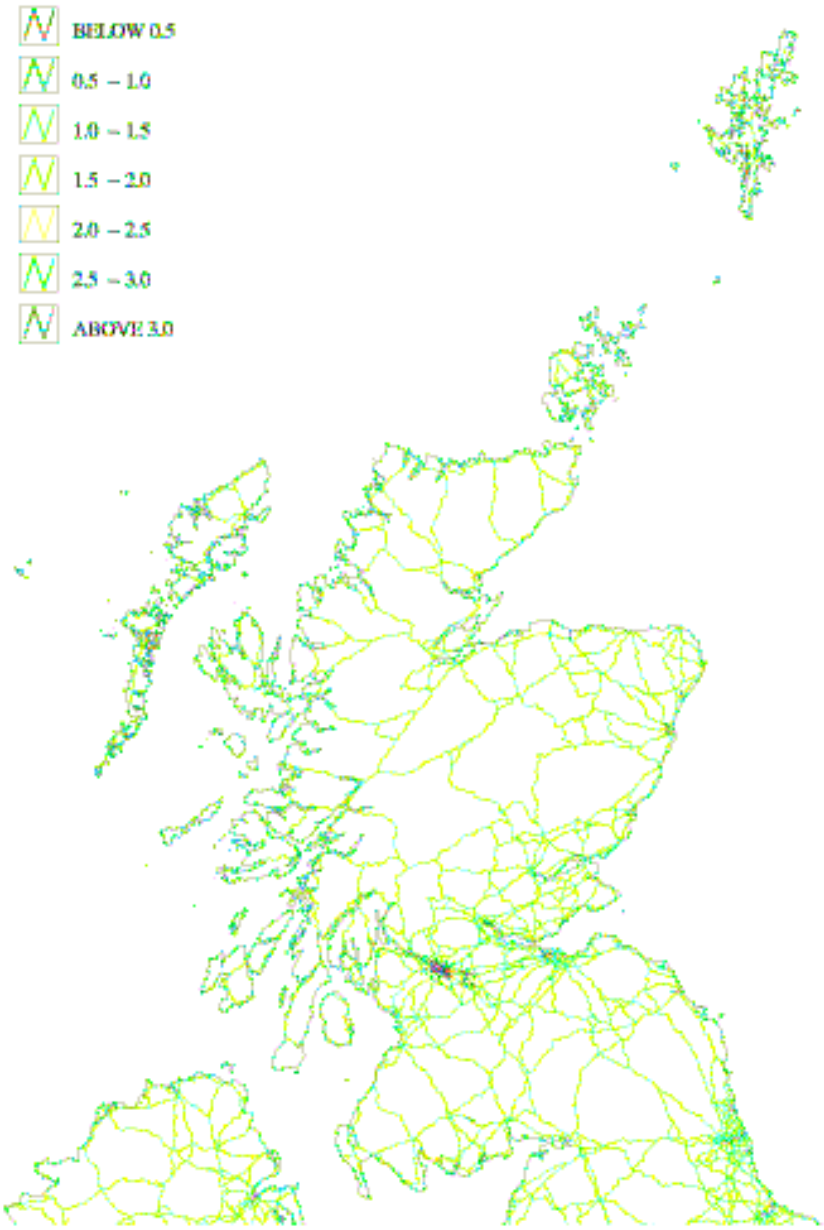
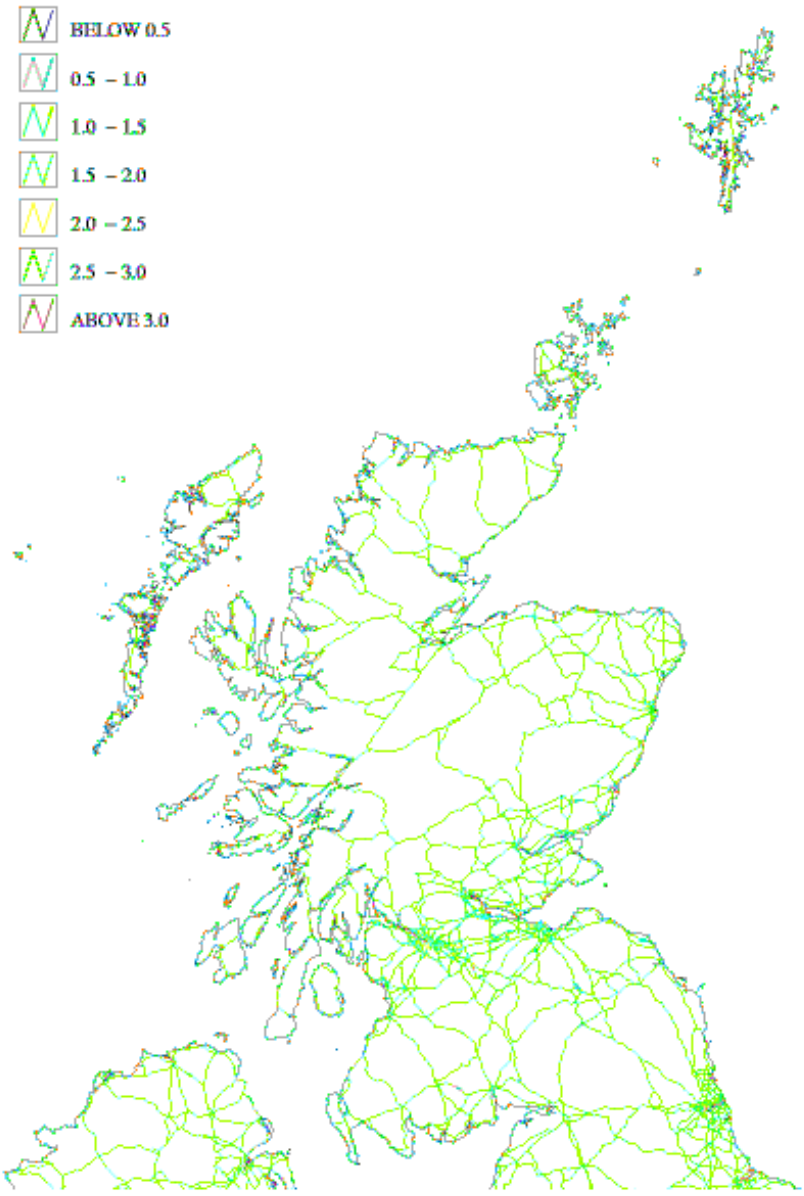


Figure 3.14 National model CO roadside maximum 8-hour 2004 map for Scotland (mg m^{-3})



4.0 NO_x and NO_2

NO_x is generally the pollutant that is best represented by the modelling process because it has the greatest number of monitoring sites on which to calibrate the model and the NAEI data upon which it is based is generally robust. NO_2 is also well represented by the model as it is derived from the NO_x output and the chemistry between NO_x and NO_2 is reasonably well understood and therefore easier to model accurately. The NO_x calibration plots for background and roadside are shown in Figures 4.1 and 4.2. There is no calibration for NO_2 concentrations. Instead, these are derived from the NO_x background and roadside model results using a chemical relationship derived by Mike Jenkin. NO_x is calibrated in the same way as CO annual mean (describe in section 3.0) – using measured NO_x concentrations (as NO_2) and comparing them against an uncalibrated area source component derived from the area source emissions grids after applying the dispersion kernel. The roadside concentrations were calibrated using the calculated roadside increment against the traffic flow adjusted emissions for each road link.

Verification plots for NO_x and NO_2 are presented in Figures 4.3 and 4.4 and the summary statistics are in Tables 4.1 and 4.2. The relationships for both models are generally good for NO_x and NO_2. NO_x annual mean R^2 values were very similar for the two models but marginally better for the national model results (R^2 = 0.83). Two of the six background sites fell outside the +/- 30% range for the Scottish model. All but one site was within this range for the national model. No R^2 could be calculated for the 2 roadside sites available. For both the Scottish and the national model one of the two roadside sites was outside the 30% DQO range. However, examination of the average modelled and measured concentrations shows that the Scottish model was closer to the measured concentrations than the national model which underestimated measured concentrations.

The NO_2 models both displayed an R^2 of 0.83 and were identical in terms of the number of sites falling within the DQO range. Both the Scottish and national models produced results that were close to the measured NO_2 average but was slightly better for the national model.

Aberdeen was underestimated by the NO_x model, falling marginally below the data quality objective for both models although the Scottish model did provide a result closer to that measured. The NO_2 Scottish model brought the Aberdeen value to just within the DQO range. However, the Scottish model appears to have overestimated the concentrations at Grangemouth and Inverness, two sites which were well represented in the national model. These sites are marginally outside the DQO range for NO_x and NO_2 for the Scottish model.

Figures 4.5 to 4.8 show the modelled background maps output from the Scottish model and the national model. Both NO_x, NO_2 background maps pick out the urban areas and large roads where the concentrations are highest. Outputs from both models are very similar with the Scottish maps showing slightly higher concentrations than the national maps.

Although roadside concentrations of NO_x are calculated as an intermediate stage in modelling roadside NO_2 roadside concentrations, this is not presented because there is no corresponding legislative objective. The roadside annual mean NO_2 maps are presented in Figures 4.9 and 4.10.

Figure 4.1 Calibration of Scottish background NO_x annual mean 2004 model ($\mu g\ m^{-3}$ as NO_2)

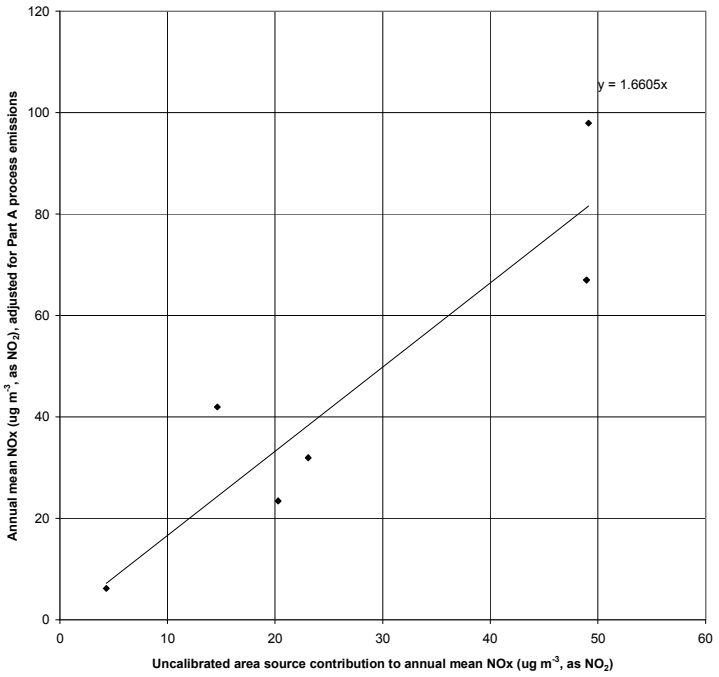


Figure 4.2 Calibration of Scottish roadside NO_x annual mean 2004 model ($\mu g\ m^{-3}$ as NO_2)

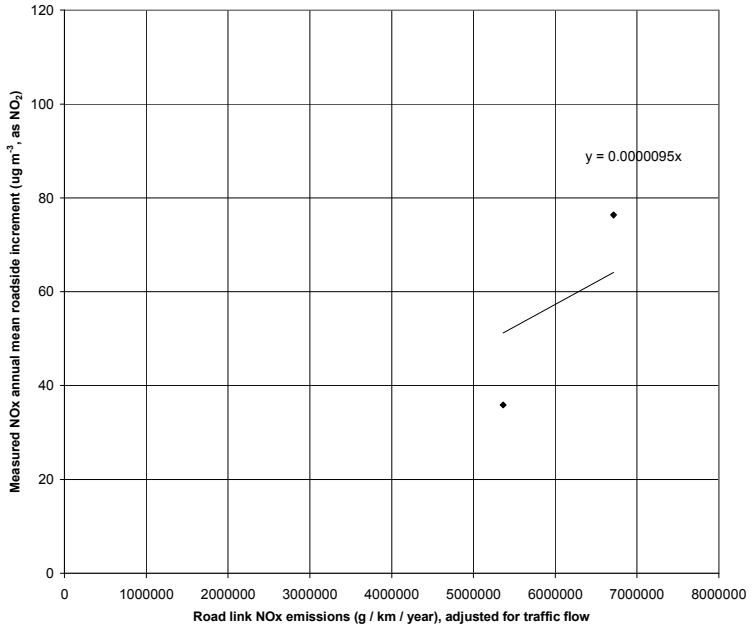


Figure 4.3 Verification of Scottish NO_x background and roadside annual mean 2004 model ($\mu g\ m^{-3}$ as NO_2)

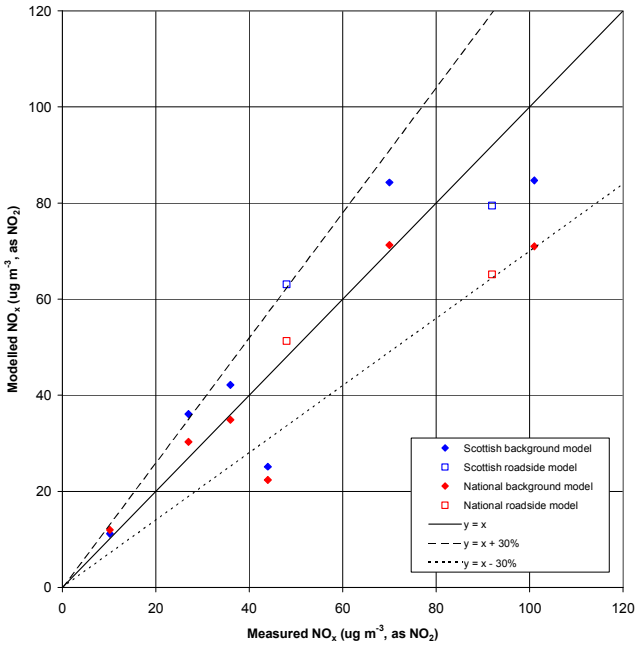


Figure 4.4 Verification of Scottish NO_2 background and roadside annual mean 2004 model ($\mu g\ m^{-3}$)

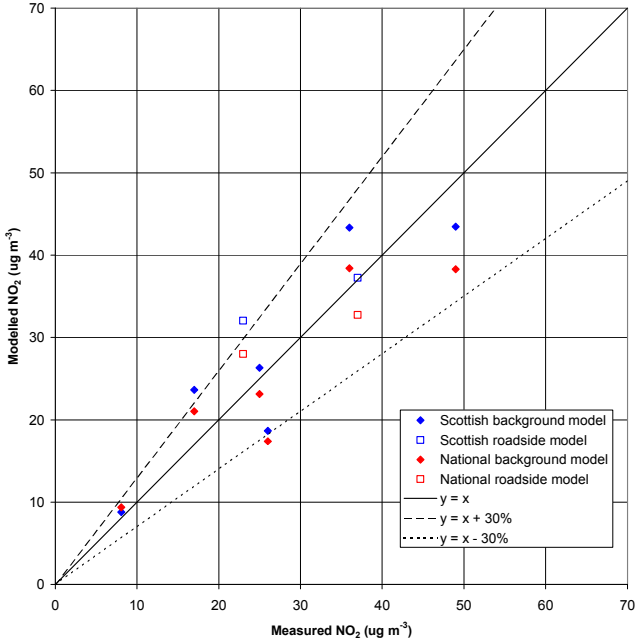


Table 4.1 NO_x annual mean 2004 verification summary ($\mu g\ m^{-3}$ as NO_2)

a) Scottish model results

	Average modelled	Average monitored	R^2	Number sites used	Number sites within range	% sites within range
Background	47.26	48.03	0.82	6	4	67
Roadside	71.27	70.0	-----	2	1	50

b) National model results

	Average modelled	Average monitored	R^2	Number sites used	Number sites within range	% sites within range
Background	40.30	48.03	0.83	6	5	83
Roadside	58.22	70.0	-----	2	1	50

Table 4.2 NO_2 annual mean 2004 verification summary ($\mu g\ m^{-3}$)

a) Scottish model results

	Average modelled	Average monitored	R^2	Number sites used	Number sites within range	% sites within range
Background	27.37	26.85	0.83	6	5	83
Roadside	34.64	30.0	-----	2	1	50

b) National model results

	Average modelled	Average monitored	R^2	Number sites used	Number sites within range	% sites within range
Background	24.60	26.85	0.83	6	5	83
Roadside	30.36	30.0	-----	2	1	50

Figure 4.5 Scottish model NO_x background annual mean 2004 map ($\mu g\ m^{-3}$ as NO_2)

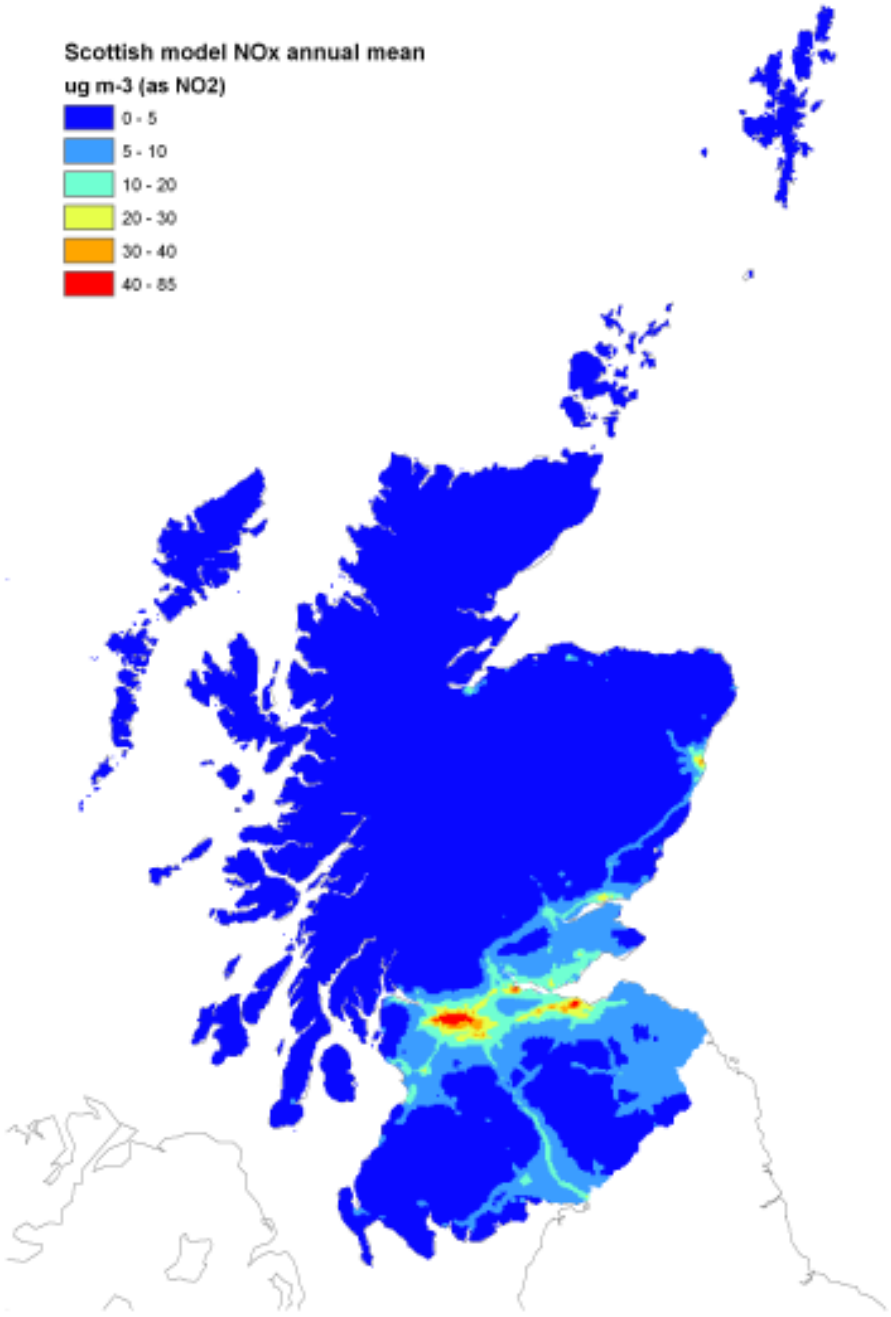


Figure 4.6 National model NO_x background annual mean 2004 map for Scotland ($\mu g\ m^{-3}$ as NO_2)

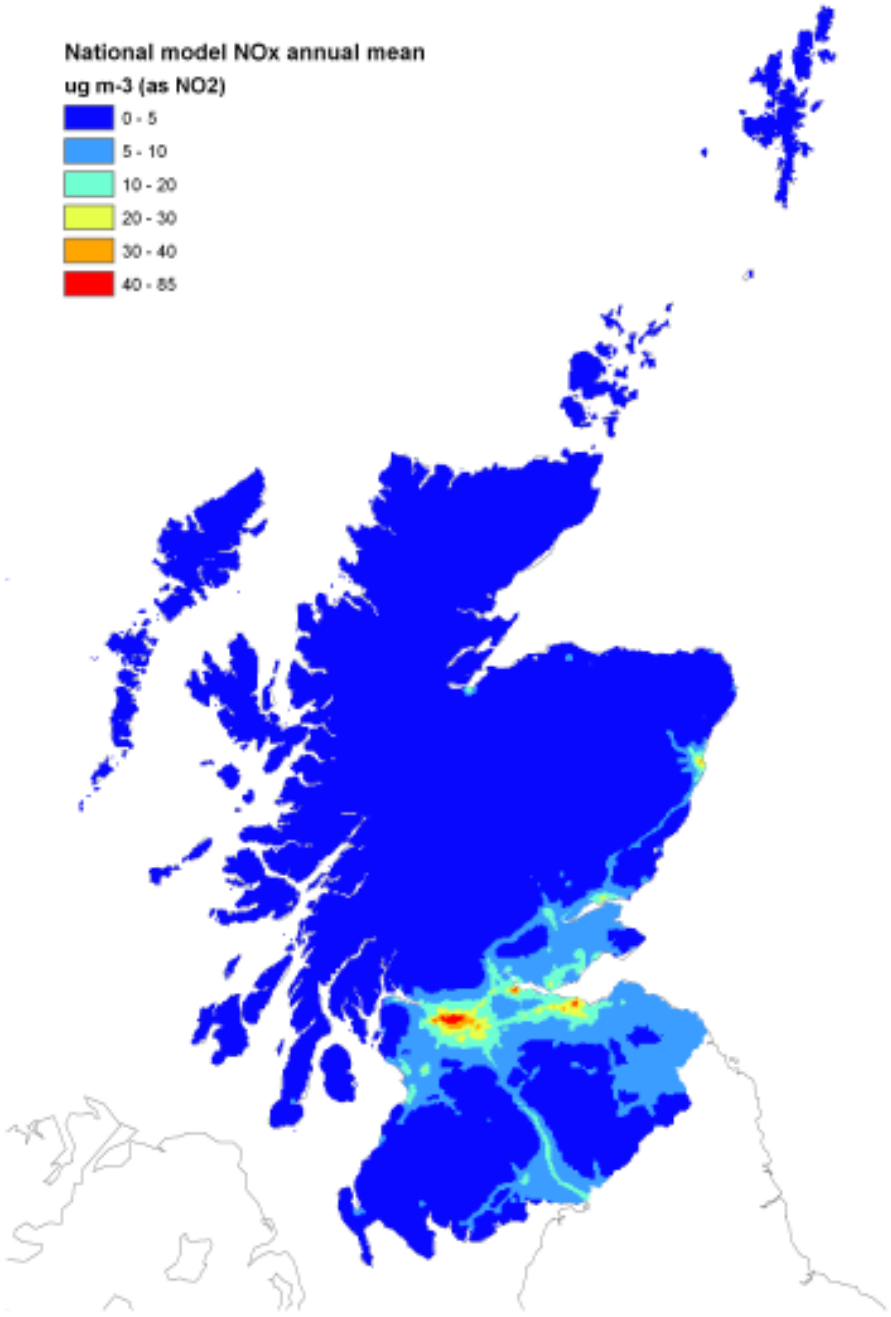


Figure 4.7 Scottish model NO_2 background annual mean 2004 map ($\mu g\ m^{-3}$)

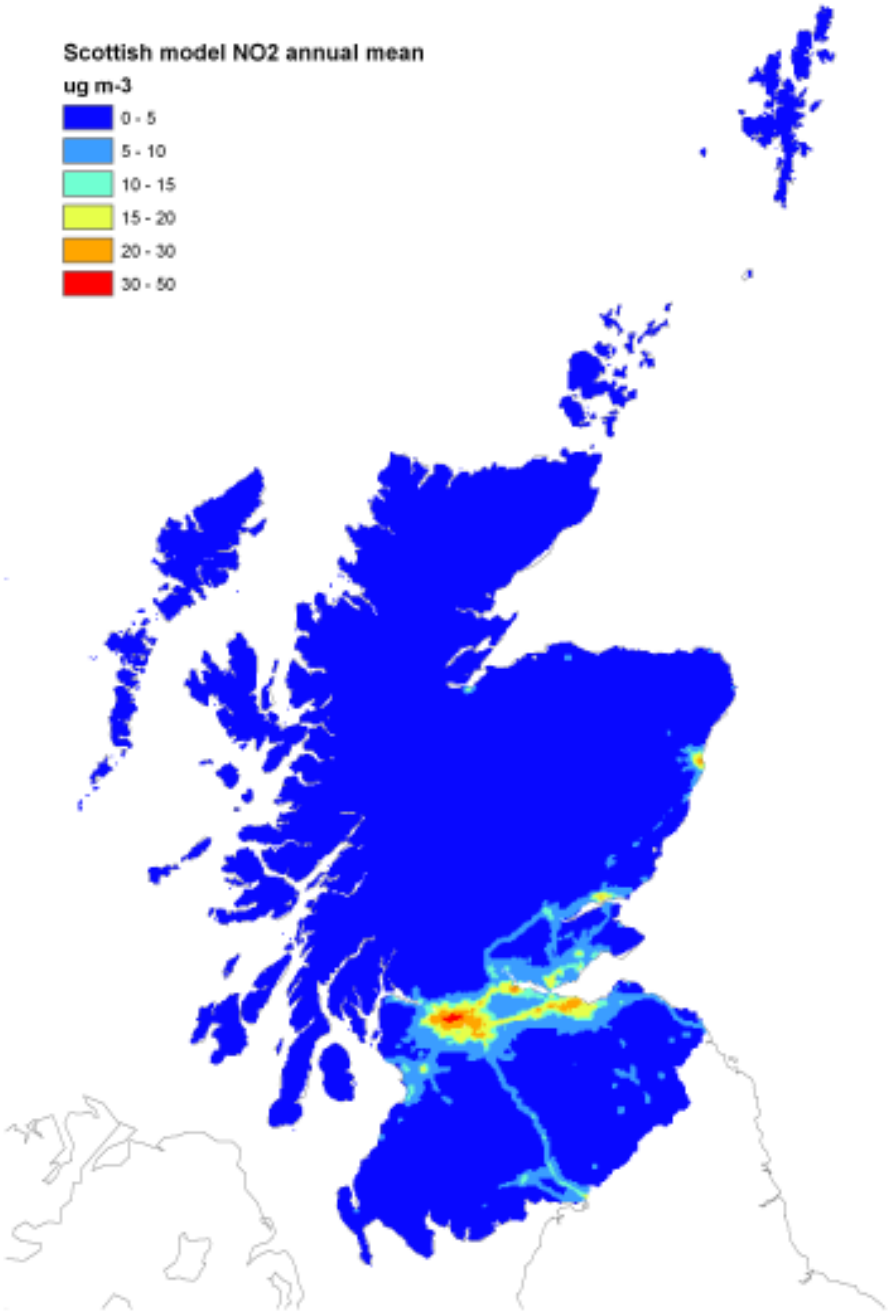


Figure 4.8 National model NO_2 background annual mean 2004 map for Scotland ($\mu g\ m^{-3}$)

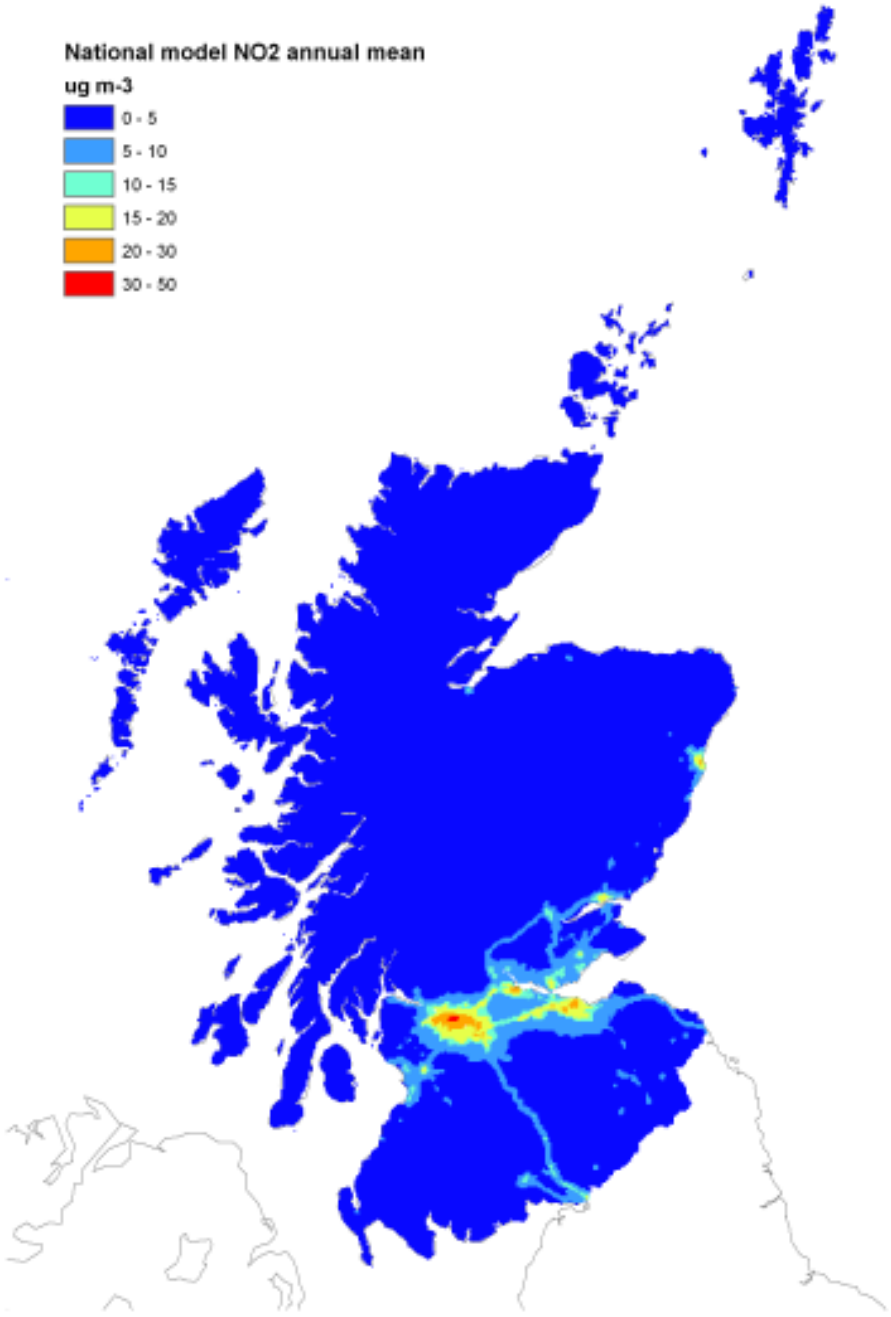


Figure 4.9 Scottish model NO_2 roadside annual mean 2004 map ($\mu g\ m^{-3}$)

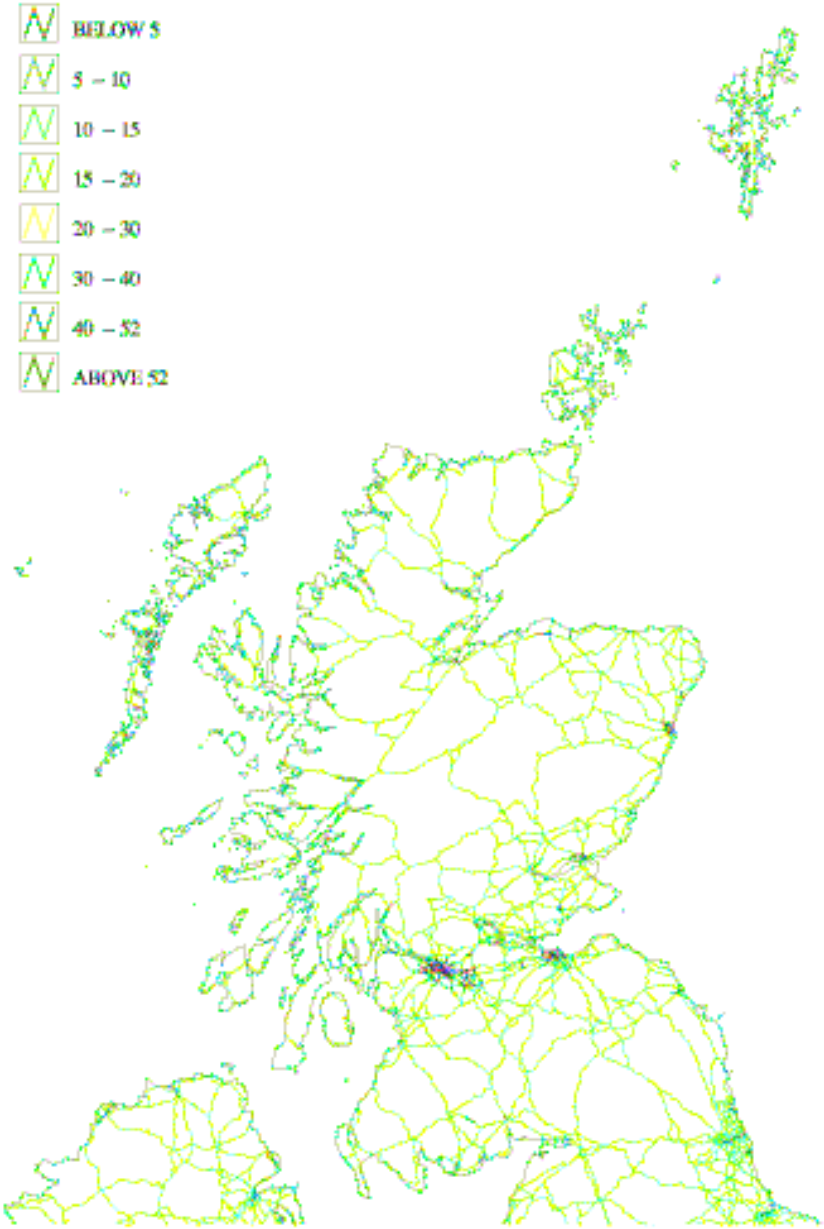
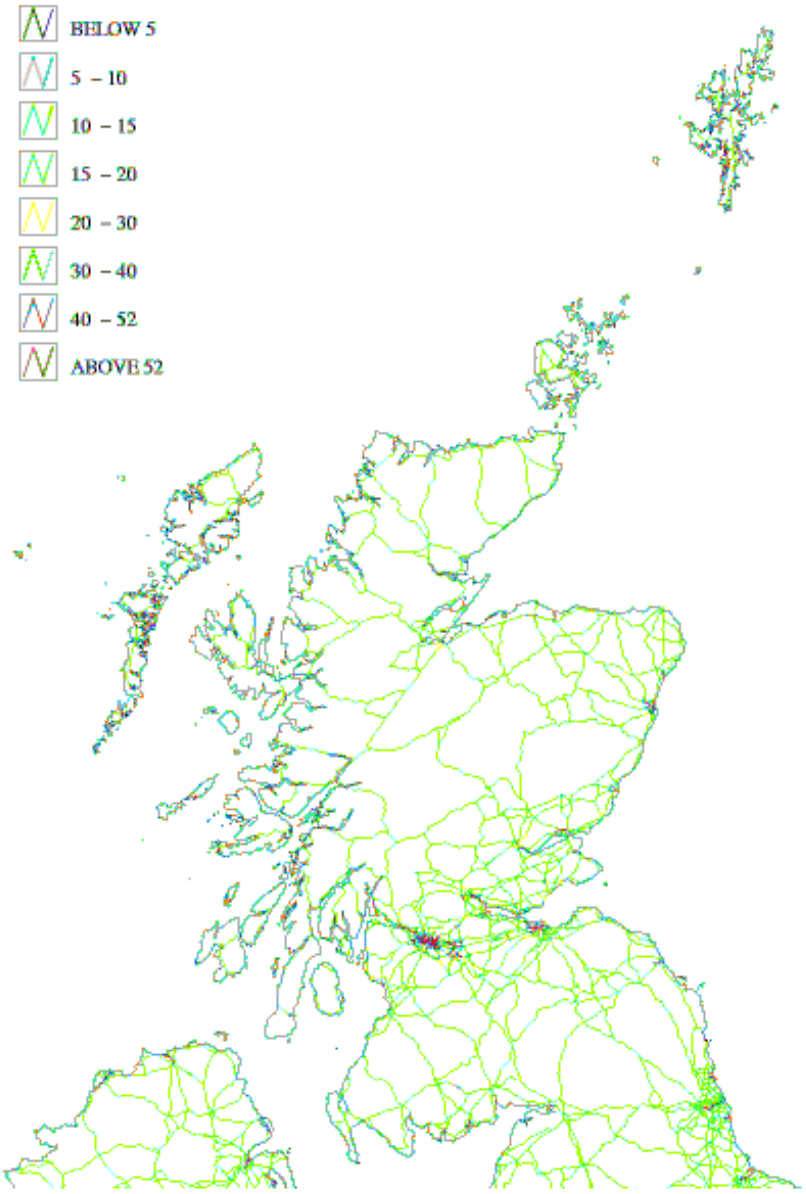


Figure 4.10 National model NO_2 roadside annual mean 2004 map for Scotland ($\mu g\ m^{-3}$)



5.0 TEOM and gravimetric PM_{10}

The PM_{10} modelling for Scotland was severely constrained by the availability of monitoring data with which to perform the calibration of the Scottish model. No gravimetric background remodelling was possible because both of the gravimetric sites were roadside sites. Despite these two roadside sites, no gravimetric roadside modelling was possible because without the gravimetric background map it is impossible to derive a roadside increment value with which to perform the roadside calibration. Although there were adequate TEOM monitoring sites to perform the background modelling, no roadside modelling was performed for Scotland because the only TEOM roadside site was Glasgow Kerbside which has been removed from the analysis as explained earlier. For these reasons, only TEOM background was remodelled using the new Scottish dispersion kernel and calibration but the national model gravimetric results for Scotland are presented here also.

Figure 5.1 shows the calibration plot for the TEOM annual mean model which was performed in a similar way as the background calibrations already described i.e. using the relationship between uncalibrated area source component (area source emissions maps with the Scottish dispersion kernel applied) and the measured TEOM annual mean adjusted for Part A process emissions, secondary components and the long-range transport primary component. The verification plots are shown in Figures 5.2 and 5.3. Figure 5.3 contains only national model results because not Scottish modelling was possible for gravimetric PM_{10} and Table 5.2a appears blank for this reason. The results are encouraging despite being based on very little data, with values around the 1:1 line in both scatterplots. Figure 5.2 illustrates that the Scottish model managed very little improvement to result over the national model. There is almost no discernible difference between the Scottish background TEOM model output and the national model output at the monitoring sites used, a feature that is confirmed by both Figure 5.2 and Table 5.1.

Figure 5.3 shows much the same as Figure 5.2 for national model background results. This is because the monitoring data used was a gravimetric equivalent based on TEOM data using the accepted factor of 1.3. The gravimetric national model roadside data in Figure 5.3 are particularly encouraging however and are based on genuine gravimetric data at Inverness and Dumfries, both of which lie very close either side of the 1:1 line.

No R^2 values are presented in Tables 5.2 or 5.3 because either there were too few points to obtain a meaningful value, the trend was negative or there was no modelled data. All sites fell within the 50% DQOs

Figures 5.4 and 5.5 show the Scottish model and national model TEOM PM_{10} maps which look very similar to each other. Both maps identify the large urban areas and busy motorways just as the maps for CO and NO_x and NO_2 did. The lower concentrations vary according to a generally south east to north west gradient. This is due to an underlying secondary particles component (typically nitrates and sulphates), which are at higher concentrations in the south and east of the UK and decline in the north westerly direction. The secondary component is also responsible for the blocky coarse resolution patterns that demark the Scottish Highlands. This is because the secondary components are modelled at a 20 x 20 km resolution before being added to the other components in the model. Figure 5.6 shows the national model gravimetric PM_{10} map and Figures 5.7 and 5.8 present the national roadside model TEOM and gravimetric PM_{10} maps.

Figure 5.1 Calibration of Scottish background TEOM PM_{10} annual mean 2004 model (μg m^{-3}, TEOM)

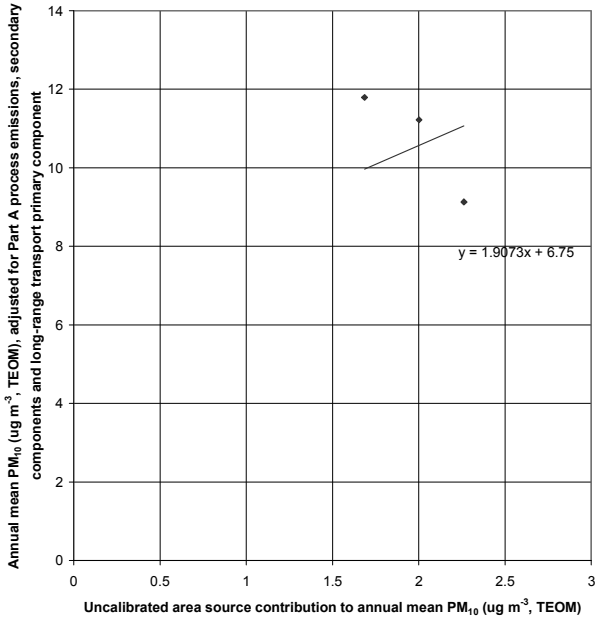


Figure 5.2 Verification of Scottish background TEOM PM_{10} annual mean 2004 model (μg m^{-3}, TEOM)

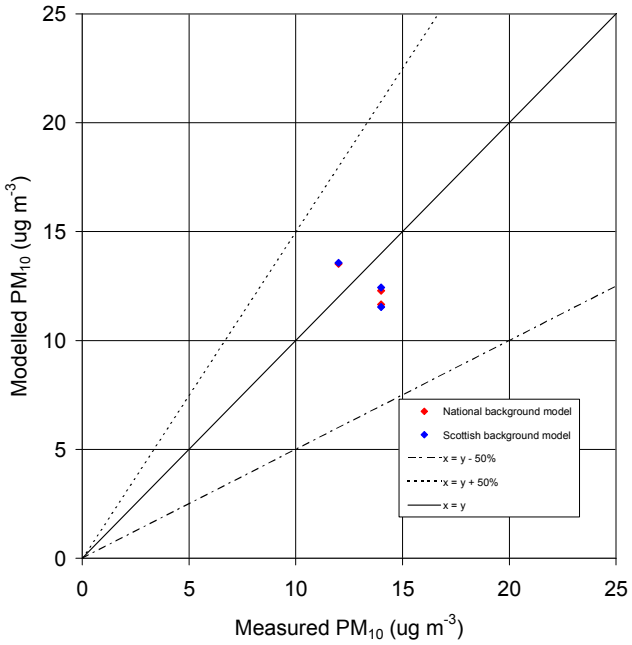


Figure 5.3 Verification of national background and roadside gravimetric PM_{10} annual mean 2004 model ($\mu g\ m^{-3}$, grav.)

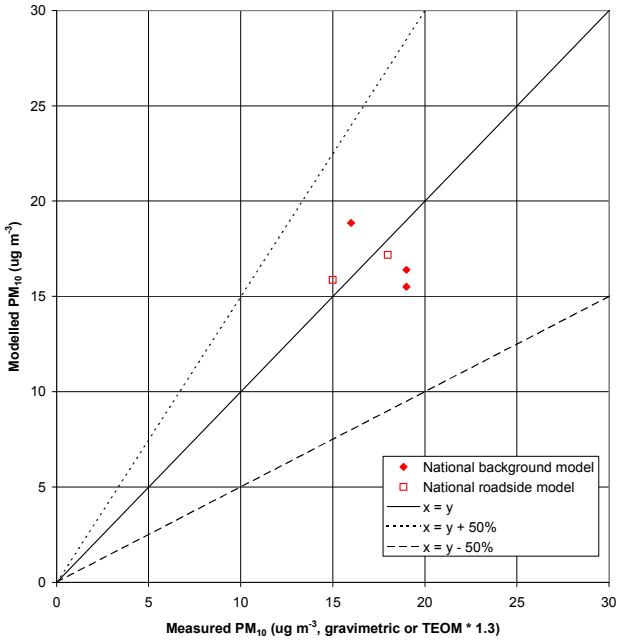


Table 5.1 TEOM PM_{10} annual mean 2004 verification summary ($\mu g\ m^{-3}$, TEOM)

a) Scottish model results

	Average modelled	Average monitored	R^2	Number sites used	Number sites within range	% sites within range
Background	12.51	13.33	-----	3	3	100
Roadside	-----	-----	-----	-----	-----	-----

b) National model results

	Average modelled	Average monitored	R^2	Number sites used	Number sites within range	% sites within range
Background	12.49	13.33	-----	3	3	100
Roadside	-----	-----	-----	-----	-----	-----

Table 5.2 Gravimetric PM_{10} annual mean 2004 verification summary ($\mu g\ m^{-3}$, grav.)

a) Scottish model results (no gravimetric Scotland model possible)

	Average modelled	Average monitored	R^2	Number sites used	Number sites within range	% sites within range
Background	-----	-----	-----	-----	-----	-----
Roadside	-----	-----	-----	-----	-----	-----

b) National model results

	Average modelled	Average monitored	R^2	Number sites used	Number sites within range	% sites within range
Background	16.9	18.0	-----	3	2	100
Roadside	16.5	16.5	-----	2	3	100

Figure 5.4 Scottish background model TEOM PM_{10} annual mean 2004 map ($\mu g\ m^{-3}$, TEOM)

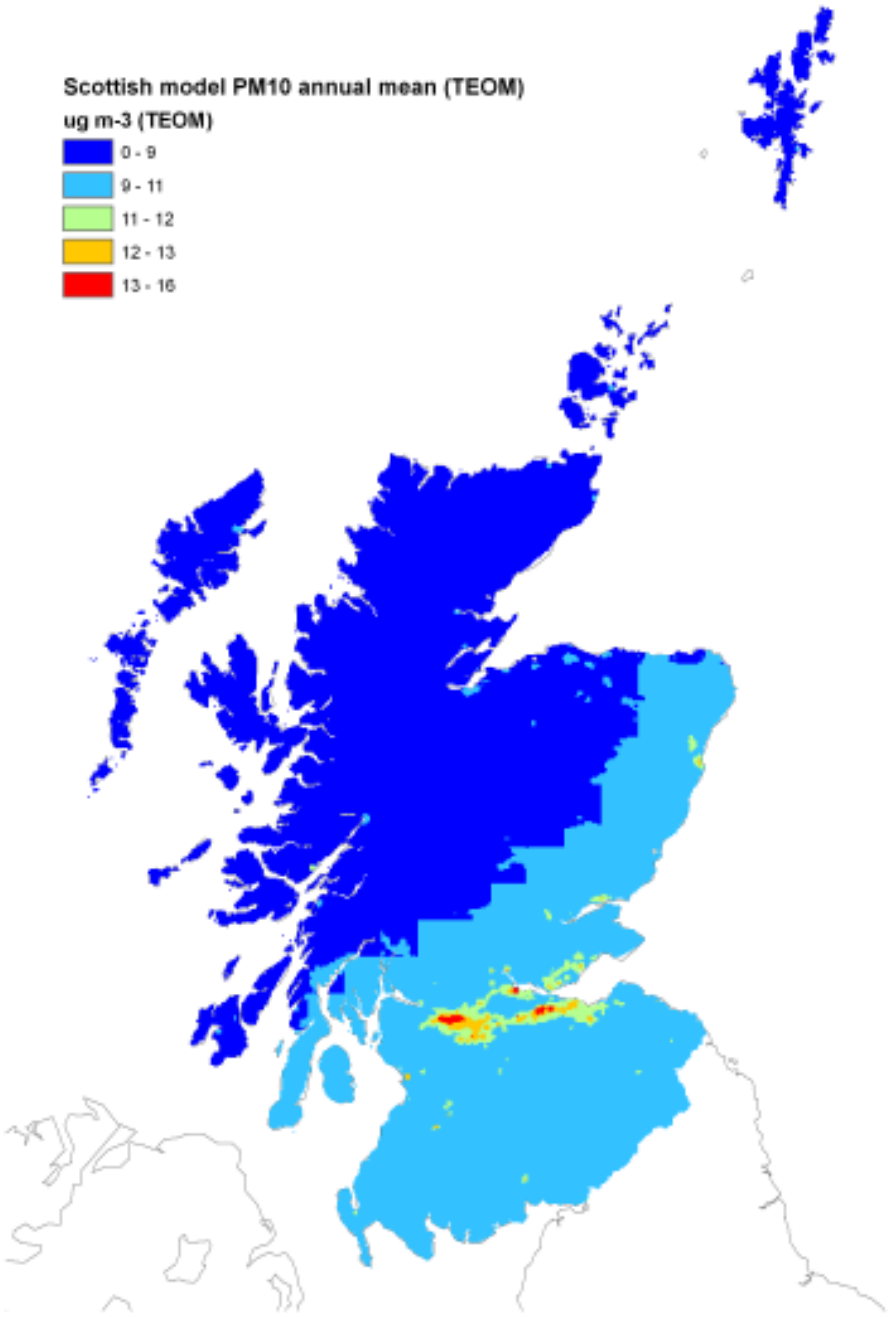


Figure 5.5 National background model TEOM PM_{10} annual mean 2004 map for Scotland ($\mu g\ m^{-3}$, TEOM)

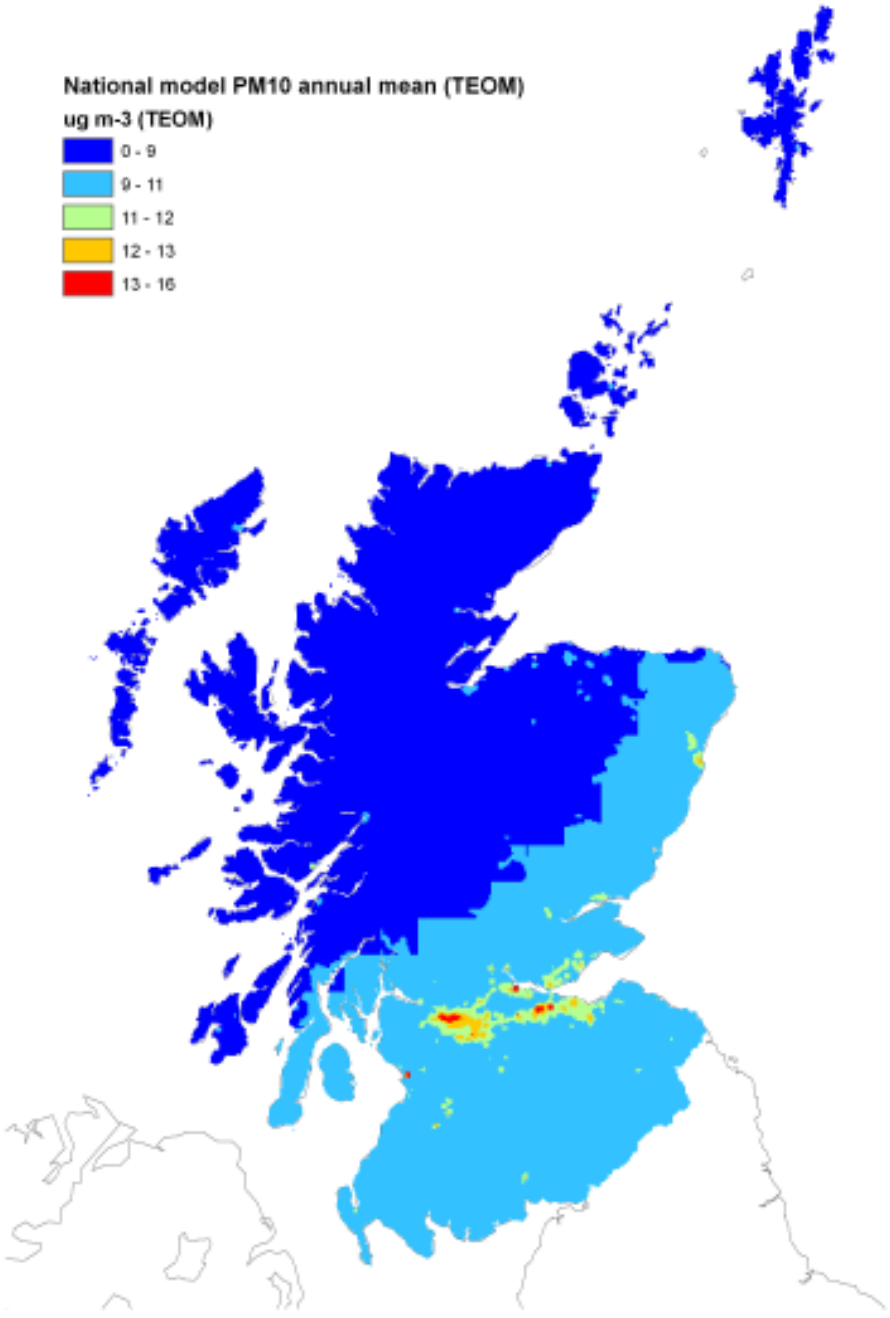


Figure 5.6 National background model gravimetric PM_{10} annual mean 2004 map for Scotland ($\mu g\ m^{-3}$, grav.)

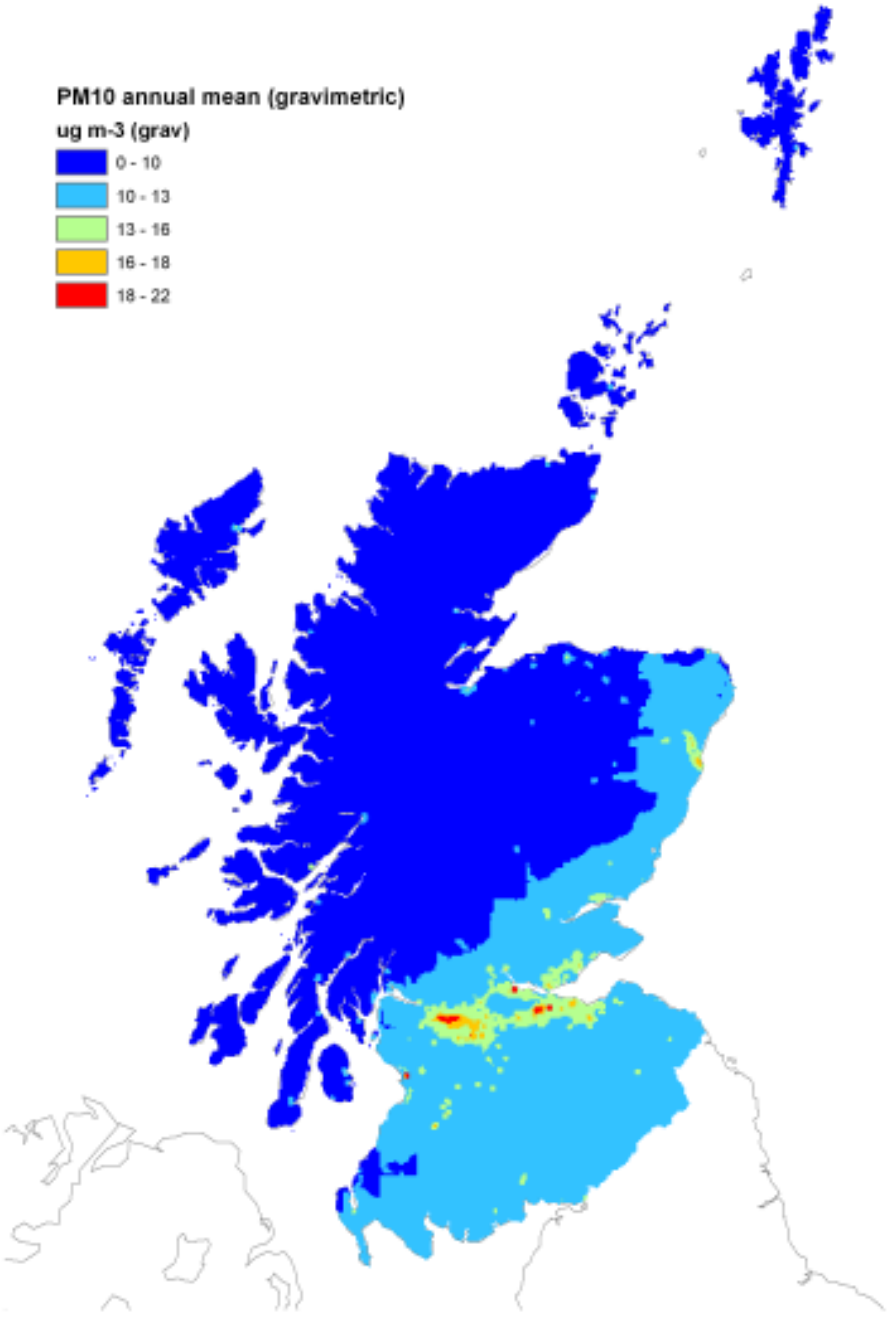


Figure 5.7 National roadside model TEOM PM_{10} annual mean 2004 map for Scotland ($\mu g\ m^{-3}$, TEOM)

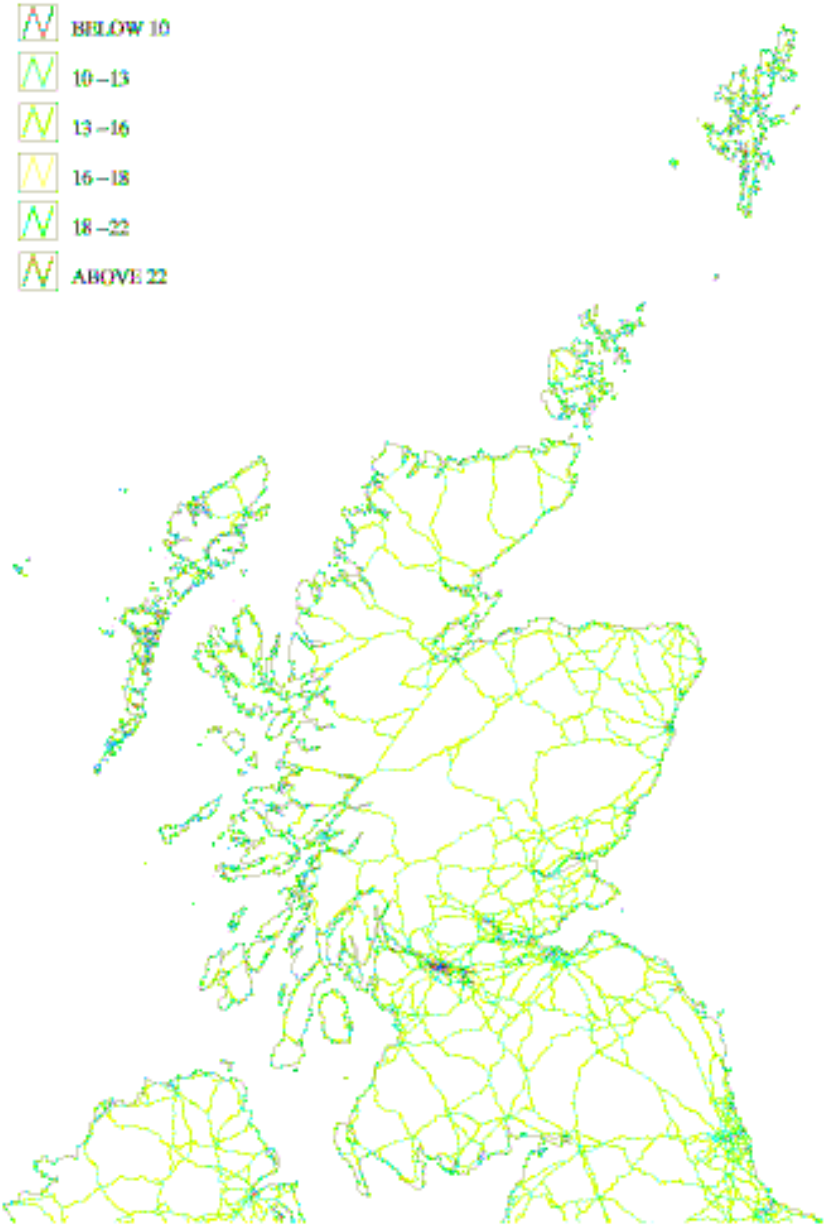
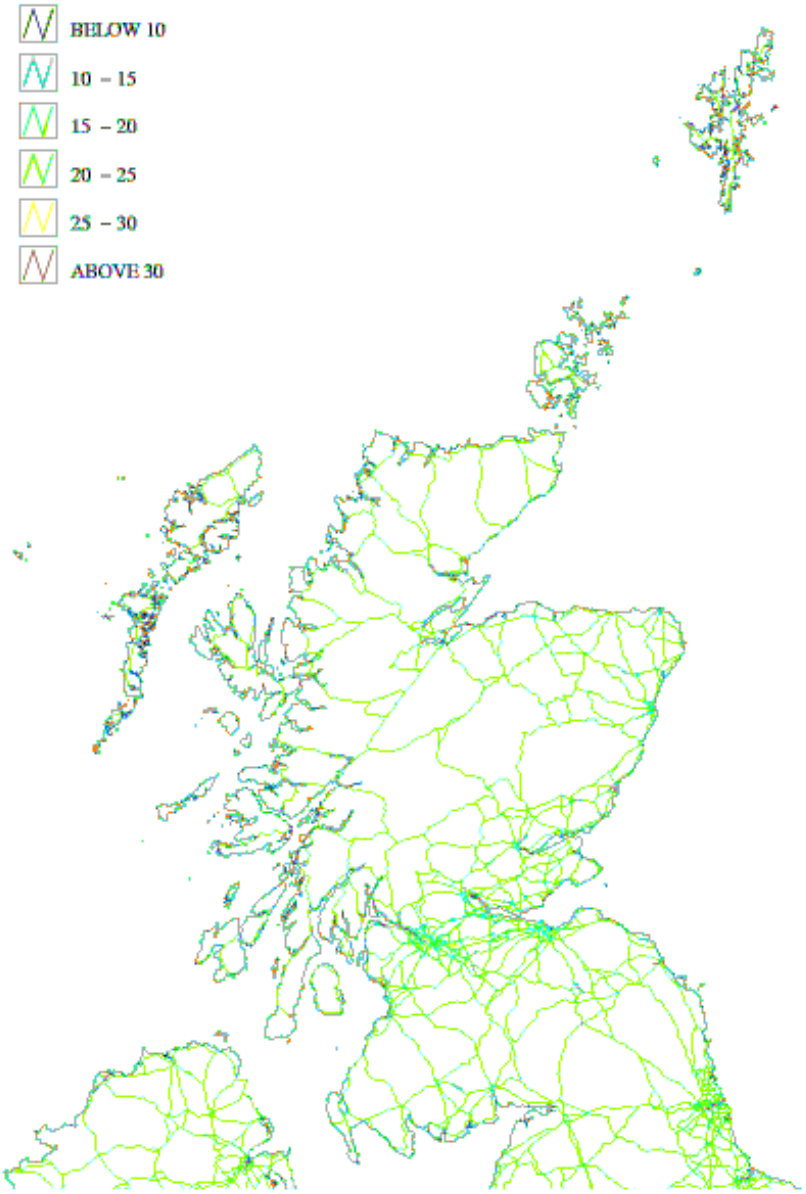


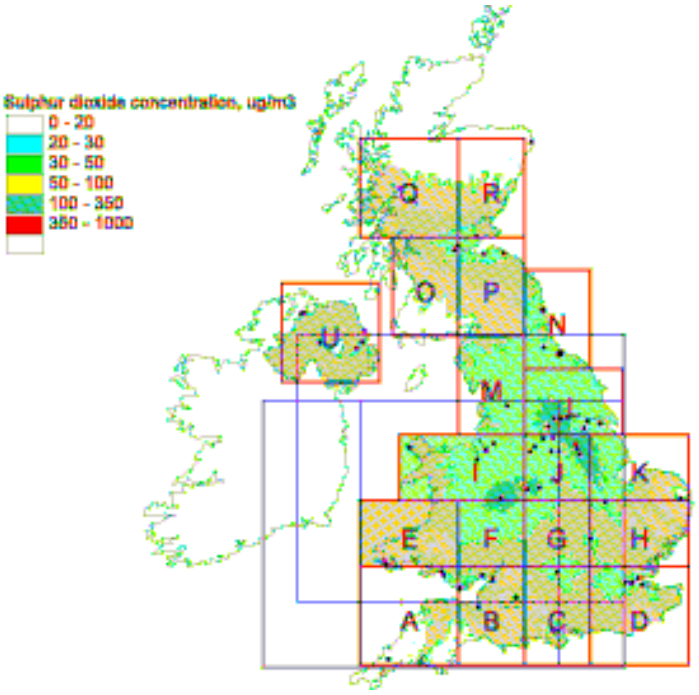
Figure 5.8 National roadside model gravimetric PM_{10} annual mean 2004 map for Scotland ($\mu g\ m^{-3}$, grav.)



6.0 SO_2

The SO_2 remodelling process for Scotland was more substantial than the case with the other pollutants. This is due to the significant influence of large point sources on SO_2 concentrations. Therefore, the model was adjusted to use the Scottish meteorological data from Edinburgh Airport for the large point sources in addition to using the Scottish dispersion kernel for the area sources and the calibration using Scottish sites. It is likely that the choice of met data will have a bigger impact on high percentile concentrations resulting from emissions from point sources than on the dispersion of low level area sources. The large point sources were modelled as a series of 6 separate tiles modelled in ADMS. Figure 6.1 shows the UK and the arrangement of these tiles used for the national mapping process. For the purpose of this exercise, the tiles labelled Q, R, O, P, M and N were used. Sources from Northern England and Northern Ireland influencing Scottish concentrations are taken into account by the tiling method because each tile includes emissions from large point sources in a 150km area surrounding the edge of the tile in addition to those within the tile.

Figure 6.1 Receptor tiles composing the UK



The calibration process for SO_2 differed from that of the other pollutants remodelled and involved reproducing the model equation in a spreadsheet and altering the coefficients used until the modelled Scottish site data represented the monitored data to a satisfactory standard in a verification plot. In addition to the measured concentrations from national automatic monitoring networks, the SO_2 model uses data supplied by rural automatic monitoring stations maintained by the electricity generating companies.

The annual mean model was modified to use a large point source coefficient of 1.1 (increased from 0.797 which was the national modelling coefficient used in 2004). This alteration of the model offered the best output result compared with the monitored data. This was also consistent with the coefficient of 1.2 used in the national model in 2005. The relationships established for the national high percentiles models were judged to provide a suitable result and so the coefficients for these metrics were retained in the models.

Verification plots of the annual mean and high percentile metrics are shown in Figures 6.2 to 6.5. The output from the Scottish SO_2 model compares reasonably well with the monitored data considering the complexity of SO_2 modelling although it should be noted that there are few data to draw robust conclusions from. Some of the monitoring sites used in the model report annual mean concentrations but do not report short-term data upon which the high percentile metrics are based – hence the reason for fewer sites in Figures 6.3 to 6.5. Of all the pollutants modelled, SO_2 is the most affected by large point sources, variations in which are hard to include in the model, particularly for the high percentile concentrations. For the higher percentile SO_2 modelling, the measured data depends greatly on the particular combination of meteorological conditions and hour by hour emissions. Hour by hour emissions are not known and reported monthly emission totals and typical profiles have been used in the modelling process.

The most favourable comparison of the national model output for SO_2 in Scotland can be seen in the annual mean metric which is less affected by emission timings and meteorology and R^2 values reflect this in both the national model (R^2 =0.81) and particularly the Scottish model (R^2 =0.93). The model appeared to under predict annual mean concentrations, particularly at the higher levels but concentrations at the lower end of the scale were overestimated and fell outside the DQO range, a feature that affected both Scottish and national models. Average modelled data from the Scottish model was closer to the average measured data than the national model was able to attain, as confirmed by Tables 6.2 to 6.4.

The 99.9th percentile of 15-minute mean Scottish model output underestimated Aberdeen but this was also underestimated to a similar extent by the national model. The Scottish model overestimated Glasgow Centre, as did the national model but the Scottish model appears to have exacerbated this and Glasgow Centre appears outside the +/- 50% range for the Scottish model. Although the model appears to have correctly predicted the exact concentration of 356 $\mu g\ m^{-3}$ at Grangemouth, this is an artefact of the modelling process. Where monitoring data used in the calibration process exceed the legislative objectives, this value is introduced into the map at the 1km square in which it has been measured, overriding any modelled value if this modelled value shows an underprediction. This is to ensure that the maps adequately represent measured exceedences where they exist (typically large industrial plant) for this pollutant. Figure 6.3 includes the Grangemouth data for illustrative purposes but since this data does not fairly represent the performance of the model it has been omitted from the calculations presented in Table 6.2. The remaining sites showed a very good agreement with the monitored data and demonstrated an improvement on the national model results.

Both the 99.73rd hourly percentile output and the 99.18th 24-hourly percentile output significantly underestimated concentrations at Grangemouth and overestimated concentrations at Glasgow Centre in both models. Grangemouth is a significant industrial source of SO_2, high percentile concentrations of which depend greatly on timing of emissions and meteorology that are not well represented in the model. The Scottish model has improved on the national model result at Grangemouth but appears to have exacerbated the over prediction of Glasgow Centre. Both these monitoring sites remain outside the 50% range shown in both models. The remaining data appears to show a favourable result for the Scottish model in both metrics which has resulted in a good fit around the 1:1 line.

Overall the Scottish maps show less of an under prediction than the national maps, showing the impact of using more local met data.

Background maps are presented for Scotland in Figures 6.6 to 6.13. Roadside maps are not prepared for SO_2 because variations in SO_2 concentrations between background and roadside locations are negligible. The SO_2 maps display similar characteristic with a particularly prominent block pattern centred on Grangemouth. This is result of large point sources (one of which is Grangemouth) being modelled using the 100 x 100 km tiles. This pattern is exhibited in the high percentile SO_2 maps and to a lesser extent in the annual mean SO_2 map.

Figure 6.2 Verification of Scottish background SO_2 annual mean 2004 model ($\mu g\ m^{-3}$)

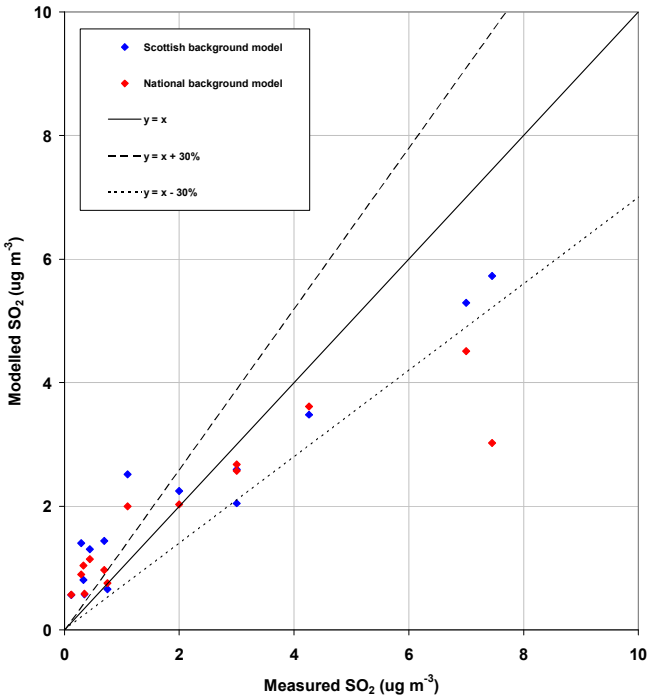


Figure 6.3 Verification of Scottish background SO_2 p99.9 15-minute mean 2004 model ($\mu g\ m^{-3}$)

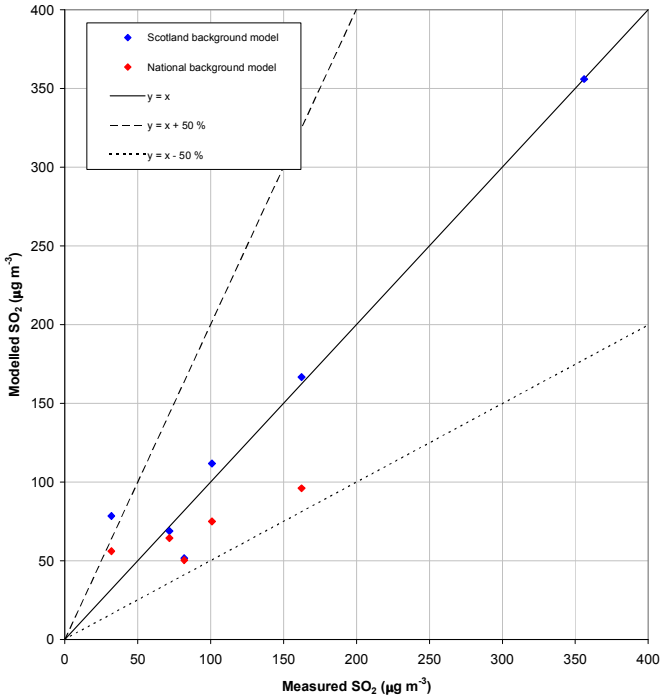


Figure 6.4 Verification of Scottish background SO_2 p99.73 1-hour mean 2004 model (μg m^{-3})

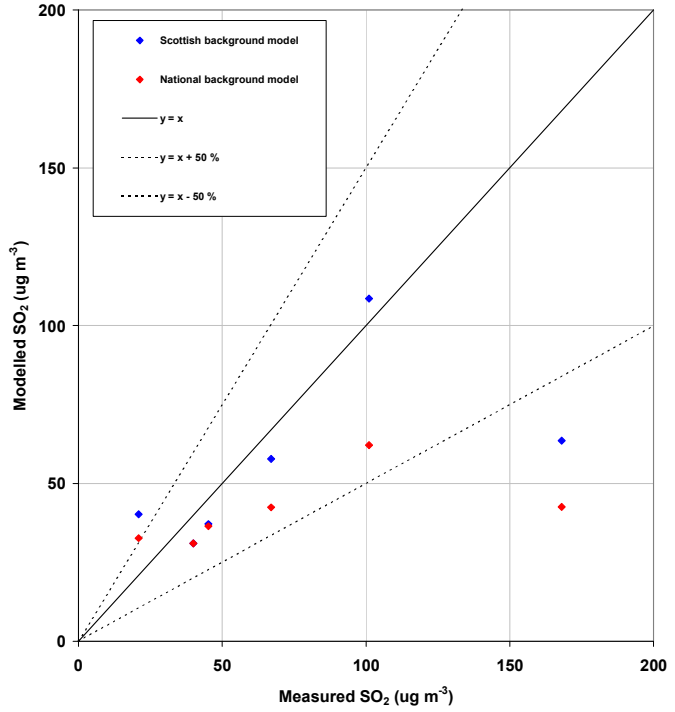


Figure 6.5 Verification of Scottish background SO_2 p99.18 24-hour mean 2004 model (μg m^{-3})

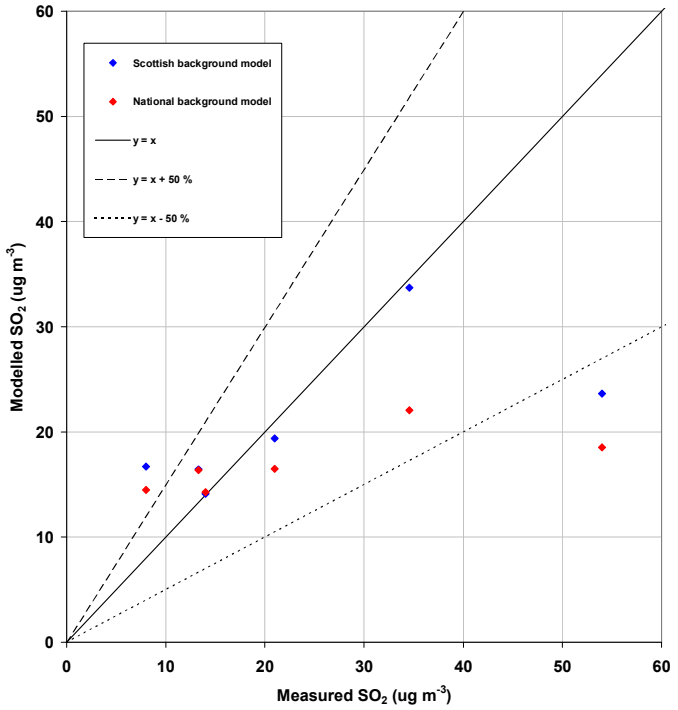


Table 6.1 SO_2 annual mean 2004 verification summary ($\mu g\ m^{-3}$)

	Average modelled	Average monitored	R^2	Number sites used	Number sites within range	% sites within range
Scottish background model	2.2	2.2	0.93	14	6	43
National background model	1.9	2.2	0.81	14	5	36

Table 6.2 SO_2 p99.9 15-minute mean 2004 verification summary ($\mu g\ m^{-3}$)

	Average modelled	Average monitored	R^2	Number sites used	Number sites within range	% sites within range
Scottish background model	95.5	89.8	0.68	5	4	80
National background model	68.4	89.8	0.76	5	5	100

Table 6.3 SO_2 p99.73 1-hour mean 2004 verification summary ($\mu g\ m^{-3}$)

	Average modelled	Average monitored	R^2	Number sites used	Number sites within range	% sites within range
Scottish background model	56.4	73.7	0.32	6	4	67
National background model	41.2	73.7	0.29	6	4	67

Table 6.4 SO_2 p99.18 24-hour mean 2004 verification summary ($\mu g\ m^{-3}$)

	Average modelled	Average monitored	R^2	Number sites used	Number sites within range	% sites within range
Scottish background model	20.7	24.1	0.43	6	4	67
National background model	17.0	24.1	0.49	6	4	67

Figure 6.6 Scottish background model SO_2 annual mean 2004 map ($\mu g\ m^{-3}$)

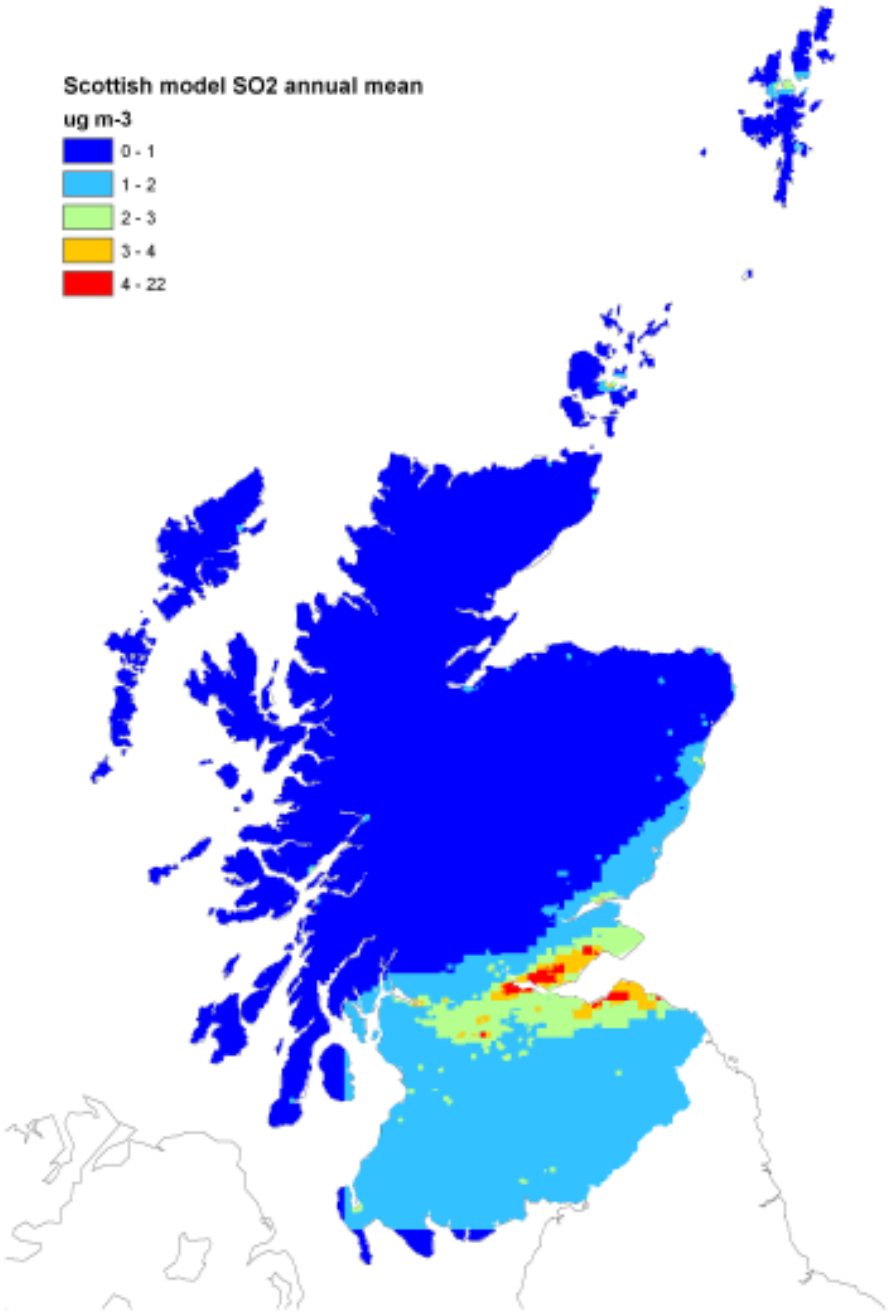


Figure 6.7 National background model SO_2 annual mean 2004 map for Scotland ($\mu g\ m^{-3}$)

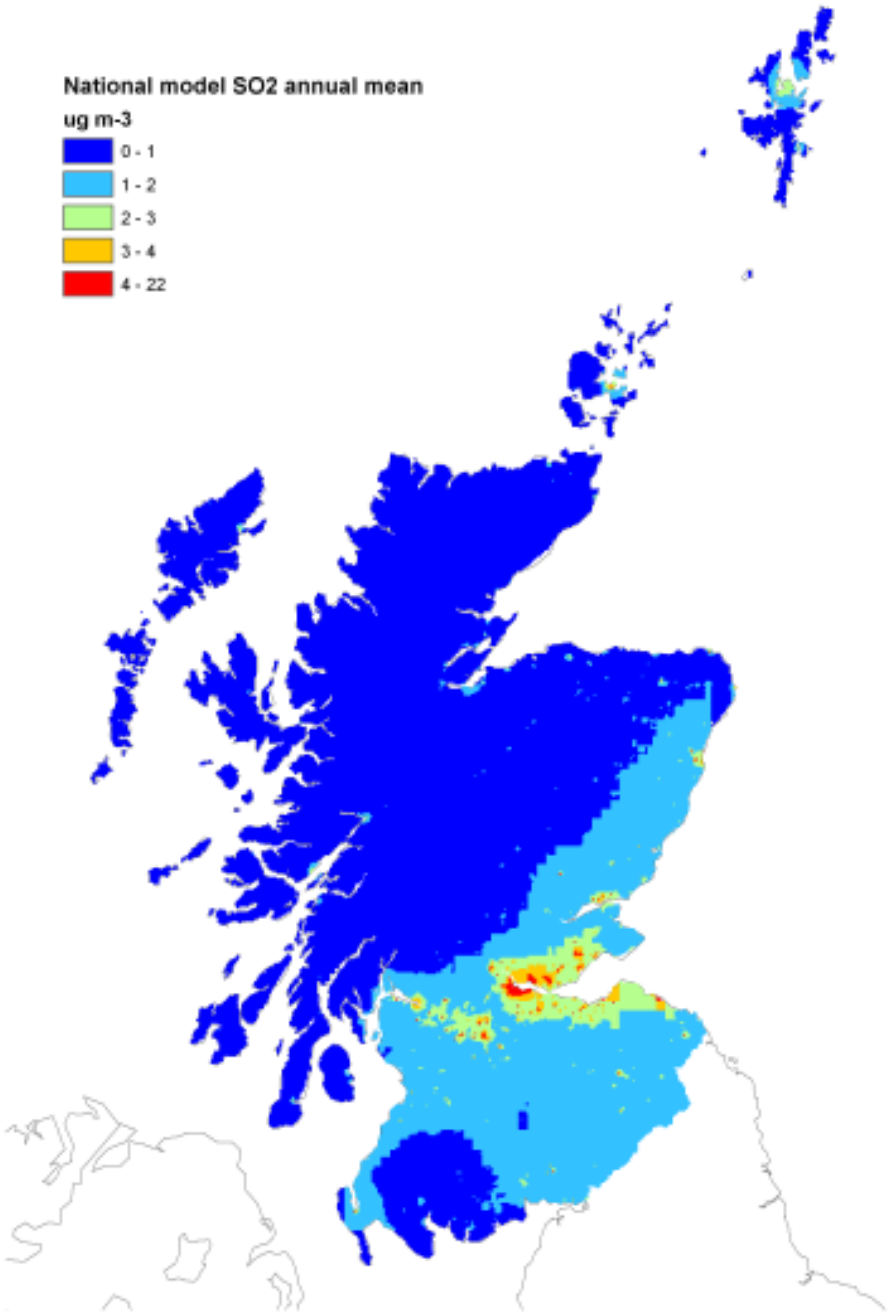


Figure 6.8 Scottish background model SO_2 p99.9 15-minute mean 2004 map ($\mu g\ m^{-3}$)

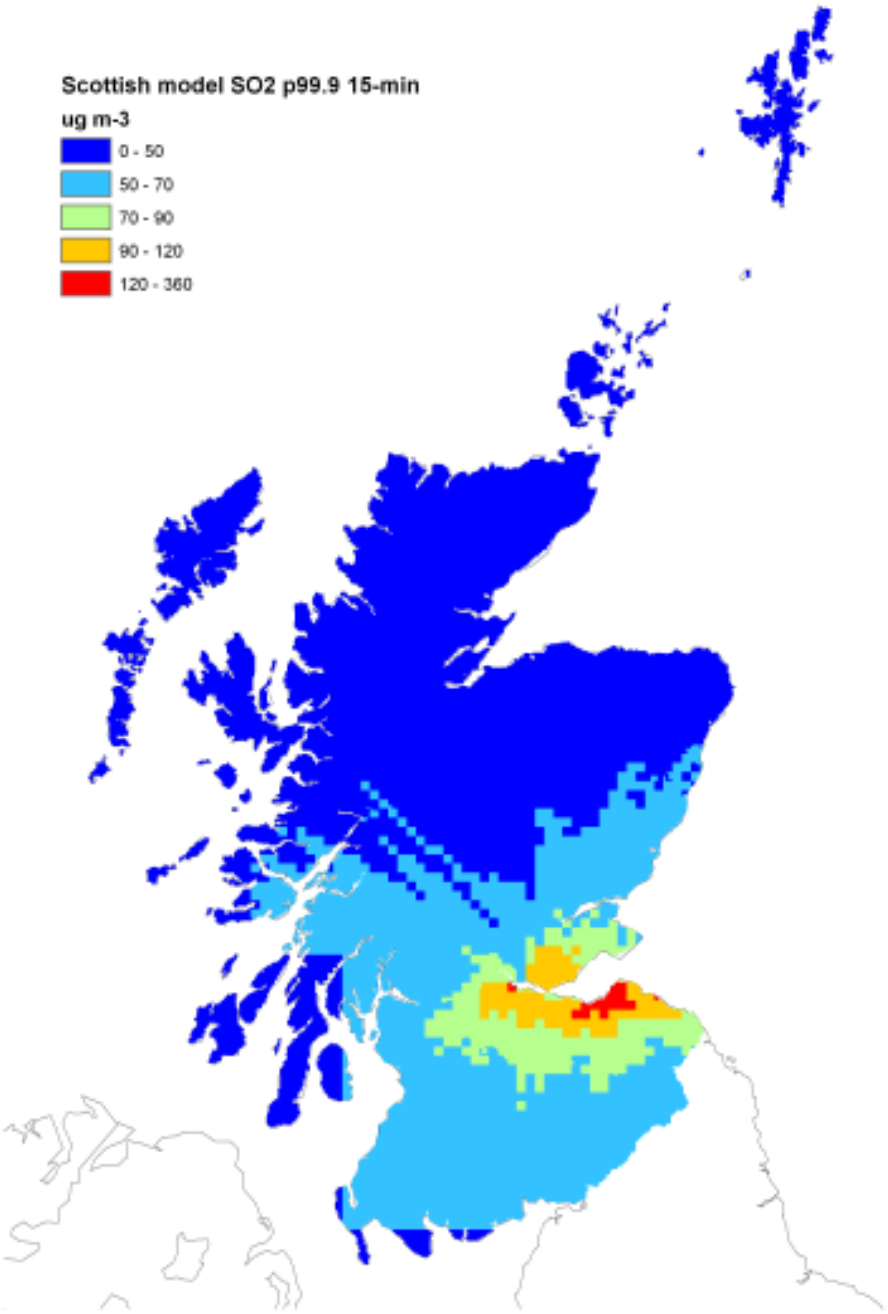


Figure 6.9 National background model SO_2 p99.9 15-minute mean 2004 map for Scotland ($\mu g\ m^{-3}$)

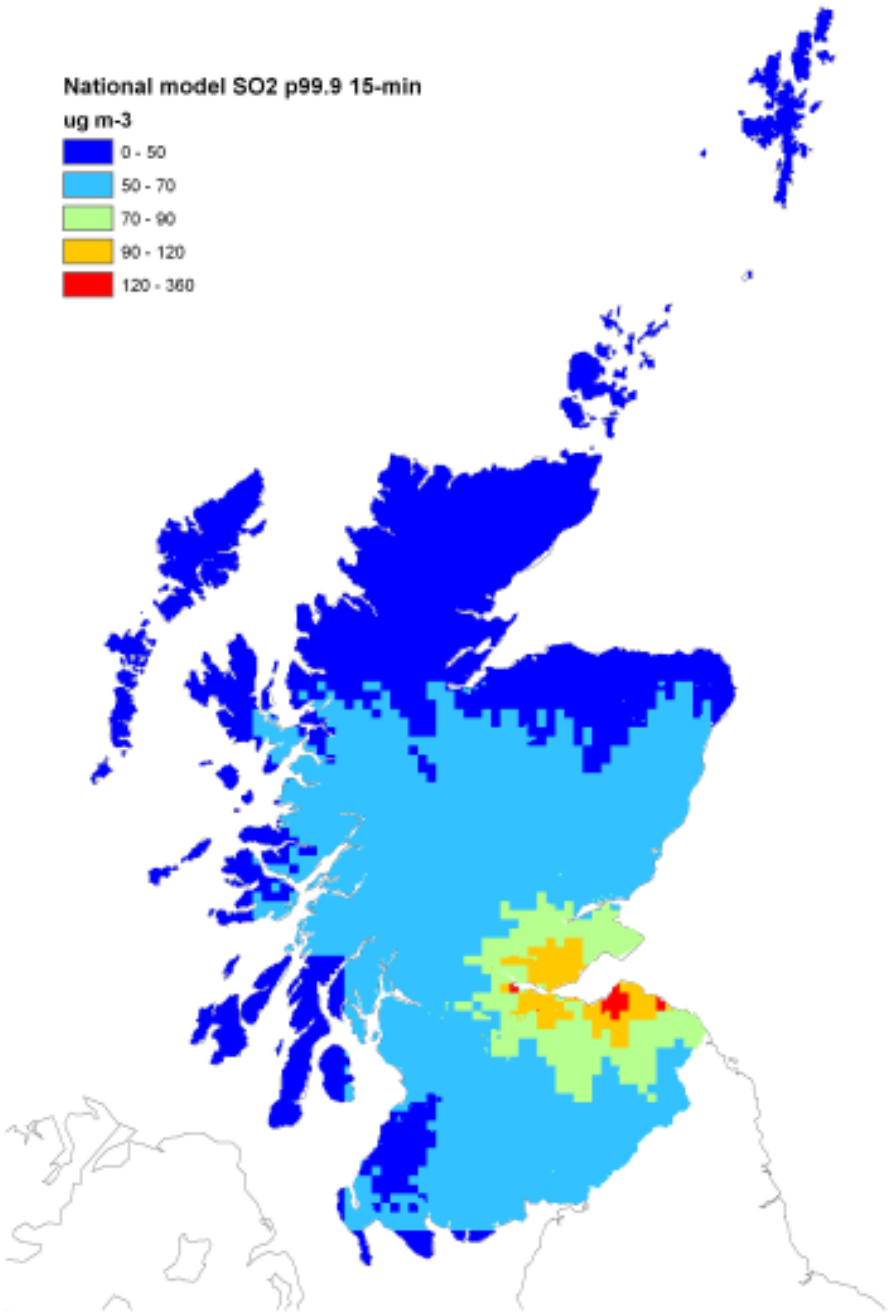


Figure 6.10 Scottish background model SO_2 p99.73 1-hour mean 2004 map ($\mu g\ m^{-3}$)

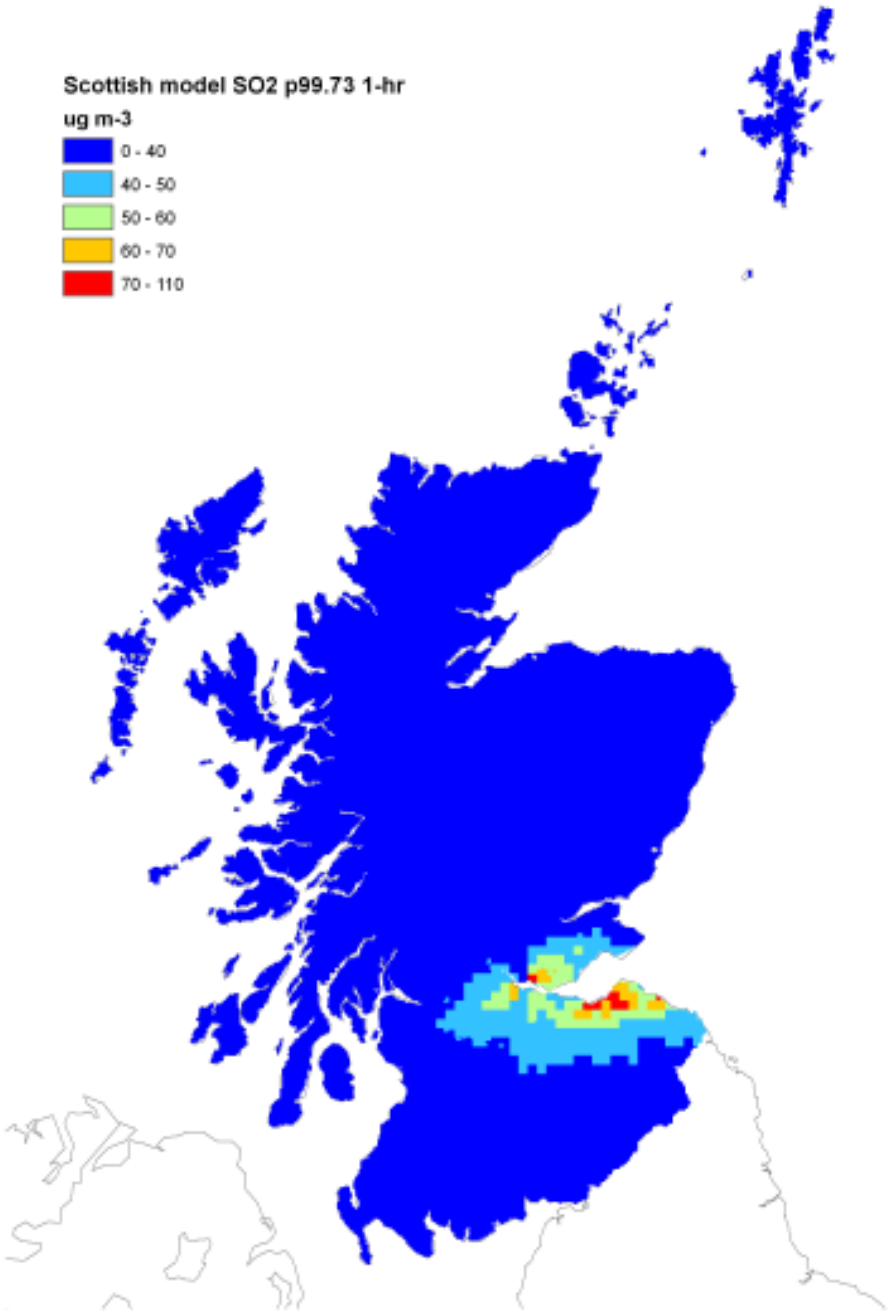


Figure 6.11 National background model SO_2 p99.73 1-hour mean 2004 map for Scotland ($\mu g\ m^{-3}$)

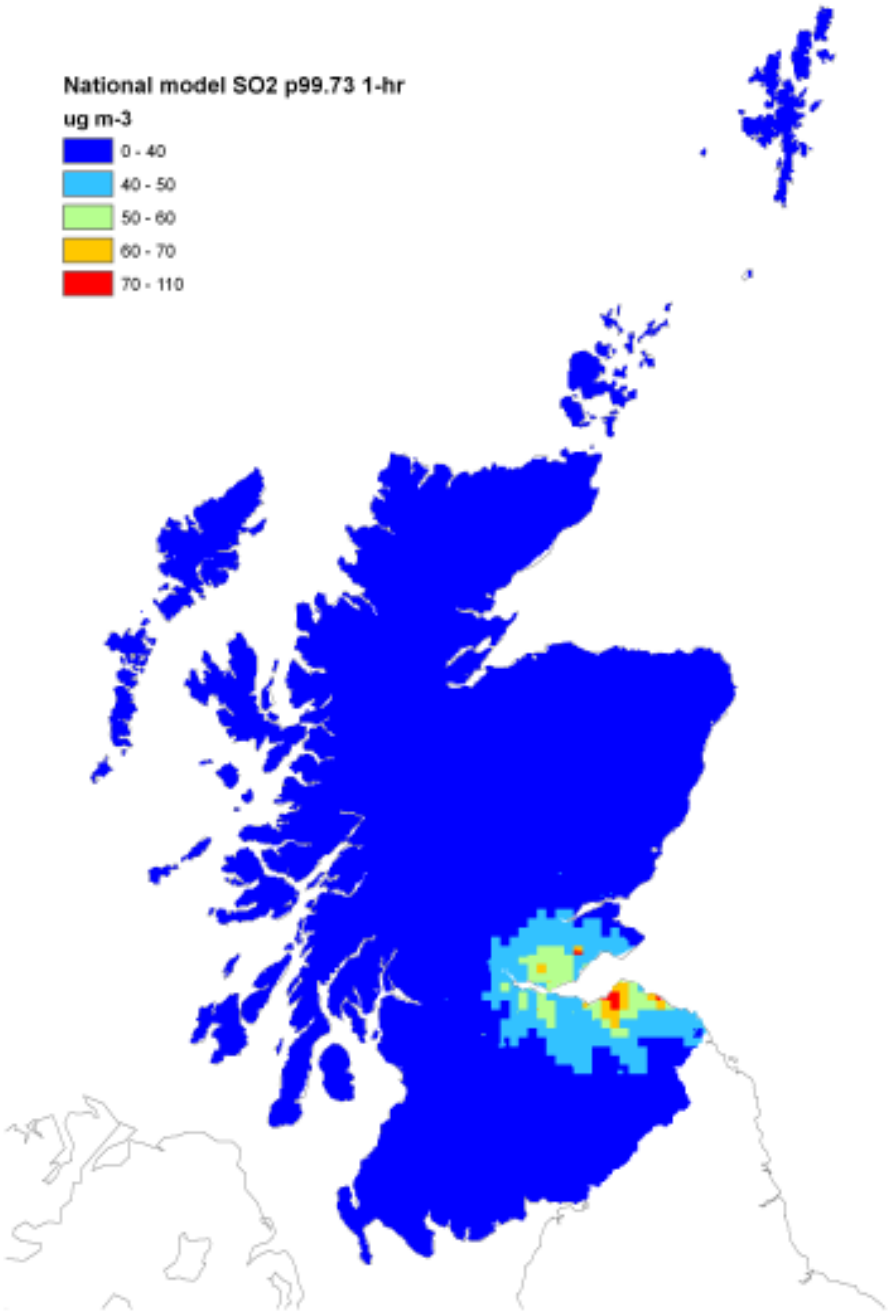


Figure 6.12 Scottish background model SO_2 p99.18 24-hour mean 2004 map ($\mu g\ m^{-3}$)

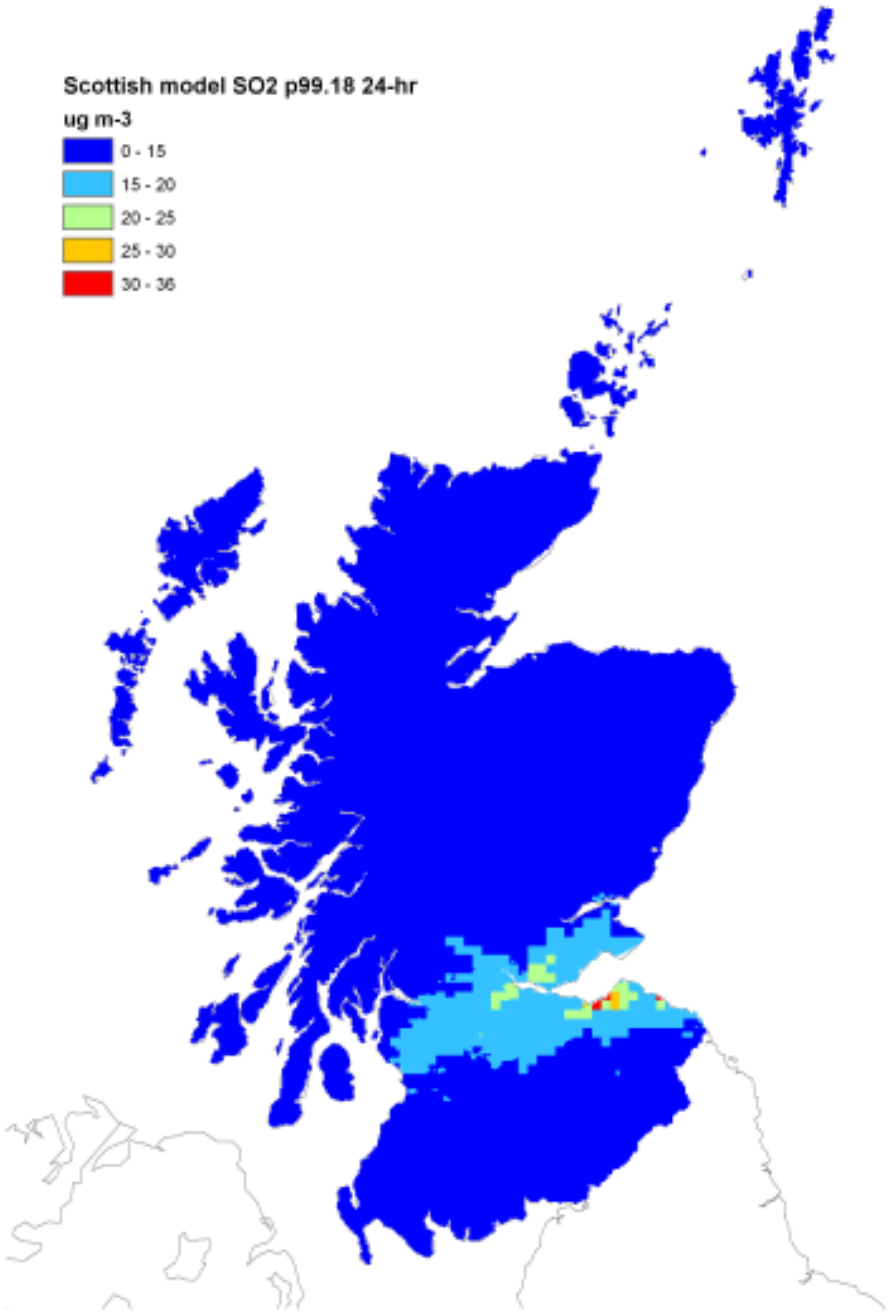
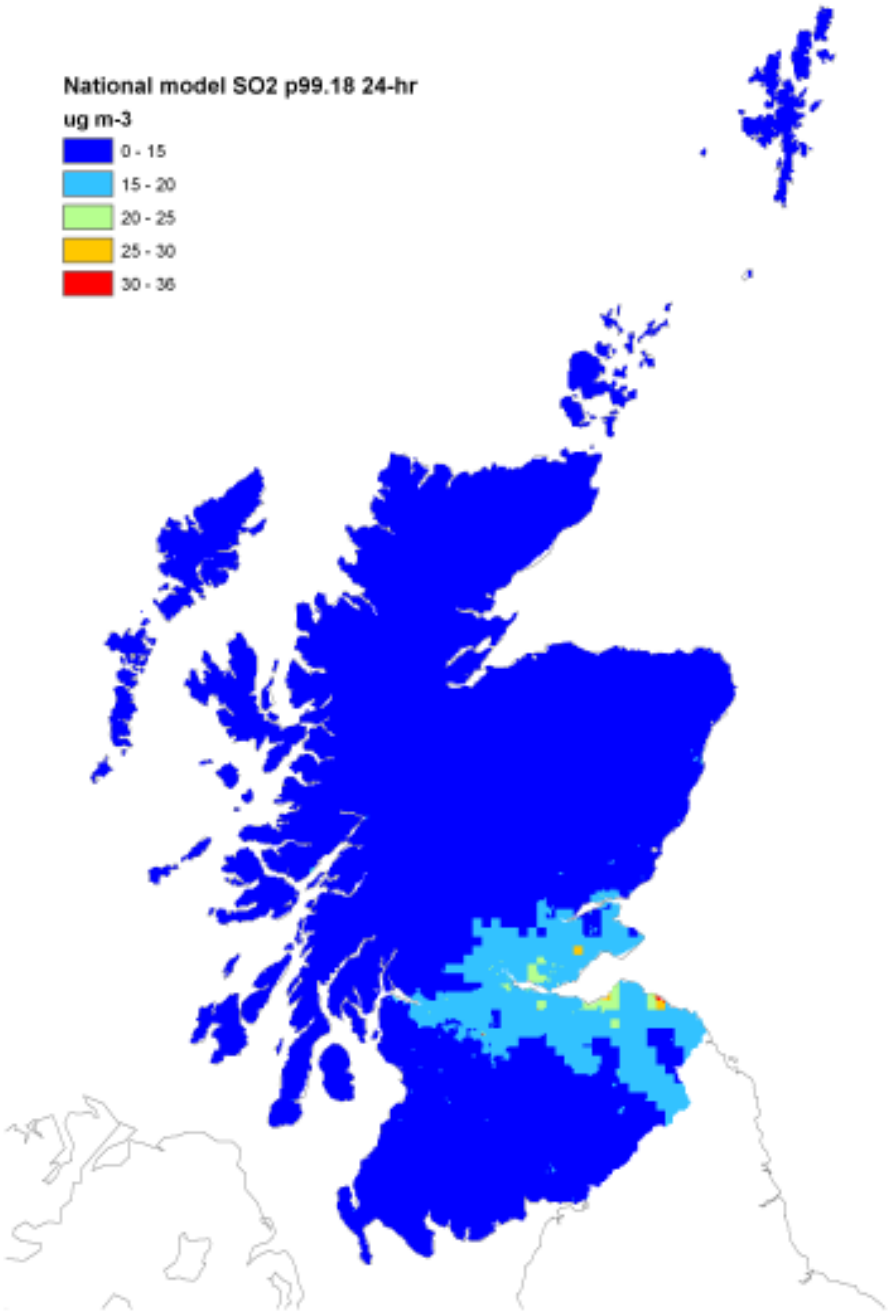


Figure 6.13 National background model SO_2 p99.18 24-hour mean 2004 map for Scotland ($\mu g\ m^{-3}$)



7.0 Conclusions

- The Scottish model demonstrated an improvement over the national model in annual mean and maximum 8-hour CO concentrations - the improvement in the maximum 8-hour metric was due to a large extent to the annual mean to maximum 8-hour relationship.

- The Scottish model results for NO_2 and NO_x were quite similar to the results provided by the national model but the Scottish model displays a marginally better fit about the 1:1 line – the result of the calibration based on these sites.

- The Scottish and national models were very similar in terms of the TEOM PM_{10} outputs. This feature is not surprising given the identical treatment of the secondary components in both models.

- For the year 2004, there is not really enough monitoring data to perform a robust calibration or to perform a fully independent verification of the Scottish model. Repeating the exercise in future is unlikely to prove any worth without more high quality monitoring data – perhaps twice as many monitoring sites.

- The exception to this is SO_2 where there are more monitoring sites to use as a result of the incorporation of rural automatic monitoring data courtesy of the electricity generating industry and where the Scotland specific meteorological data appears to have yielded the largest improvement.

8.0 References

Stedman, J R, Bush, T J, Grice, S E, Kent, A J, Vincent K J, Abbott, J and Derwent, R G (2006). UK air quality modelling for annual reporting 2004 on ambient air quality assessment under Council Directives 96/62/EC, 1999/30/EC and 2000/69/EC. AEA Technology, National Environmental Technology Centre (Ref. AEAT/ENV/R/2052 Issue 1)