Technical report on UK supplementary assessment under the Air Quality Directive (2008/50/EC), the Air Quality Framework Directive (96/62/EC) and Fourth Daughter Directive (2004/107/EC) for 2013

Report for Report for The Department for Environment, Food and Rural Affairs, Welsh Government, the Scottish Government and the Department of the Environment for Northern Ireland

Ricardo-AEA/R/3421 Issue 1
ED57728
Date 15/10/2015

Customer:

The Department for Environment, Food and Rural Affairs, Welsh Government, the Scottish Government and the Department of the Environment for Northern Ireland

Customer reference:

AQ0650

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15 October 2015

Ricardo-AEA reference:

Ref: Ricardo-AEA/R/3421 Issue 1 ED57728

Executive summary

European Union directives on ambient air quality require member states including the UK to undertake air quality assessments, and to report the findings of these assessments to the European Commission on an annual basis:

- The Directive on ambient air quality and cleaner air for Europe (2008/50/EC), which is known as the ‘Air Quality Directive’ (AQD)
- The fourth Daughter Directives 2004/107/EC (AQDD4) under the Air Quality Framework Directive (1996/62/EC).

The UK annual air quality assessment for the year 2013 has been undertaken in accordance with the requirements of the AQD and the AQDD4. The assessment takes the form of comparisons of measured and modelled air pollutant concentrations with the limit values, critical levels, target values and long term objectives set out in the directives. The AQD includes a requirement to deduct the contribution to ambient PM from natural sources. The results were submitted to the European Commission in September 2014 in the form of e-Reporting Data flows (specifically Data flow G on attainment) that each member state must complete and upload onto the Central Data Repository of the European Environment Agency: http://cdr.eionet.europa.eu/gb/eu/aqd/ (CDR, 2014).

The AQD sets limit values for the ambient concentrations to be achieved for:

- sulphur dioxide (SO_2)
- nitrogen dioxide (NO_2)
- particles (PM_{10})
- lead (Pb)
- benzene (C_6H_6)
- carbon monoxide (CO)

The AQD also includes:

- critical levels for the protection of vegetation to be achieved for ambient concentrations of sulphur dioxide (SO_2) and oxides of nitrogen (NO_x)
- a target value, limit values, an exposure concentration obligation and exposure reduction targets for fine particles ($PM_{2.5}$)
- target values and long-term objectives for ozone (O_3)

AQDD4 sets target values for the ambient concentrations to be achieved for:

- Arsenic (As)
- Cadmium (Cd)
- Nickel (Ni)
- Benzo(a)Pyrene (B(a)P)

This report provides a summary of key attainment results from the e-reporting submission for the AQD and AQDD4 pollutants and technical information on the modelling methods that have been used.

The UK has been divided into 43 zones for air quality assessment. There are 28 agglomeration zones (large urban areas) and 15 non-agglomeration zones. The status of the zones in relation to the limit values, critical levels, target values and long term objectives has been assessed.

The results of the assessment against limit values are summarised in Table E1. The table shows no exceedance of the daily mean limit value for PM_{10} for the Greater London Urban Area. However, it should be noted that there was one exceedance of the daily mean limit value for PM_{10} before subtraction of natural sources. Table E1 also shows that 38 zones have not achieved full compliance with the annual NO_2 limit value in 2013. One zone was also non-compliant with the hourly limit value in 2013. The UK has been granted a time extension for the annual mean limit value for 12 zones in 2013.

Table E2 summarises the results of the assessment for O_3 in terms of the numbers of zones with exceedances of the target values and long term objectives. Table E3 shows that there were no exceedances of the target value or stage 1 limit value for $PM_{2.5}$. There was an exceedance of the stage 2 indicative limit value for $PM_{2.5}$, which is not currently in force, in one zone. Table E4 lists no exceedances of old directives in 2013.

The results of the assessment against the target values for AQDD4 pollutants are presented in Table E5.

Table E1. Summary results of air quality assessment for 2013: comparison with limit values and critical levels

Pollutant	Averaging time	Number of zones exceeding limit value
SO_2	1-hour	none
SO_2	24-hour	none
SO_2	Annual[1]	none
SO_2	Winter[1]	none
NO_2	1-hour[2]	1 zone measured (Greater London Urban Area)
NO_2	Annual	38 zones (9 measured + 29 modelled)
NO_x	Annual[1]	none
PM_{10}	24-hour	none (*1 zone modelled, Greater London Urban Area before subtraction of natural contribution*)
PM_{10}	Annual	none
Lead	Annual	none
Benzene	Annual	none
CO	8-hour	none

1 - Critical levels rather than LVs applying to vegetation and ecosystem areas only.
2 - No modelling for 1-hour LV

Table E2. Summary results of air quality assessment for 2013 for O_3: comparison with target values and long term objectives

Pollutant	Averaging time	Number of zones exceeding target value	Number of zones exceeding long term objective
O_3	8-hour	none	33 zones (21 measured + 12 modelled)
O_3	AOT40	none	8 zones (6 measured + 2 modelled)

Table E3. Summary results of air quality assessment for 2013 for $PM_{2.5}$: comparison with target value and limit value and exposure concentration obligation

Pollutant	Averaging time	Number of zones exceeding target value
$PM_{2.5}$	Annual target value (25 µg m^{-3})	none
$PM_{2.5}$	Annual limit value (25 µg m^{-3})	none
$PM_{2.5}$	Annual limit value (Indicative Stage 2, 20 µg m^{-3})	1 zone (modelled, Greater London Urban Area) *Remains after subtraction of natural contribution*
$PM_{2.5}$	Exposure concentration obligation (20 µg m^{-3})	Not exceeded

Table E4. Exceedances of old Directives

Pollutant	Directive	Averaging time (limit value)	Concentration (µg m^{-3})
NO_2	85/203/EEC	1-hour 98%ile (200 µg m^{-3})	none

Table E5. Summary results of AQDD4 air quality assessment for 2013: comparison with target values

Pollutant	Averaging time	Number of zones exceeding target value
As	Annual	None
Cd	Annual	None
Ni	Annual	2 zones (1 measured Swansea, 1 modelled South Wales)
B(a)P	Annual	6 zones (1 measured + 5 modelled)

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1 Introduction

1.1 The EU ambient air quality directives

European Union directives on ambient air quality require member states including the UK to undertake air quality assessments, and to report the findings of these assessments to the European Commission on an annual basis. Historically this was done according to:

- The Air Quality Framework Directive (1996/62/EC)
- The four Daughter Directives 1999/30/EC, 2000/69/EC, 2002/3/EC and 2004/107/EC.

In June 2008, a new directive came into force: the Council Directive on ambient air quality and cleaner air for Europe (2008/50/EC), which is known as the ‘Air Quality Directive’ (AQD). This directive consolidates the first three Daughter Directives, and was transposed into Regulations in England, Scotland, Wales and Northern Ireland in June 2010. The 4th Daughter Directive (AQDD4), 2004/107/EC, remains in force.

The UK annual air quality assessment for the year 2013 has been undertaken in accordance with the requirements of the AQD and the AQDD4. The assessment takes the form of comparisons of measured and modelled air pollutant concentrations with the limit values, critical levels, target values and long term objectives set out in the directives. The results were submitted to the European Commission in September 2014 in the form of e-Reporting Data flows (specifically Data flow G on attainment) that each member state must complete and upload onto the Central Data Repository of the European Environment Agency: http://cdr.eionet.europa.eu/gb/eu/aqd/ (CDR, 2014).

The air quality assessment has been reported via the following e-Reporting Data flows required by decision 2011/850/EU:

- B: Zones and agglomerations
- C: Assessment regime
- D: Assessment methods
- E: Primary validated assessment data
- G: Attainment

Information on the supplementary assessment methods (modelling and objective estimations) has been provided in Data flows C and D and model results have been provided in Data flows E and G. Data flow G effectively replaces forms 8, 9 and 19 of the questionnaire previously compiled according to decision 2004/461/EC.

An important change between the Framework and Daughter Directives and the AQD has been a requirement to deduct the contribution to ambient PM from a wider range of natural sources prior to the comparison with limit values than specified in the Framework and Daughter Directives. This requirement was included for the first time in the assessment of concentrations for 2008 and in accordance with the AQD has also been included in the annual assessments from 2009 to 2013.

The AQD sets limit values (LV) for the ambient concentrations to be achieved for:

- sulphur dioxide (SO_2)
- nitrogen dioxide (NO_2)
- particles (PM_{10})
- lead (Pb)
- benzene (C_6H_6)
- carbon monoxide (CO)

The AQD also includes:

- critical levels (CL) for the protection of vegetation to be achieved for ambient concentrations of sulphur dioxide (SO_2) and oxides of nitrogen (NO_x)
- a target value (TV), limit values, an exposure concentration obligation (ECO) and national exposure reduction targets (NERT) for fine particles ($PM_{2.5}$)
- target values (TVs) and long-term objectives (LTOs) for ozone (O_3)

AQDD4 sets target values to be achieved for:

- arsenic (As)
- cadmium (Cd)
- nickel (Ni)
- polycyclic aromatic hydrocarbons with benzo(a)pyrene (B(a)P) as an indicator species

The number of monitoring sites required for compliance defined within the directives is significantly reduced if other means of assessment, in addition to fixed monitoring sites, are available for inclusion in the annual air quality assessment. Air quality modelling has therefore been carried out to supplement the information available from the UK national air quality monitoring networks.

1.2 This report

This report covers assessments required under the AQD and AQDD4. Specifically it provides detailed information on the modelling methods used to assess relevant metrics throughout the UK and a summary of the key attainment results of the assessment. The 2013 UK submission on air quality to the European Commission is summarised by the annual Air Pollution in the UK reports (Air Pollution in the UK 2013) which comprise a compliance assessment summary report and a full report, which in addition presents air quality modelling data and measurements from the UK national air quality monitoring networks.

Sections 3 to 11 of this report describe the Pollution Climate Mapping (PCM) modelling methods that have been used to calculate concentrations of SO_2, NO_x, NO_2, PM_{10}, $PM_{2.5}$, C_6H_6, O_3, heavy metals (Pb, As, Cd, Ni) and B(a)P. This includes:

- A summary of the limit values, critical levels, target values and long term objectives set out in the directives for each pollutant
- Details of the modelling methods
- Information on the verification of the models used and comparisons with data quality objectives

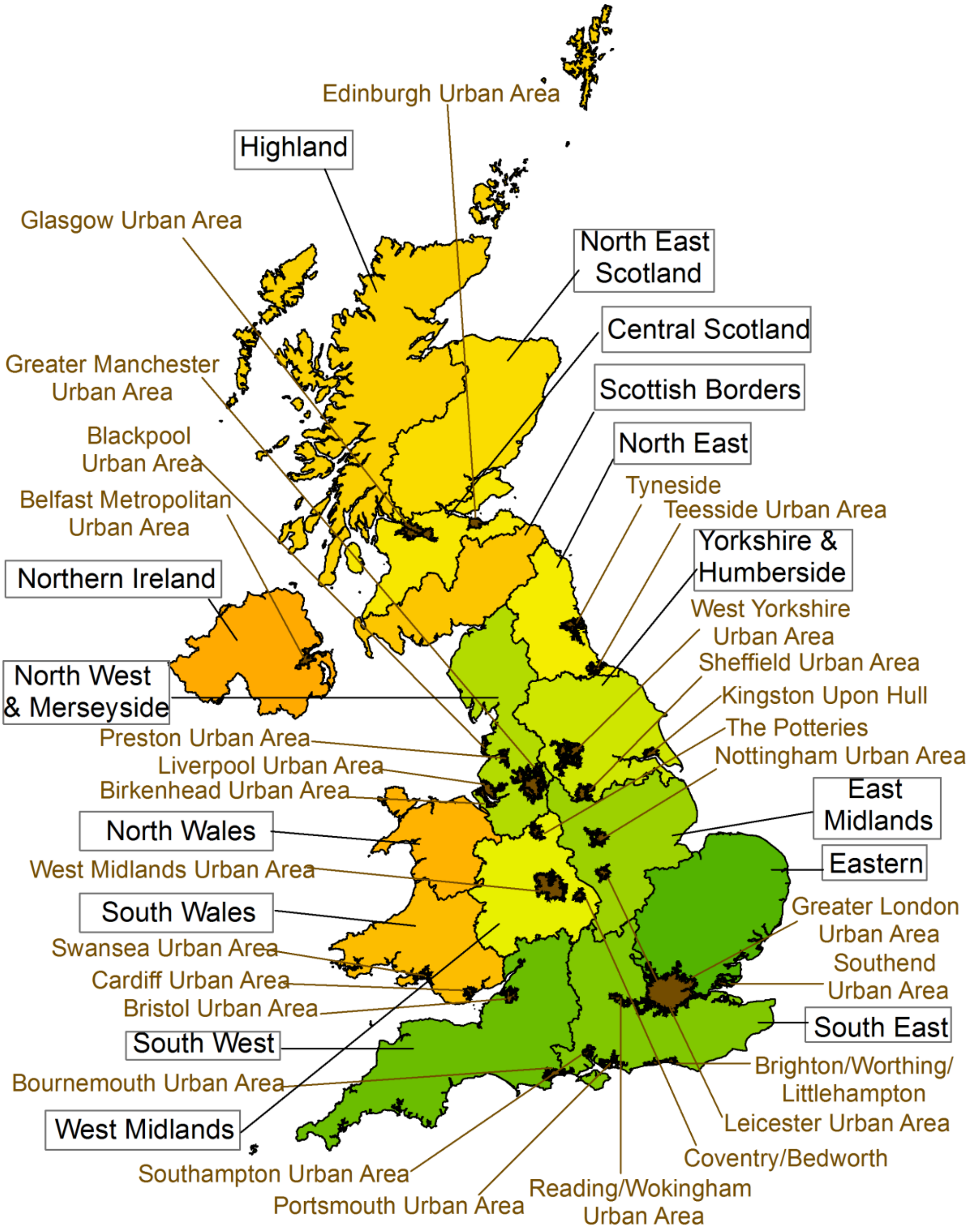
The assessment for CO is described in Section 8. Prior to 2011 a modelling assessment was completed for CO. However, as ambient concentrations throughout the UK have been well below the limit value and assessment threshold for many years, models are no longer required for CO and the supplementary assessment for 2013 has been based on objective estimation, as it was for 2011 and 2012.

The status of zones in relation to the limit, target values, critical levels and long term objectives for the AQD pollutants have been reported to the EU via e-Reporting (CDR, 2014) and a summary of the results of the assessments are included in Section 2. The status has been determined from a combination of monitoring data and model results. A comparison of the results of similar assessments carried out since 2001 (Stedman et al., 2002, 2003, 2005 and 2006; Bush et al., 2006 and 2007; Kent and Stedman, 2007 and 2008; Kent et al., 2007a, 2007b and 2010; Yap et al., 2009; Grice et al., 2009, 2010a and 2010b; Walker et al., 2010 and 2011; Brookes et al., 2011 and 2012, 2013) has been reported in Air Pollution in the UK 2013.

1.3 Assessment regime and definition of zones

The Framework Directive included a requirement for member states to undertake preliminary assessments of ambient air quality, prior to the implementation of the Daughter Directives under Article 5 of this Directive. The objectives of these assessments were to establish estimates for the overall distribution and levels of pollutants, and to identify additional monitoring required to fulfil obligations within the Framework Directive. The preliminary assessment (Bush, 2000) carried out for 1st Daughter Directive (AQDD1), 1999/30/EC, defined a set of zones to be used for air quality assessment in the UK. The preliminary assessment for the UK for AQDD4 was reported by Bush (2007). The AQD includes a similar requirement for continued assessment under Article 5, the preliminary assessment for the UK fulfilling this requirement was reported by Vincent et al. (2010). The AQD continues the requirement for the establishment of zones and agglomerations under Article 4. Table 1.1 contains details of area, population (from the 2011 census) and urban road length contained in each UK zone and agglomeration. The zones and agglomerations map for the UK is presented in Figure 1.1.

Figure 1.1 - UK zones and agglomerations for 2013



Agglomeration zones (brown)
Non-agglomeration zones (green, yellow and orange)

Table 1.1 - Zones for Air Quality Directive reporting

Zone	Zone code	Ag or non-ag*	Population	Area (km^2)	Number of urban road links	Length of urban road links (km)
Greater London Urban Area	UK0001	ag	8921189	1618	1914	1883
West Midlands Urban Area	UK0002	ag	2295744	605	386	529
Greater Manchester Urban Area	UK0003	ag	2078782	554	580	638
West Yorkshire Urban Area	UK0004	ag	1308189	352	303	402
Tyneside	UK0005	ag	770536	221	185	195
Liverpool Urban Area	UK0006	ag	744225	198	256	210
Sheffield Urban Area	UK0007	ag	577551	163	112	150
Nottingham Urban Area	UK0008	ag	599524	155	134	126
Bristol Urban Area	UK0009	ag	536979	139	123	121
Brighton/Worthing/Littlehampton	UK0010	ag	420590	94	62	85
Leicester Urban Area	UK0011	ag	432018	101	73	82
Portsmouth Urban Area	UK0012	ag	399206	96	59	73
Teesside Urban Area	UK0013	ag	315067	119	66	69
The Potteries	UK0014	ag	285366	91	115	126
Bournemouth Urban Area	UK0015	ag	378544	121	55	71
Reading/Wokingham Urban Area	UK0016	ag	300142	82	67	68
Coventry/Bedworth	UK0017	ag	304515	76	35	38
Kingston upon Hull	UK0018	ag	278695	85	37	52
Southampton Urban Area	UK0019	ag	298793	79	66	73
Birkenhead Urban Area	UK0020	ag	284975	97	71	76
Southend Urban Area	UK0021	ag	243360	67	32	52
Blackpool Urban Area	UK0022	ag	230342	73	51	63
Preston Urban Area	UK0023	ag	214302	60	39	41
Glasgow Urban Area	UK0024	ag	1105095	367	283	340
Edinburgh Urban Area	UK0025	ag	468399	134	60	99
Cardiff Urban Area	UK0026	ag	327129	86	44	62
Swansea Urban Area	UK0027	ag	210269	83	34	63
Belfast Metropolitan Urban Area	UK0028	ag	545493	216	51	227
Eastern	UK0029	non-ag	5364958	19498	600	789
South West	UK0030	non-ag	4396528	24396	440	649
South East	UK0031	non-ag	6682607	19108	881	1301
East Midlands	UK0032	non-ag	3503120	15458	429	654
North West & Merseyside	UK0033	non-ag	3501924	13507	634	858
Yorkshire & Humberside	UK0034	non-ag	3120522	15019	396	587
West Midlands	UK0035	non-ag	2713684	12221	386	523
North East	UK0036	non-ag	1510704	8377	216	257
Central Scotland	UK0037	non-ag	1942272	9984	238	353
North East Scotland	UK0038	non-ag	1121019	19024	133	233
Highland	UK0039	non-ag	393586	43514	11	37
Scottish Borders	UK0040	non-ag	265466	11400	36	47
South Wales	UK0041	non-ag	1772244	12645	182	302
North Wales	UK0042	non-ag	749704	8747	81	152
Northern Ireland	UK0043	non-ag	1265360	14540	84	248
Total			63178714	253570	10040	13003

* ag = agglomeration zone; non-ag = non-agglomeration zone

1.4 Monitoring sites

The monitoring stations operating during 2013 for the purpose of AQD and AQDD4 reporting have been listed within e-Reporting Data flow C (Assessment Regimes), which can be found on the CDR (CDR, 2014). Not all sites had sufficient data capture during 2013 for data to be reported. The data quality objective (DQO) for AQD/AQDD4 measurements is 90% data capture. The Implementing Provisions on Reporting (IPR) guidance states that when checking for compliance the minimum data quality objective can be reduced to take into account the proportion of time taken in a calendar year for planned maintenance and calibration. The IPR states that an estimation of this time is 5% which makes the data quality objective 85%. For the purposes of compliance reporting all measurements from monitoring sites with at least 85% data capture for the entire year have been included. The IPR also states that measurements can be included in compliance reporting as indicative values where the data capture is at least 14%. Monitoring stations with at least 75% data capture have been included in the modelling analysis to ensure that a greater number of operational monitoring sites have been used for model calibration and verification purposes.

The monitoring data for the sites used in the assessment for heavy metals and B(a)P are summarised in Appendix 2.

1.5 Data quality objectives for modelling results and model verification

The AQD sets data quality objectives (DQOs) for modelling uncertainty, within supplementary assessment under the AQD. AQDD4 sets DQOs in terms of uncertainty, which acts as a guide for quality assurance programmes when identifying an acceptable level of uncertainty for assessment methods appropriate for supplementary assessment under the AQDD4. Uncertainty is defined in the AQD as the maximum deviation of the measured and calculated concentration levels for 90% of individual monitoring points over the period considered by the limit value (or target value), without taking into account the timing of events. The uncertainty of modelling should be interpreted as applicable in the region of the appropriate LV or TV. The fixed measurements that have been selected for comparison with the modelling results should be representative of the scale covered by the model. Final guidance clarifying the recommended methods for assessing model performance with respect to the DQOs has yet to be agreed. The comparisons with monitoring data presented in this report have therefore included data from all sites including those with measured values not in the vicinity of the LVs or TVs and a highly detailed assessment of the spatial representativity of the sites has not been carried out.

Under the AQD, DQOs have been set at 50% for hourly averages, daily averages and 8 hour averages of SO_2, NO_2, NO_x, CO and O_3. DQOs have been set at 30% for annual averages of SO_2, NO_2 and NO_x. For PM_{10}, $PM_{2.5}$ and Pb the DQO for annual averages is 50%. DQOs have not been defined for daily averages of PM_{10}. Under the AQDD4 DQOs have been set at 60% for annual averages of As, Cd, Ni and B(a)P.

The models used to calculate the maps of NO_x, NO_2, PM_{10}, $PM_{2.5}$, C_6H_6, O_3, and B(a)P presented in this report have been calibrated using data from the national monitoring network sites. Data from these sites alone does not allow an independent assessment of the validity of the mapped estimates in relation to the DQOs for modelling. Measurement data from sites not included in the calibration are used in addition to the national monitoring network sites to make this assessment, except for C_6H_6 and B(a)P where no independent data are available. Data from sites quality assured by Ricardo-AEA under contract and not part of the national network, including Local Authority sites with data available from the Air Quality England website, Scottish Air Quality Archive monitoring sites, Welsh Air Quality Forum monitoring sites, Northern Ireland Automatic Urban Network sites and sites from the Kent and Medway Air Quality Monitoring Network, have therefore been used for the verification of the modelled estimates. The description ‘Verification Sites’ is used to describe the independent monitoring sites included in the verification analysis. Monitoring data has also been obtained for the London Air Quality Network (LAQN) and other local authority monitoring networks for which data have been provided by Kings College London (ERG). The ‘Verification Sites’ used for the 2013 assessment are listed in Appendix 1.

The model used to calculate maps of SO_2 presented in this report is not calibrated so has been compared to and verified using a combination of national network monitoring data along with the ‘Verification Sites’ listed in Appendix 1. Similarly, the models used to calculate maps of air pollution from heavy metals (Pb, As, Cd, Ni) presented in this report are not calibrated so have been compared to and verified using national network monitoring data for those sites that are listed Appendix 2. Sites with data capture of at least 75% have been included in the verification analysis. Model verification results are listed in the sections on each pollutant.

1.6 Air quality modelling

Full details of the modelling methods implemented are given in Sections 3 to 11. A brief introduction is presented here.

1.6.1 Background concentration maps

Maps showing background concentrations for NO_X, SO_2 and C_6H_6 have been calculated at a 1 km x 1 km resolution for the relevant metrics set out in the AQD. These maps have been calculated by summing concentrations from the following layers:

- Large point sources[1] – modelled using the air dispersion model ADMS and emissions estimates from the UK National Atmospheric Emissions Inventory 2012 (NAEI 2012)
- Small point sources – modelled using the small points model and emissions estimates from the NAEI 2012
- EU Emissions Trading Scheme[2] (ETS) point sources – modelled using the small points model and emissions estimates from the NAEI 2012
- Distant sources – characterised by the rural background concentration
- Area sources[3] related to domestic combustion – modelled using a time varying dispersion kernel and emissions estimates from the NAEI 2012
- Area sources related to combustion in industry – modelled using the small points model and emissions estimates from the NAEI 2012
- Area sources related to road traffic – modelled using a dispersion kernel using time varying emissions and emissions estimates from the NAEI 2012
- Other area sources – modelled using a dispersion kernel and annual emissions estimates from the NAEI 2012
- Fugitive point source emissions – modelled using fugitive source kernel model and an estimate of the fugitive component of emissions derived from the NAEI 2012 (C_6H_6 only).

1 km x 1 km background concentration maps for B(a)P have been calculated using a similar approach except that a regional background has not been included and area sources related

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[1] Point source emissions are defined as emissions of a known amount from a known location (e.g. a power station).

[2] Emissions Trading Scheme point emissions estimates for Air Quality pollutants based on reported carbon emissions

[3] Area source emissions are defined as ‘diffuse emissions’ from many unspecified locations (e.g. emissions from domestic heating, or from shipping).

to industrial combustion and ETS point sources have been modelled using an area source dispersion kernel.

For PM_{10} and $PM_{2.5}$ a similar approach has been used to generate 1 km x 1 km background concentration maps. For these pollutants, the following additional layers have also been included:

- Secondary inorganic aerosol – derived by interpolation and scaling of measurements of SO_4, NO_3 and NH_4 at rural sites
- Secondary organic aerosol – semi-volatile organic compounds formed by the oxidation of non-methane volatile organic compounds. Estimates derived from results from the NAME model
- Regional primary particles – from results from the TRACK model and emissions estimates from the NAEI 2012 and EMEP
- Regional calcium rich dusts from re-suspension of soils – modelled using a dispersion kernel and information on land use
- Urban calcium rich dusts from re-suspension of soils due to urban activity – estimated from a combination of measurements made in Birmingham and population density
- Regional iron rich dusts from re-suspension – assumed to be a constant value, estimated measurements made in the vicinity of Birmingham
- Iron rich dusts from re-suspension due to vehicle activity – modelled using a dispersion kernel and vehicle activity data for heavy duty vehicles
- Sea salt – derived by interpolation and scaling of measurements of chloride at rural sites
- Residual – assumed to be a constant value

For Pb, As, Cd and Ni a similar approach has been used to generate 1 km x 1 km background concentration maps. For these pollutants, the following additional layers have also been included:

- Regional concentrations – derived from estimates of primary PM from regional sources calculated using the TRACK model and emissions estimates from the NAEI 2012 and EMEP
- Re-suspension from bare soils – derived from estimates of re-suspension of PM modelled using a dispersion kernel and information on land use
- Re-suspension as a result of vehicle movements – derived from estimates of re-suspension of PM modelled using a dispersion kernel and vehicle activity data for heavy duty vehicles

1.6.2 Roadside concentration maps

Maps showing modelled roadside concentrations of NO_X, PM_{10}, $PM_{2.5}$ and C_6H_6 have been calculated for 9336 urban major road receptors (A-roads and motorways) across the UK. These have been calculated by adding a ‘roadside increment’ concentration component to the modelled background concentration for each road. This roadside increment concentration is calculated as a function of a road link emission that has been adjusted to take into account traffic flow. The roadside increment model is then calibrated using monitoring data from the AURN. This is a similar approach to that used within the DMRB Screening Model (Boulter, Hickman, and McCrae, 2003). Some of the lengths of road associated with each receptor cross zone boundaries and thus a total of 10040 road links have been included in the analysis.

1.6.3 NO_2 maps

Background and roadside NO_2 concentration maps have been calculated by applying a calibrated version of the updated oxidant-partitioning model. This model describes the complex inter-relationships between NO, NO_2 and O_3 as a set of chemically coupled species (Jenkin, 2004; Murrells et al., 2008; Jenkin, 2012).

1.6.4 Key input data

Emissions inventory data used in this modelling is taken from the NAEI 2012 (Passant et al., 2014). Emission estimates for area and point sources (taking into account plant closure) have been scaled forward from 2012 to 2013. Work carried out to calculate emissions from aircraft and shipping within the PCM model is described in Appendix 5. Dispersion modelling has been done using ADMS 5.0 using meteorological data from Waddington for 2013. UK national network monitoring data has been used to calibrate the background and roadside models.

1.6.5 Ozone maps

Maps of the O_3 metrics specified in the AQD have been calculated using a different modelling approach to the approach used for other pollutants in this report. This is because of the complex chemistry involved in the production and destruction of O_3. The more empirical methods used to model O_3 concentrations are described in Section 9.

1.7 Air quality in Gibraltar in 2013

Air quality monitoring and assessments are also undertaken in Gibraltar and the results of the assessment are submitted to the Commission each year via a separate e-Reporting Data flows to those compiled for the UK (CDR, 2014). Further information on air quality monitoring in Gibraltar can be found at http://www.gibraltarairquality.gi/.

2 Results of air quality assessments for 2013

The results of the air quality assessments for AQD pollutants SO_2, NO_2 and NO_X, PM_{10}, $PM_{2.5}$, Pb, C_6H_6, CO and O_3 have been listed in Table 2.1 to Table 2.5. $PM_{2.5}$ is additionally reported against a TV, summarised here in Table 2.3. Results of the air quality assessments for AQDD4 pollutants As, Cd, Ni and B(a)P are summarised here in Table 2.6. These tables summarise information from e-Reporting Data flow G (Attainment) submitted to the CDR (CDR, 2014) relating to compliance with the respective Limit Value (LV), Target Value (TV) or Long-term Objective (LTO). The tables have been completed as follows:

- Where all measurements were within the relevant LVs in 2013, the table shows this as “OK”.
- Where compliance was determined by supplementary assessment (modelling), this is shown as “OK (m)”. In general where the status of a location was determined by supplementary assessment, this is indicated by (m) as done here for compliance.
- Where locations were identified as exceeding a LV, this is identified with “>LV”.
- Where locations have a time extension in place compliance is assessed against the LV plus the maximum margin of tolerance (MOT), this is shown as either “≤ LV + MOT” or “> LV + MOT”.

A similar approach has been used to summarise results in relation to critical levels (CLs), TVs and LTOs. Zones that complied with the relevant CLs, LVs, TVs or LTOs are shaded blue, while those in exceedance are shaded red. Where locations have a time extension in place exceedances of the LV + MOT are shaded red, exceedances of the LV but not the LV + MOT are shaded orange. For O_3, exceedances of the LTO but not the TV are also shaded orange. “n/a” means that an assessment is not relevant for a zone, such as for the vegetation critical level in agglomeration zones.

Measurements are regarded as the primary basis for the compliance status if both measurements and supplementary assessment estimates show that a threshold has been exceeded. Where locations have been identified as exceeding by modelling this indicates that modelled concentrations were higher than measured concentrations or that measurements were not available (or not required for that zone as determined by a 5-yearly assessment of concentrations relative to lower and upper assessment thresholds in the AQD) and modelled values were therefore used. Modelled concentrations may be higher than measured concentrations because the modelling studies provide estimates of concentrations over the entire zone. It is possible that the locations of the monitoring sites do not correspond to the location of the highest concentration in the zone, for example, there may be no roadside monitoring sites in a zone. Compliance can be determined by modelling where measurements are not available for a zone.

CO concentrations were not modelled for 2013; therefore in zones where measurements were not available compliance has been determined through objective estimation. The objective estimation process is explained further in Section 8.

In 2013 there were time extensions in place in nine zones for the annual mean limit value for NO_2 until 1 January 2015 and in three zones until 1 January 2014. The exposure concentration obligation for the average of annual mean $PM_{2.5}$ concentrations measured in urban areas of 20 µg m^{-3} was met. Table 2.3 shows no exceedance of the daily mean limit value for PM_{10} for the Greater London Urban Area. However, it should be noted that there was one exceedance of the daily mean limit value for PM_{10} before subtraction of natural sources, as is required by the AQD (Article 20). There was an exceedance of the stage 2 indicative limit value for $PM_{2.5}$, which is not currently in force, in the Greater London Urban Area.

The 1-hour limit value of 200 µg m^{-3} as a 98th percentile specific in Directive 85/203/EEC was not exceeded in 2013.

The UK Government is currently (October 2015) consulting on air quality plans for compliance with the limit values for nitrogen dioxide. The reference year for these air quality plans for NO_2 is 2013. The air quality modelling assessments carried out to support the air quality plans are based on the modelling methods and base year modelling carried out for the 2013 air quality assessment described in this report. The base data has, however, been updated for the 2015 air quality plans to incorporate updated information on emission factors for road traffic emissions of NO_X and an improved modelling method for traffic (roadside) locations. These updates have only become available during the period since the original assessment for 2013 was reported. These revisions were made in order to ensure that the best possible evidence is available to support the development of the 2015 air quality plans. The revised 2013 data will be re-submitted to the Commission in due course. Details of the updates to the model will be provided in the technical document that will accompany the finalised 2015 air quality plans. A short summary of the revisions is included in section 3.6 of this report. The compliance status of all air quality zones in 2013 with respect to the annual limit value for NO_2 is unchanged for this revised assessment.

Table 2.1 - List of zones and agglomerations in relation to limit value and critical level exceedances for SO_2 in 2013

Zone	Zone code	SO_2 LV for health (1hr mean)	SO_2 LV for health (24hr mean)	SO_2 CL for vegetation (annual mean)	SO_2 CL for vegetation (winter mean)
Greater London Urban Area	UK0001	OK	OK	n/a	n/a
West Midlands Urban Area	UK0002	OK	OK	n/a	n/a
Greater Manchester Urban Area	UK0003	OK	OK	n/a	n/a
West Yorkshire Urban Area	UK0004	OK	OK	n/a	n/a
Tyneside	UK0005	OK (m)	OK (m)	n/a	n/a
Liverpool Urban Area	UK0006	OK	OK	n/a	n/a
Sheffield Urban Area	UK0007	OK (m)	OK (m)	n/a	n/a
Nottingham Urban Area	UK0008	OK	OK	n/a	n/a
Bristol Urban Area	UK0009	OK (m)	OK (m)	n/a	n/a
Brighton/Worthing/Littlehampton	UK0010	OK (m)	OK (m)	n/a	n/a
Leicester Urban Area	UK0011	OK (m)	OK (m)	n/a	n/a
Portsmouth Urban Area	UK0012	OK (m)	OK (m)	n/a	n/a
Teesside Urban Area	UK0013	OK	OK	n/a	n/a
The Potteries	UK0014	OK (m)	OK (m)	n/a	n/a
Bournemouth Urban Area	UK0015	OK (m)	OK (m)	n/a	n/a
Reading/Wokingham Urban Area	UK0016	OK (m)	OK (m)	n/a	n/a
Coventry/Bedworth	UK0017	OK (m)	OK (m)	n/a	n/a
Kingston upon Hull	UK0018	OK	OK	n/a	n/a
Southampton Urban Area	UK0019	OK	OK	n/a	n/a
Birkenhead Urban Area	UK0020	OK (m)	OK (m)	n/a	n/a
Southend Urban Area	UK0021	OK (m)	OK (m)	n/a	n/a
Blackpool Urban Area	UK0022	OK (m)	OK (m)	n/a	n/a
Preston Urban Area	UK0023	OK (m)	OK (m)	n/a	n/a
Glasgow Urban Area	UK0024	OK (m)	OK (m)	n/a	n/a
Edinburgh Urban Area	UK0025	OK	OK	n/a	n/a
Cardiff Urban Area	UK0026	OK	OK	n/a	n/a
Swansea Urban Area	UK0027	OK	OK	n/a	n/a
Belfast Urban Area	UK0028	OK	OK	n/a	n/a
Eastern	UK0029	OK	OK	OK (m)	OK (m)
South West	UK0030	OK (m)	OK (m)	OK (m)	OK (m)
South East	UK0031	OK	OK	OK	OK
East Midlands	UK0032	OK	OK	OK	OK
North West & Merseyside	UK0033	OK (m)	OK (m)	OK (m)	OK (m)
Yorkshire & Humberside	UK0034	OK	OK	OK (m)	OK (m)
West Midlands	UK0035	OK (m)	OK (m)	OK (m)	OK (m)
North East	UK0036	OK (m)	OK (m)	OK (m)	OK (m)
Central Scotland	UK0037	OK	OK	OK (m)	OK (m)
North East Scotland	UK0038	OK (m)	OK (m)	OK (m)	OK (m)
Highland	UK0039	OK (m)	OK (m)	OK (m)	OK (m)
Scottish Borders	UK0040	OK (m)	OK (m)	OK (m)	OK (m)
South Wales	UK0041	OK	OK	OK	OK
North Wales	UK0042	OK	OK	OK (m)	OK (m)
Northern Ireland	UK0043	OK	OK	OK (m)	OK (m)

Table 2.2 - List of zones and agglomerations in relation to limit value and critical level exceedances for NO_2 and NO_X in 2013 (zones for which time extensions apply, * = 2015, ** = 2014)

Zone	Zone code	NO_2 LV for health (1-hr mean)	NO_2 LV for health (annual mean)	NO_x CL for vegetation (annual mean)
Greater London Urban Area	UK0001	> LV	> LV	n/a
West Midlands Urban Area	UK0002	OK	> LV	n/a
Greater Manchester Urban Area	UK0003	OK	> LV (m)	n/a
West Yorkshire Urban Area	UK0004	OK	> LV	n/a
Tyneside	UK0005	OK	> LV	n/a
Liverpool Urban Area	UK0006	OK	> LV (m)	n/a
Sheffield Urban Area	UK0007	OK	> LV (m)	n/a
Nottingham Urban Area*	UK0008	OK	> LV + MOT (m)	n/a
Bristol Urban Area	UK0009	OK	> LV (m)	n/a
Brighton/Worthing/Littlehampton	UK0010	OK	> LV (m)	n/a
Leicester Urban Area*	UK0011	OK	> LV + MOT (m)	n/a
Portsmouth Urban Area*	UK0012	OK	≤ LV + MOT (m)	n/a
Teesside Urban Area	UK0013	OK	> LV (m)	n/a
The Potteries	UK0014	OK	> LV (m)	n/a
Bournemouth Urban Area	UK0015	OK	> LV (m)	n/a
Reading/Wokingham Urban Area	UK0016	OK	> LV (m)	n/a
Coventry/Bedworth	UK0017	OK	> LV (m)	n/a
Kingston upon Hull	UK0018	OK	> LV (m)	n/a
Southampton Urban Area	UK0019	OK	> LV (m)	n/a
Birkenhead Urban Area*	UK0020	OK	≤ LV + MOT (m)	n/a
Southend Urban Area*	UK0021	OK	≤ LV + MOT (m)	n/a
Blackpool Urban Area	UK0022	OK	OK	n/a
Preston Urban Area**	UK0023	OK	OK	n/a
Glasgow Urban Area	UK0024	OK	> LV	n/a
Edinburgh Urban Area*	UK0025	OK	≤ LV + MOT (m)	n/a
Cardiff Urban Area*	UK0026	OK	> LV + MOT (m)	n/a
Swansea Urban Area**	UK0027	OK	≤ LV + MOT (m)	n/a
Belfast Urban Area	UK0028	OK	> LV (m)	n/a
Eastern	UK0029	OK	> LV (m)	OK
South West	UK0030	OK	> LV	OK
South East	UK0031	OK	> LV	OK
East Midlands	UK0032	OK	> LV	OK
North West & Merseyside	UK0033	OK	> LV (m)	OK (m)
Yorkshire & Humberside	UK0034	OK	> LV (m)	OK
West Midlands	UK0035	OK	> LV (m)	OK (m)
North East	UK0036	OK	> LV (m)	OK (m)
Central Scotland*	UK0037	OK	≤ LV + MOT (m)	OK (m)
North East Scotland	UK0038	OK	> LV	OK (m)
Highland	UK0039	OK	OK	OK (m)
Scottish Borders	UK0040	OK	OK	OK
South Wales	UK0041	OK	> LV (m)	OK
North Wales*	UK0042	OK	≤ LV + MOT (m)	OK
Northern Ireland**	UK0043	OK	OK	OK (m)

Table 2.3 - List of zones and agglomerations in relation to limit value exceedances for PM_{10}, limit value and target value exceedances for $PM_{2.5}$ in 2013 (after subtraction of contribution from natural sources where applicable)

Zone	Zone code	PM_{10} LV for health (24-hr mean)	PM_{10} LV for health (annual mean)	$PM_{2.5}$ LV for health (annual mean) Stage 1	$PM_{2.5}$ LV for health (annual mean) Stage 2*	$PM_{2.5}$ TV for health (annual mean)
Greater London Urban Area	UK0001	OK (m)	OK	OK	> LV (m)	OK
West Midlands Urban Area	UK0002	OK	OK	OK	OK	OK
Greater Manchester Urban Area	UK0003	OK	OK	OK	OK	OK
West Yorkshire Urban Area	UK0004	OK	OK	OK	OK	OK
Tyneside	UK0005	OK	OK	OK	OK	OK
Liverpool Urban Area	UK0006	OK	OK	OK	OK	OK
Sheffield Urban Area	UK0007	OK	OK	OK	OK	OK
Nottingham Urban Area	UK0008	OK	OK	OK	OK	OK
Bristol Urban Area	UK0009	OK	OK	OK	OK	OK
Brighton/Worthing/Littlehampton	UK0010	OK (m)	OK (m)	OK	OK	OK
Leicester Urban Area	UK0011	OK	OK	OK	OK	OK
Portsmouth Urban Area	UK0012	OK	OK	OK	OK	OK
Teesside Urban Area	UK0013	OK	OK	OK	OK	OK
The Potteries	UK0014	OK	OK	OK	OK	OK
Bournemouth Urban Area	UK0015	OK (m)	OK (m)	OK	OK	OK
Reading/Wokingham Urban Area	UK0016	OK	OK	OK	OK	OK
Coventry/Bedworth	UK0017	OK (m)	OK (m)	OK	OK	OK
Kingston upon Hull	UK0018	OK	OK	OK	OK	OK
Southampton Urban Area	UK0019	OK	OK	OK	OK	OK
Birkenhead Urban Area	UK0020	OK (m)	OK (m)	OK	OK	OK
Southend Urban Area	UK0021	OK (m)	OK (m)	OK	OK	OK
Blackpool Urban Area	UK0022	OK (m)	OK (m)	OK	OK	OK
Preston Urban Area	UK0023	OK (m)	OK (m)	OK	OK	OK
Glasgow Urban Area	UK0024	OK	OK	OK	OK	OK
Edinburgh Urban Area	UK0025	OK	OK	OK	OK	OK
Cardiff Urban Area	UK0026	OK	OK	OK	OK	OK
Swansea Urban Area	UK0027	OK	OK	OK	OK	OK
Belfast Urban Area	UK0028	OK	OK	OK	OK	OK
Eastern	UK0029	OK	OK	OK	OK	OK
South West	UK0030	OK	OK	OK	OK	OK
South East	UK0031	OK	OK	OK	OK	OK
East Midlands	UK0032	OK	OK	OK	OK	OK
North West & Merseyside	UK0033	OK	OK	OK	OK	OK
Yorkshire & Humberside	UK0034	OK	OK	OK	OK	OK
West Midlands	UK0035	OK	OK	OK	OK	OK
North East	UK0036	OK	OK	OK	OK	OK
Central Scotland	UK0037	OK	OK	OK	OK	OK
North East Scotland	UK0038	OK	OK	OK	OK	OK
Highland	UK0039	OK	OK	OK	OK	OK
Scottish Borders	UK0040	OK (m)	OK (m)	OK (m)	OK (m)	OK (m)
South Wales	UK0041	OK	OK	OK	OK	OK
North Wales	UK0042	OK	OK	OK	OK	OK
Northern Ireland	UK0043	OK	OK	OK	OK	OK

* The stage 2 indicative limit value for $PM_{2.5}$ is not currently in force.

Table 2.4 - List of zones and agglomerations in relation to limit value exceedances for lead, benzene and CO in 2013

Zone	Zone code	Lead LV for health (annual mean)	Benzene LV for health (annual mean)	CO LV for health (8-hr mean)
Greater London Urban Area	UK0001	OK	OK	OK
West Midlands Urban Area	UK0002	OK	OK	OK (m)
Greater Manchester Urban Area	UK0003	OK	OK	OK (m)
West Yorkshire Urban Area	UK0004	OK (m)	OK	OK
Tyneside	UK0005	OK (m)	OK	OK (m)
Liverpool Urban Area	UK0006	OK (m)	OK	OK (m)
Sheffield Urban Area	UK0007	OK	OK	OK (m)
Nottingham Urban Area	UK0008	OK (m)	OK	OK (m)
Bristol Urban Area	UK0009	OK (m)	OK (m)	OK (m)
Brighton/Worthing/Littlehampton	UK0010	OK (m)	OK (m)	OK (m)
Leicester Urban Area	UK0011	OK (m)	OK (m)	OK (m)
Portsmouth Urban Area	UK0012	OK (m)	OK (m)	OK (m)
Teesside Urban Area	UK0013	OK (m)	OK	OK (m)
The Potteries	UK0014	OK (m)	OK	OK (m)
Bournemouth Urban Area	UK0015	OK (m)	OK (m)	OK (m)
Reading/Wokingham Urban Area	UK0016	OK (m)	OK (m)	OK (m)
Coventry/Bedworth	UK0017	OK (m)	OK (m)	OK (m)
Kingston upon Hull	UK0018	OK (m)	OK (m)	OK (m)
Southampton Urban Area	UK0019	OK (m)	OK	OK (m)
Birkenhead Urban Area	UK0020	OK (m)	OK (m)	OK (m)
Southend Urban Area	UK0021	OK (m)	OK (m)	OK (m)
Blackpool Urban Area	UK0022	OK (m)	OK (m)	OK (m)
Preston Urban Area	UK0023	OK (m)	OK (m)	OK (m)
Glasgow Urban Area	UK0024	OK	OK	OK (m)
Edinburgh Urban Area	UK0025	OK (m)	OK (m)	OK
Cardiff Urban Area	UK0026	OK	OK (m)	OK
Swansea Urban Area	UK0027	OK	OK (m)	OK
Belfast Urban Area	UK0028	OK	OK	OK
Eastern	UK0029	OK	OK	OK (m)
South West	UK0030	OK	OK	OK (m)
South East	UK0031	OK	OK	OK (m)
East Midlands	UK0032	OK	OK	OK (m)
North West & Merseyside	UK0033	OK	OK	OK (m)
Yorkshire & Humberside	UK0034	OK	OK	OK (m)
West Midlands	UK0035	OK (m)	OK	OK (m)
North East	UK0036	OK	OK	OK (m)
Central Scotland	UK0037	OK	OK	OK (m)
North East Scotland	UK0038	OK	OK (m)	OK (m)
Highland	UK0039	OK (m)	OK (m)	OK (m)
Scottish Borders	UK0040	OK	OK (m)	OK (m)
South Wales	UK0041	OK	OK	OK (m)
North Wales	UK0042	OK (m)	OK (m)	OK (m)
Northern Ireland	UK0043	OK (m)	OK (m)	OK (m)

Table 2.5 - List of zones and agglomerations in relation to target value and long term objective exceedances for ozone in 2013

Zone	Zone code	O_3 TV and LTO for health (8-hr mean)	O_3 TV and LTO for vegetation (AOT40)
Greater London Urban Area	UK0001	Met TV, > LTO	Met TV, > LTO
West Midlands Urban Area	UK0002	Met TV, > LTO	OK
Greater Manchester Urban Area	UK0003	Met TV, > LTO	OK
West Yorkshire Urban Area	UK0004	OK	OK
Tyneside	UK0005	OK	OK
Liverpool Urban Area	UK0006	Met TV, > LTO	OK
Sheffield Urban Area	UK0007	OK	OK
Nottingham Urban Area	UK0008	Met TV, > LTO (m)	OK
Bristol Urban Area	UK0009	Met TV, > LTO	Met TV, > LTO (m)
Brighton/Worthing/Littlehampton	UK0010	Met TV, > LTO	Met TV, > LTO
Leicester Urban Area	UK0011	Met TV, > LTO (m)	OK
Portsmouth Urban Area	UK0012	Met TV, > LTO (m)	OK (m)
Teesside Urban Area	UK0013	OK	OK
The Potteries	UK0014	Met TV, > LTO (m)	OK
Bournemouth Urban Area	UK0015	Met TV, > LTO	Met TV, > LTO
Reading/Wokingham Urban Area	UK0016	Met TV, > LTO	OK
Coventry/Bedworth	UK0017	Met TV, > LTO	OK
Kingston upon Hull	UK0018	OK	OK
Southampton Urban Area	UK0019	Met TV, > LTO (m)	OK
Birkenhead Urban Area	UK0020	Met TV, > LTO (m)	OK
Southend Urban Area	UK0021	Met TV, > LTO	OK
Blackpool Urban Area	UK0022	Met TV, > LTO	OK
Preston Urban Area	UK0023	Met TV, > LTO (m)	OK
Glasgow Urban Area	UK0024	OK (m)	OK (m)
Edinburgh Urban Area	UK0025	OK	OK
Cardiff Urban Area	UK0026	Met TV, > LTO	OK
Swansea Urban Area	UK0027	Met TV, > LTO	OK
Belfast Urban Area	UK0028	Met TV, > LTO (m)	OK
Eastern	UK0029	Met TV, > LTO	OK
South West	UK0030	Met TV, > LTO	Met TV, > LTO
South East	UK0031	Met TV, > LTO	Met TV, > LTO
East Midlands	UK0032	Met TV, > LTO	OK
North West & Merseyside	UK0033	Met TV, > LTO	OK
Yorkshire & Humberside	UK0034	Met TV, > LTO (m)	OK
West Midlands	UK0035	Met TV, > LTO	Met TV, > LTO
North East	UK0036	OK	OK
Central Scotland	UK0037	OK	OK
North East Scotland	UK0038	OK	OK
Highland	UK0039	Met TV, > LTO (m)	OK
Scottish Borders	UK0040	Met TV, > LTO (m)	OK
South Wales	UK0041	Met TV, > LTO	Met TV, > LTO (m)
North Wales	UK0042	Met TV, > LTO	OK
Northern Ireland	UK0043	Met TV, > LTO (m)	OK

Table 2.6: List of zones and agglomerations where levels exceed or do not exceed target values for arsenic, cadmium, nickel and benzo(a)pyrene in 2013

Zone	Zone code	As TV	Cd TV	Ni TV	B(a)P TV
Greater London Urban Area	UK0001	OK	OK	OK	OK
West Midlands Urban Area	UK0002	OK	OK	OK	OK
Greater Manchester Urban Area	UK0003	OK	OK	OK	OK
West Yorkshire Urban Area	UK0004	OK (m)	OK (m)	OK (m)	OK
Tyneside	UK0005	OK (m)	OK (m)	OK (m)	OK
Liverpool Urban Area	UK0006	OK (m)	OK (m)	OK (m)	OK
Sheffield Urban Area	UK0007	OK	OK	OK	OK (m)
Nottingham Urban Area	UK0008	OK (m)	OK (m)	OK (m)	OK (m)
Bristol Urban Area	UK0009	OK (m)	OK (m)	OK (m)	OK (m)
Brighton/Worthing/Littlehampton	UK0010	OK (m)	OK (m)	OK (m)	OK
Leicester Urban Area	UK0011	OK (m)	OK (m)	OK (m)	OK (m)
Portsmouth Urban Area	UK0012	OK (m)	OK (m)	OK (m)	OK (m)
Teesside Urban Area	UK0013	OK (m)	OK (m)	OK (m)	> TV (m)
The Potteries	UK0014	OK (m)	OK (m)	OK (m)	OK (m)
Bournemouth Urban Area	UK0015	OK (m)	OK (m)	OK (m)	OK (m)
Reading/Wokingham Urban Area	UK0016	OK (m)	OK (m)	OK (m)	OK (m)
Coventry/Bedworth	UK0017	OK (m)	OK (m)	OK (m)	OK (m)
Kingston upon Hull	UK0018	OK (m)	OK (m)	OK (m)	OK (m)
Southampton Urban Area	UK0019	OK (m)	OK (m)	OK (m)	OK (m)
Birkenhead Urban Area	UK0020	OK (m)	OK (m)	OK (m)	OK (m)
Southend Urban Area	UK0021	OK (m)	OK (m)	OK (m)	OK (m)
Blackpool Urban Area	UK0022	OK (m)	OK (m)	OK (m)	OK (m)
Preston Urban Area	UK0023	OK (m)	OK (m)	OK (m)	OK (m)
Glasgow Urban Area	UK0024	OK	OK	OK	OK
Edinburgh Urban Area	UK0025	OK (m)	OK (m)	OK (m)	OK
Cardiff Urban Area	UK0026	OK	OK	OK	OK
Swansea Urban Area	UK0027	OK	OK	> TV	> TV (m)
Belfast Urban Area	UK0028	OK	OK	OK	OK
Eastern	UK0029	OK	OK	OK	OK
South West	UK0030	OK	OK	OK	OK (m)
South East	UK0031	OK	OK	OK	OK
East Midlands	UK0032	OK	OK	OK	> TV (m)
North West & Merseyside	UK0033	OK	OK	OK	OK
Yorkshire & Humberside	UK0034	OK	OK	OK	> TV
West Midlands	UK0035	OK (m)	OK (m)	OK (m)	OK (m)
North East	UK0036	OK	OK	OK	> TV (m)
Central Scotland	UK0037	OK	OK	OK	OK
North East Scotland	UK0038	OK	OK	OK	OK (m)
Highland	UK0039	OK (m)	OK (m)	OK (m)	OK
Scottish Borders	UK0040	OK	OK	OK	OK (m)
South Wales	UK0041	OK	OK	> TV (m)	> TV (m)
North Wales	UK0042	OK (m)	OK (m)	OK (m)	OK (m)
Northern Ireland	UK0043	OK (m)	OK (m)	OK (m)	OK

3 NO_2/NO_X

3.1 Introduction

3.1.1 Limit values

Two limit values for ambient NO_2 concentrations are set out in the Air Quality Directive (AQD). These have been specified for the protection of human health and came into force from 01/01/2010. These limit values are:

- An annual mean concentration of 40 µg m^{-3}.
- An hourly concentration of 200 µg m^{-3}, with 18 permitted exceedances each year

A critical level for NO_X for the protection of vegetation has also been specified in the Directive:

- An annual mean concentration 30 µg m^{-3} (NO_X as NO_2).

Because this critical level is designed to protect vegetation, it only applies in vegetation areas as defined in the Directive. This critical level has been in force since 2001.

It should be noted that the UK has been granted a time extension for compliance with the annual mean NO_2 limit value in twelve zones (Nottingham Urban Area, Leicester Urban Area, Portsmouth Urban Area, Birkenhead Urban Area, Southend Urban Area, Preston Urban Area, Edinburgh Urban Area, Cardiff Urban Area, Swansea Urban Area, Central Scotland zone, North Wales zone and Northern Ireland Zone). This exemption applies until 1st January 2015 for all but Preston Urban Area, Swansea Urban Area and Northern Ireland zones, for which they apply until 1st January 2014. The time extension for Reading/Wokingham Urban Area expired on 1st January 2013. These time extensions mean that the maximum margin of tolerance for this limit value (annual mean of 60 µg m^{-3}) is in force for the duration of the time extension in these zones.

Results of the assessment in terms of comparisons of the modelled concentrations with the annual mean limit value for NO_2 and critical level for NO_X have been reported in e-Reporting Data flow G (CDR, 2014).

3.1.2 Annual mean modelling

Annual mean concentrations of NO_X and NO_2 have been modelled for the UK for 2013 at background and roadside locations. Figure 3.1 and Figure 3.2 present maps of annual mean NO_2 concentrations for these locations in 2013. These maps have been used for comparison with the annual mean NO_2 limit value described above. To calculate NO_2 annual mean maps, NO_X annual mean concentration maps at background and roadside locations were first calculated.

The modelling methods for annual mean NO_X and NO_2 have been developed over a number of years (Stedman and Bush, 2000, Stedman et al., 2001a, Stedman et al., 2001b, Stedman et al., 2002, 2003, 2005 and 2006, Kent et al., 2007a, Kent et al., 2007b, Grice et al., 2009, 2010a and 2010b, Brookes et al., 2011, 2012 and 2013).

3.1.3 Outline of the annual mean model for NO_X

The 1 km x 1 km annual mean background NO_X concentration map has been calculated by summing the contributions from:

- Large point sources
- Small point sources

- Distant sources (characterised by the rural background concentration)
- Local area sources
- Point sources with emissions estimates for air quality pollutants based on reported carbon emissions (ETS points)

The area source model has been calibrated using data from the national automatic monitoring networks (AURN) for 2013. At locations close to busy roads an additional roadside contribution has been added to account for contributions to total NO_X from road traffic sources. The contributions from each of these components are described in Section 3.3.

3.1.4 Outline of the annual mean model for NO_2

NO_2 concentrations have been calculated from the modelled NO_X concentrations derived from the approach outlined above using a calibrated version of the updated oxidant-partitioning model. This model describes the complex inter-relationships between NO, NO_2 and ozone as a set of chemically coupled species (Jenkin, 2004; Murrells et al., 2008, Jenkin, 2012). This approach provides additional insights into the factors controlling ambient levels of NO_2 (and O_3), and how they may vary with NO_X concentration.

3.1.5 Annual mean NO_X concentration in vegetation areas

The background NO_X map has also been used to generate a map of annual mean NO_X concentrations in vegetation areas for comparison with the NO_X critical level described above; this map is shown in Figure 3.3. This map has been calculated by removing non-vegetation areas from the background NO_X map and calculating the zonal mean of the 1 km x 1 km grid squares for a 30 km x 30 km grid so that it complies with the criteria set out in the AQD. Mean concentrations on a 30 km x 30 km grid have been used to prevent the influence of any urban area appearing unrealistically large on adjacent vegetation areas. Thus the modelled concentrations in vegetation areas should be representative of approximately 1000 km^2 as specified in the AQD for monitoring sites used to assess concentrations for the vegetation critical level.

3.1.6 Assessment for the 1-hour limit value

Hourly concentrations for comparison with the 1-hour limit value have not been modelled due to the considerable uncertainties involved in modelling at such a fine temporal scale.

The annual mean limit value is expected to be more stringent than the 1-hour limit value in the majority of situations (AQEG, 2004). This is illustrated in Figure 3.4, which is a scatter plot of annual mean NO_2 in 2013 against the 99.8th percentile of hourly mean concentration (equivalent to 18 exceedances in the same year). This plot shows a significantly higher number of sites exceeding the annual mean limit value of 40 $\mu g\ m^{-3}$ than the 200 $\mu g\ m^{-3}$ hourly limit value.

An objective estimation method has been applied for the Leicester Urban Area zone by combining the measured number of 1-hour exceedances for two monitoring stations with low data capture, which was the result of a site relocation during the year.

3.1.7 Chapter structure

This chapter describes modelling work carried out for 2013 to assess compliance with the NO_X critical level and NO_2 limit values. Emission estimates for NO_X are described in Section 3.2. Section 3.3 describes the NO_X modelling methods. Details of the methods used to estimate ambient NO_2 from NO_X are presented in Section 3.4. Verification of and source apportionment for the modelling results are presented in Section 3.5.

Figure 3.1 - Annual mean background NO_2 concentration, 2013 ($\mu g\ m^{-3}$)

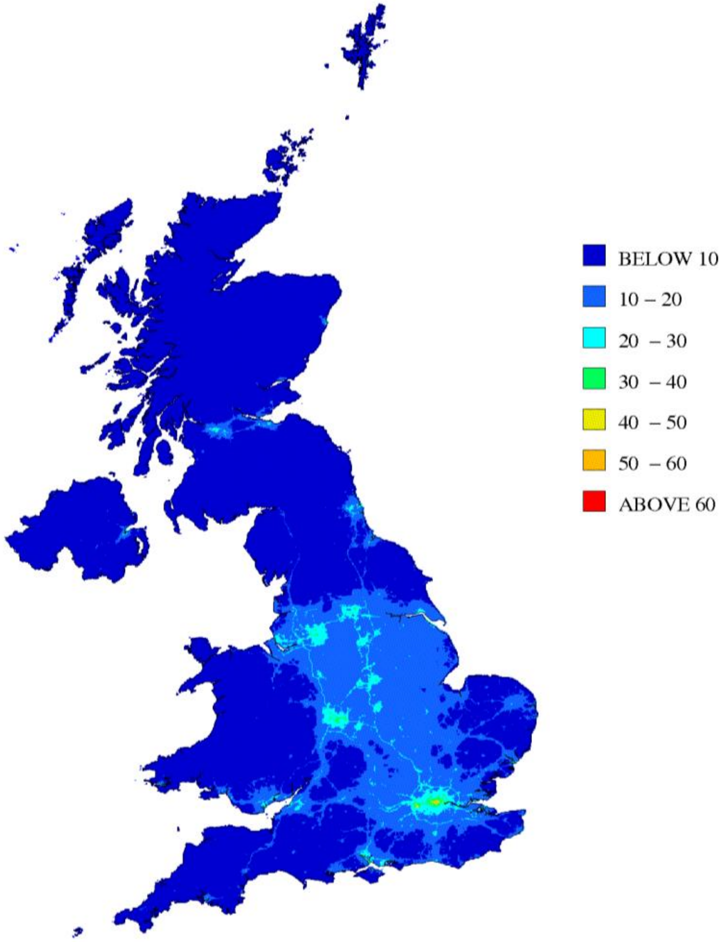


Figure 3.2 - Urban major roads, annual mean roadside NO_2 concentration, 2013 ($\mu g\ m^{-3}$)

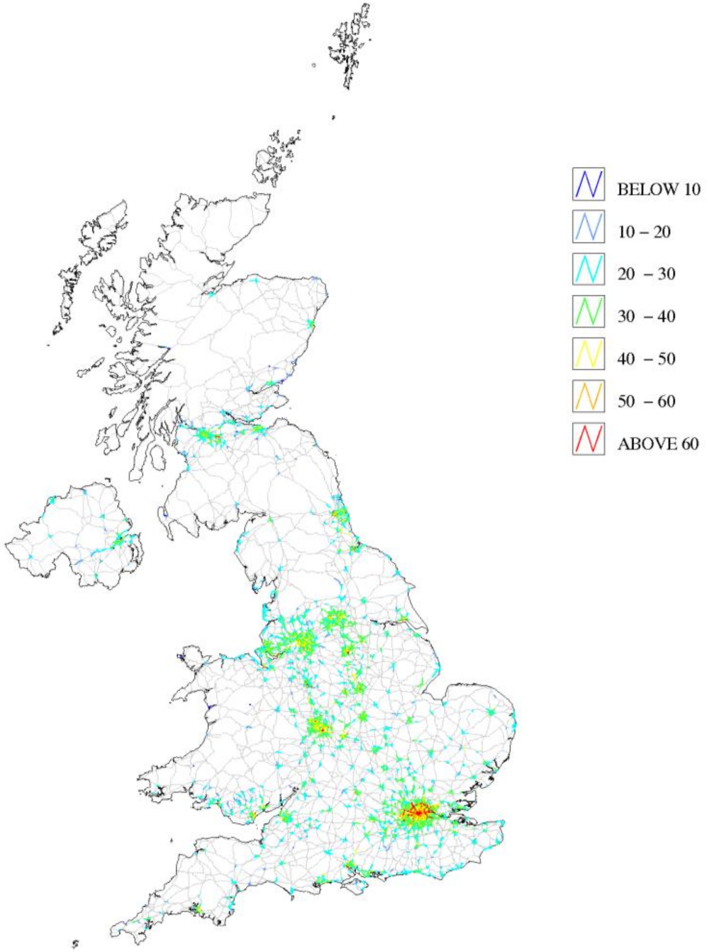


Figure 3.3 - Annual mean map of NO_X concentrations for comparison with the NO_X vegetation critical level, 2013 (µg m^{-3}, as NO_2)

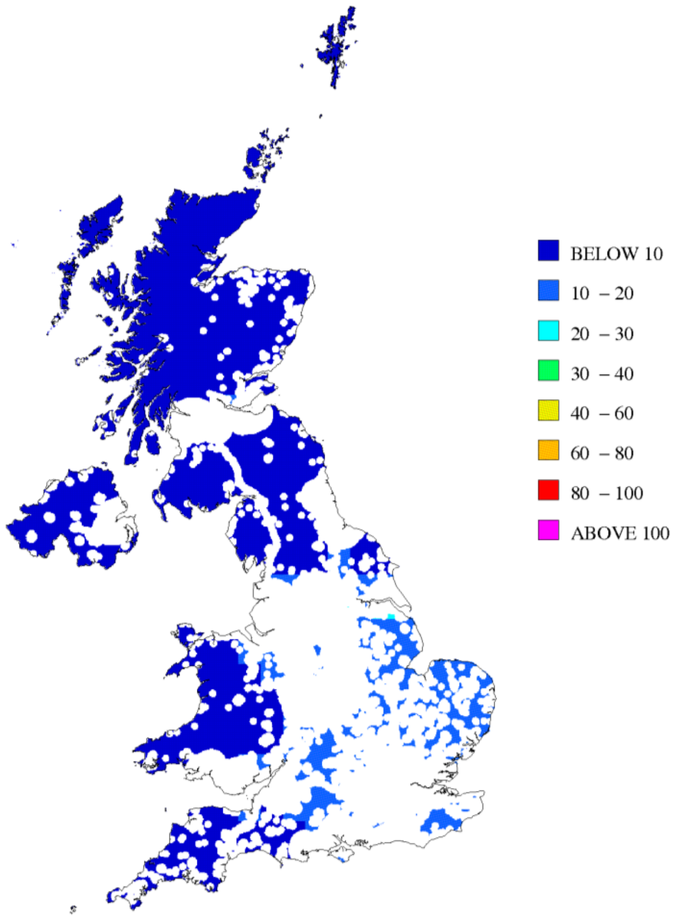
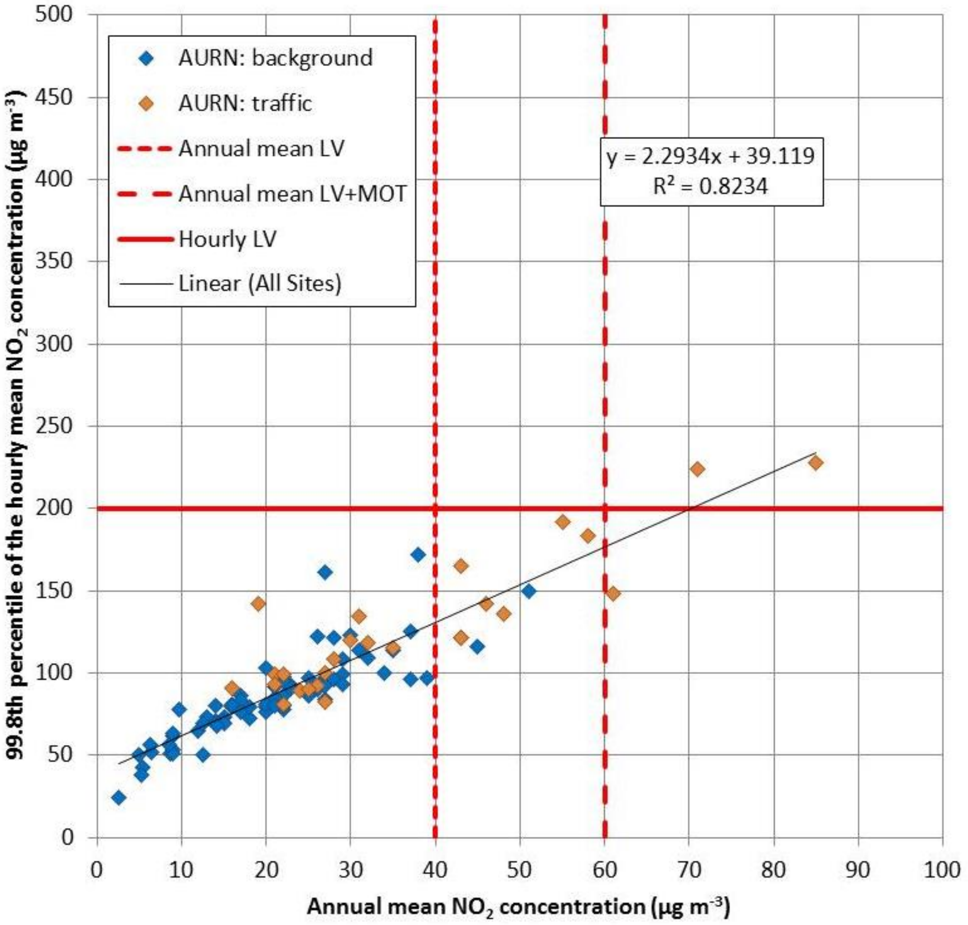


Figure 3.4 - Plot of annual mean against 99.8th percentile hourly NO_2 concentrations in 2013



3.2 NO_X emissions

The NO_X modelling is underpinned by the UK National Atmospheric Emissions Inventory 2012 (NAEI 2012) NO_X emissions estimates (Passant et al., 2014). Emissions projections have been provided by the NAEI (Passant pers. comm. 2014a) based on DECCs UEP48 energy and emissions projections (DECC, 2013). Figure 3.5 shows the UK total NO_X emissions for 2012 and emissions projections for 2015, 2020, 2025 and 2030 split by SNAP code, with the coding described in Table 3.1. Values for intermediate years have been interpolated in this figure. The figure shows that NO_X emissions in 2013 are dominated by three main sources:

- SNAP 7: road transport (exhaust emissions)
- Combustion point sources (SNAP codes 1, 2 and 3)
- SNAP 8: other transport & mobile machinery (ships)

NO_X emissions are predicted to decrease by just over a third between 2012 and 2030, with a particularly steep decline from road transport exhaust emissions and combustion point sources over this period.

Figure 3.5 - Total UK NO_X emissions for 2012 and emissions projections up to 2030 by SNAP code from NAEI 2012

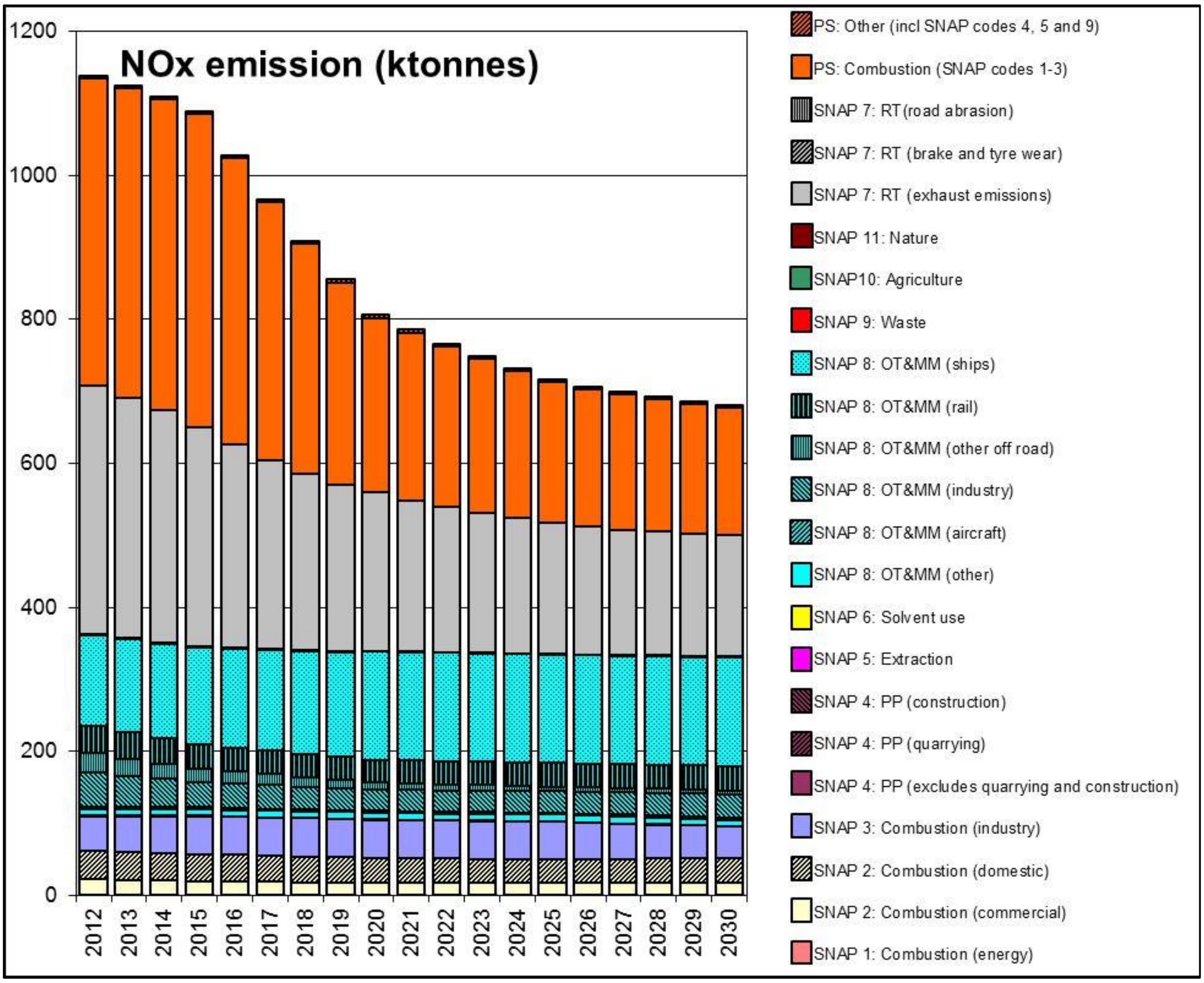


Table 3.1 - Description of SNAP sector coding

Short code	Description
SNAP 1: Combustion (energy)	SNAP 1: Combustion in energy production & transformation
SNAP 2: Combustion (commercial)	SNAP 2: Combustion in Commercial, Institutional & residential & agriculture (excludes domestic)
SNAP 2: Combustion (domestic)	SNAP 2: Combustion in Commercial, Institutional & residential & agriculture (domestic only)
SNAP 3: Combustion (industry)	SNAP 3: Combustion in industry
SNAP 4: PP (excludes quarrying and construction)	SNAP 4: Production processes (excludes quarrying and construction)
SNAP 4: PP (quarrying)	SNAP 4: Production processes (quarrying)
SNAP 4: PP (construction)	SNAP 4: Production processes (construction)
SNAP 5: Extraction	SNAP 5: Extraction & distribution of fossil fuels
SNAP 6: Solvent use	SNAP 6: Solvent use
SNAP 8: OT&MM (other)	SNAP 8: Other Transport & mobile machinery (other)
SNAP 8: OT&MM (aircraft)	SNAP 8: Other Transport & mobile machinery (aircraft)
SNAP 8: OT&MM (industry)	SNAP 8: Other Transport & mobile machinery (industry off road mobile machinery)
SNAP 8: OT&MM (other off road)	SNAP 8: Other Transport & mobile machinery (other off road mobile machinery)
SNAP 8: OT&MM (rail)	SNAP 8: Other Transport & mobile machinery (rail)
SNAP 8: OT&MM (ships)	SNAP 8: Other Transport & mobile machinery (ships)
SNAP 9: Waste	SNAP 9: Waste treatment and disposal
SNAP10: Agriculture	SNAP10: Agriculture forestry & land use change
SNAP 11: Nature	SNAP 11: Nature
SNAP 7: RT (exhaust emissions)	SNAP 7: Road transport (exhaust emissions)
SNAP 7: RT (brake and tyre wear)	SNAP 7: Road transport (brake and tyre wear)
SNAP 7: RT(road abrasion)	SNAP 7: Road transport (road abrasion)
PS: Combustion (SNAP codes 1-3)	Combustion point sources (SNAP codes 1-3)
PS: Other (incl SNAP codes 4, 5 and 9)	Other point sources (including SNAP codes 4, 5 and 9)

3.3 NO_X modelling

3.3.1 NO_X contributions from large point sources

Point sources in the NAEI 2012 have been classified as large if they fulfil either of the following criteria:

- Annual NO_X emissions in the NAEI 2012 are greater than 500 tonnes for any given plant
- Stack parameters are already available for any given plant in the PCM stack parameters database (described in more detail below)

Contributions to ground level annual mean NO_X concentrations from large point sources in the NAEI 2012 were estimated by modelling each source explicitly using the atmospheric dispersion model ADMS 5.0 and sequential meteorological data for 2013 from Waddington. A total of 378 large point sources were modelled. Surface roughness was assumed to be 0.1 m at both the dispersion and meteorological sites. Concentrations were calculated for a 99 km x 99 km square composed of a regularly spaced 1 km x 1 km resolution receptor grid. Each receptor grid was centred on the point source. For each large point source information was retrieved from the PCM stack parameters database. This database has been developed over a period of time under the current Modelling of Ambient Air Quality (MAAQ) contract and its predecessors. The database is updated annually as required. Data sources for this database include a survey of Part A authorisation notices held by the Environment Agency and previously collated datasets on emission release parameters from large SO_2 point sources (Abbott and Vincent, 1999). Parameters used in the modelling from the stack parameters database include:

- Stack height
- Stack diameter
- Discharge velocity
- Discharge temperature

Where release parameters were unavailable, engineering assumptions have been applied.

The NAEI emissions for large point sources are for the year 2012; however, the year 2013 has been modelled for the assessment. The modelled concentrations for 2012 have been scaled to 2013 using projection factors calculated from NAEI source sector specific emissions total for point sources for 2012 and NAEI emissions projections for 2013 (described in Section 3.3.5). Closure of particular plant or activities are taken into account when deriving the source sector projection factors by subtracting the base year emissions associated with plant closure from the relevant source sector total for point sources for the NAEI base year. Any point sources in the NAEI base year which closed before the start or early on in the current assessment year are removed from the modelling, based on recommendations from the NAEI team (Passant pers. comm. 2014b).

3.3.2 NO_X contributions from small point sources

Contributions from NO_X point sources in the NAEI 2012 which were not classified as large point sources (see above) were modelled using the small point source model described in Appendix 3. In line with the method applied for the large point sources the NAEI 2012 emissions for small point sources have been scaled to 2013 using the same source sector specific projection factors applied to the large point sources.

3.3.3 NO_X contributions from ETS point sources

In common with the NAEI 2011 additional point source emissions data have been provided in the NAEI 2012. These emissions estimates have been derived from carbon emissions data reported under the EU-Emissions Trading Scheme (ETS), most recently described in Tsagatakis et al. (2014). These point sources are referred to as ETS points in this report. To model the contribution to background annual mean NO_x concentrations from ETS points the emissions have been treated as an additional set of small point sources. As such they have been modelled using the small points approach (described in Appendix 3). These derived air quality pollutant emissions estimates are particularly uncertain, hence the emissions for particular sources have been capped at reporting thresholds given by the Scottish Pollutant Release Inventory (SPRI). Typically more than 90% of the ETS points do not exceed the SPRI reporting threshold, which for NO_x is 100 tonnes per year.

3.3.4 NO_X contribution from rural background concentrations

Rural annual mean background NO_X concentrations have been estimated using:

- NO_X measurements at 9 selected rural AURN sites.
- NO_X estimated from NO_2 measurements at 19 rural NO_2 diffusion tube sites from the UK Eutrophying and Acidifying Atmospheric Pollutants Network.

Figure 3.6 shows the locations of these monitoring sites and the interpolated rural map.

Rural NO_X was estimated from rural NO_2 at diffusion tube sites by dividing by 0.7835. This factor, which is a typical NO_X/NO_2 ratio measured at rural automatic monitoring sites (Stedman et al., 2003), does not vary significantly between years or across the country. Measurements have then been corrected to remove the contribution from point source and local area sources to avoid double counting these contributions later in the modelling process.

The correction procedure is as follows:

Corrected rural background ($\mu g\ m^{-3}$) *= Uncorrected rural background* ($\mu g\ m^{-3}$) *– (A + B + C)*,

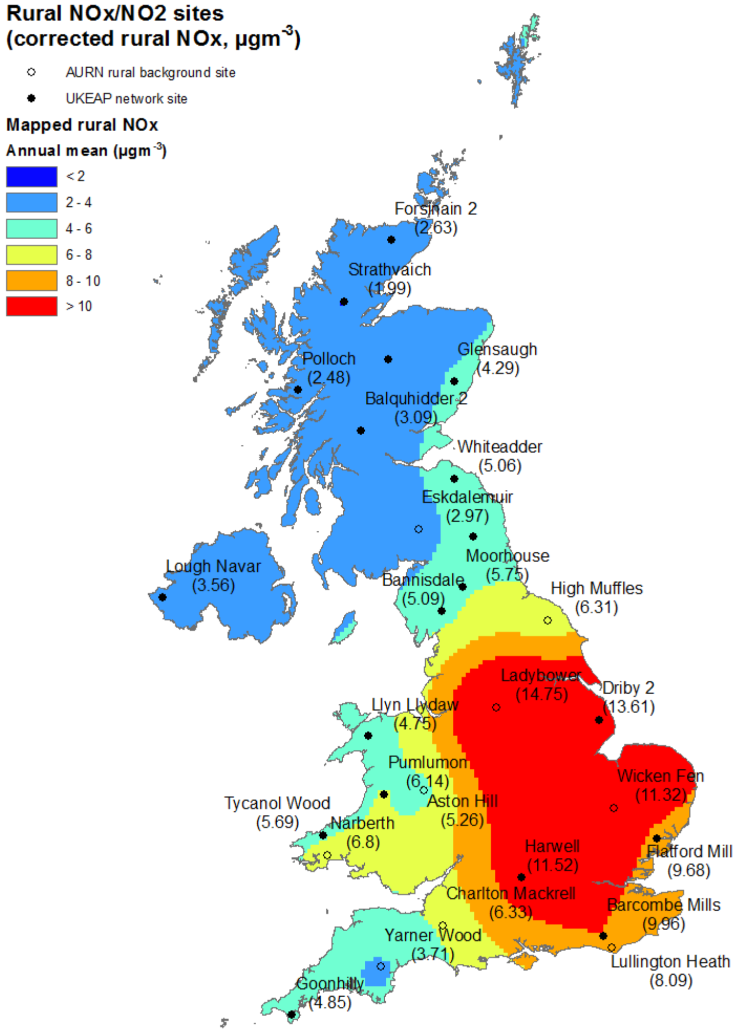
where: *A* is an estimate of the contribution from area source components, derived using the area source contributions from the 2012 modelling (scaled using the ratio of 2012 and 2013 emissions),

B is the sum of contributions from large point sources in 2012 modelling,

C is the sum of contributions from small point sources in 2012 modelling.

Automatic sites, where available have been used in preference to diffusion tubes as these are considered to be more accurate. An interpolation of corrected rural measurement data by Kriging has been used to map regional background concentrations throughout the UK.

Figure 3.6 - Rural background NO_X concentrations map with monitoring sites used in the interpolation (annual mean NO_X concentrations for 2013 ($\mu g\ m^{-3}$, as NO_2) are shown below the site name)



3.3.5 NO_X contributions from local area sources

In the NAEI 2012, NO_X area source emissions maps have been calculated for each source code-activity code combination using distribution grids that have been generated using appropriate surrogate statistics. These NO_X emissions grids are then added together to give SNAP code sector NO_X area source emission grids. The full method is described in Tsagatakis et al. (2014). To calculate NO_X area source emission grids for 2013 emissions projections from the NAEI (Passant pers. comm. 2014a) for each source code-activity code combination have been used to scale 2012 emissions forwards to 2013. The emissions projections are based on DECCs UEP48 energy and emissions projections (DECC, 2013). The 2013 area source NO_X emissions have been mapped using updated distribution grids produced for the NAEI 2012 (Tsagatakis et al. 2014).

The 2013 area source emissions maps have then been used to calculate uncalibrated area source concentration maps for each SNAP code sector. With the exception of SNAP sector 3 (combustion in industry), this has been done by applying an ADMS 5.0 derived dispersion kernel to the emission maps to calculate the contribution to ambient concentrations on a 1 km x 1 km receptor grid, from the area source emissions within a 33 km x 33 km square surrounding each receptor. Hourly sequential meteorological data from Waddington in 2013 have been used to construct the dispersion kernels. Appendix 4 describes these kernels in more detail and explains how they have been calculated.

For 2011, 2012 and 2013 a new dispersion kernel approach has been applied to the SNAP 2 domestic area sources sector for the whole of the UK in order to weight these emissions more realistically by time of day and meteorological conditions. The approach has been to develop a time varying emission profile based on degree days, which is described in Appendix 4. A degree day scaling factor has also been applied to all of SNAP 2 to project changes in combustion activity related to year to year variations in meteorology. This scaling factor was derived from the ratio of the summed degree days for 2013 to the summed degree days for 2012. A degree day is unit used to determine the heating requirements of buildings, representing a fall of one degree below a specified average outdoor temperature.

A development introduced for the 2011 assessment (and also used in the 2012 and 2013 assessments) was a revision to the methodology for treating the SNAP 3 (combustion in industry) area source component (i.e. the component of the UK SNAP 3 national total not accounted for by regulated processes). This sector was formerly modelled as a volume source with emissions at a fixed release height, using the area source dispersion kernel approach described in Appendix 4. This over simplified real world release conditions; the magnitudes of emission observed in the emissions inventory are such that in operational terms they would be expected to occur under some sort of authorised release at height and with thermal buoyancy which would impart greater dispersion on the plume. In recognition of this, the small points model (described in Appendix 3) has been applied to derive concentrations resulting from SNAP 3 area source emissions. By using the small points method for this sector a more realistic release height, buoyancy and momentum of discharge is used based on the magnitude of the emission for small industrial chimneys.

Figure 3.7 shows the calibration of the area source model. The modelled concentrations from all point sources, SNAP 3 area sources and corrected rural NO_X concentrations have been subtracted from the measured annual mean NO_X concentration at background sites. This concentration is compared with the modelled area source contribution (excluding SNAP 3) to annual mean NO_X concentrations to calculate the calibration coefficients used in the area source modelling.

As part of the calibration process emission caps have been applied to certain sectors; this is because the use of surrogate statistics for mapping area source emissions sometimes results in unrealistically large concentrations in some grid squares for a given sector. The emission caps applied are given in Table 3.2.

The modelled area source contributions for each sector except SNAP 3 were multiplied by the coefficient to calculate the calibrated area source contribution for each grid square in the country. The point source contributions, SNAP 3 area source component and regional rural concentrations were then added, resulting in a map of background annual mean NO_X concentrations.

Figure 3.7 - Calibration of area source NO_X model, 2013 ($\mu g\ m^{-3}$, as NO_2)

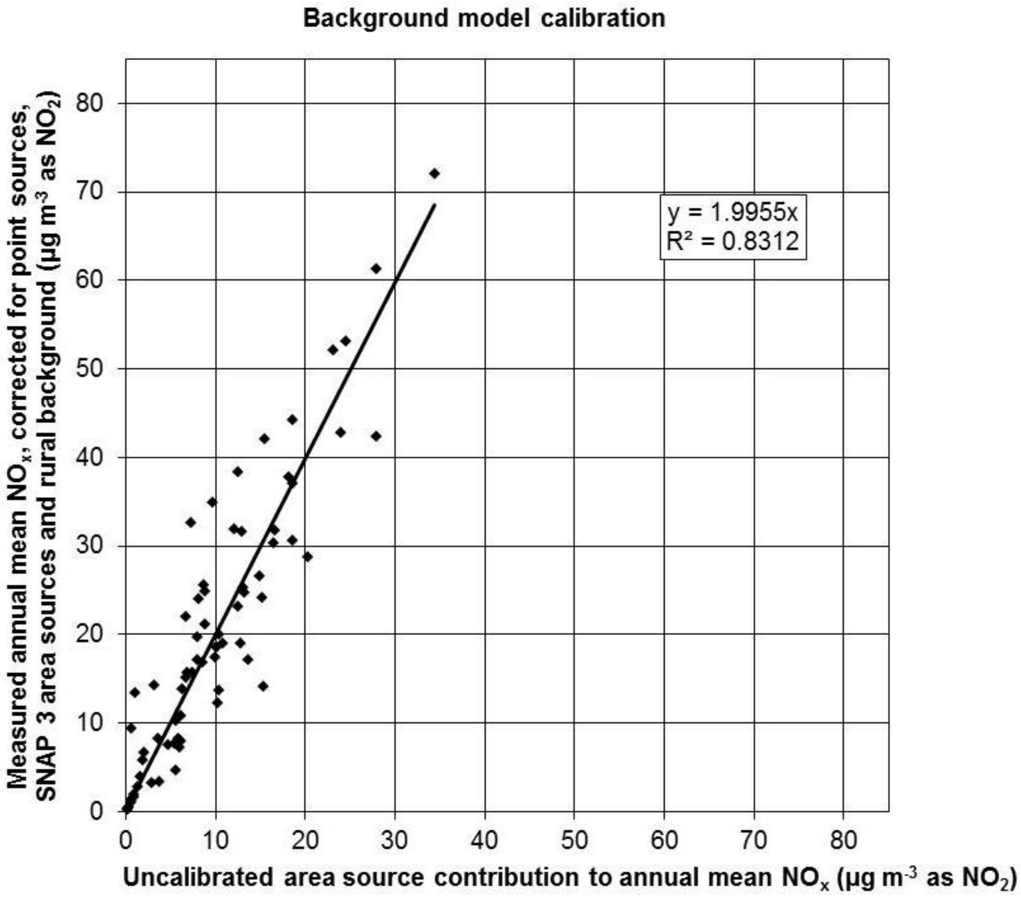


Table 3.2 - Emission caps applied to NO_X sector grids

SNAP code	Description	Cap applied (t/a/km^2)
SNAP 1 (Upstream oil and gas production, combustion at gas separation plant LPG)	Combustion in energy production & transformation	30
SNAP 1 (Upstream oil and gas production, combustion at gas separation plant OPG)	Combustion in energy production & transformation	30
SNAP 1 (Gas production, natural gas)	Combustion in energy production & transformation	30
SNAP 1 (Refineries combustion, natural gas)	Combustion in energy production & transformation	75
SNAP 2 (Public sector combustion, natural gas)	Combustion in Commercial, Institutional & residential & agriculture	75
SNAP 8 (shipping only)	Other Transport & Mobile Machinery	100

3.3.6 NO_X Roadside concentrations

The annual mean concentration of NO_X at roadside locations has been assumed to be made up of two parts: the background concentration (as described above) and a roadside increment:

roadside NO_X concentration = background NO_X concentration + NO_X roadside increment.

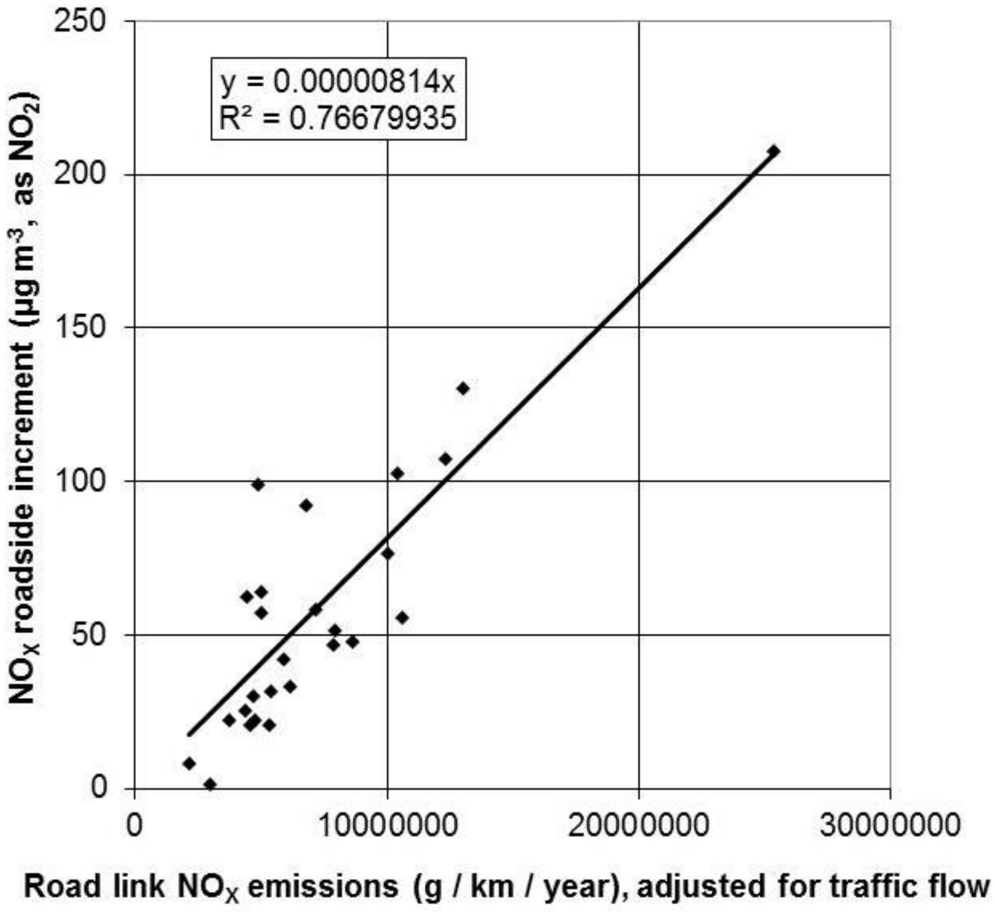
The NAEI provides estimates of NO_X emissions for major road links in the UK for 2012 (Passant et al., 2014) and these have been adjusted to provide estimates of emissions in 2013. The projections for NO_X were updated with the following changes (Passant et al., 2014):

- The Department for Transport (DfT) 2013 traffic forecasts;
- Updated NO_x assumptions for Euro 5/6 diesel cars and LGVs based on COPERT 4 v10.0
- The uptake of low carbon passenger cars and LGVs with electric and hybrid electric propulsion systems is included for the first time, according to figures provided by DfT.
- Slightly lower diesel car penetration rates are assumed compared with previous projections, reaching 41% of all new car sales by 2020, compared with 43% previously assumed.
- Some measures specific for London are also included, such as updated fleet composition projections for TfL buses and updated traffic projections (2013) for London provided by Transport for London (TfL).
- Inclusion of new EU Directive on motorcycle emissions covering stricter emissions standards.

Figure 3.8 shows the roadside increment of annual mean NO_X concentrations (i.e. measured roadside NO_X concentration minus modelled background NO_X concentration) at roadside AURN monitoring sites plotted against NO_X emission estimates adjusted for traffic flow for the individual road links alongside which these sites are located. The background NO_X component at these roadside monitoring sites is taken from the background map described in Section 3.3.5 above.

The calibration coefficient derived is then used to calculate the roadside increment on each road link by multiplying it by an adjusted road link emission (see Figure 3.8). The average distance from the kerb for the roadside and kerbside monitoring sites used to calibrate the roadside increment model is approximately 4 m. The calculated roadside concentrations are therefore representative of this distance from the kerb. Roadside concentrations for urban major road links (A-roads and motorways) only are reported to the EU and included in this report.

Figure 3.8 - Calibration of NO_X roadside increment model, 2013 ($\mu g\ m^{-3}$, as NO_2)



The dispersion of emissions from vehicles travelling along an urban road is influenced by a number of factors. These factors generally contribute to make the dispersion of emissions less efficient on urban roads with lower flows. Factors include:

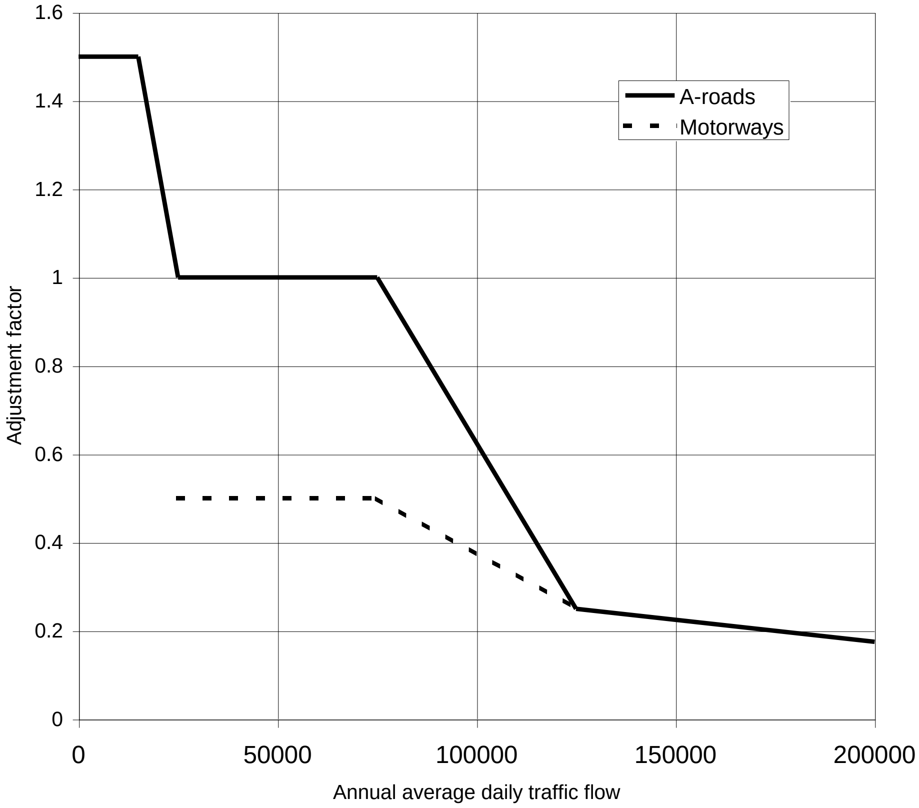
- Traffic speed (urban roads with lower flows are more likely to have slower moving traffic and thus cause less initial dispersion due to mechanical and thermal turbulence)
- Road width (dispersion will tend to be more efficient on wider roads, such as motorways than on smaller roads in town centres)
- Proximity of buildings to the kerbside (buildings close to the road result in a more confined setting and hence reduced dispersion)

Only urban roads have been considered here because the model does not cover rural roads.

Detailed information on the dispersion characteristics of each urban major road link within the NAEI is not available. An approach similar to that used within the DMRB Screening Model (Boulter, Hickman and McCrae, 2003) has therefore been adopted and adjustment factors applied to the estimated emissions. These adjustment factors are illustrated in Figure 3.9 and depend on the total traffic flow on each link and are higher for the roads with the lowest flow and lower for roads with the highest flow. Thus the traffic flow is used as a surrogate for road width and other factors influencing dispersion. Motorways are generally wider than A-roads and the emission have therefore been adjusted accordingly, as illustrated in Figure 3.9.

An improved modelling method for traffic (roadside) locations, the PCM Roads Kernel Model, has been adopted for an update to the assessment for NO_2, see Section 3.6.

Figure 3.9 - The adjustment factors applied to road link emissions



3.4 NO_2 Modelling

3.4.1 Introduction

Maps of estimated annual mean NO_2 concentrations (Figure 3.1 and Figure 3.2) have been calculated from the modelled NO_X concentrations using a calibrated version of the updated oxidant-partitioning model (Jenkin, 2004; Murrells et al., 2008, Jenkin, 2012). This model uses representative equations to account for the chemical coupling of O_3, NO and NO_2 within the atmosphere. A key advantage of this approach for modelling NO_2 concentrations is that emission scenarios can be directly addressed by varying regional oxidant levels and/or primary NO_2 emissions.

3.4.2 The updated oxidant-partitioning model

The oxidant-partitioning model, developed by Jenkin (2004), enables NO_2 concentrations to be calculated using the following equations:

$$[NO_2] = [OX].f(NO_x) \qquad (i)$$
$$[OX] = f\text{-}NO_2.[NO_x] + [OX]_B \qquad (ii)$$

Where [OX] is the total oxidant (the sum of NO_2 and O_3), f-NO_2 is the primary NO_2 emission fraction (defined as the proportion of NO_X emitted directly as NO_2), $[OX]_B$ is the regional oxidant and f(NO_x) is a function, the value of which is determined by the concentration of NO_x. NO_X, NO_2, O_3 and OX are all expressed as ppb in these equations: 1 ppb of O_3 = 2 µg m^{-3}; 1 ppb of NO_2 = 1.91 µg m^{-3}. By convention when NO_X is expressed in µg m^{-3} it is expressed as “µg m^{-3} as NO_2” therefore 1 ppb of NO_X = 1.91 µg m^{-3} of NO_X as NO_2.

In Jenkin (2004), $[NO_2]/[OX]$ was calculated using two equations, one of which represented background locations and the other roadside locations. Updated equations for $[NO_2]/[OX]$

were subsequently developed in (Murrells et al., 2008). More recently, Jenkin (2012) found that short term variability in NO_x concentrations is a major cause of the scatter in the relationship between $[NO_2]/[OX]$ and $[NO_X]$. The ratio of the upper to the lower quartile of hourly concentrations is a good indicator of this variability and this ratio increases with decreasing NO_x concentrations at roadside and background sites. This dependence has been used to interpolate between equations based on a constant NO_x quartile ratio. This led to two equations for calculating $[NO_2]/[OX]$, one of which represents background locations and the other roadside locations. These are the equations that are currently used in the modelling. These are an improvement over the equations presented in Murrells et al. (2008) because the background equation requires less adjustment in the background adjustment calibration and the roadside equation enables linear calibration adjustment for roadside.

Jenkin (2012) presented two equations for calculating $[NO_2]/[OX]$ as a function of $[NO_X]$. These are:

- One background relationship, which has been derived using data from background sites.
- One roadside relationship, which has been derived using data from roadside sites.

The two relationships are presented in Table 3.3 below.

Table 3.3 - The two relationships in the updated oxidant-partitioning model (Jenkin, 2012)

PCM Category	Relationship (where y = $[NO_2]/[OX]$ and x = $[NO_X]$, in ppb)
Background	y = -2.5124E-13x^6 + 1.5805E-10x^5 – 4.1429E-08x^4 + 5.8239E-06x^3 – 4.8076E-04x^2 + 2.5916E-02x
Roadside	y = -2.0901E-13x^6 + 1.5001E-10x^5 – 4.2894E-08x^4 + 6.2659E-06x^3 – 5.0720E-04x^2 + 2.5322E-02x

The following sections describe the method for calculating an average regional oxidant value for the UK (Section 3.4.3), local oxidant calculations for background and roadside locations (Section 3.4.4), calculating $[NO_2]/[OX]$ in the PCM model and how the updated oxidant-partitioning model has been applied in the UK to background and roadside locations (Section 3.4.5).

3.4.3 UK regional oxidant

In 2013 a map of 2012 UK regional oxidant was produced using the method outlined in Murrells et al. (2008). This map was compared to the average measured regional oxidant. It was found that there was little difference between using the map and using the average measured regional oxidant. Therefore for modelling 2013 the average measured regional oxidant has been calculated and this has been used in the model as a fixed regional oxidant value for the whole of the UK.

The regional oxidant value for 2013 was calculated to be 32.5 ppb. This value was derived from an analysis of annual mean data for O_3, NO_2 and total nitrogen oxides (NO_x) at 49 AURN sites. These sites were selected using the criterion that the annual mean $[NO_X]$ in 2013 was less than 25 ppb, so that the contribution to [OX] derived from primary NO_2 was comparatively small. A constant value f-NO_2 value of 0.093 was used to correct for the contribution from local oxidant

3.4.4 Local oxidant calculations

Local oxidant is calculated in the updated oxidant-partitioning model as:

$$\textit{Local oxidant} = f\text{-}NO_2.[NO_X]. \qquad (iv)$$

Where $f\text{-}NO_2$ is the fraction of NO_x emissions emitted as primary NO_2 (by volume). Therefore, to calculate local oxidant levels, the $f\text{-}NO_2$ levels from different local sources need to be understood. In general it is possible to make a distinction between $f\text{-}NO_2$ from road traffic sources and *f-NO_2* from non-road traffic sources. *f-NO_2* from road traffic sources is thought to have risen since the early 2000s, although this trend displays considerable variation with location (AQEG, 2007; Carslaw et al., 2011). By comparison, *f-NO_2* from non-traffic sources has remained relatively constant with time.

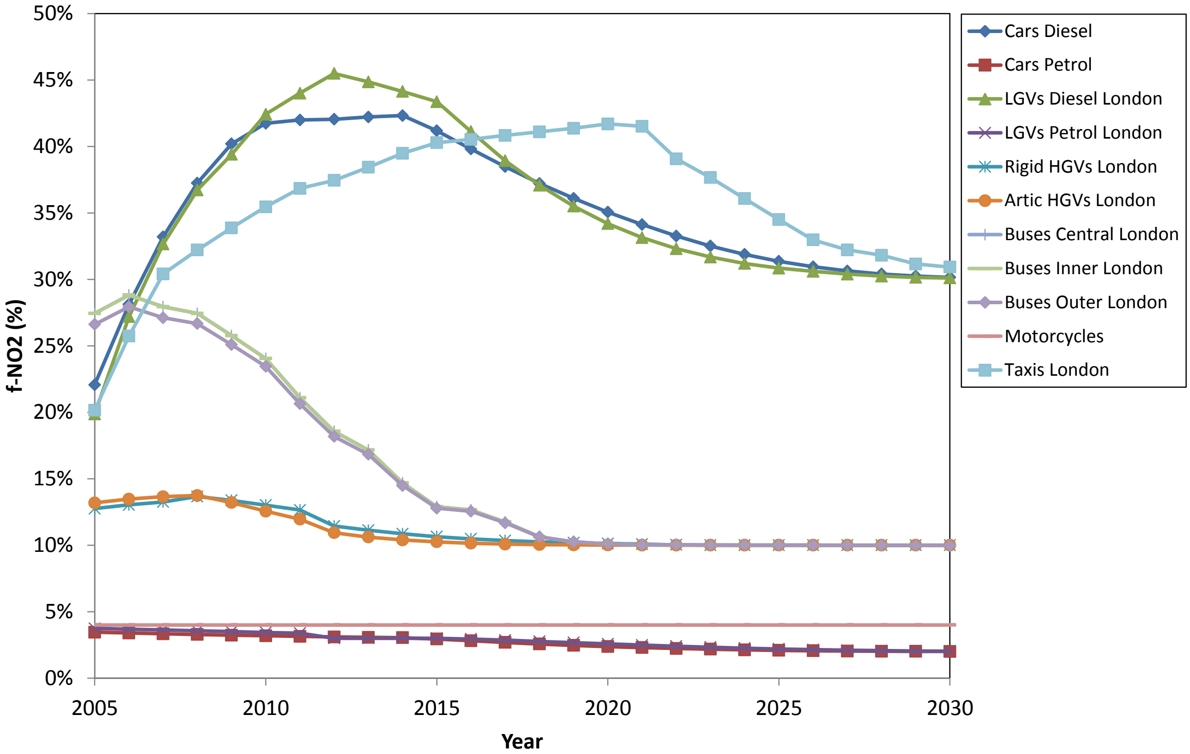
3.4.4.1 *f-NO_2 for road traffic sources on individual road links*

Figure 3.10 shows fleet average *f-NO_2* projections by vehicle type for London and the rest of the UK from the NAEI 2012.

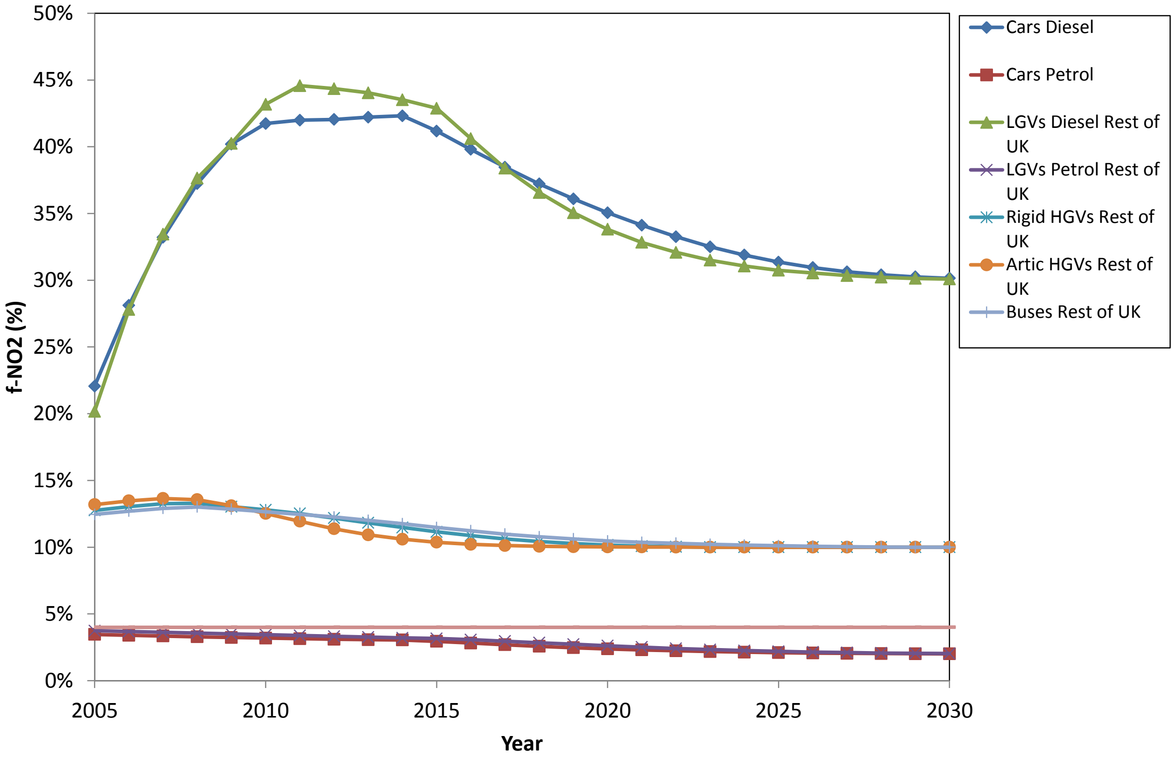
f-NO_2 for all petrol vehicles is very low (less than 5%). f-NO_2 for diesel cars and LGVs rose steeply between 2005 and about 2010 and is expected to decline somewhat from 2020 onwards. A gentle decline in f-NO_2 is expected for HGVs and buses outside London. Buses in London had higher f-NO_2 than in the rest of the UK in 2005 and this is expected to decline and be similar to the rest of the UK before 2020. f-NO_2 for London taxis is expected to peak in about 2020.

Figure 3.10 - Fleet average f-NO_2 projections by vehicle type for a) London and b) rest of the UK from NAEI 2012

a) London



b) Rest of the UK



3.4.4.2 f-NO_2 for background sources

Table 3.4 shows the *f-NO_2* values used for background sources in 2013.

The non-road *f-NO_2* values used for background calculations in Table 3.4 have been taken directly from Jenkin (2004), as there is little evidence that this has changed significantly over the past few years.

The road traffic *f-NO_2* values for background calculations have been calculated using the average of the major road link *f-NO_2* values for each area type.

Table 3.4 - Local oxidant coefficients (f-NO_2) for background concentrations in 2013

DfT Area type[1]	Region	Non-road *f-NO_2* for background calculations	Road *f-NO_2* for background calculations
1	Central London	0.140	0.268
2	Inner London	0.128	0.293
3	Outer London	0.093	0.326
4	Inner Conurbations	0.093	0.322
5	Outer Conurbations	0.093	0.339
6	Urban (population > 250,000)	0.093	0.344
7	Urban (population > 100,000)	0.093	0.350
8	Urban (population > 25,000)	0.093	0.354
9	Urban (population > 10,000)	0.093	0.351
10	Rural	0.093	0.345

[1] Locations in Northern Ireland have been assigned area types according to how built up the local environment is because the DfT area types map does not cover Northern Ireland. A map of the distribution of DfT area types is included in Appendix 4.

3.4.4.3 Local oxidant calculations

A map of local oxidant for the background NO_2 calculations was generated by splitting the background annual mean NO_X map into its two constituent components:

- NO_X from background non-road traffic emissions (includes rural background component)
- NO_X from background road-traffic emissions

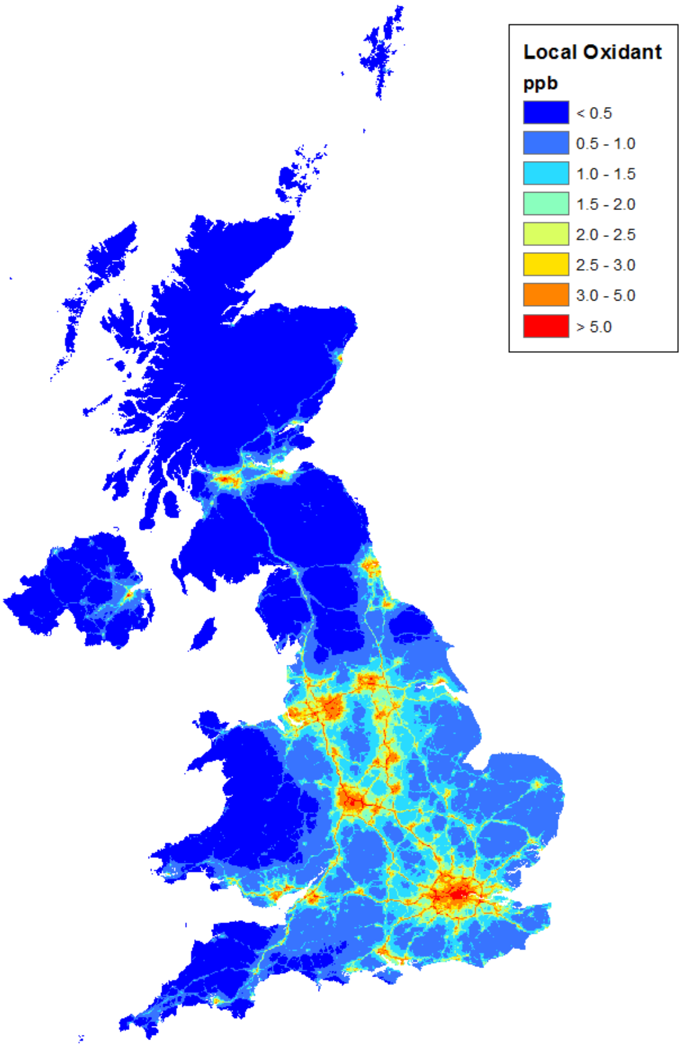
These components were multiplied by the relevant $f\text{-}NO_2$ value from Table 3.4 and then added together to give a total local oxidant. Figure 3.11 shows the UK background local oxidant map for 2013.

Local oxidant on individual road links was calculated by splitting the total annual mean NO_X for the road link into its three constituent components:

- NO_X from background non-road traffic emissions (includes rural background component)
- NO_X from background road-traffic emissions
- Roadside increment NO_X concentrations from emissions on the specific road link under consideration

The background components were then multiplied by the relevant $f\text{-}NO_2$ value from Table 3.4 and the roadside increment NO_X was multiplied by the specific $f\text{-}NO_2$ calculated for that road link. These local oxidant values were then added together to give a total local oxidant for the road.

Figure 3.11 - Background local oxidant map for 2013 (ppb)



3.4.5 Calculating $[NO_2]/[OX]$ in the PCM model

As described in Section 3.4.2, two relationships for calculating $[NO_2]/[OX]$ have been derived in Jenkin (2012). The ratio of $[NO_2]/[OX]$ has been considered separately for background and roadside locations in this analysis as there are separate relationships for these locations. Background and roadside sites tend to behave differently because of differences in the ‘age’ of the NO_X at these locations.

3.4.5.1 Background

For background locations, the background relationship has been calibrated using data from AURN background sites for 2013. The calibration plot for background sites is shown in Figure 3.12. Figure 3.13a and Figure 3.13b show verification plots of measured NO_2 against modelled NO_2 calculated from measured NO_X using the uncalibrated background relationship and calibrated background relationship respectively. The agreement is better for the calibrated model. The background oxidant partitioning curves are only valid for annual mean NO_X concentrations up to 267.4 µg m^{-3} hence NO_X concentrations above this value have been set to 267.4 µg m^{-3}.

Figure 3.12 - Background NO_2 calibration curve (NB verification sites are shown for reference here, but were not used in calculating the calibration), 2013

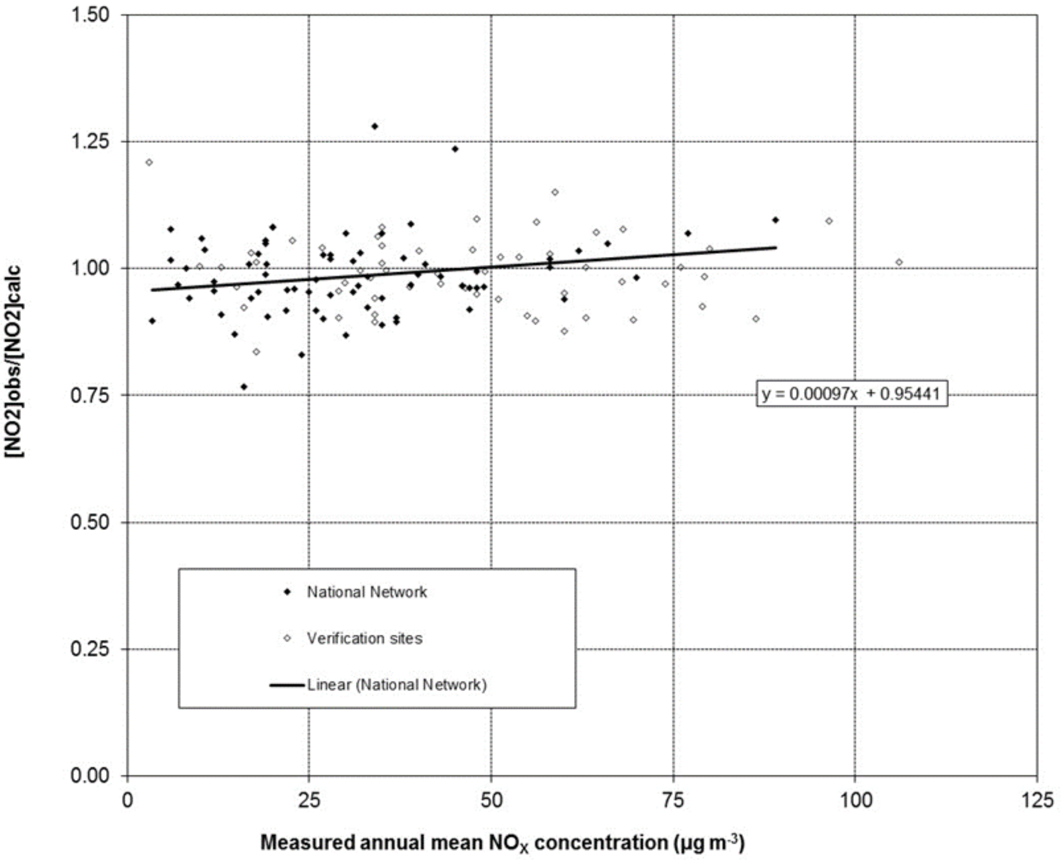
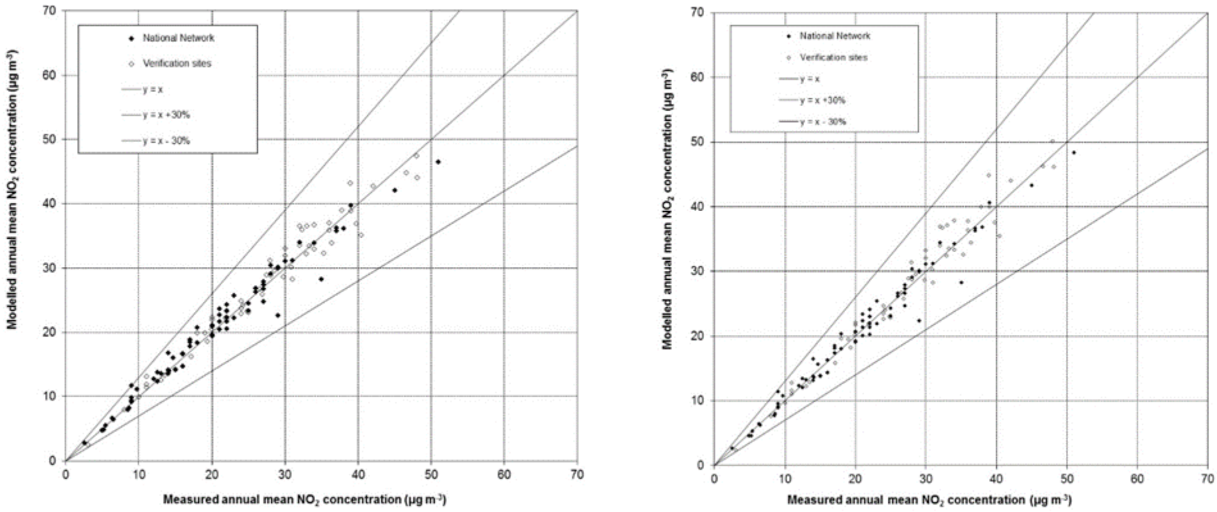


Figure 3.13 - Verification of background relationship at background locations in 2013

a) Uncalibrated **b)** ***Calibrated***



3.4.5.2 Roadside

For roadside locations, the roadside relationship has been selected and an additional calibration has been applied using data from AURN roadside sites for 2013. The model has been calibrated by plotting the ratio of measured NO_2 to modelled NO_2 as a function of NO_X for each AURN roadside sites for 2013 and then fitting a straight line through these points.

Figure 3.14 shows this ratio for each site and also the straight line that was fitted though the data. The verification sites are also shown on this plot for reference although they were not used to calibrate the model.

Figure 3.14 - Roadside NO_2 calibration curve (NB verification sites are shown for reference here, but were not used in calculating the calibration factors), 2013

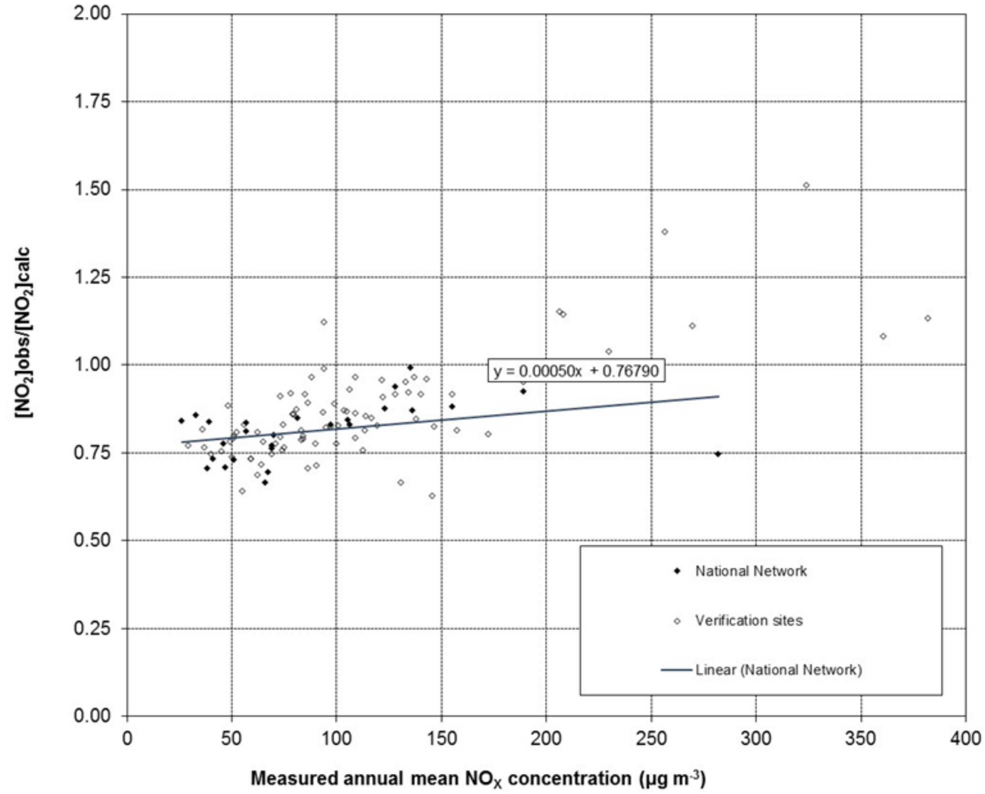
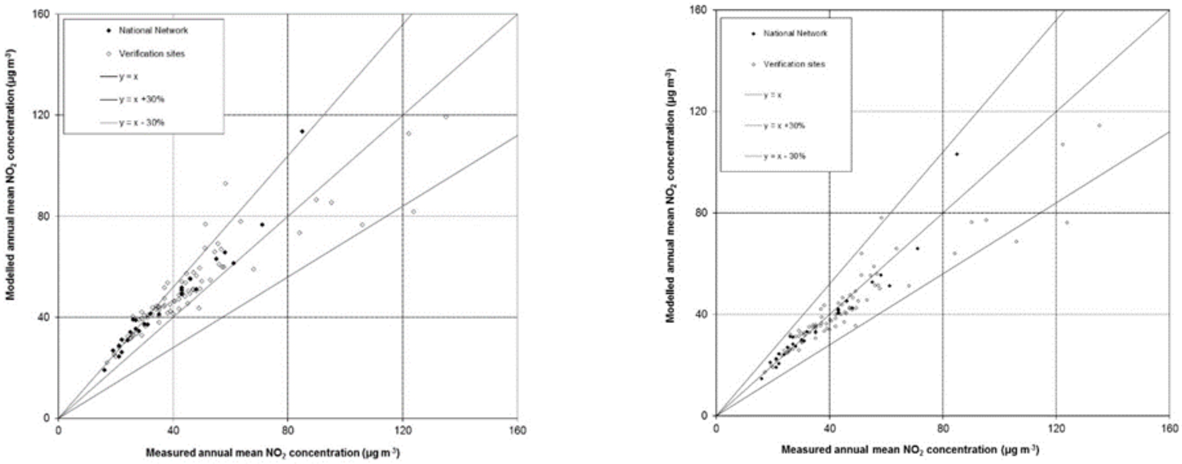


Figure 3.15a shows a verification plot of measured NO_2 against modelled NO_2 calculated from measured NO_X using the uncalibrated roadside relationship. Figure 3.15b shows the same information, but using the calibrated roadside relationship. It is clear that the calibrated model provides a better fit to the monitoring data in the vicinity of the limit value of 40 µg m^{-3}. The roadside oxidant partitioning curves are only valid for annual mean NO_X concentrations up to 382 µg m^{-3} hence NO_X concentrations above this value have been set to 382 µg m^{-3}.

Figure 3.15 - Verification of roadside relationship at roadside locations in 2013



***a)* Uncalibrated** ***b)* Calibrated**

3.5 Results

3.5.1 Verification of mapped values

Figure 3.16 and Figure 3.17 show comparisons of modelled and measured annual mean NO_X and NO_2 concentration in 2013 at background monitoring site locations. Figure 3.18 and Figure 3.19 show similar comparisons for roadside sites. Both the national network sites used to calibrate the models and the verification sites are shown. Lines representing y = x – 30 % and y = x + 30% are also shown (this is the AQD data quality objective for modelled annual mean NO_2 and NO_X concentrations – see Section 1.5). There is no requirement under the AQD to report modelled annual mean NO_X concentrations for comparison with limit values for the protection of human health (the NO_X limit value for the protection of vegetation only applies in vegetation areas). However, comparisons of modelled and measured NO_X concentrations and of the modelled NO_X concentrations with the data quality objectives are presented here alongside the comparisons for NO_2. This provides an additional check on the reliability of the modelled estimates of NO_2 because the non-linear relationships between NO_X and NO_2 tend to cause modelled NO_2 concentrations to be relatively insensitive to errors in the dispersion modelling of NO_X.

Summary statistics for the comparison between modelled and measured NO_X and NO_2 concentrations are listed in Table 3.5 and Table 3.6. The percentages of monitoring sites for which the modelled annual mean concentrations fall outside the data quality objectives is generally greater for NO_X than for NO_2, for the reasons discussed above.

Figure 3.16 - Verification of background annual mean NO_X model 2013

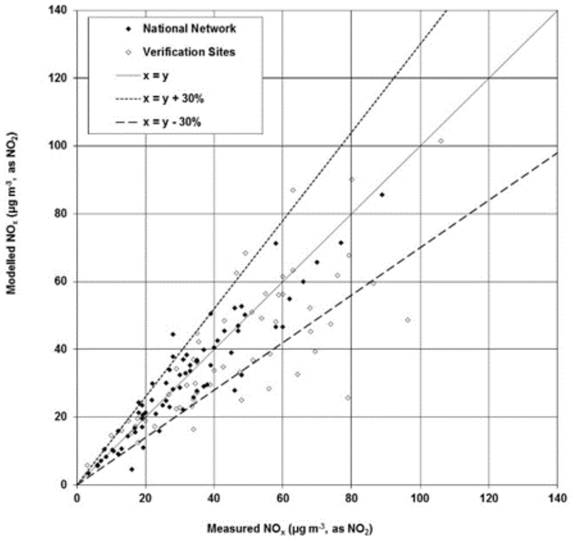


Figure 3.17 - Verification of background annual mean NO_2 model 2013

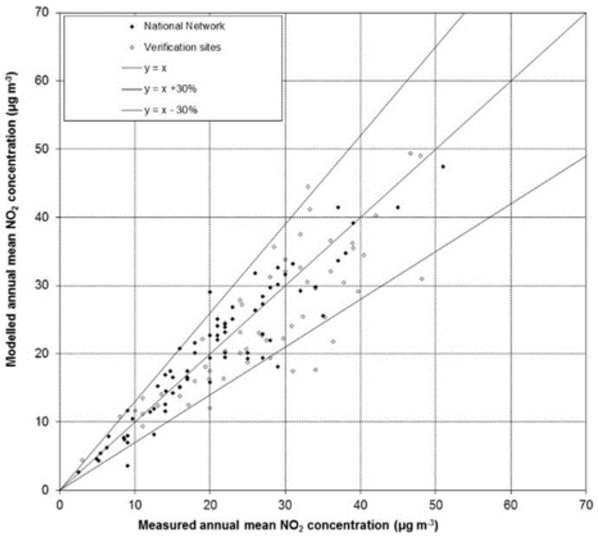


Figure 3.18 - Verification of roadside annual mean NO_X model 2013

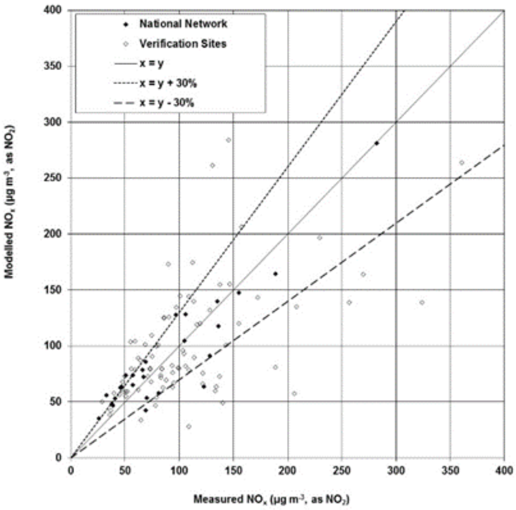


Figure 3.19 - Verification of roadside annual mean NO_2 model 2013

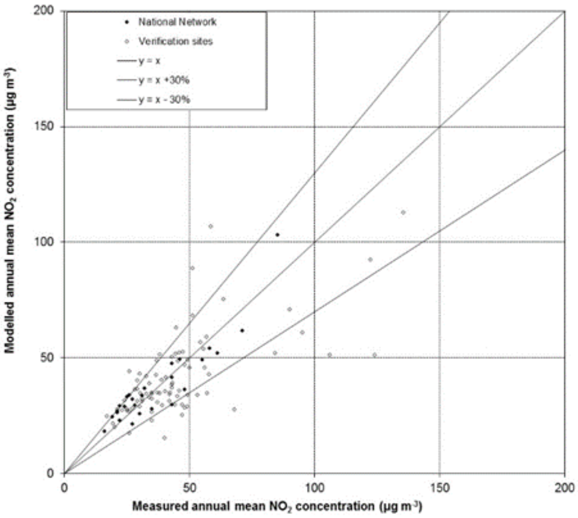


Table 3.5 - Summary statistics for comparison between modelled and measured NO_X and NO_2 concentrations at background sites (µg m^{-3}, as NO_2)

		Mean of measurements (µg m^{-3}, as NO_2)	Mean of model estimates (µg m^{-3}, as NO_2)	R^2	% outside data quality objectives	Number of sites in assessment
NO_X	National Network	31.5	30.9	0.88	14.1	71
	Verification Sites	46.4	39.4	0.61	33.3	57
NO_2	National Network	20.6	20.3	0.88	7.0	71
	Verification Sites	27.1	24.7	0.71	15.8	57

Table 3.6 - Summary statistics for comparison between modelled and measured NO_X and NO_2 concentrations at roadside sites (µg m^{-3}, as NO_2)

		Mean of measurements (µg m^{-3}, as NO_2)	Mean of model estimates (µg m^{-3}, as NO_2)	R^2	% outside data quality objectives	Number of sites in assessment
NO_X	National Network	89.0	89.9	0.86	30.8	26
	Verification Sites	110.8	102.8	0.45	48.2	83
NO_2	National Network	36.9	37.7	0.83	15.4	26
	Verification Sites	45.3	41.7	0.45	34.9	83

3.5.2 Source apportionment

Figure 3.20 and Figure 3.21 show the modelled NO_X source apportionment at AURN background and roadside sites respectively for 2013. This shows that while road transport is the dominant source in the majority of locations (background and roadside), contributions from other sectors such as domestic, commercial, off road mobile machinery and industry are also significant at many sites. Contributions from aircraft and shipping are evident at some sites. No source apportionment is given for NO_2 because this is not a physically meaningful concept because of the non-linear relationship between NO_X and NO_2.

Figure 3.20 - Annual mean NO_X source apportionment at background AURN monitoring sites (area type of each site is shown in parenthesis after its name – see Table 3.4)

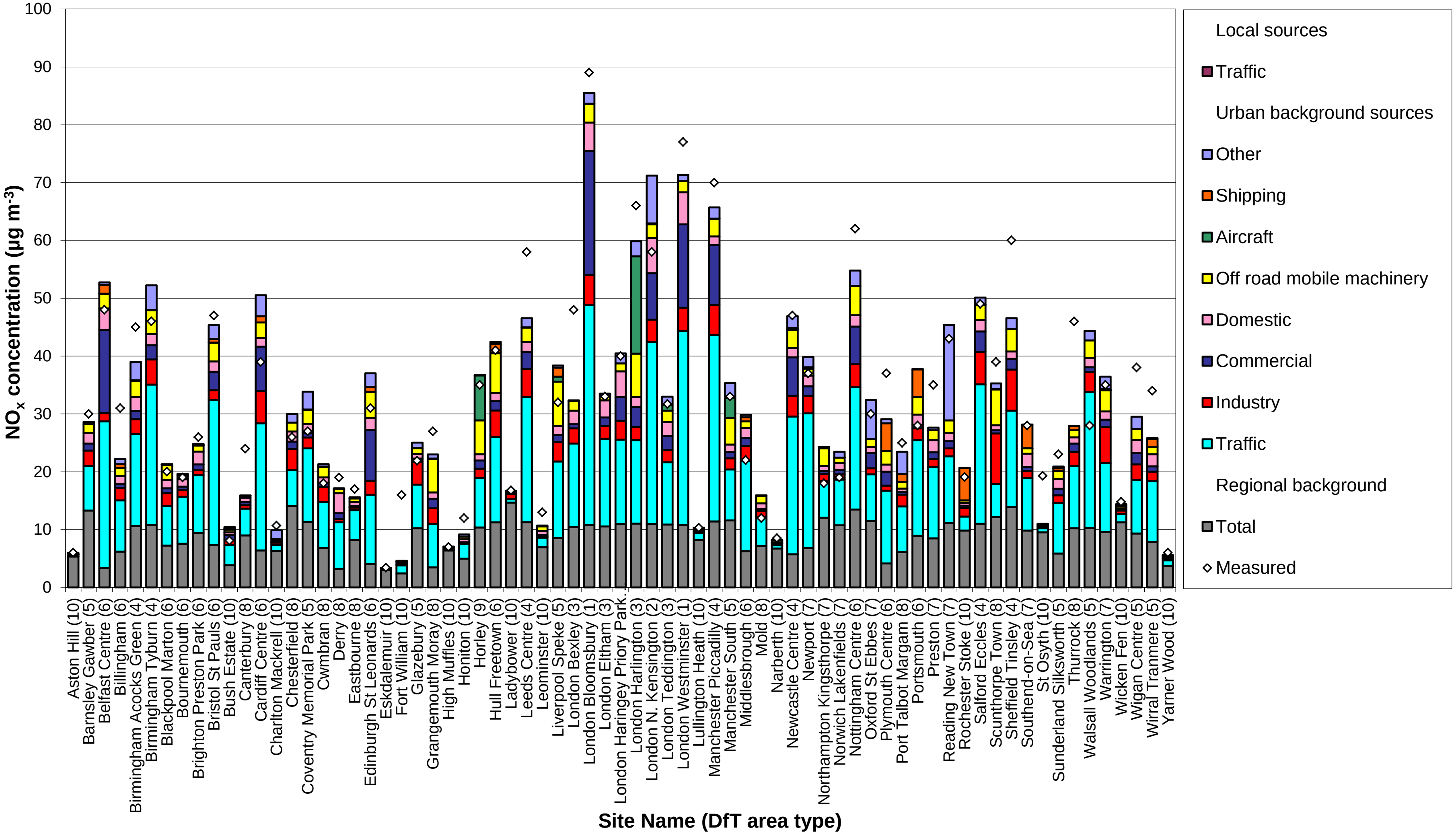
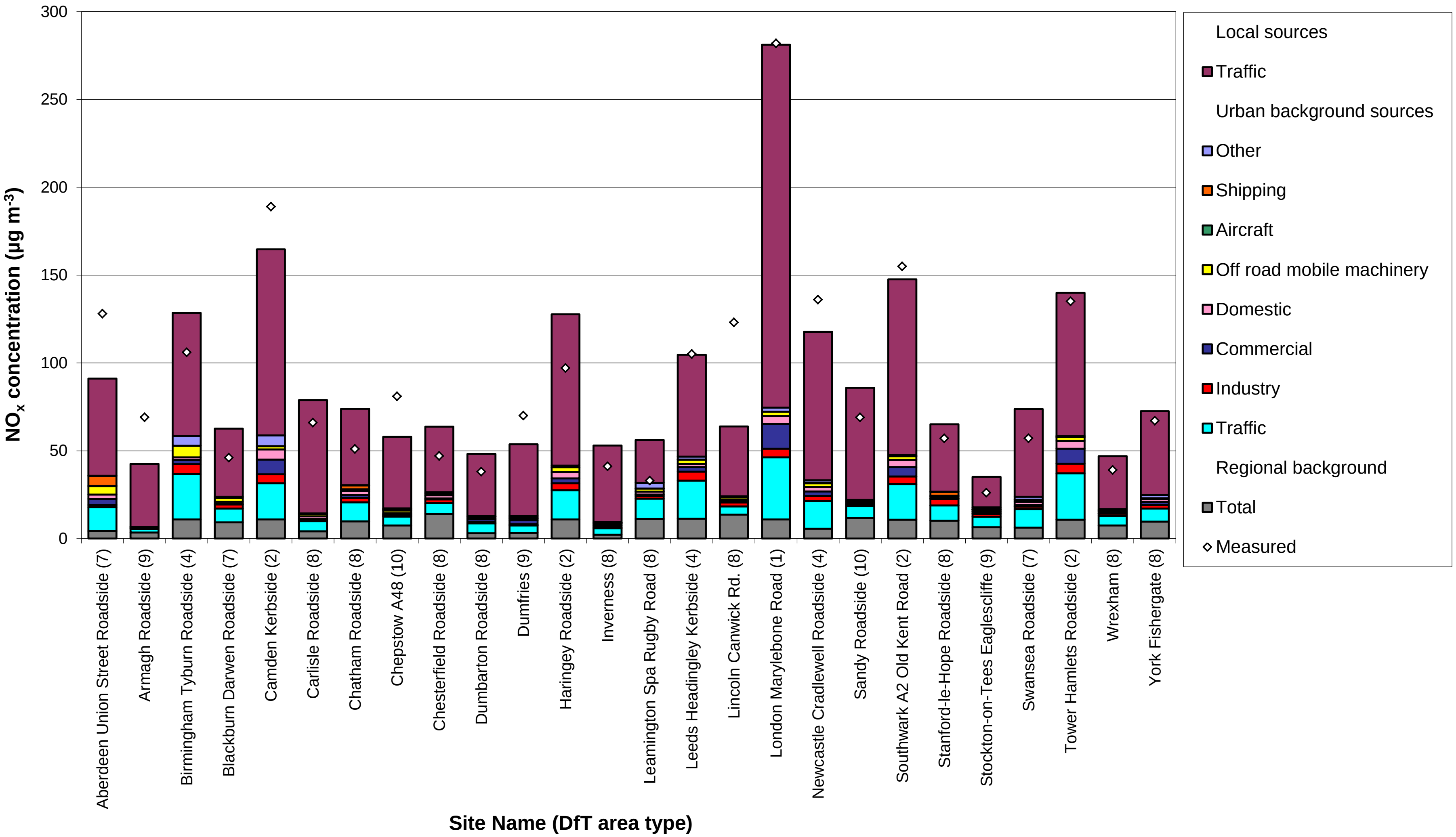


Figure 3.21 - Annual mean NO_X source apportionment at roadside AURN monitoring sites (area type of each site is shown in parenthesis after its name – see Table 3.4)



3.6 Updates to the 2013 NO_2 assessment for the 2015 air quality plans

3.6.1 Introduction

The UK Government is currently (October 2015) consulting on air quality plans for compliance with the limit values for nitrogen dioxide. The reference year for these 2015 air quality plans for NO_2 is 2013. The air quality modelling assessments carried out to support the air quality plans are based on the modelling methods and base year modelling carried out for the 2013 air quality assessment described in this report. The base data has, however, been updated for the 2015 air quality plans to incorporate updated information on emission factors for road traffic emissions of NO_X and an improved modelling method for traffic (roadside) locations. These updates have only become available during the period since the original assessment for 2013 was reported. These revisions were made in order to ensure that the best possible evidence is available to support the development of the 2015 air quality plans. The revised 2013 data will be re submitted to the Commission in due course. The compliance status of all air quality zones in 2013 with respect to the annual limit value for NO_2 is unchanged for this revised assessment.

Full details of the updates to the model will be provided in the technical document that will accompany the finalised 2015 air quality plans. A summary of the revisions is provided below.

3.6.2 Emission factors for NO_X from road traffic

Emissions estimates in the original 2013 compliance assessment were calculated using vehicle emissions factors from COPERT 4v10[4] as these represented the best available evidence at the time. Updated emission factors for road traffic have since become available from COPERT 4v11[5]. These updated emission factors have been used in the revised reference year calculation for 2013, and in the projections for future years used in the 2015 plans.

3.6.3 Primary NO_2 emission fractions from road transport

The primary NO_2 emission fraction (f-NO_2) for individual road links within the PCM model has been calculated from a combination of traffic counts for each vehicle type and fuel and fleet weighted f-NO_2 values for each vehicle type and fuel. The f-NO_2 values used for the updated modelling have been revised to reflect the updated emission factors for NO_X from COPERT 4v11 and f-NO_2 values from the EMEP/EEA Emissions Inventory Guidebook 2013, updated July 2014[6]. The resulting fleet weighted f-NO_2 values for different vehicle types, fuels and different years are presented in the technical document that will accompany the finalised 2015 air quality plans.

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[4] COPERT 4 v10.0 released in November 2012 and the accompanying report "Description of new elements in COPERT 4 v10.0" can be downloaded at http://emisia.com/sites/default/files/COPERT4_v10_0.pdf

[5] COPERT 4 v11.0 released in September 2014 and the accompanying report "Update of the Air Emissions Inventory Guidebook – Road Transport 2014 Update" can be downloaded at http://www.emisia.com/sites/default/files/files/COPERT4_v11_0.pdf and emission factors are provided directly via personal communication.

[6] http://www.eea.europa.eu/publications/emep-eea-guidebook-2013/part-b-sectoral-guidance-chapters/1-energy/1-a-combustion/1-a-3-b-road-transport (Table 3.113)

3.6.4 PCM Roads Kernel Model

A revised method has been used to calculate the additional roadside contribution to total ambient NO_X concentration from road traffic sources at locations close to busy roads. The PCM Roads Kernel Model (PCM-RKM) has been used. Full details of the PCM-RKM are provided in the technical document that will accompany the finalised 2015 air quality plans.

The revised method, based upon dispersion kernels generated by the ADMS-Roads dispersion model, represents a more process-based approach than the previous empirical method. It provides a more robust assessment, whilst retaining the link with measurement data provided by the use of AURN measurement data to calibrate this component of the model.

4 SO_2

4.1 Introduction

4.1.1 Limit values

Two limit values for ambient SO_2 concentrations are set out in the AQD for the protection of human health. These limit values have been in force since 1st January 2005 and are specified as follows:

- An hourly concentration of 350 µg m^{-3}, with 24 permitted exceedances each year
- A 24-hour mean concentration of 125 µg m^{-3}, with 3 permitted exceedances each year.

A critical level for SO_2 for the protection of vegetation has also been specified in the AQD:

- An annual mean and winter mean concentration of 20 µg m^{-3}.

The critical level is designed to protect vegetation so it only applies in vegetation areas as defined in the Directive. The critical level has been in force since 2001.

4.1.2 Annual mean and winter mean modelling

A map of annual mean SO_2 concentration for 2013 in vegetation areas has been calculated for comparison with the annual mean critical level described above; this map is shown in Figure 4.1. This map has been calculated by removing non-vegetation areas from the background SO_2 annual mean map and calculating the zonal mean of the 1 km x 1 km grid squares for a 30 km x 30 km grid so that it complies with the criteria set out in the AQD. Mean concentrations on a 30 km x 30 km grid have been used to prevent the influence of any urban area appearing unrealistically large on adjacent vegetation areas. Thus the modelled concentrations in vegetation areas should be representative of approximately 1000 km^2 as specified in the AQD for monitoring sites used to assess concentrations for the vegetation critical level.

A map of winter mean SO_2 concentrations for the period October 2012 to March 2013 has also been calculated for comparison with the winter mean critical level and is shown in Figure 4.2. This map was calculated by multiplying the annual mean map for 2013 by 1.27, which is the ratio between the average concentration measured at rural SO_2 monitoring sites during the 2012-2013 winter period and the annual concentration for 2013. By comparison the ratio between winter and annual means for 2008, 2009, 2010, 2011 and 2012 respectively were 1.30, 1.23, 1.01, 1.60 and 1.10.

4.1.3 Outline of annual mean and winter mean modelling

The 1 km x 1 km annual mean background SO_2 concentration map has been calculated by summing the contributions from:

- Large point sources
- Small point sources
- Local area sources
- Distant sources (characterised by a residual)
- Point sources with emissions estimates for air quality pollutants based on reported carbon emissions (ETS points)

The contributions from each of the above components were modelled as described in Section 4.3.1.

4.1.4 Modelling for comparison with the hourly and 24-hour limit values

Maps of the 99.73 percentile of the hourly mean and the 99.18 percentile of the 24-hour mean SO_2 concentrations have been calculated for 2013. They are shown in Figure 4.3 and Figure 4.4 respectively. These percentile concentrations correspond to the number of allowed exceedances of the 1-hour and 24-hour limit values for SO_2 described above.

4.1.5 Outline of modelling for comparison with the hourly and 24-hour limit values

The 1 km x 1 km percentile SO_2 concentration maps have been calculated by combining the contributions from:

- Large point sources
- Small point sources
- Local area sources
- Distant sources (characterised by a residual)
- Point sources with emissions estimates for air quality pollutants based on reported carbon emissions (ETS points)

Details of the method can be found in Section 4.3.2.

4.1.6 Chapter structure

This chapter describes modelling work carried out for 2013 to assess compliance with the SO_2 limit values and critical levels described above. Emission estimates for SO_2 are described in Section 4.2. Section 4.3.1 describes the SO_2 modelling methods for the annual and winter means. Section 4.3.2 describes the SO_2 modelling methods for the percentile metrics (for comparison with the hourly and 24-hour limit values). Model verification and source apportionment information are presented in Section 4.4.

Figure 4.1 - Annual mean SO_2 concentration, 2013 ($\mu g\ m^{-3}$) in vegetation areas

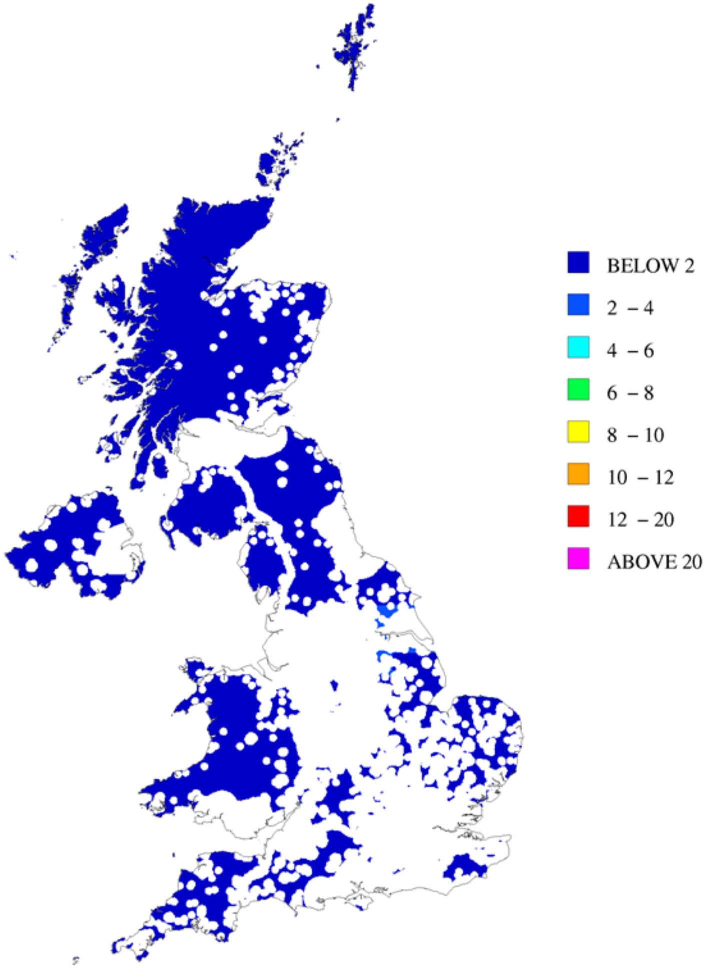


Figure 4.2 - Winter mean SO_2 concentration, 2012-2013 ($\mu g\ m^{-3}$) in vegetation areas

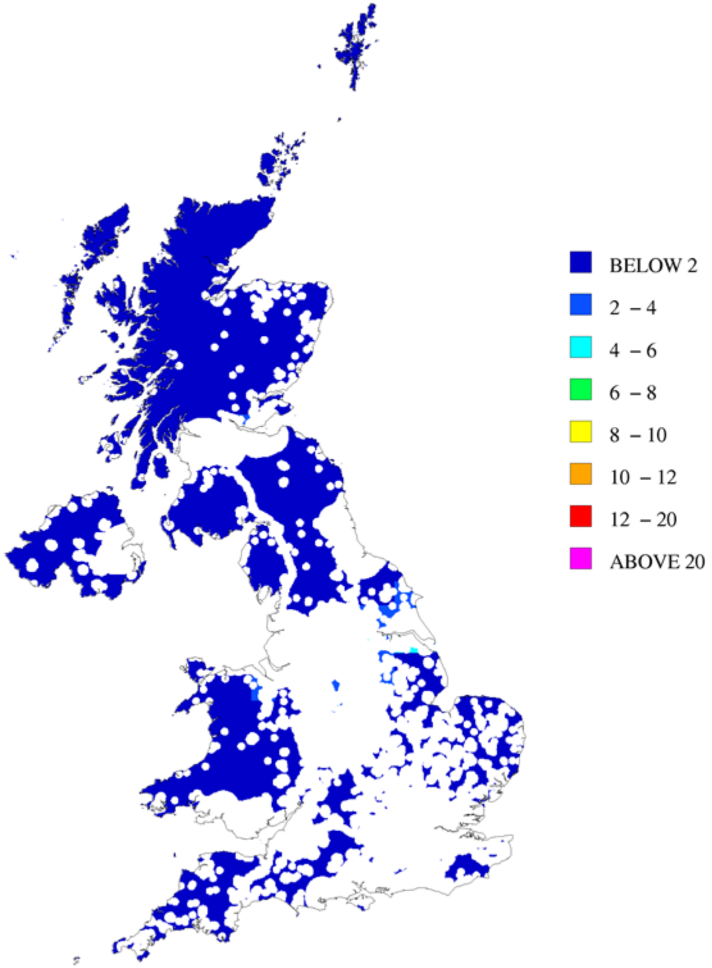


Figure 4.3 - 99.73 percentile of 1-hour mean SO_2 concentration, 2013 (µg m^{-3})

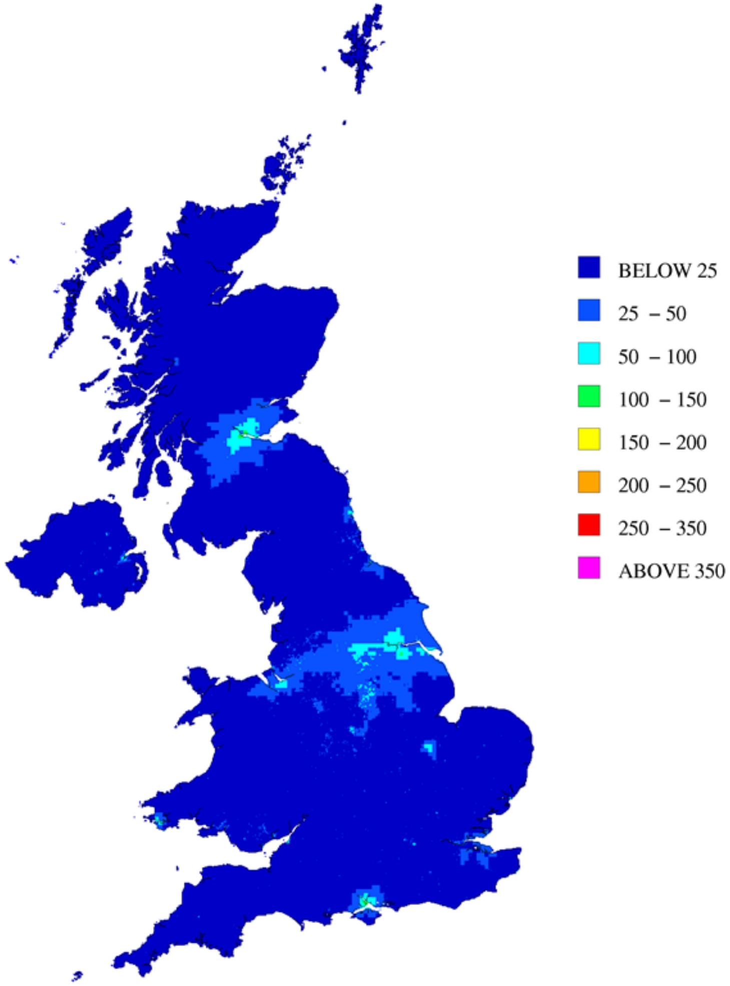
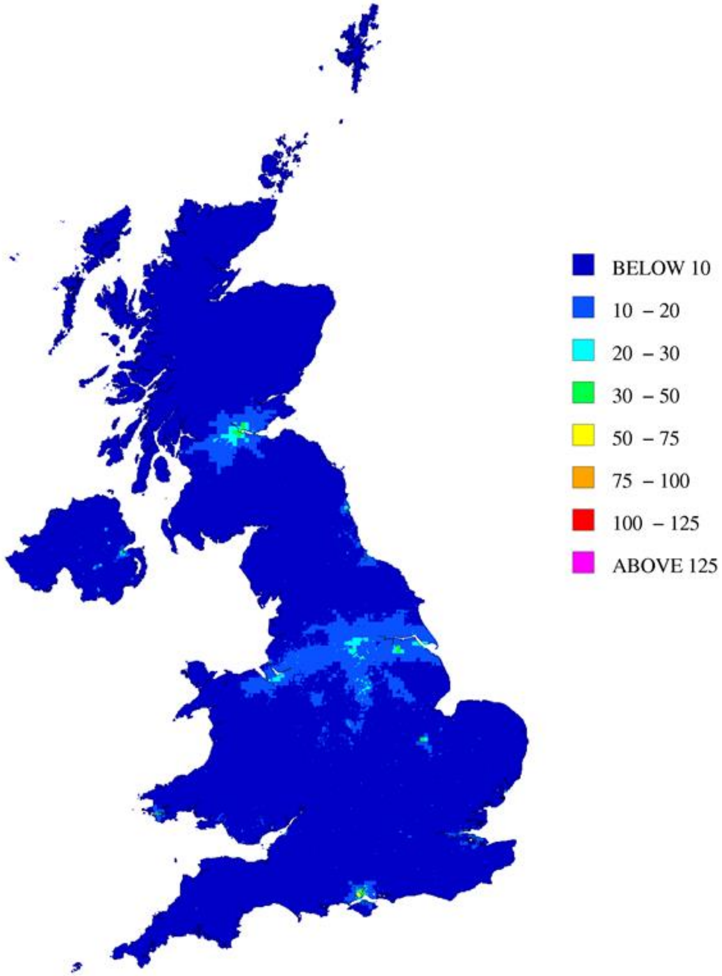


Figure 4.4 - 99.18 percentile of 24-hour mean SO_2 concentration, 2013 (µg m^{-3})

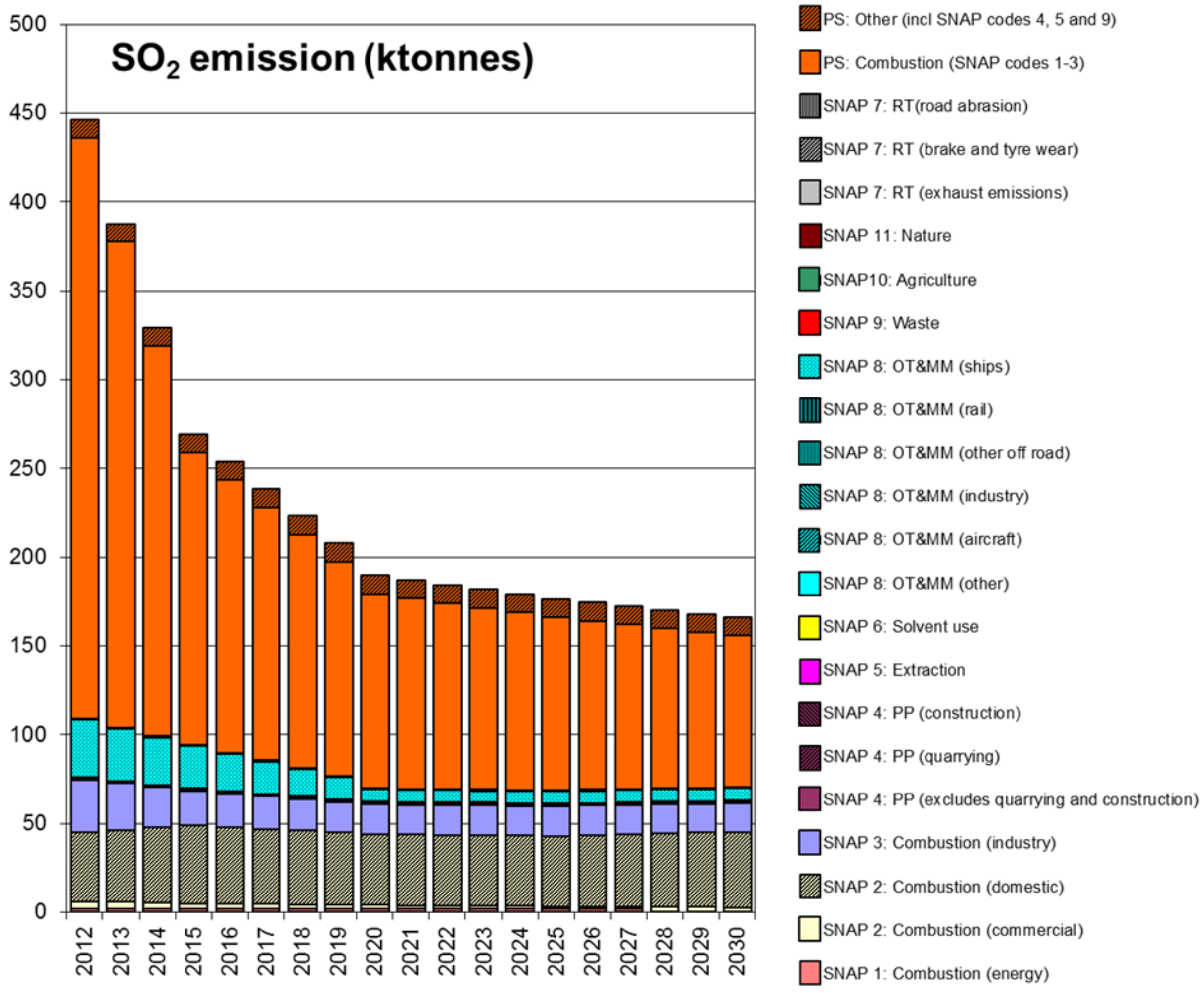


4.2 SO_2 emissions

Estimates of the emissions of SO_2 from the UK National Atmospheric Emissions Inventory 2012 (NAEI 2012) have been used in this study (Passant et al., 2014). Emissions projections have been provided by the NAEI (Passant pers. comm. 2014a) based on DECCs UEP48 energy and emissions projections (DECC, 2013). Figure 4.5 shows the UK total SO_2 emissions for 2012 and emissions projections for 2015, 2020, 2025 and 2030 split by SNAP code, with the coding described in Table 3.1. Values for intermediate years have been interpolated in this figure.

The emissions are dominated by point source emissions from combustion in energy production and transformation. The predicted trend in total emissions is for a decrease in SO_2 emissions from 2012 onwards, dominated by a reduction in emissions from combustion point sources.

Figure 4.5 - Total UK SO_2 emissions for 2012 and emissions projections up to 2030 by SNAP code from NAEI 2012



4.3 SO_2 modelling

The modelling methods for SO_2 were developed by Abbott and Vincent (1999, 2006). Emissions from point and area sources have been modelled separately and the results combined within a geographical information system to produce the concentration maps.

4.3.1 Annual mean and winter mean modelling

4.3.1.1 SO_2 contributions from large and small point sources

Point sources in the NAEI 2012 have been classified as large if they fulfil either of the following criteria:

- Annual SO_2 emissions in the NAEI 2012 are greater than 500 tonnes for any given plant
- Stack parameters are already available for any given plant in the PCM stack parameters database (described in Section 3.3.1)

The contribution to ambient concentrations resulting from emissions from large point sources in the NAEI 2012 was estimated by modelling each source explicitly using the atmospheric dispersion model ADMS 5.0. Surface roughness was assumed to be 0.1 m at both dispersion and meteorological sites. A total of 340 large point sources were modelled using emission release characteristics from the PCM stack parameters database.

Hourly emissions profiles for the power stations in England and Wales for 2013 were provided by the Environment Agency. Scottish Power provided an hourly emissions profile for one power station in Scotland. Some power stations were closed during the year 2013 where they were opted out of the Large Combustion Plant Directive (2001/80/EC). Care has been taken to reflect the expected level and timing of emissions for these plant by applying the time varying emissions profiles provided or otherwise estimating the level of activity up to the closure date from the most recent period in the previous year. The NAEI emission estimates for the power stations in Northern Ireland and one power station in Scotland, non-power station large and small point sources are for the year 2012. To model concentrations a year ahead of the NAEI these emissions have been scaled to values appropriate to 2013, using projection factors derived from NAEI source sector total emissions for point sources for 2012 and NAEI emissions projections for 2013 (described in Section 3.3.5). Closure of particular plant or activities are taken into account when deriving the source sector projection factors by subtracting the base year emissions associated with plant closure from the relevant source sector total for point sources for the NAEI base year. The concentrations resulting from emissions from all power stations in Northern Ireland and one power station in Scotland were modelled using the projected NAEI emissions in combination with time varying emissions profiles typical of electricity generation in summer and winter. Concentrations resulting from emissions from large non-power station point sources were modelled using the projected NAEI emissions without time varying emissions.

Concentrations resulting from the projected emissions from small point sources were modelled using the small point source model described in Appendix 3. In line with the method applied for the large point sources the NAEI 2012 emissions for small point sources have been scaled to 2013 using the same source sector specific projection factors applied to the large point sources. Any point sources in the NAEI base year which closed before the start or early on in the current assessment year are removed from the modelling, based on recommendations from the NAEI team (Passant pers. comm. 2014b).

In common with the NAEI 2011 additional point source emissions data have been provided in the NAEI 2012. These emissions estimates have been derived from carbon emissions data reported under the EU-Emissions Trading Scheme (ETS), most recently described in Tsagatakis et al. (2014). These point sources are referred to as ETS points in this report. To model the contribution to background annual mean SO_2 concentrations from ETS points the emissions have been treated as an additional set of small point sources. As such they have been modelled using the SO_2 small points approach described above. These derived air quality pollutant emissions estimates are particularly uncertain, hence the emissions for particular sources have been capped at reporting thresholds given by the Scottish Pollutant Release Inventory (SPRI). Typically more than 90% of the ETS points do not exceed the SPRI reporting threshold, which for SO_2 is 100 tonnes per year.

For the large point sources, concentrations were predicted for 5 km x 5 km resolution receptor grids within a number of receptor areas (or tiles), which together cover the UK. The size of the receptor areas was typically 100 km x 100 km, extending out to 150 km where appropriate. All sources within the receptor area and extending out 100 km from the tile border were assumed to influence concentrations within the receptor area. Concentrations have been modelled using sequential meteorological data for 2013 from Waddington in Lincolnshire. This site has been chosen as the most representative of meteorology in the vicinity of the largest point sources in the UK. This approach ensures that the combined impact of several sources on ambient high percentile concentrations is estimated correctly. While not essential for the estimation of the annual mean this method enables both the annual mean and high percentiles to be calculated from the same set of dispersion model calculations.

4.3.1.2 SO_2 contributions from local area sources

The 2013 area source SO_2 emissions maps have been calculated from the NAEI 2012 emissions maps following the method described in Section 3.3.5. With the exception of SNAP sector 3 (combustion in industry), the contribution to ambient SO_2 concentrations from area sources was calculated using a dispersion kernel approach. Concentrations are predicted for a 1 km x 1 km receptor grid, from the area source emissions within a 33 km x 33 km square surrounding each receptor. Dispersion kernels were calculated using ADMS 5.0 and hourly sequential meteorological data for 2013 from Waddington. Modelling of the area sources is described in more detail in Appendix 4.

Revised methods introduced in the 2012 assessment (Brookes et al., 2013) for modelling the contributions to SO_2 from SNAP 2 (domestic and non-domestic combustion) and SNAP 3 (combustion in industry) area sources were used and have been described in Section 3.3.5.

As part of the calibration process emission caps have been applied to certain sectors. This is because the use of surrogate statistics for mapping area source emissions sometimes results in unrealistically large concentrations in some grid squares for a given sector. The emission caps applied are given in Table 4.1.

Table 4.1 - Emissions caps applied to SO_2 sector grids

SNAP code	Description	Cap applied (t/a/km2)
SNAP 2 (Non-industrial combustion plants)	Public sector combustion	50
SNAP 2 (Domestic combustion, petroleum coke)	Domestic combustion	35
SNAP 2 (Domestic combustion, SSF)	Domestic combustion	25
SNAP 8 (Shipping only)	Other Transport & Mobile Machinery	30

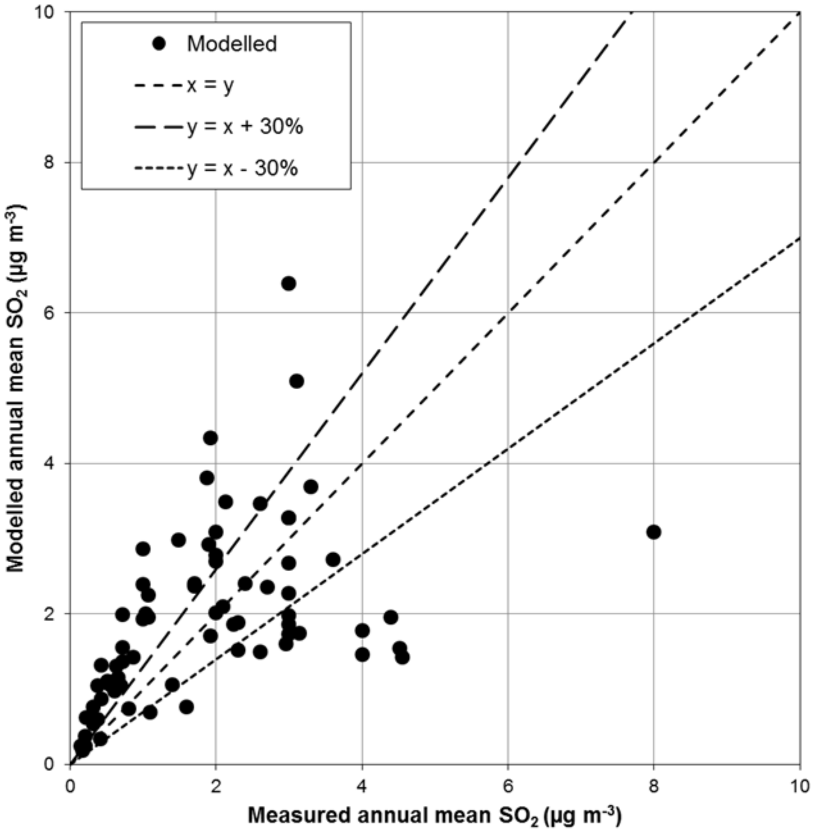
4.3.1.3 Calculating the total concentrations

Details of the method to combine the model components are described below. The map of winter mean SO_2 concentrations was derived from the annual mean map by scaling using a factor of 1.27, which is the ratio between the average concentration measured at rural SO_2 monitoring sites during the 2012-2013 winter periods and annual concentration for 2013.

The point source and area source contributions are summed without calibration, along with a residual concentration of 0.19 µg m^{-3} to derive the annual mean concentration. The residual is added to account for background SO_2 due to long-range transport of SO_2 from transboundary sources, e.g., SO_2 sources in continental European sources that are not explicitly modelled. The residual was derived by a linear least squares fit between the measured and modelled concentrations in the work of Abbott and Vincent (2006).

Measured concentrations from UK Acid Gases and Aerosols Monitoring Network (AGANet) sites (Tang, 2014), selected rural and urban background sites in the national automatic monitoring networks and rural automatic monitoring sites maintained by the electricity generating companies were used to check the results from the method used to combine the modelled components. A list of the additional sites used in model verification is included in Appendix 1. The comparison plot for 2013 is shown in Figure 4.6.

Figure 4.6 - Comparison plot for 2013 annual mean SO_2 concentration



4.3.2 Modelling percentile concentrations for comparison with the 1-hour and 24-hour limit values

The methodology to produce the percentile maps is based on research on combining concentrations arising from area and industrial sources undertaken for the Environment Agency (Abbott and Vincent, 2006). This methodology aims to derive an estimate of the percentile concentrations at locations distant from the industrial sources. A weighted regression analysis was carried out by Abbott and Vincent assuming that the variance of the residuals was proportional to the modelled concentration.

The regression model was of the form:

$$c_{measured} = \max\begin{bmatrix} Ac_{modelled\_industrial,\%ile} + 2(c_{modelled\_area} + c_{long\_range})_{annual} \\ 2Ac_{modelled\_industrial,annual} + k(c_{modelled\_area} + c_{long\_range})_{annual} \end{bmatrix}$$

The constant *A* was obtained from the regression analysis. The background multiplier factor, *k*, was derived from monitoring data. The factor “2”, used to scale the $(c_{modelled\_area} + c_{long\_range})_{annual}$ and $c_{modelled\_industrial,annual}$ components, has been shown to be a robust factor that allows short-term average concentrations to be estimated from modelled annual mean concentrations arising from non-industrial or industrial sources (Abbott et al., 2005). Table 4.2 presents the *A* and *k* factors used in the derivation of the maps.

Table 4.2 - Factors for percentile models

Metric	Constant (*A*)	Background multiplier factor (*k*)	c_{long_range}
99.73 percentile of 1-hour values	1.09	10.1	0.19
99.18 percentile of 24-hour values	1.23	3.3	0.19

The justification for treating industrial sources and area emissions separately is because peaks in high percentile modelled contributions may not coincide with peaks in high percentile background concentrations – a problem that is more pronounced in emissions from large industrial point sources because the meteorological conditions that give rise to high concentrations from tall stacks can be very different from those that produce high concentrations from emissions at low level. Figure 4.7 and Figure 4.8 provide an intermediate quality check at selected rural and urban background sites which form part of the national network and at sampling sites operated by the electricity generating companies.

An alternative method was used to derive the high percentile concentrations in Northern Ireland. This was required because area sources, predominately emissions from domestic solid and liquid fuel use, make a more significant contribution to observed high percentile concentrations in Northern Ireland than in the rest of the United Kingdom. Additionally, the smaller number of point sources in Northern Ireland means that these sources make a much smaller contribution to the observed high percentile concentrations.

Maps of high percentile concentrations in Northern Ireland have been calculated from the mapped annual mean SO_2 concentrations using a linear least squares fit between measured annual mean and measured high percentile concentrations in Northern Ireland over a six year period from 2008 to 2013 at AURN National Network and Ricardo-AEA Calibration Club monitoring sites. Six years of data have been used in order to enable the calculation of robust estimates. Figure 4.9 and Figure 4.10 show the relationship between the annual mean and the 99.73 percentile of 1-hour mean values and the 99.18 percentile of 24-hour mean values at the sampling sites in Northern Ireland.

The equations used to derive the high percentile maps are:

Predicted 99.73%ile in Northern Ireland = 8.35 × Modelled Annual Mean + 2.04 µg m^{-3}*, and*

Predicted 99.18%ile in Northern Ireland = 4.23 × Modelled Annual Mean + 0 µg m^{-3}*.*

Figure 4.7 - Comparison plot for 2013 99.73 percentile of 1-hour mean SO_2 concentrations

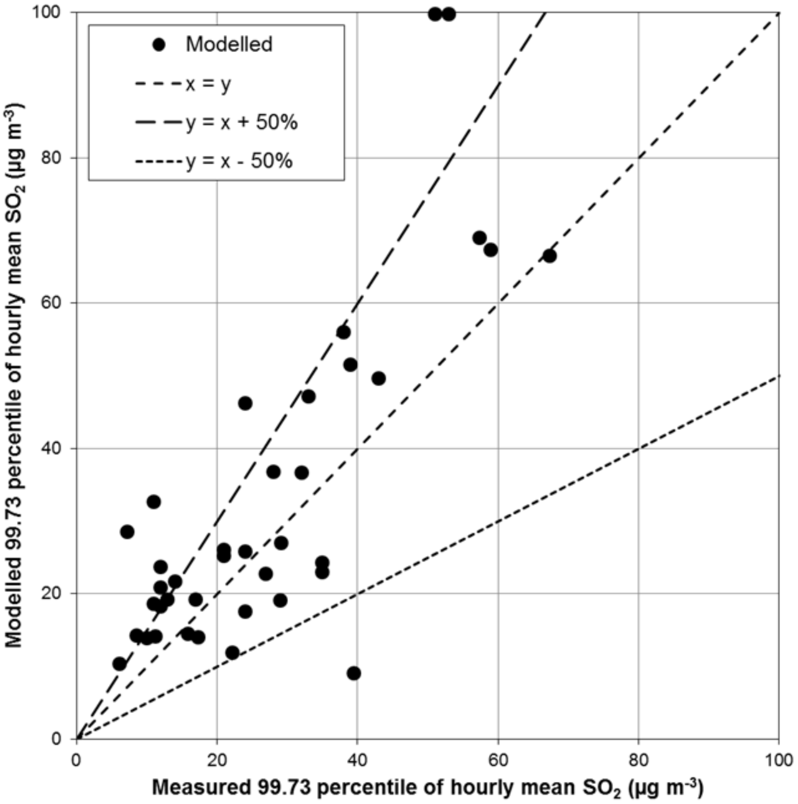


Figure 4.8 - Comparison plot for 2013 99.18 percentile of 24-hour mean SO_2 concentrations

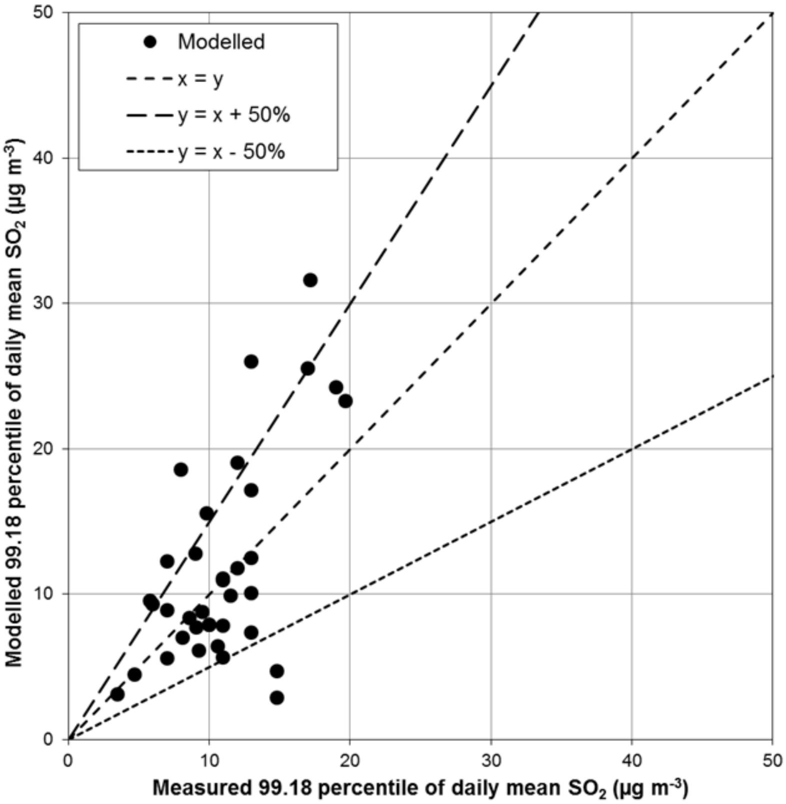


Figure 4.9 - Relationship between mean concentration and 99.73 percentile of 1-hour concentrations at sampling sites in Northern Ireland, 2008-2013

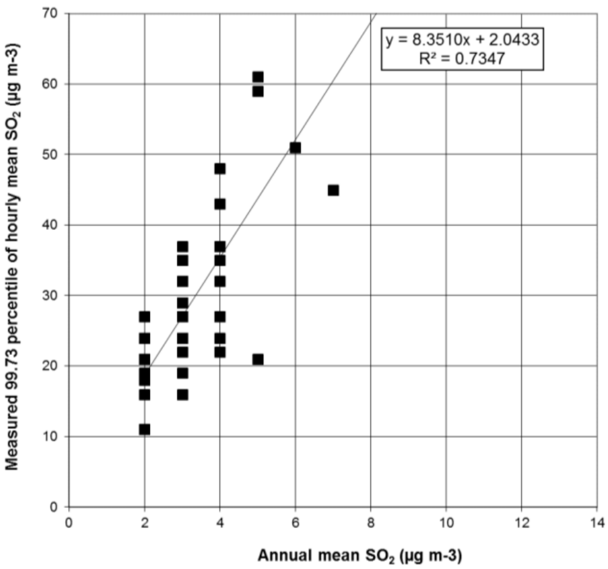
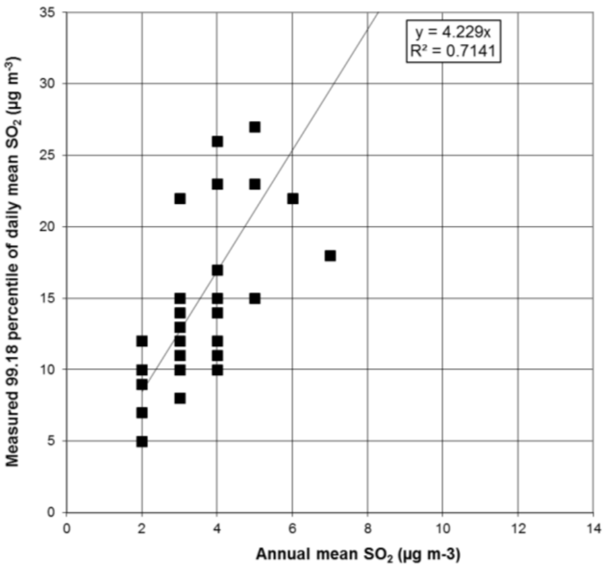


Figure 4.10 - Relationship between mean concentration and 99.18 percentile of 24-hour concentrations at sampling sites in Northern Ireland, 2008-2013



4.4 Results

4.4.1 Verification of mapped values

Figure 4.11, Figure 4.12 and Figure 4.13 show comparisons of modelled and measured annual mean, 99.73 percentile of 1-hour mean and 99.18 percentile of 24-hour mean SO_2 concentrations in 2013 at monitoring site locations in the UK. Both the national network sites and the verification sites are shown. Lines representing y = x – 30 % and y = x + 30% or y = x – 50 % and y = x + 50% are also shown (the AQD data quality objective for modelled annual mean and percentile SO_2 concentrations respectively – see Section 1.5). The 'Quality Check Sites' include the electricity generating company sites, selected AURN sites and (for annual means only) Acid Gases and Aerosols Monitoring Network sites (Tang, 2013). Urban background and urban centre AURN sites not used in the checking process are also presented along with 'verification sites' that include ad-hoc monitoring sites and Ricardo-AEAs Calibration Club monitoring sites. A complete list of the AURN sites used is presented in Data flow E of the e-Reporting submission (CDR, 2014). Details of other verification sites are presented in Table A1.1 of Appendix 1 and sites maintained by the electricity generating companies and Hanson Building Products Ltd are listed in Table A1.3.

Figure 4.11 - Verification of annual mean SO_2 model, 2013

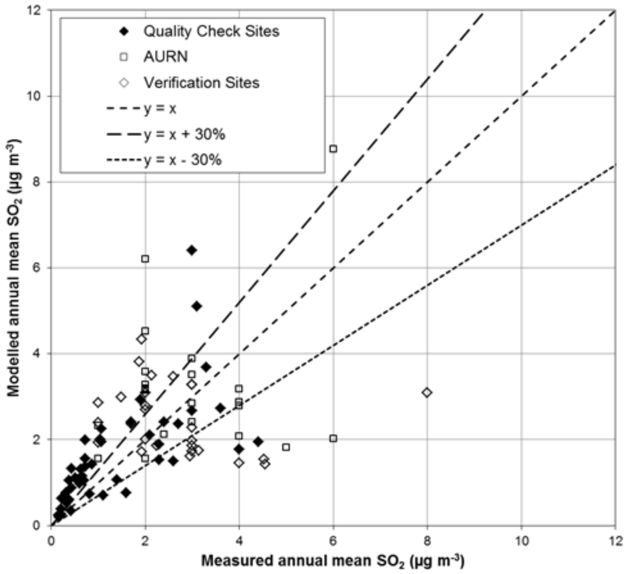


Figure 4.12 - Verification of 99.73 percentile of 1-hour mean SO_2 model, 2013

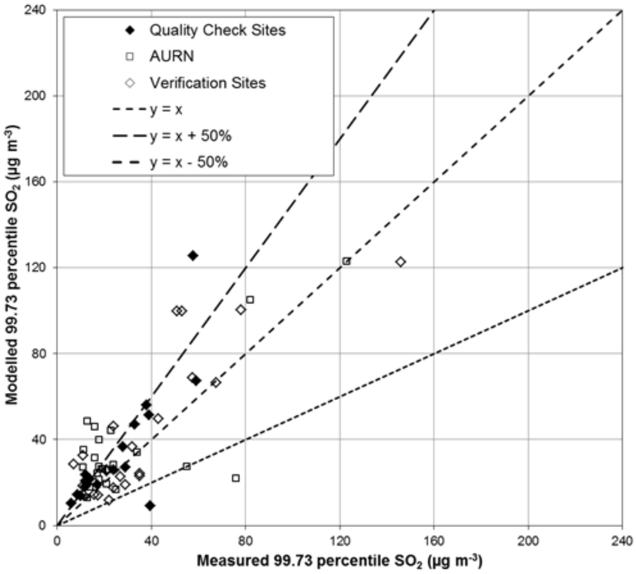
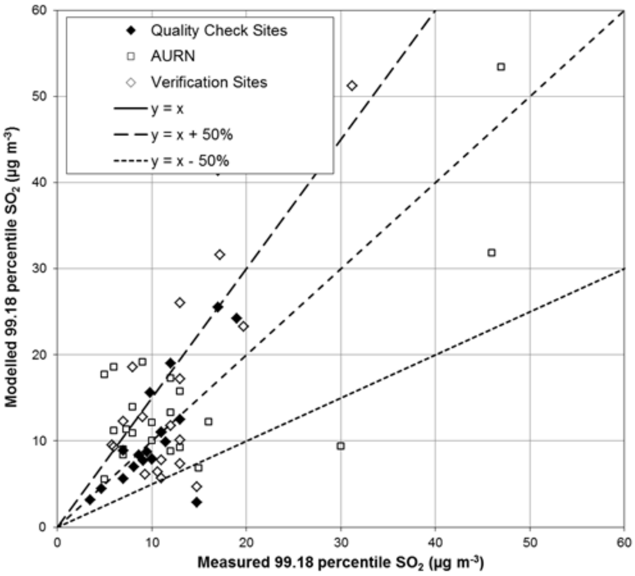


Figure 4.13 -Verification of 99.18 percentile of 24-hour mean SO_2 model, 2013



Summary statistics for modelled and measured SO_2 concentrations, the percentage of sites for which the modelled values are outside the data quality objectives (DQOs) and the total number of sites included in the analysis are listed in Table 4.3, Table 4.4 and Table 4.5. Note that the 1 km x 1 km grid annual mean map is not compared directly with the annual mean limit value; the zonal mean of the 1 km x 1 km grid squares in vegetation areas has been calculated for a 30 km x 30 km grid, as discussed above.

The mean measured and modelled concentration for each averaging time is within reasonable agreement, with some outliers in particular for the verification sites. The agreement between measured and modelled concentrations on a site-by-site basis (quantified using R^2) is relatively poor for all metrics for sites in the national network and in particular the verification sites.

Historically it has been difficult to capture the variability in measured concentrations and reasons for the poor agreement include:

- Emissions from large industrial emission sources are decreasing. This will result in an increase in the relative contribution from other sources. The emission characteristics of these sources are less well known;
- The receptor grid used in the model predictions for point sources (concentrations are predicted at 5 km intervals) may be too coarse for the smaller emission sources; and,
- The modelling method does not explicitly model concentrations arising from non-UK sources.

Table 4.3 - Summary statistics for comparison between modelled and measured annual mean concentrations of SO_2 at background sites

	Mean of measurements (µg m^{-3})	Mean of model estimates (µg m^{-3})	R^2	% of sites outside DQO of ±30%	Number of sites in assessment
National Network[a]	1.7	2.0	0.41	75%	55
Verification Sites	2.7	2.5	0.03	78%	27

a includes measurement data from sites in Defra's AURN and AGANet

Table 4.4 - Summary statistics for comparison between modelled and measured 99.73 percentile of 1-hour mean concentrations of SO_2 at background sites

	Mean of measurements (µg m^{-3})	Mean of model estimates (µg m^{-3})	R^2	% of sites outside DQO of ±50%	Number of sites in assessment
National Network[b]	28.7	33.5	0.55	46%	28
Verification Sites	31.1	43.0	0.55	37%	27

b includes measurement data from sites in Defra's AURN only

Table 4.5 - Summary statistics for comparison between modelled and measured 99.18 percentile of 24-hour mean concentrations of SO_2 at background sites

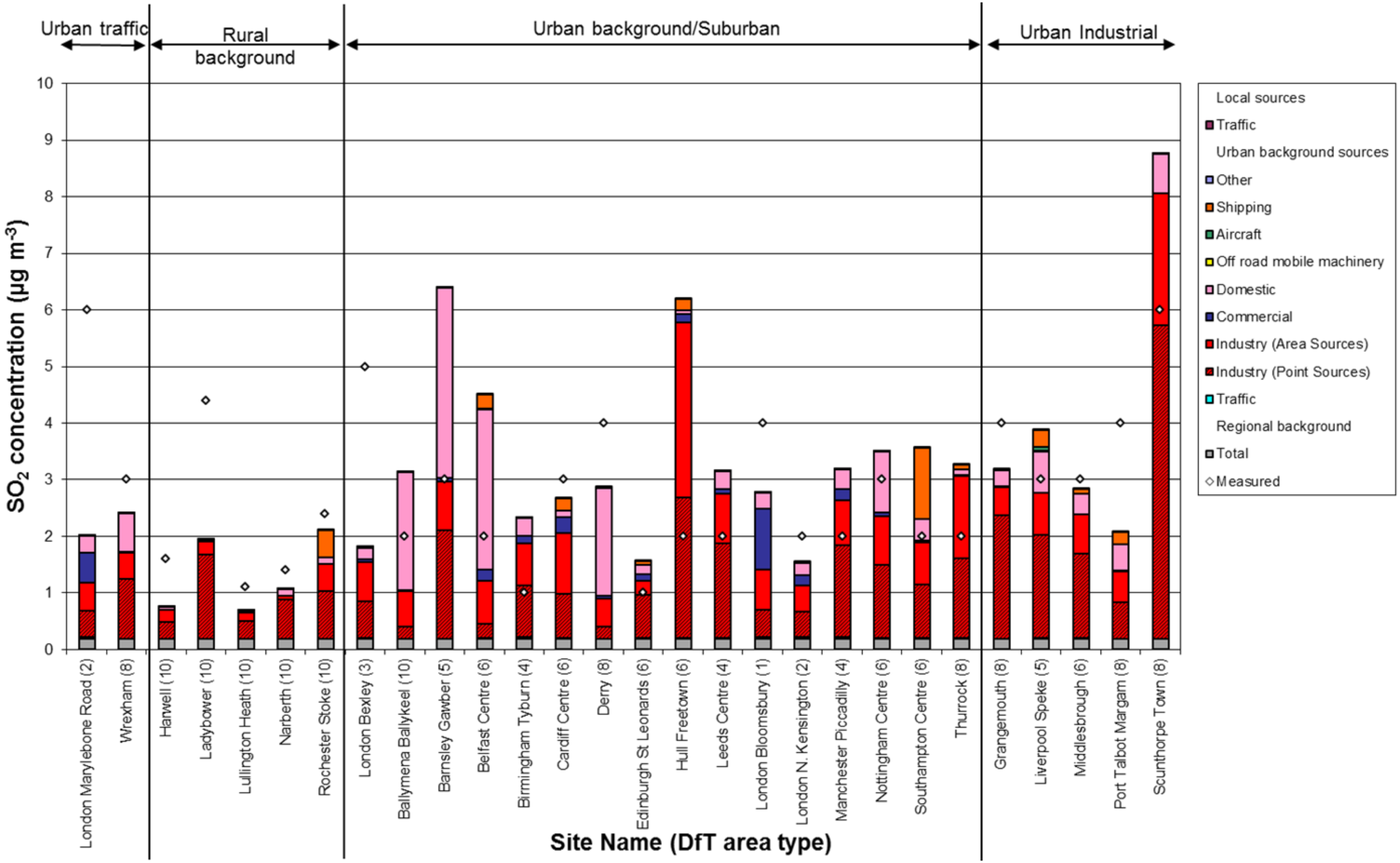
	Mean of measurements (µg m^{-3})	Mean of model estimates (µg m^{-3})	R^2	% of sites outside DQO of ±50%	Number of sites in assessment
National Network[c]	13.0	13.6	0.55	36%	28
Verification Sites	14.3	17.0	0.16	56%	27

c includes measurement data from sites in Defra's AURN only

4.4.2 Source apportionment

Figure 4.14 shows the source apportionment for modelled annual mean concentrations of SO_2 at AURN monitoring sites for 2013. Measured annual mean concentrations at each site are shown for reference. The figure shows that annual mean SO_2 concentrations at most sites are dominated by contributions from industrial emissions treated as either point sources or area sources. Some sites also have significant contributions from shipping, commercial and domestic sources of emissions. Modelled concentrations are noticeably over-estimated at Barnsley Gawber, Belfast Centre, Hull Freetown, Scunthorpe Town and Southampton Centre. For Barnsley Gawber and Belfast Centre this appears to be driven by domestic SO_2 emissions, while for Hull Freetown and Scunthorpe Town estimated industrial SO_2 emissions are driving the over-estimate, as are shipping emissions at Southampton Centre.

Figure 4.14 - Annual mean SO_2 source apportionment at AURN monitoring sites (the area type of each site is shown in parenthesis after its name – see Table 3.4)



5 PM_{10}

5.1 Introduction

5.1.1 Limit values

Two limit values for ambient PM_{10} concentrations are set out in the AQD. These have been specified for the protection of human health and came into force from 01/01/2005. These limit values are:

- An annual mean concentration of 40 µg m^{-3}.
- A 24-hour mean concentration of 50 µg m^{-3}, with 35 permitted exceedances each year

Results of the assessment in terms of comparisons of the modelled concentrations with the annual mean and 24-hour mean limit values for PM_{10} have been reported in e-Reporting Data flow G (CDR, 2014).

5.1.2 Annual mean model

Maps of annual mean PM_{10} in 2013 at background and roadside locations are shown in Figure 5.1 and Figure 5.2. These maps have been calibrated using measurements from TEOM FDMS instruments within the national network for which co-located $PM_{2.5}$ measurements are also available for 2013. The models for PM_{10} and $PM_{2.5}$ are designed to be fully consistent. Each component is either derived from emission estimates for PM_{10} or $PM_{2.5}$ or the contributions to the fine and coarse particle size fractions are estimated separately. This enables us to carry out an additional reality check that the calibration parameters for the two pollutants are reasonably consistent. Measurements from national network sites without collocated $PM_{2.5}$ instruments have been used as an additional verification dataset (and similarly $PM_{2.5}$ sites without PM_{10} have been used as an additional verification dataset for $PM_{2.5}$). Measurements from gravimetric instruments, TEOM monitors and TEOM monitors adjusted using the VCM model (http://www.volatile-correction-model.info/) have been used to verify the mapped estimates by applying the appropriate scaling factors prior to comparison.

A detailed description of the Pollution Climate Mapping (PCM) models for PM in 2004 has been provided by Stedman et al. (2007). The methods used to derive the maps for 2013 are largely the same as was adopted for the 2012 maps described in Brookes et al. (2013).

5.1.3 Outline of the annual mean model

The maps of annual mean background PM_{10} concentrations have been calculated by summing contributions from different sources:

- Secondary inorganic aerosol
- Secondary organic aerosol
- Large point sources of primary particles
- Small point sources of primary particles
- Point sources with emissions estimates for air quality pollutants based on reported carbon emissions (ETS points)
- Regional primary particles
- Area sources related to domestic combustion
- Area sources related to combustion in industry
- Area sources related to road traffic

- Other area sources
- Regional calcium rich dusts from re-suspension of soils
- Urban calcium rich dusts from re-suspension of soils due to urban activity
- Regional iron rich dusts from re-suspension
- Iron rich dusts from re-suspension due to vehicle activity
- Sea salt
- Residual

The concentrations of many of these components have been estimated separately for the fine and coarse fraction. This enables a consistent method to be adopted for estimation of PM_{10} (the sum of the fine and coarse fractions) and $PM_{2.5}$ (fine fractions only). These component pieces are aggregated to a single 1 km x 1 km background PM_{10} grid. An additional roadside increment is added for roadside locations.

The results from the annual mean model can be directly compared with the annual mean limit value in order to carry out the air quality assessment.

Figure 5.1 - Annual mean background PM$_{10}$ concentration, 2013 (µg m-3, gravimetric)

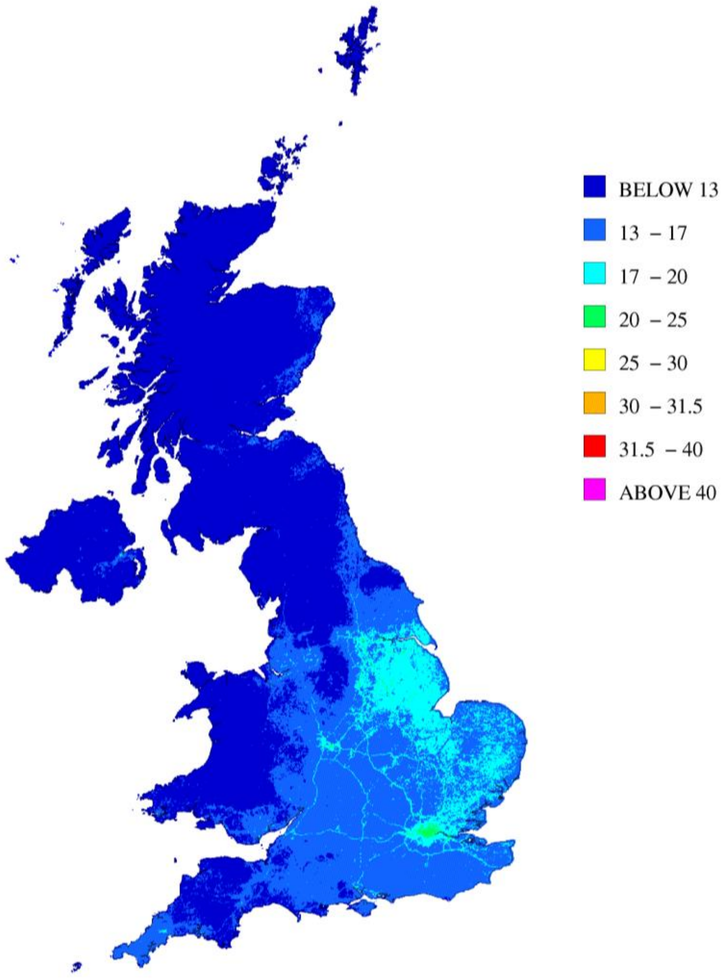
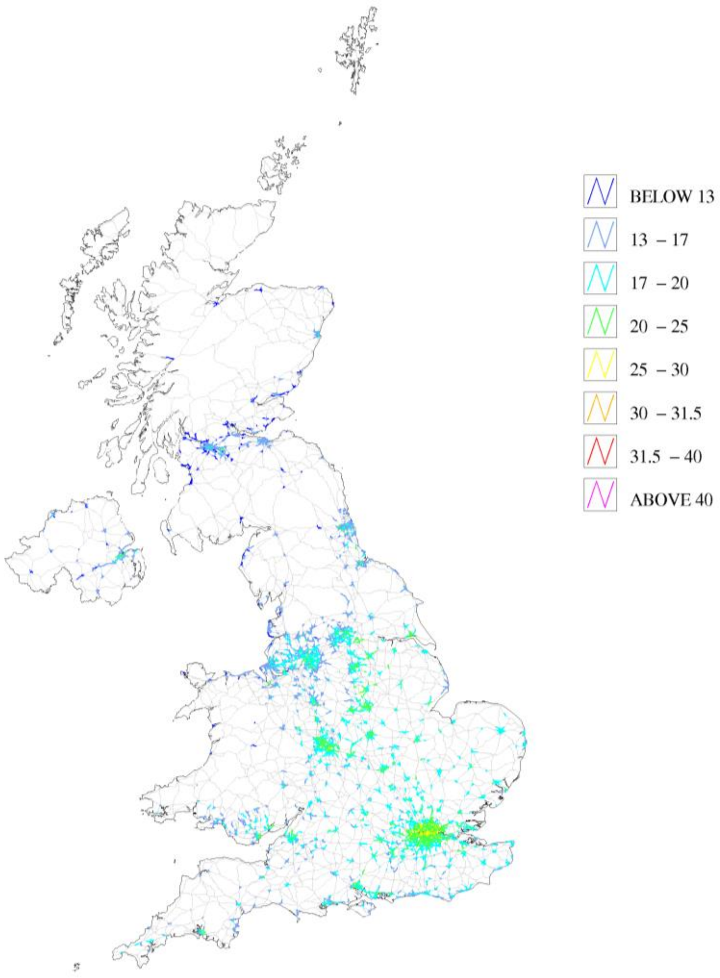


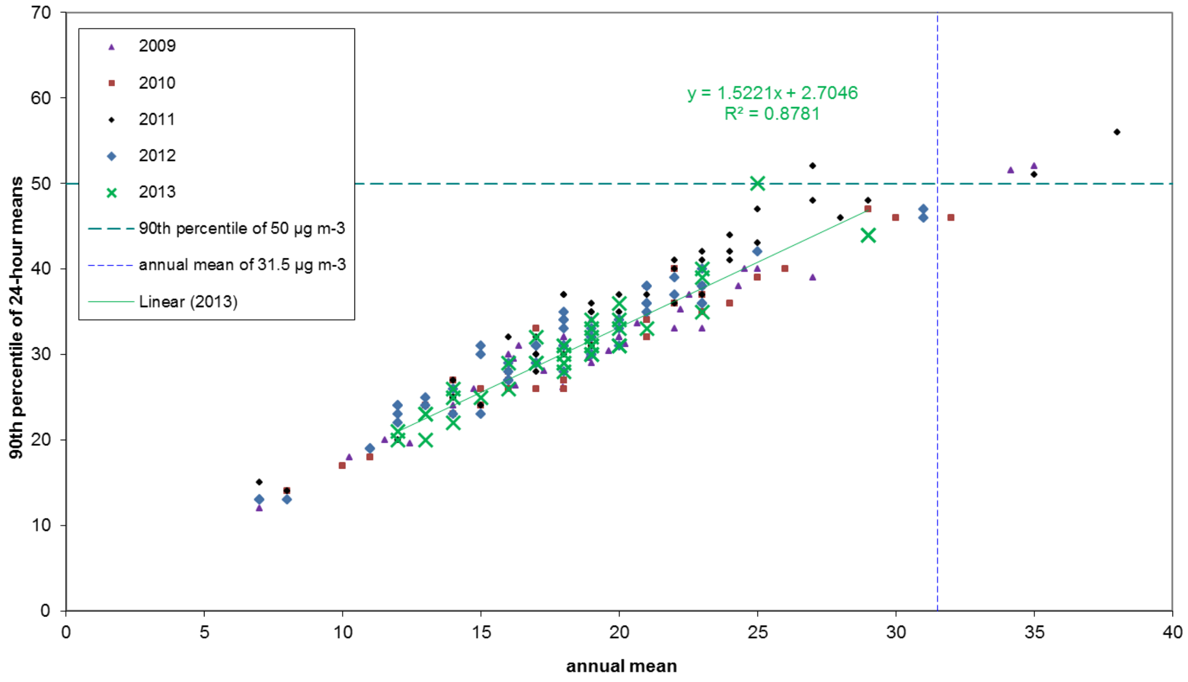
Figure 5.2 - Urban major roads, annual mean roadside PM$_{10}$ concentration, 2013 (µg m^{-3}, gravimetric)



5.1.4 Compliance assessment for the 24-hour limit value

24-hour mean concentrations have not been explicitly modelled for comparison with the 24-hour limit value. An annual mean concentration of 31.5 µg m^{-3}, gravimetric has been taken to be equivalent to 35 days with 24-hour mean concentrations greater than 50 µg m^{-3} gravimetric (the 24-hour limit value) for 2013. A modelled annual mean concentration of greater than this value has been taken to indicate a modelled exceedance of the 24-hour mean limit value. This approach was initially proposed by Stedman et al. (2001a) who recommended a value of 31.5 µg m^{-3} based on an analysis of monitoring data for the period 1992 to 1999. An analysis of more recent monitoring data (Brookes et al., 2011) showed that the value of 31.5 µg m^{-3} was still valid up to and including 2010 and an analysis of monitoring data for 2013 shown in Figure 5.3 confirms that this value is valid for 2013.

Figure 5.3 - The relationship between the 90th percentile of 24-hour mean PM$_{10}$ concentration and annual mean concentration (µg m^{-3}) for 2013



5.1.5 Chapter structure

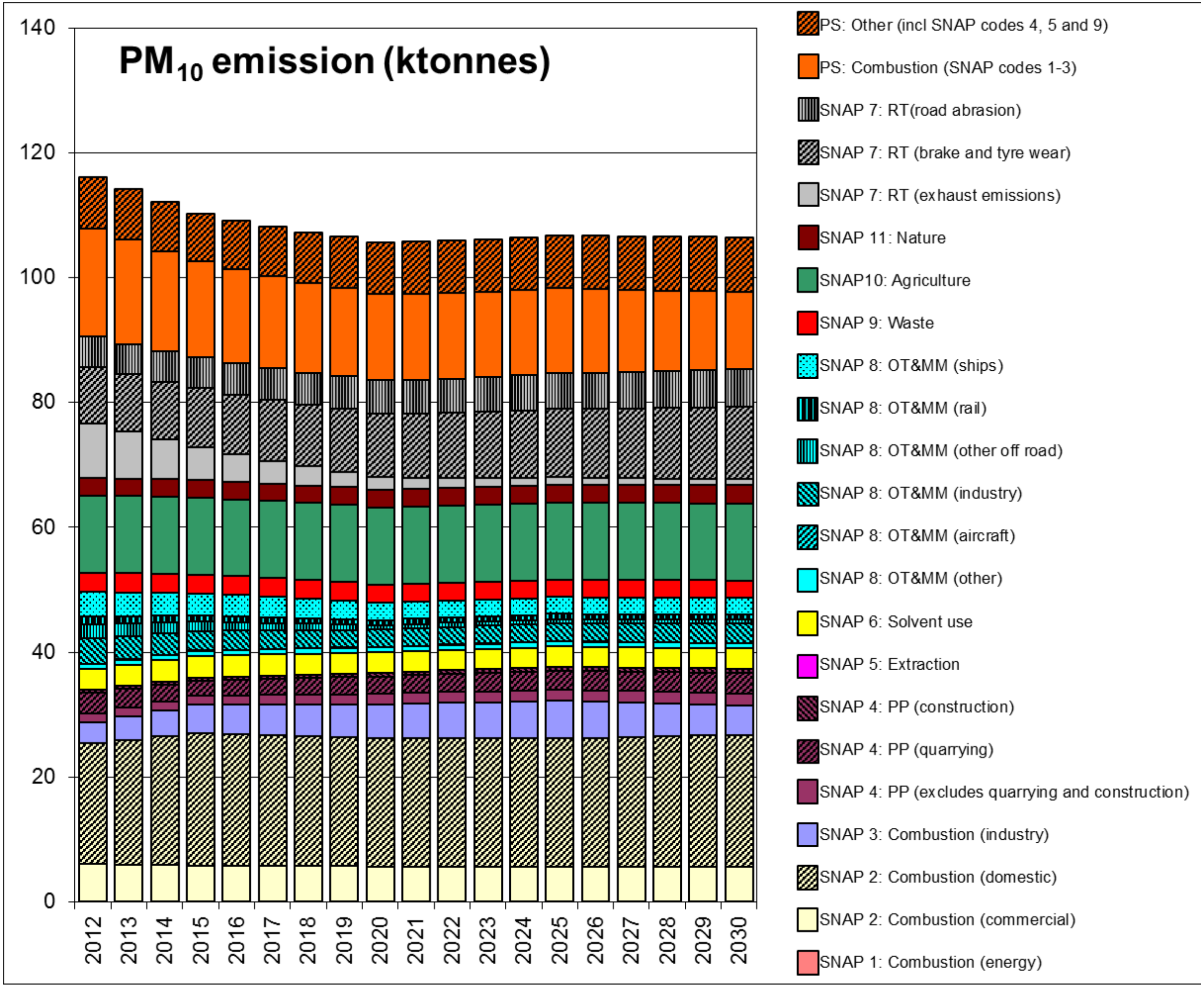
This chapter describes modelling work carried out for 2013 to assess compliance with the PM$_{10}$ limit values described above. Emission estimates for primary PM are described in Section 5.2, Section 5.3 describes the PM$_{10}$ modelling methods, the modelling results are presented in Section 5.4.The methods used to subtract the contribution from natural sources (sea salt) and the results of this subtraction are presented in Section 5.5.

5.2 PM$_{10}$ emissions

Estimates of the emissions of primary PM from the UK National Atmospheric Emission Inventory 2012 (NAEI 2012) have been used in this study (Passant et al., 2014). Emissions projections have been provided by the NAEI (Passant pers. comm. 2014a) based on DECCs UEP48 energy and emissions projections (DECC, 2013). Figure 5.4 shows UK total PM$_{10}$ emissions for 2012 and emissions projections for 2015, 2020, 2025 and 2030 split by SNAP code, with the coding described in Table 3.1. Values for intermediate years have been interpolated in this figure. Figure 5.4 shows that PM$_{10}$ emissions in 2012 include contributions from a wide range of different source sectors. Some of the sectors with the largest contribution to the total in 2012 include road traffic (exhaust and brake and tyre wear), off-road mobile machinery, agriculture and domestic combustion.

Maps of emissions from area sources for 2013 were derived from the 2012 inventory maps using specific scaling factors derived for each combination of source and activity (typically fuel type), as described for NO_X (Section 3.3.5). The emissions from point sources were scaled in a similar way, see Section 3.3.1. The methods used to calculate ambient concentrations from the estimates of primary PM emissions are described below for point, area and regional sources.

Figure 5.4 - Total UK PM_{10} emissions for 2012 and emissions projections up to 2030 by SNAP code from NAEI 2012



5.3 PM_{10} modelling

5.3.1 Contributions from secondary inorganic aerosol

Maps of secondary inorganic aerosol (SIA) concentrations across the UK have been calculated from rural measurements of sulphate, nitrate and ammonium concentrations by interpolation, followed by the application of scaling factors derived from mass closure modelling. Measurements on a monthly basis are available for 28 rural monitoring sites within the UKEAP AGAnet for 2013 (Tang, 2014). Concentration surfaces on a 5 km x 5 km grid were calculated from the measurement data using Kriging.

These secondary components were then split into fine and coarse fractions and non-volatile and volatile components using coefficients derived with reference to the detailed PM sampling carried out during the PUMA campaign at the University of Birmingham urban background monitoring site in June and July 1999 (Harrison et al., 2006 and summarised by Kent et al., 2007a). The non-volatile secondary PM has been assumed to be sampled by a TEOM instrument, a gravimetric instrument should sample the sum of the non-volatile and volatile components. These secondary components were also scaled according to ‘bound water’ associated with the mass of water embedded within the particles (AQEG, 2005). Particle bound water is associated with the hygroscopic anions (Harrison et al., 2006). This has been assumed to contribute to the fine and coarse components gravimetric but not the TEOM. Therefore a particle bound water scaling factor of 1.279 has been applied to the SIA components for the gravimetric maps (see Table 5.1). The scaling factors for bound water and counter ions (non-volatile) have not been used in this study but would be appropriate for mapping TEOM concentrations. The factor for coarse mode nitrate is higher as this includes the mass of the counter-ion (sodium or calcium).

The split between coarse and fine nitrate was revised for the 2006 modelling assessment with reference to measurement data from the TRAMAQ (Abdalmogith et al., 2006) and Birmingham (Harrison and Yin, 2006) studies. The revised method has also been used in this assessment. Fine PM is used to describe $PM_{2.5}$ and coarse PM is used to describe $PM_{2.5\text{-}10}$ in this report. The split between fine and coarse PM is simple to interpret for most PM constituents but is more complex for nitrate PM because there are two modes. The fine nitrate mode consists of ammonium nitrate, which is volatile, and is all in the fine $PM_{2.5}$ fraction. The coarse mode consists of sodium nitrate, which is split roughly half and half between fine $PM_{2.5}$ and coarse $PM_{2.5\text{-}10}$ fractions (Abdalmogith et al., 2006). Measurement data from the Birmingham study (Harrison and Yin, 2006) shows that the fine $PM_{2.5}$ nitrate to coarse $PM_{2.5\text{-}10}$ ratio was 3.5. Thus the fine mode nitrate to coarse mode nitrate ratio was 1.25. The factors for nitrate in Table 5.1 have been derived from a combination of this factor of 1.25 and the half and half split of the coarse mode nitrate into the fine $PM_{2.5}$ and coarse $PM_{2.5\text{-}10}$ fractions.

Table 5.1 - Scaling factors for size fraction, bound water and counter ion mass for secondary inorganic and organic aerosol

Pollutant	Size fraction	Scaling factor for size fraction	Scaling factor for bound water and counter-ion mass	Scaling factor for bound water and counter-ion mass (non-volatile)
SO_4	Fine	0.94	1.279	1.00
	Coarse	0.06	1.279	1.00
NO_3	Fine mode	0.556	1.279	0.00
	Coarse mode fine	0.222	1.60	1.32
	Coarse mode coarse	0.222	1.60	1.32
NH_4	Fine	0.97	1.279	0.86
	Coarse	0.03	1.279	1.00
SOA	Fine	1.00	1.0	0.00
	Coarse	0.0	1.0	0.00

5.3.2 Contributions from secondary organic aerosol

Estimates of annual mean secondary organic aerosol (SOA) concentrations in 2008 from the NAME Model for 20 km x 20 km across the UK have been provided by Redington and Derwent (2013). SOA concentrations are assumed to have remained at 2008 levels in 2013. NAME is a Lagrangian dispersion model that simulates the dispersion, chemistry and deposition processes occurring in the atmosphere, utilising three dimensional meteorological fields from the Met Office Unified Model (Redington et al. 2009). The chemistry scheme has been recently updated to include the formation of anthropogenic and biogenic SOA, the details of which can be found in Redington and Derwent (2013). The SOA component has been assumed to fall within the $PM_{2.5}$ fraction.

5.3.3 Contributions from large and small point sources

Contributions to ground level annual mean primary PM concentrations from large point sources (those with annual emission greater than 200 tonnes, or for which emission release characteristics are known) in the NAEI 2012 have been estimated by modelling each source explicitly using the atmospheric dispersion model ADMS 5.0. Hourly sequential meteorological data for 2013 from Waddington was applied. Surface roughness was assumed to be 0.1 m at the dispersion site and 0.1 m at the meteorological site. Concentrations were calculated for a 99 km x 99 km square composed of a regularly spaced 1 km x 1 km resolution receptor grid. Each receptor grid was centred on the point source. A total of 290 point sources were modelled using emission release characteristics from the PCM stack parameters database (described in Section 3.3.1). The NAEI emissions for point sources for 2012 were scaled in order to provide values for 2013 as described in Section 3.3.1.

Contributions from PM point sources with less than 200 tonnes per annum release and for which emission characteristics were not known were modelled using the ‘small points’ model originally described by Stedman et al. (2005) and summarised in Appendix 3. This model consists of separate ‘in-square’ and ‘out-of-square’ components, in which concentrations are estimated using dispersion kernels, which have been calculated by using ADMS to model the dispersion of unit emissions from a central source to a grid of receptors at a spatial resolution of 1 km x 1 km squares. In line with the method applied for the large point sources the NAEI 2012 emissions for small point sources of PM have been scaled to 2013 using the same source sector specific projection factors applied to the large point sources.

In common with the NAEI 2011 additional point source emissions data have been provided in the NAEI 2012. These emissions estimates have been derived from carbon emissions data reported under the EU-Emissions Trading Scheme (ETS), most recently described in Tsagatakis et al. (2014). These point sources are referred to as ETS points in this report. To model the contribution to background annual mean PM_{10} concentrations from ETS points the emissions have been treated as an additional set of small point sources. As such they have been modelled using the PM_{10} small points approach described above. These derived air quality pollutant emissions estimates are particularly uncertain, hence the emissions for particular sources have been capped at reporting thresholds given by the Scottish Pollutant Release Inventory (SPRI). Typically more than 75% of the ETS points do not exceed the SPRI reporting threshold for PM_{10} and $PM_{2.5}$, which is 1 tonne per year for both PM_{10} and $PM_{2.5}$.

5.3.4 Contributions from distant sources of primary particles

Contributions from long-range transport of primary particles on a 20 km x 20 km grid have been estimated using the TRACK receptor oriented, Lagrangian statistical model (Lee et al., 2000). Emissions of primary PM were taken from the NAEI for UK sources and from EMEP (Webdab data, http://www.ceip.at/) for sources in the rest of Europe. Primary PM was modelled as an inert tracer. All sources within 10 km of the receptor point were excluded from the TRACK model to allow the area source model and the point source model to be nested within this long-range transport model without duplicating source contributions.

5.3.5 Iron and calcium rich dusts

5.3.5.1 Introduction

The NAEI does not include estimates of the emissions of iron or calcium rich dusts. Various process-based or more empirically based models have therefore been applied to estimate the contribution of these dusts to ambient PM_{10} concentrations across the UK.

The contributions have been split into four categories:

- Regional calcium rich dusts from re-suspension of soils
- Urban calcium rich dusts from re-suspension of soils due to urban activity
- Regional iron rich dusts from re-suspension
- Iron rich dusts from re-suspension due to vehicle activity

A method for estimating the mass of iron (Fe) and calcium (Ca) rich dusts was included in the modelling method for PM_{10} for the first time in 2006. The PCM models were revised for 2008 in order to incorporate a more process-based modelling approach for regional calcium rich dusts from re-suspension of soils and iron rich dusts from re-suspension due to vehicle activity. The revised models developed from those proposed by Abbott (2008) were also used for this 2013 assessment. The models for urban calcium rich dusts and regional iron rich dusts remain largely unchanged and are based a more empirical approach.

The starting point for the assessment of iron and calcium rich dusts is the measurements of a range of PM components including Fe and Ca reported by Harrison and Yin (2006) for three monitoring sites in the Birmingham area. Measurements were made and urban background site (BCCS) from May 2004 to May 2005, an urban roadside site (BROS) from May 2005 to November 2005 and at a rural site about 20 km from the city (CPSS) from November 2005 to May 2006. Measurements were not made at the different sites simultaneously but the measurement periods were sufficiently long that they can be used to provide reasonable estimates of the urban and roadside increments of various PM components. The measurement data for Fe and Ca are summarised in Table 5.2.

Table 5.2 - Measured concentration of iron and calcium and derived estimates of iron and calcium rich dusts (µg m^{-3})

	CPSS (rural)	BCCS (urban)	conversion factor	rural x factor	Urban increment x factor
Fe fine	0.06	0.10	9.0	0.54	0.36
Fe coarse	0.14	0.24	9.0	1.26	0.89
Ca fine	0.03	0.09	4.3	0.13	0.26
Ca coarse	0.12	0.30	4.3	0.52	0.77

Table 5.2 also includes the conversion factors suggested by Harrison et al., (2006) for use within their pragmatic mass closure model. This factor converts the mass of elemental Fe to iron related dusts and the mass of elemental Ca to calcium related dusts. The urban increment in the table has been calculated by subtracting the data for CPSS from that for the urban BCCS site. It is clear that there is an urban increment for both fine and coarse iron and calcium rich dusts. Measurement data for the BROS roadside site indicates that there is a roadside increment on top of the urban increment for Fe but not for Ca. Thus it is reasonable to assume that the urban increment for iron rich dusts is associated with emissions generated by road traffic but that the urban increment for calcium rich dusts is associated with urban emissions that are not related to traffic activity.

5.3.5.2 Regional calcium rich dusts

The regional concentration of Ca rich dusts was assumed to be a constant value across the UK in the 2006 and 2007 assessments (Kent et al., 2007b; Grice et al., 2009). Abbott (2008) developed a method to estimate the ambient concentration of Ca rich PM_{10} dusts resulting from the re-suspension of soils in rural areas. The starting points for this method are the proportion of bare soil, root crops and cereal crops in 1 km x 1 km grid squares across the UK within the Land Cover Map 2000 (2009). The concentration of Ca rich dusts cannot be calculated using the standard approach of using an estimate of the annual emissions and an air dispersion model. This is because the rate of re-suspension and the atmospheric dispersion of these emissions are both dependant on the meteorological conditions. The emission rate will be higher when the wind is stronger but the dispersion of these emissions will also be more efficient under these conditions.

The method presented by Abbott (2008) makes use of combined emission and dispersion kernels for cereal and root crop fields and for bare soils. Concentrations were calculated for each hour of the year based on hourly sequential meteorological data from twelve sites throughout the UK for 1999. This year was selected because the data were readily available.

The method of Abbott (2008) has been adapted for use within the PCM models by using an inverse distance weighted average of the results from the different kernels for each receptor location. This revised method avoids the discontinuities caused by the use of a simpler nearest met site to the receptor method used in the original work.

Figure 5.5a shows the results for regional Ca rich dusts. The highest concentrations are predicted to be in eastern areas where bare soils, root and arable crops are more common and there is less rainfall. A maximum value for this component has been set as 5 µg m^{-3} within the map. This value has been chosen as an estimate of the maximum likely concentration for a grid square average based on a comparison of this map with available PM_{10} measurements in the locations with the highest predicted contributions.

5.3.5.3 Urban calcium rich dusts

A more empirical method has been used to estimate the urban increment for Ca rich dusts. The normalized distribution of resident population on a 1 km x 1 km grid has been used as a surrogate for urban emissions within the area source model. The model has been calibrated to provide good agreement with the urban increment for Ca rich dusts found by Harrison and Yin (2006) and listed in Table 5.2.

Figure 5.5b shows the results for urban Ca rich dusts. The highest concentrations are in the major urban areas since this is a re-scaled population density map. A maximum value for this component has been set as 2 µg m^{-3} within the map. This value has been chosen as an estimate of the maximum likely concentration for a grid square average based on a comparison of this map with available PM_{10} measurements in the locations with the highest predicted contributions.

5.3.5.4 Regional iron rich dusts

A constant value for the regional contribution to Fe rich dusts of 1 µg m^{-3} has been applied across the UK. This residual value has been chosen to provide the best fit to the measurements from the Birmingham study (Harrison and Yin, 2006) and available urban background particulate Fe measurements once the estimated contribution from re-suspension due to vehicle movements has been taken into account. Figure 5.5c shows this constant contribution across the UK.

5.3.5.5 Iron rich dusts from re-suspension associated with vehicle movements

The assessments for 2006 and 2007 used an empirical method for the Fe rich dusts associated with re-suspension from vehicle movements based on the use of vehicle km statistics for 1 km x 1 km squares (Grice et al., 2009). Abbott (2008) developed a more process-based approach to estimating this contribution, which takes vehicle km statistics for heavy-duty vehicles (heavy good vehicles and buses) as its starting point. These estimates are likely to be subject to greater uncertainty than the estimates for re-suspension from soils because there is little information on the availability of material on road surfaces to be re-suspended.

Abbott (2008) calculated two sets of combined emission and dispersion kernels for each of the 12 meteorological stations for 1999: one to represent rural conditions and one to represent urban conditions. The estimated re-suspension rate was considerably higher for rural conditions due to the higher speeds assumed. These two sets of kernels were then used to calculate the contribution to PM_{10} concentrations according to the proportion of urban and rural land cover in each 1 km x 1 km grid square. A detailed examination of the results from this assessment has shown that the concentrations in urban areas were largely driven by the small proportion of rural land cover in these urban areas. The urban kernels have therefore been chosen to apply to all roads within the PCM model.

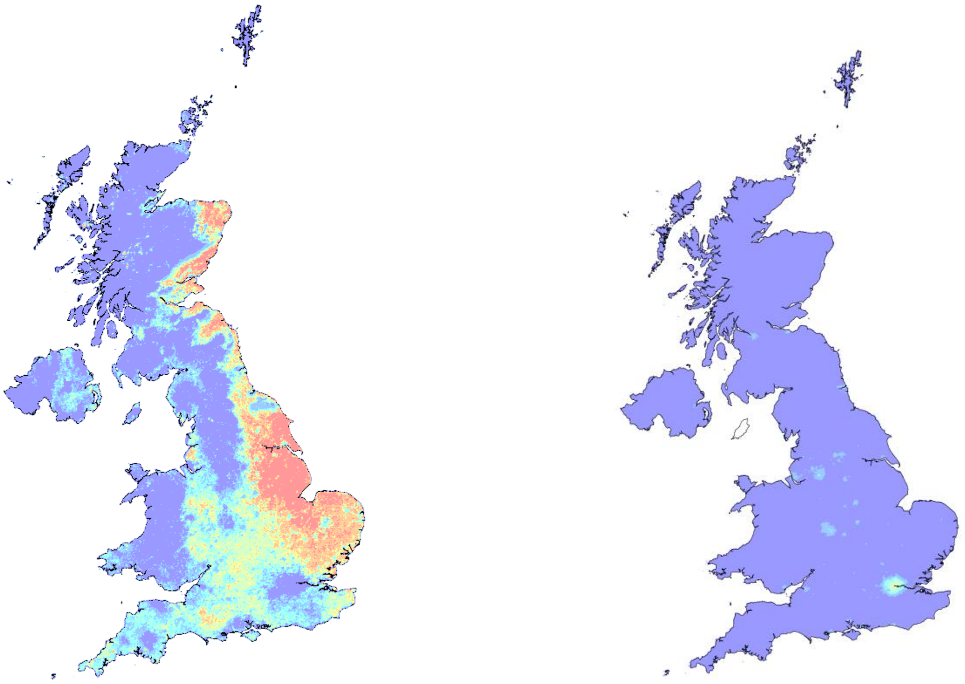
Figure 5.5d shows the results for Fe rich dusts from vehicle movements. The highest concentrations are associated with the roads with the highest flows of heavy-duty vehicles. A maximum value for this component has been set as 2.5 $\mu g\ m^{-3}$ within the map. This value has been chosen as an estimate of the maximum likely concentration for a grid square average based on a comparison of this map with available PM_{10} measurements in the locations with the highest predicted contributions.

An indication that the method is providing reasonable estimates the total of Fe rich dusts is provided by Figure 5.6, which shows a comparison of modelled annual mean Fe (the sum of regional and vehicle related Fe) with ambient Fe measurements at non-industrial and non-roadside sites for 2013 from the national metals monitoring network. The modelled estimates are clearly of the correct magnitude and provide a reasonable description of the rural to urban gradients.

Figure 5.5

a) Contribution to PM_{10} from regional Ca rich dusts associated with re-suspension from soils ($\mu g\ m^{-3}$)

b) Contribution to PM_{10} from urban Ca rich dusts associated with urban activities ($\mu g\ m^{-3}$)



c) Contribution to PM_{10} from regional Fe rich dusts ($\mu g\ m^{-3}$)

d) Contribution to PM_{10} from Fe rich dusts associated with vehicle movements ($\mu g\ m^{-3}$)

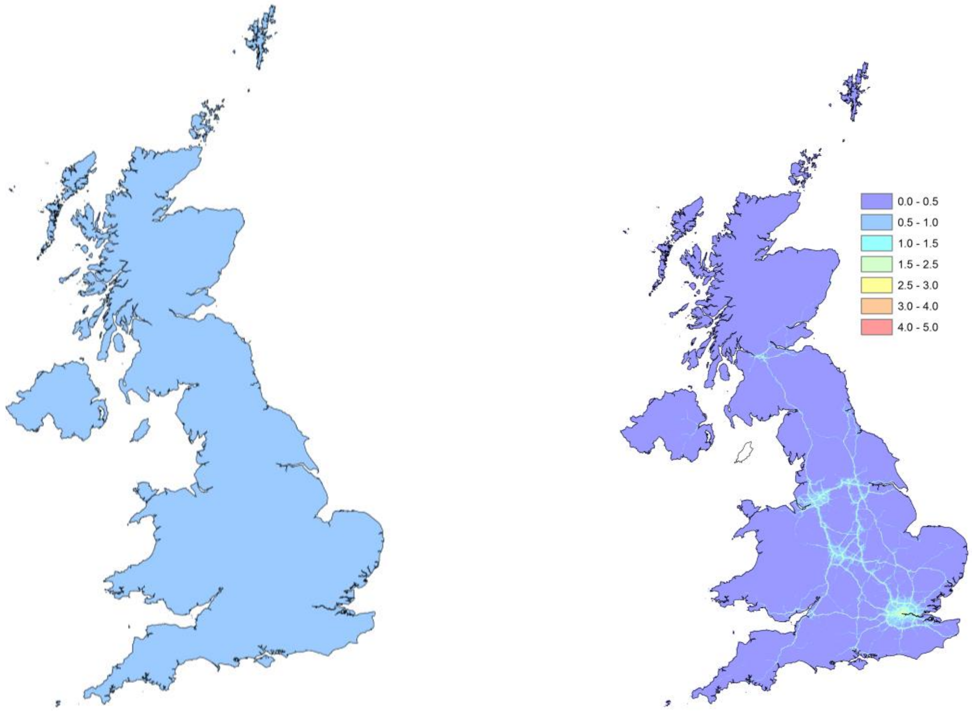
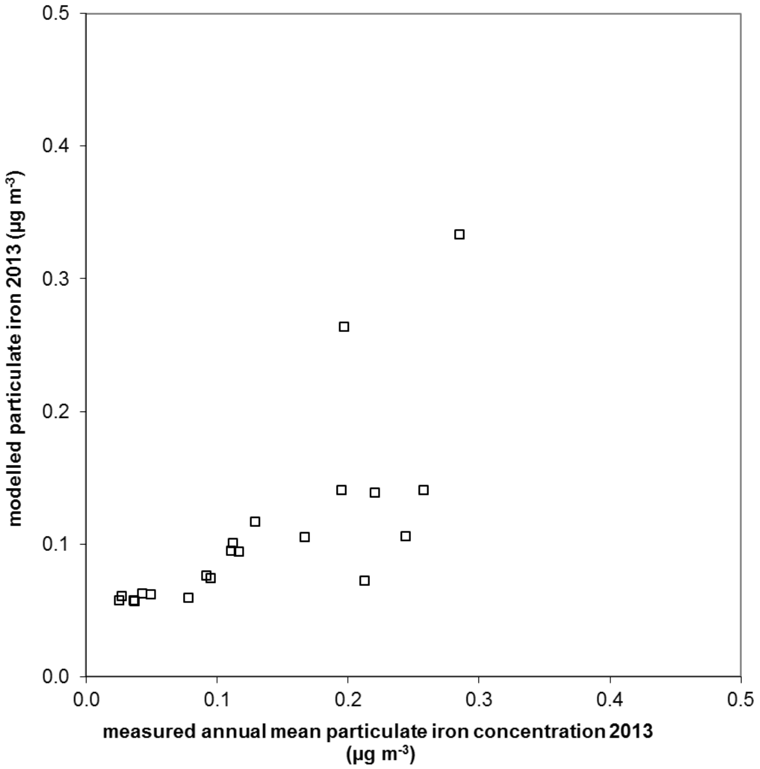


Figure 5.6 - Comparison of modelled and measured annual mean elemental Fe concentrations 2013 (µg m^{-3})



5.3.5.6 Application to the mapping of heavy metal concentrations

Abbott (2008) also suggested a method for estimating the contributions to the ambient concentrations of heavy metals from soil and vehicle related re-suspension processes. Section 10.3 on the modelling of heavy metal concentrations describe how the maps of PM mass from rural re-suspension of soils and re-suspension associated with vehicle movements have been used to estimate the contributions to the ambient concentration of heavy metals using a combination of information on the heavy metal content of soils and enhancement factors.

5.3.6 Sea salt

The contribution to ambient PM from sea salt has been derived directly from measurements of particulate chloride (Tang, 2013). Data from 28 rural sites were interpolated by Kriging onto a 5 km x 5 km grid. A scaling factor of 1.648 was applied to convert elemental chloride mass to sodium chloride mass. 73% of the sea salt mass was assumed to be in the coarse fraction and 27% in the fine fraction. This split was derived from measurement data presented by APEG (1999) and Harrison and Yin (2006).

The use of chloride is potentially subject to both positive and negative artefacts. Sea salt is not the only source of particulate chloride in the atmosphere. HCl is emitted from coal burning but reductions in coal use and flue gas abatement are likely to have reduced atmospheric HCl and ammonium chloride concentrations considerably. There will also be loss of chloride from marine aerosol due to reactions with nitric acid. The resulting sodium nitrate PM has been considered to be of anthropogenic origin and the contribution to PM mass from this sodium nitrate is explicitly included in the modelled concentrations presented. If sodium were used as the marker for sea salt rather than chloride then this sodium nitrate would tend to be included in the natural component.

In addition to selecting chloride as the marker for sea salt, the analysis was simplified by assuming that the sea salt consists of sodium chloride only. Thus the measured chloride concentration has been scaled by a factor of 1.648. An alternative approach would be to scale by 1.809 to take account of the full composition of sea salt. The composition of sea salt is dominated by chloride and sodium. Other components contributing more than 1% by mass are sulphate, magnesium, calcium and potassium. Sulphate is already explicitly included in the modelled concentrations and a sea salt correction has not been applied to the measured concentrations used in the PCM model. Adding a further sea salt sulphate component would lead to double counting. The other components (magnesium, calcium and potassium) have, in effect, been treated as sodium by the use of a scaling factor of 1.648. The ratio of (chloride + sodium) to chloride in sea salt is 1.552, while the ratio of (chloride + sodium + magnesium + calcium + potassium) to chloride is 1.658. Thus the simplification of sea salt as pure sodium chloride has not had a large impact on the total mass assumed apart from the contribution from sea salt sulphate, which, as a simplification, has been included with the rest of the sulphate as anthropogenic.

5.3.7 Contributions from area sources

Figure 5.7 shows the calibration of the area source model. The modelling method makes use of an ADMS derived dispersion kernel to calculate the contribution to ambient concentrations at a central receptor location from area source emissions within a 33 km x 33 km square surrounding each receptor. Hourly sequential meteorological data from Waddington in 2013 was used to construct the dispersion kernels, as described in Appendix 4. A total of 20 background FDMS monitoring sites within the national network had sufficient data capture for PM_{10} and $PM_{2.5}$ in 2013 to be used to calibrate the model. Only sites with valid data for PM_{10} and $PM_{2.5}$ have been used to calibrate the PM_{10} and $PM_{2.5}$ models, as described in Section 5.1.

Revised methods introduced in the 2011 assessment (Brookes et al., 2012) for modelling the contributions to PM_{10} from SNAP 2 (domestic and non-domestic combustion) and SNAP 3 (combustion in industry) area sources were used and have been described in Section 3.3.5.

As part of the calibration process emission caps have been applied to certain sectors; this is because the use of surrogate statistics for mapping area source emissions sometimes results in unrealistically large concentrations in some grid squares for a given sector. The emission caps applied are given in Table 5.3.

With the exception of area sources associated with SNAP sector 3 (combustion in industry), the area source model has been calibrated using FDMS ambient PM monitoring data from the UK national networks. The modelled large point and small point source, SIA, SOA, iron and calcium rich dust, long range transport primary PM, sea salt and the residual concentrations have been subtracted from the measured annual mean PM concentration at background sites and compared with the modelled area source contribution to annual mean PM concentration. A residual concentration of 1.5 $\mu g\ m^{-3}$ was found to provide the best fit to the monitoring data for both PM_{10} and $PM_{2.5}$ in 2013.

The modelled area source contribution (excluding SNAP 3) was multiplied by the relevant empirical coefficient to calculate the calibrated area source contribution for each grid square in the country. The area source contribution was then added to the contributions from SNAP 3 area sources, secondary organic and inorganic particles, from small and large point sources, from regional primary particles, from sea salt, from calcium and iron rich dusts and the residual, resulting in a map of background annual mean gravimetric PM_{10} concentrations.

Figure 5.7 - Calibration of PM_{10} area source model 2013 ($\mu g\ m^{-3}$, gravimetric)

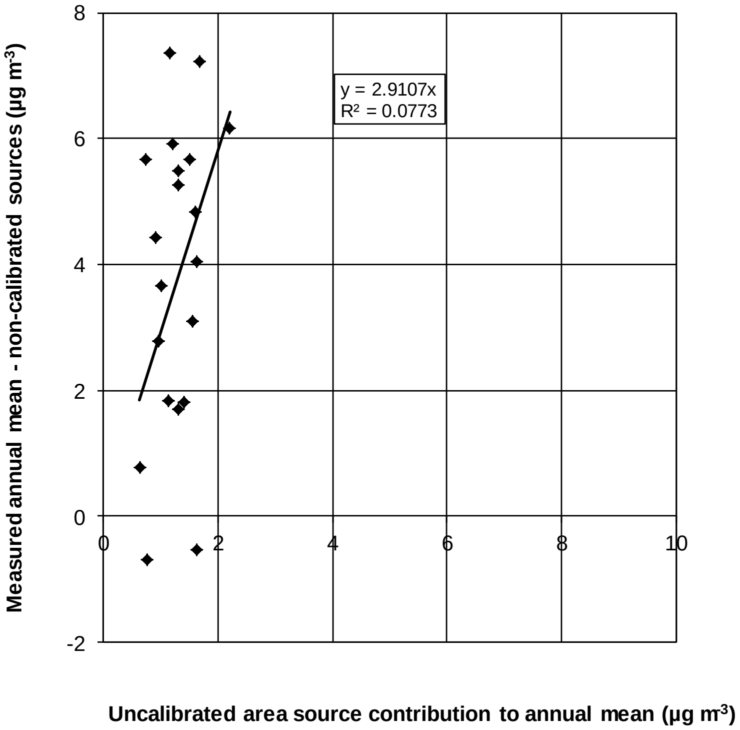


Table 5.3 - Emission caps applied to PM10 sector grids

SNAP code	Description	Cap applied (t/a/km^2)
SNAP 6 (Solvent use)	Industrial coatings - metal and plastic Metal and plastic coatings	6
SNAP 6 (Solvent use)	Industrial coatings - high performance High performance coatings	6
SNAP 6 (Solvent use)	Industrial coatings - marine Marine coatings	10
SNAP 6 (Solvent use)	Industrial coatings - commercial vehicles Commercial vehicle coatings	10
SNAP 6 (Solvent use)	Industrial coatings - aircraft Aircraft coatings	10
SNAP 6 (Solvent use)	Industrial coatings - agricultural and construction Ace coatings	10
SNAP 8 (Other Transport &	Industrial off-road mobile machinery DERV	3
SNAP 8 (Other Transport & mobile machinery)	Industrial off-road mobile machinery Gas oil	3
SNAP 8 (Other Transport & mobile machinery)	Industrial off-road mobile machinery Petrol	3
SNAP10 (Agriculture forestry & land use change)	Agriculture livestock - pigs Housed livestock	6
SNAP10 (Agriculture forestry & land use change)	Agriculture livestock - laying hens Housed livestock	3
SNAP10 (Agriculture forestry & land use change)	Agriculture livestock - broilers Housed livestock	3
SNAP10 (Agriculture forestry & land use change)	Agriculture livestock - other poultry Housed livestock	3

SNAP code	Description	Cap applied (t/a/km^2)
SNAP 1 (Combustion in energy production & transformation)	Upstream oil and gas production - combustion at gas separation plant LPG	2
SNAP 1 (Combustion in energy production & transformation)	Upstream oil and gas production - combustion at gas separation plant OPG	2
SNAP 2 Combustion (commercial)	Public sector combustion Coal	10
SNAP 6 (Solvent use)	Industrial coatings - automotive Automotive coatings	10

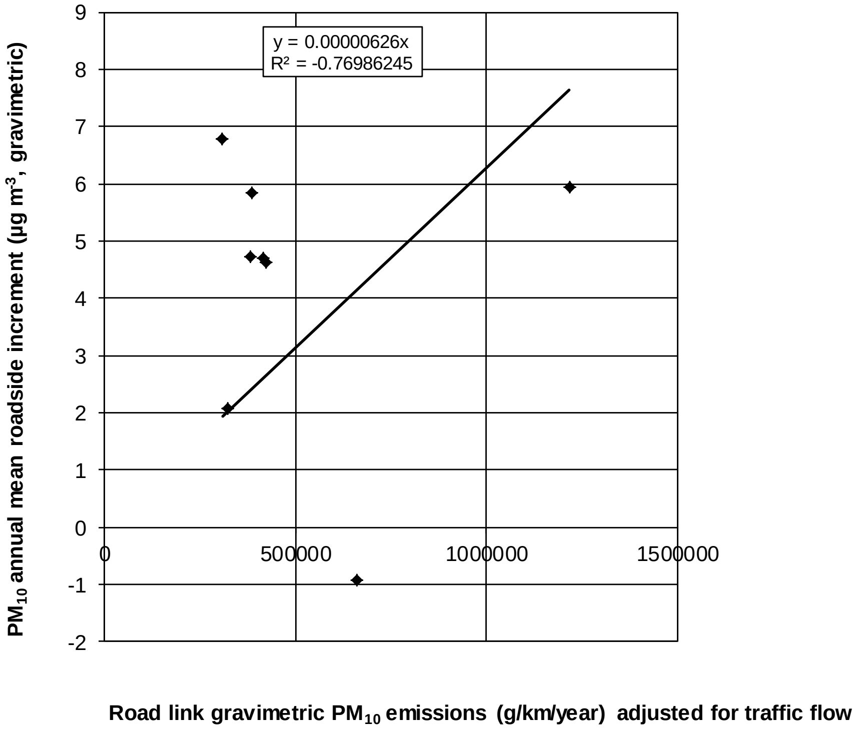
5.3.8 Roadside concentrations

The annual mean concentration of PM_{10} at a roadside location has been considered to be made up of two parts: the background concentration (as described above) and a roadside increment:

roadside PM_{10} *concentration = background* PM_{10} *concentration +* PM_{10} *roadside increment*.

The NAEI provides estimates of PM_{10} emissions for major road links in the UK for 2012 (Passant et al., 2014) and these have been adjusted to provide estimates of emissions in 2013. The roadside increment model for PM_{10} has been calibrated using data from FDMS and Partisol monitoring sites with valid data for both PM_{10} and $PM_{2.5}$ in 2013. Figure 5.8 shows a comparison of the roadside increment of annual mean PM_{10} concentrations at roadside monitoring sites with PM_{10} emission estimates for the individual road links alongside which these sites are located. The regression line has been forced through zero to provide a reasonable model output without imposing an unrealistic high residual to the roadside increment. Emissions were adjusted for annual average daily traffic flow using the method described in Section 3.3.6. Roadside concentrations for urban major road links (A-roads and motorways) only are reported to the EU and included in this report.

Figure 5.8 - Calibration of PM_{10} roadside increment model 2013 (µg m^{-3}, gravimetric)



5.4 Results

5.4.1 Verification of mapped values

Figure 5.9 and Figure 5.10 show comparisons of modelled and measured annual mean PM_{10} concentration in 2013 at background and roadside monitoring site locations. Lines representing y = x – 50 % and y = x + 50% are also shown because 50% is the AQD data quality objective for modelled annual mean PM_{10} concentrations – see Section 1.5. Summary statistics for the comparison between modelled and measured PM_{10} concentrations are presented in Table 5.4 and Table 5.5.

There are a number of different categories of monitoring sites within these tables and graphs. This is because there are some sites in the national network at which only PM_{10} or $PM_{2.5}$ are measured, but not both. TEOM PM_{10} data adjusted using the VCM model (http://www.volatile-correction-model.info/), are available for some verification sites.

The agreement between the FDMS and TEOM VCM measurement data and the modelled values is generally good. The TEOM x 1.3 measurement data for verification sites are higher than the modelled estimates. This is as expected since TEOM x 1.3 is known to over predict in comparison to the reference gravimetric monitoring method. The measured values for gravimetric (Partisol) sites are lower than the modelled values at two background sites; this is because the measured gravimetric annual means are lower than the measured FDMS annual means at these sites.

Figure 5.9 - Verification of background annual mean PM_{10} model 2013

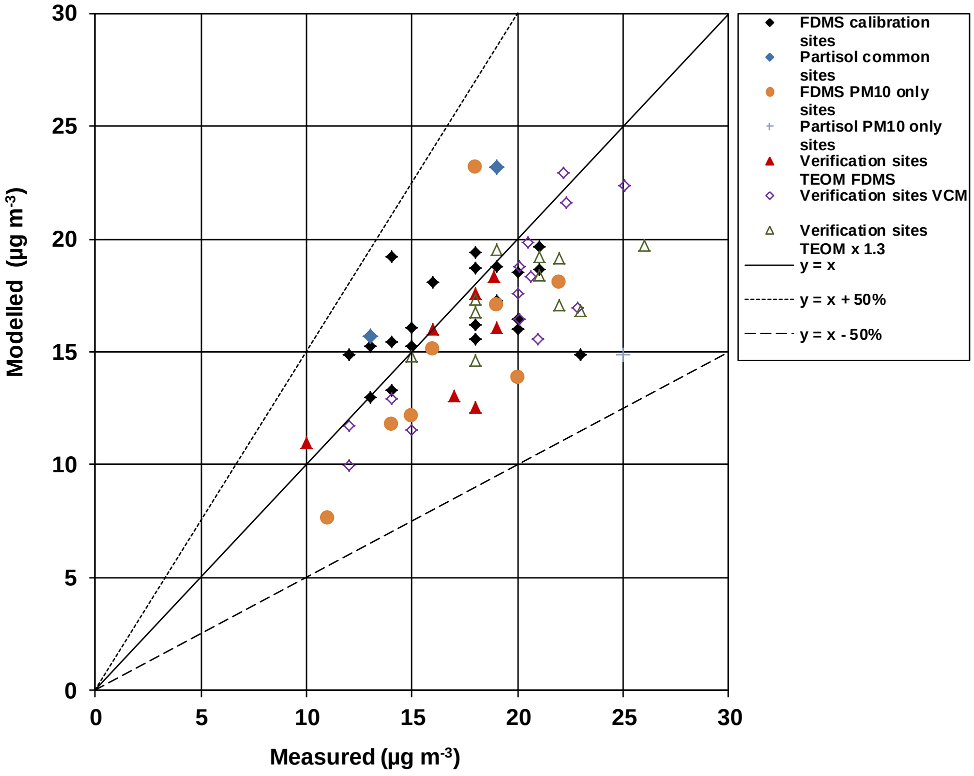


Figure 5.10 - Verification of roadside annual mean PM_{10} model 2013

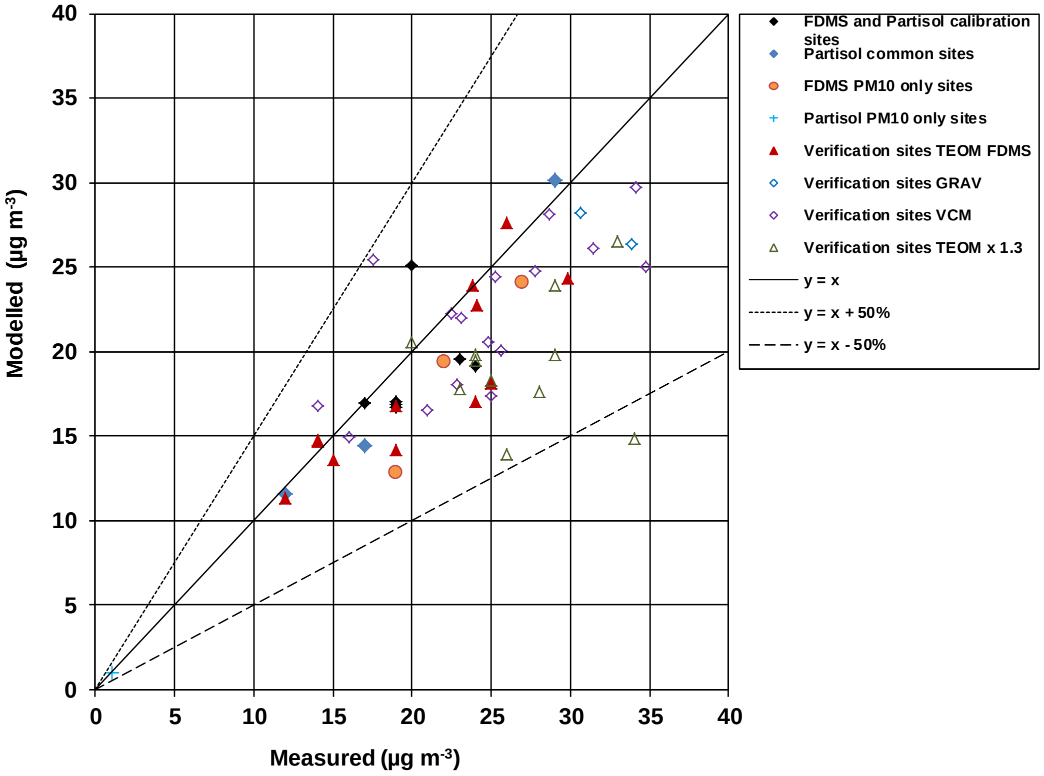


Table 5.4 - Summary statistics for comparison between gravimetric modelled and measured concentrations of PM_{10} at background sites

	Mean of measurements ($\mu g\ m^{-3}$, grav)	Mean of model estimates ($\mu g\ m^{-3}$, grav)	R^2	% outside data quality objectives	Number of sites
National network FDMS (Calibration)	17.2	16.7	0.22	0	21
National network Partisol	16.0	19.4	1.00	0	2
National network FDMS PM10 only sites	16.9	14.9	0.51	0	8
National network Partisol PM10 only sites	25.0	14.9	-	0	1
Verification sites FDMS	16.7	14.9	0.47	0	7
Verification sites gravimetric	-	-	-	-	-
Verification sites VCM	19.1	16.9	0.80	0	14
Verification sites TEOM x 1.3	20.3	17.6	0.42	0	11

Table 5.5 - Summary statistics for comparison between gravimetric modelled and measured concentrations of PM_{10} at roadside sites

	Mean of measurements (µg m^{-3}, grav)	Mean of model estimates (µg m^{-3}, grav)	R^2	% outside data quality objectives	Number of sites
National network FDMS (Calibration)	21.3	20.2	0.60	0	8
National network Partisol	19.3	18.7	0.98	0	3
National network FDMS PM10 only sites	22.7	18.8	0.94	0	3
National network Partisol PM10 only sites	-	-	-	-	-
Verification sites FDMS	20.5	18.3	0.72	0	12
Verification sites gravimetric	32.2	27.3	1.00	0	2
Verification sites VCM	24.6	22.0	0.50	0	16
Verification sites TEOM x 1.3	26.8	19.3	0.02	9	11

5.4.2 PM_{10} source apportionment at monitoring sites

Figure 5.11 and Figure 5.12 show the modelled annual mean PM_{10} source apportionment for 2013 at national network background and roadside monitoring sites respectively. The measured concentration at each site is also shown for reference.

At background locations, the contributions from non-emissions inventory sources (i.e. regional background sources and urban dusts), which are shown in grey on the figures, dominate with a particularly large contribution from secondary aerosols. The smaller contribution from urban background emissions sources, shown in colour on the figures, is dominated in most locations by traffic (exhaust emissions, brake and tyre wear and road abrasion), industry and off road mobile machinery.

At roadside locations the source apportionment follows a very similar pattern to background locations, except that there is an extra local road traffic component composed of local exhaust emissions and local brake and tyre wear and local road abrasion emissions. Depending on the magnitude of the local traffic emissions, local traffic emissions can contribute up to about 8 µg m^{-3} of PM_{10} at the roadside monitoring sites.

Figure 5.11 - Annual mean PM_{10} source apportionment at background national network monitoring sites in 2013

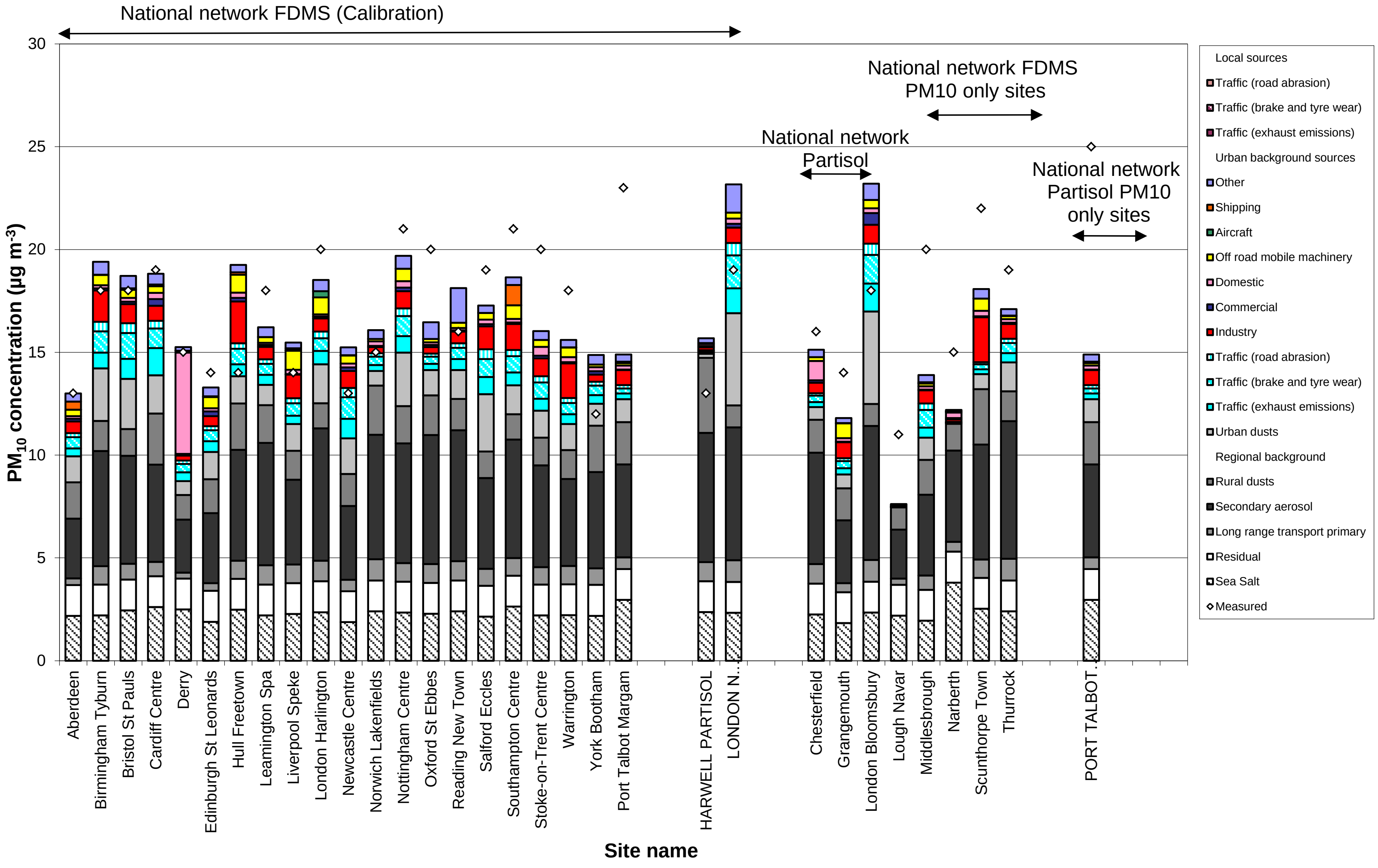
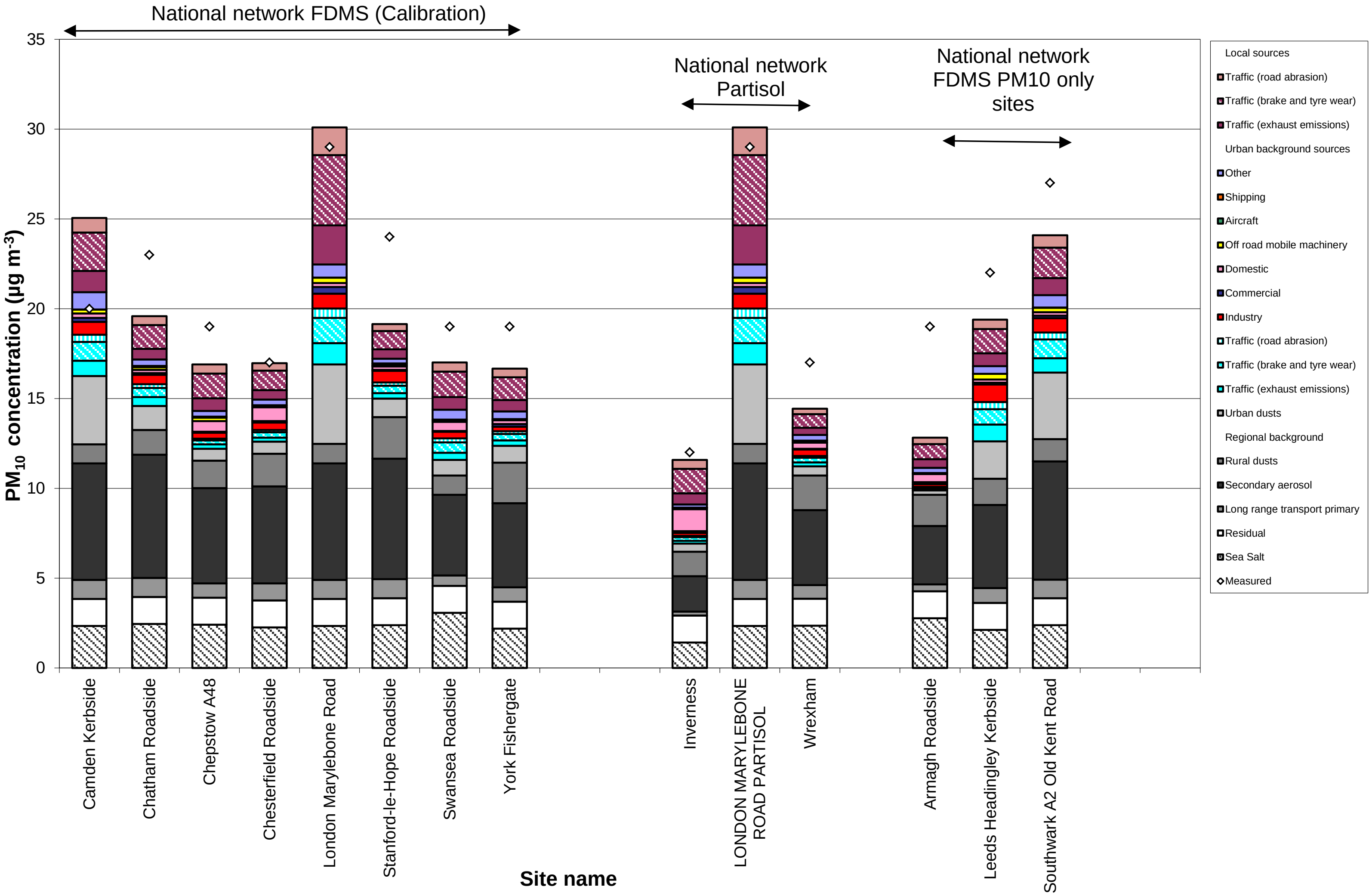


Figure 5.12 - Annual mean PM_{10} source apportionment at national network roadside monitoring sites in 2013



5.5 Subtraction of sea salt component

5.5.1 Introduction

The AQD (Article 20) requires member states to attribute exceedances of limit values due to natural sources when reporting the results of air quality assessments. The definition of natural sources in this directive includes sea spray. An assessment of concentrations with the contribution from natural sources subtracted is provided in e-reporting Data flow G (CDR, 2014) for locations with measured or modelled exceedances of the limit values. 2013 is the sixth year for which the contribution from natural sources has been subtracted. Where exceedances are attributed to natural sources, subtraction is a requirement of the Directive.

5.5.2 Map of annual mean sea salt PM_{10}

The method used to estimate the sea salt contribution to annual mean PM_{10} concentrations across the UK has been described in Section 5.3.6. The map of annual mean sea salt PM_{10} can be used to subtract this contribution directly from measured or modelled annual mean concentrations. The uncertainties associated with estimating the sea salt contribution to annual mean PM_{10} from measurements of particulate chloride have been discussed in Section 5.3.6. It is recognised that the interpolated map of sea salt concentrations will not capture the steep gradients in sea salt concentration very close to the coast. Thus the analysis presented may underestimate the sea salt contribution to exceedances in coastal areas.

5.5.3 Method for the 24-hour limit value

A method has also been developed to estimate the contribution from sea salt to exceedances of the 24-hour limit value for PM_{10} of no more than 35 days with concentration greater than 50 µg m^{-3}. This method has been described in detail by Defra (2009). This method makes use of the relationship between the number of days with concentrations greater than 50 µg m^{-3} and annual mean concentrations described by Stedman et al. (2001a). There is some scatter around the best-fit line of the relationship shown in Figure 5.3. Using the best-fit line relationship within the annual method for subtracting sea salt has been considered appropriate since this should give the best central estimate of the sea salt contribution.

An estimate of the number of days with a PM_{10} concentration greater than 50 µg m^{-3} associated with the contribution to annual mean concentration from sea salt has been calculated by applying the relationship of Stedman et al. (2001a) in the vicinity of the limit value. This has been done by calculating the difference between the number of days corresponding to 31.5 µg m^{-3} minus half the sea salt concentration and the number of days corresponding to 31.5 µg m^{-3} plus half the sea salt concentration.

Daily chloride measurements are available for three sites in the south east of the UK. These measurements can be used to calculate a daily sea salt subtraction for PM_{10} monitoring data. This method is not applicable to model results and will be less reliable for sites not in the south east of the UK. For these reasons the method based on annual mean sea salt concentrations has been used across the UK as described above. Defra (2009) have provided a comparison of the annual and daily methods for the years 2005, 2006 and 2007 which shows that the agreement between the methods is reasonably good.

5.5.4 Results

The results of the assessment of number of days with a PM_{10} concentration greater than 50 µg m^{-3} with the contribution from sea salt subtracted in zones with measured or modelled exceedances of the 24-hour limit value are shown in Table 5.6. The modelled exceedance in the Greater London Urban Area is no longer present after the subtraction of the contribution from sea salt. S8 in this table refers to natural sources, sea salt in this instance.

There were no reported exceedances of the annual mean limit value for PM_{10} in 2013.

Table 5.6 - Exceedance of limit values of PM_{10} due to natural events or natural contributions - Contribution of natural events to exceedance of the PM_{10} limit value (24-hr mean)

Zone code	Zone	EoI station code	Number of exceedances measured	Natural event code(s)	Estimated number of exceedances after subtraction of natural contribution
UK0001	Greater London Urban Area	n/a	40	S8	30

6 $PM_{2.5}$

6.1 Introduction

6.1.1 Limit and Target values

The Air Quality Directive (AQD) includes a target value (TV) for annual mean $PM_{2.5}$ which came into force from 01/01/2010. This target value is:

- An annual mean concentration of 25 µg m^{-3}.

Two limit values have also been set for ambient $PM_{2.5}$ concentrations in the AQD. These limit values are:

- Stage 1 limit value – An annual mean concentration of 25 µg m^{-3}.
- Stage 2 indicative limit value – An annual mean concentration of 20 µg m^{-3}

The Stage 1 limit value is due to come into force on 01/01/2015, the Stage 2 limit value is due to come into force 01/01/2020. There were no measured or modelled exceedances of the annual mean target value and Stage 1 limit value for $PM_{2.5}$ in 2013. There was one modelled exceedance of the annual mean Stage 2 indicative limit value for $PM_{2.5}$ in 2013 and this exceedance remained after subtraction of the contribution from natural sources (sea salt). Note that this indicative limit value is not currently in force.

An exposure reduction target and an exposure concentration obligation have also been set for $PM_{2.5}$.

6.1.2 Annual mean model

Maps of annual mean $PM_{2.5}$ in 2013 at background and roadside locations are shown in Figure 6.1 and Figure 6.2.

Full details of the models used to calculate concentrations of PM_{10} and $PM_{2.5}$ are provided in Chapter 5. The maps have been calibrated using measurements from TEOM FDMS instruments within the national network for which co-located PM_{10} measurements are also available for 2013. The models for PM_{10} and $PM_{2.5}$ are designed to be fully consistent, with each component either derived from emission estimates for PM_{10} or $PM_{2.5}$, or the contributions to the fine and coarse particle size fractions are estimated separately. This enables us to carry out an additional reality check that the calibration parameters for the two pollutants are reasonably consistent. Measurements from national network sites without collocated $PM_{2.5}$ instruments have been used as an additional verification dataset.

The concentrations of many of the modelled components have been estimated separately for the fine and coarse fraction. This enables a consistent method to be adopted for estimation of PM_{10} (the sum of the fine and coarse fractions) and $PM_{2.5}$ (fine fractions only). The mass fractions of each component assigned to $PM_{2.5}$ are listed in Section 6.3.1. The component pieces are then aggregated to a single 1 km x 1 km background $PM_{2.5}$ grid. An additional roadside increment is added for roadside locations.

The results from the annual mean model can be directly compared with the annual mean target and limit values in order to carry out the air quality assessment.

6.1.3 Chapter Structure

This chapter describes modelling work carried out for 2013 to assess compliance with the $PM_{2.5}$ limit and target values described above. Emission estimates for primary PM are described in Section 6.2, Section 6.3 describes the $PM_{2.5}$ modelling methods, the modelling results in terms of verification and source apportionment are presented in Section 6.4. The methods used to subtract the contribution from natural sources (sea salt) and the results of this subtraction are presented in Section 6.5. The method used to calculate the average exposure indicator (AEI) for annual mean $PM_{2.5}$ and an assessment of compliance with the exposure concentration obligation is presented in Section 6.6.

Figure 6.1 - Annual mean background PM$_{2.5}$ concentration, 2013 (µg m^{-3}, gravimetric)

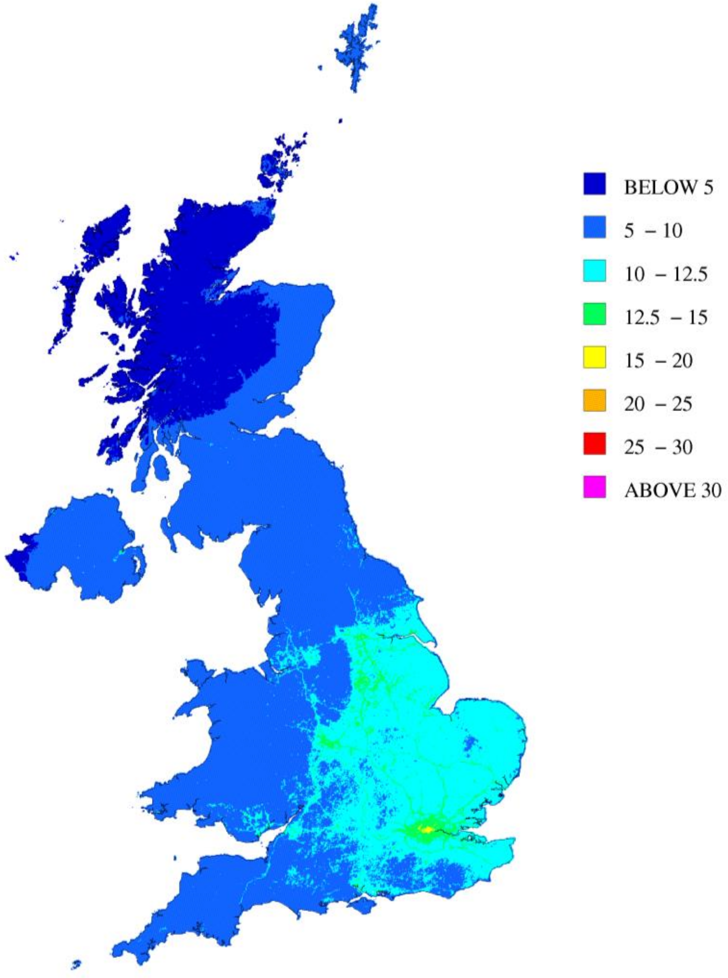
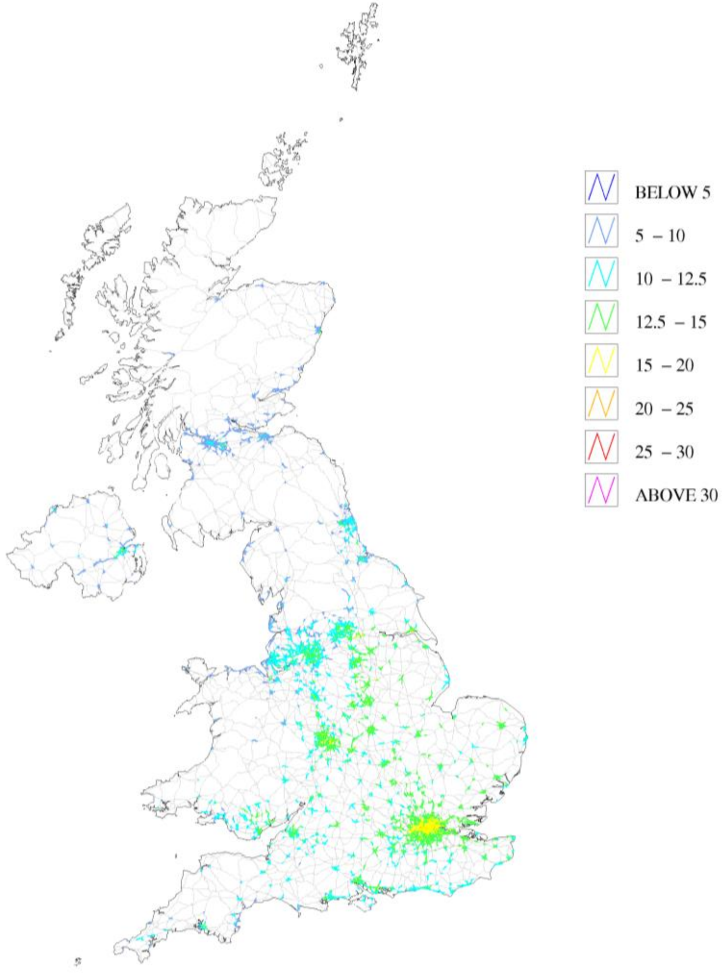


Figure 6.2 - Urban major roads, annual mean roadside PM$_{2.5}$ concentration, 2013 (µg m^{-3}, gravimetric)

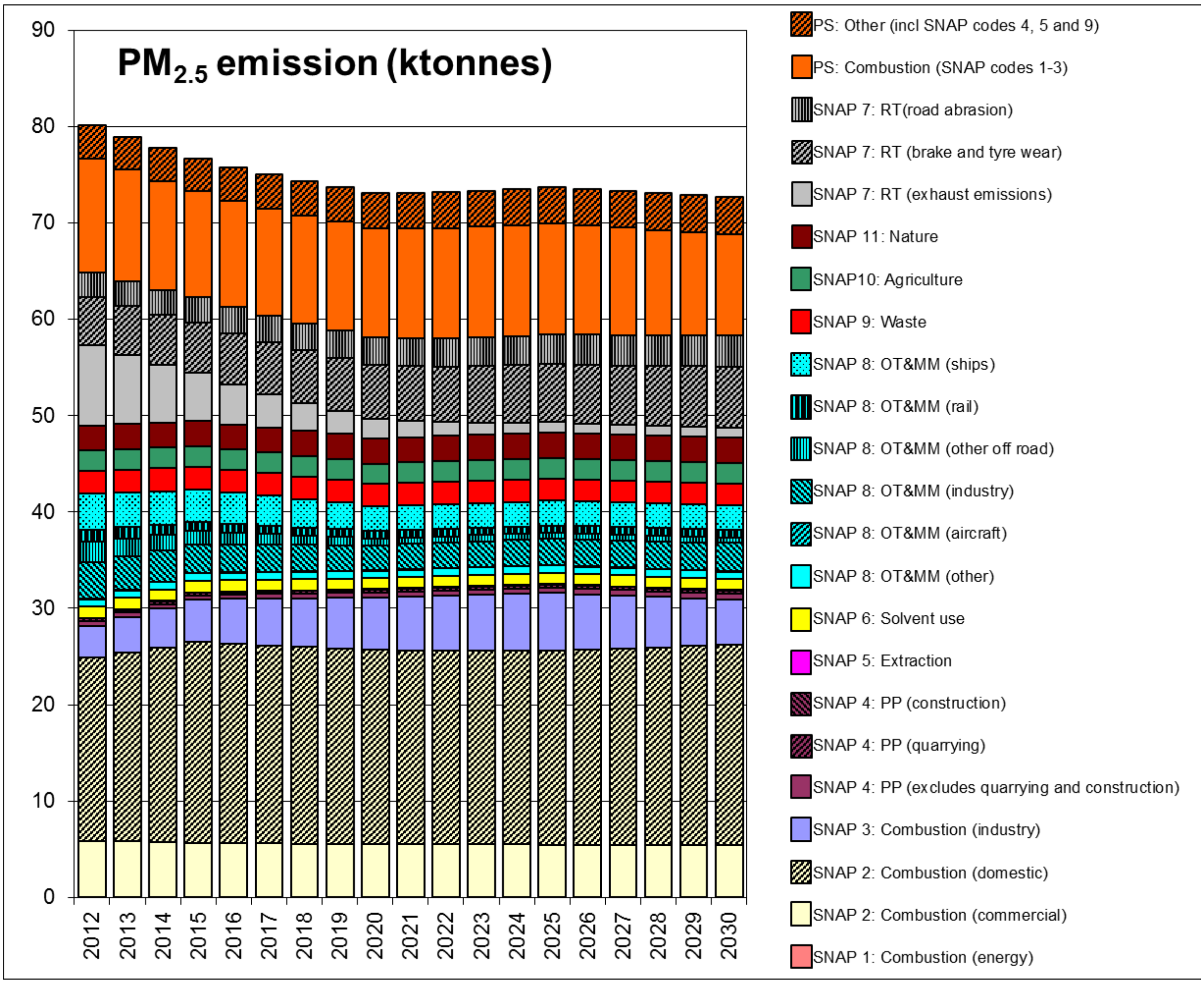


6.2 $PM_{2.5}$ emissions

Estimates of the emissions of primary PM from the UK National Atmospheric Emission Inventory 2012 (NAEI 2012) have been used in this study (Passant et al., 2014). Emissions projections have been provided by the NAEI (Passant pers. comm. 2014a) based on DECCs UEP48 energy and emissions projections (DECC, 2013). Figure 6.3 shows UK total $PM_{2.5}$ emissions for 2012 and emissions projections for 2015, 2020, 2025 and 2030 split by SNAP code, with the coding described in Table 3.1. Values for intermediate years have been interpolated in this figure. Figure 6.3 shows that $PM_{2.5}$ emissions in 2012 include contributions from a wide range of different source sectors. Some of the sectors with the largest contribution to the total in 2012 include road traffic exhaust, off-road mobile machinery and domestic combustion.

Maps of emissions from area sources for 2013 were derived from the 2012 inventory maps using specific scaling factors derived for each combination of source activity (typically fuel type), as described for NO_X (Section 3.3.5). The emissions from point sources were scaled in a similar way, see Section 3.3.1. The methods used to calculate ambient concentrations from the estimates of primary PM emissions are described below for point, area and regional sources.

Figure 6.3 - Total UK $PM_{2.5}$ emissions for 2012 and emissions projections up to 2030 by SNAP code from NAEI 2012



6.3 $PM_{2.5}$ modelling

6.3.1 $PM_{2.5}$ mass fractions

The proportions of the PM mass for each component assigned to the $PM_{2.5}$ fraction within the PCM models are listed in Table 6.1. The proportions for secondary inorganic aerosols have been derived as described in Section 5.3. The proportions for local point and area sources are based on the NAEI emission inventories for $PM_{2.5}$ and PM_{10} (Passant et al., 2014). The NAEI $PM_{2.5}$ emission inventory has been derived from the PM_{10} emission inventory by the application of estimates of the mass fraction represented by $PM_{2.5}$ for different sources and fuels. Overall the UK total mass emissions for $PM_{2.5}$ for 2013 were about 70% of the value for PM_{10}. The proportions for calcium and iron rich dusts have been derived with reference to the monitoring data presented in Section 5.3.5 and to provide good fit to the available co-located $PM_{2.5}$ and PM_{10} measurements. The proportion for sea salt has been derived as described in Section 5.3.6.The proportions for secondary organic aerosol, regional primary particles and the residual have been set at 1.0 for $PM_{2.5}$ so as to provide best fit to the available measurements.

Table 6.1 - The proportion of PM mass assigned to the $PM_{2.5}$ and $PM_{2.5\text{-}10}$ size fractions

Component	Fine fraction ($PM_{2.5}$)	Coarse fraction ($PM_{2.5\text{-}10}$)
SO_4	0.94	0.06
NO_3	0.556 (fine mode), 0.222 (coarse mode)	- (fine mode), 0.222 (coarse mode)
NH_4	0.97	0.03
SOA	1.0	-
Large point sources of primary particles	$PM_{2.5}$ emission inventory*	PM_{10} emission inventory
Small point sources of primary particles	$PM_{2.5}$ emission inventory*	PM_{10} emission inventory
Regional primary particles	1.00	-
Area sources of primary particles	$PM_{2.5}$ emission inventory*	PM_{10} emission inventory
Rural calcium rich dusts from re-suspension of soils	0.50	0.50
Urban calcium rich dusts from re-suspension of soils due to urban activity	0.50	0.50
Regional iron rich dusts from re-suspension	0.50	0.50
Iron rich dusts from re-suspension due to vehicle activity	0.50	0.50
Sea salt	0.27	0.73
Residual	1.00	-

* The NAEI $PM_{2.5}$ emission inventory has been derived from the PM_{10} emission inventory by the application of estimates of the mass fraction represented by $PM_{2.5}$ for different sources and fuels.

6.3.2 Contributions from large and small point sources

The contributions from large and small point sources have been calculated in the same way as for the PM_{10} model described in Section 5.3.3. A total of 289 point sources were modelled explicitly.

6.3.3 Contributions from area sources

Figure 6.4 shows the calibration of the area source model for $PM_{2.5}$. The calibration coefficient for $PM_{2.5}$ is quite similar to the calibration coefficient for PM_{10} and the difference is considered to be well within the uncertainty of the PM_{10} and $PM_{2.5}$ measurements and $PM_{2.5}$ mass fractions within the emission inventory. A reasonably good agreement between the calibration coefficients for area sources is one of the criteria for the choice of mass fraction parameters for $PM_{2.5}$ within the PCM model.

As part of the calibration process emission caps have been applied to certain sectors; this is because the use of surrogate statistics for mapping area source emissions sometimes results in unrealistically large concentrations in some grid squares for a given sector. The emission caps applied are given in Table 6.2.

Figure 6.4 - Calibration of $PM_{2.5}$ area source model 2013 (µg m^{-3}, gravimetric)

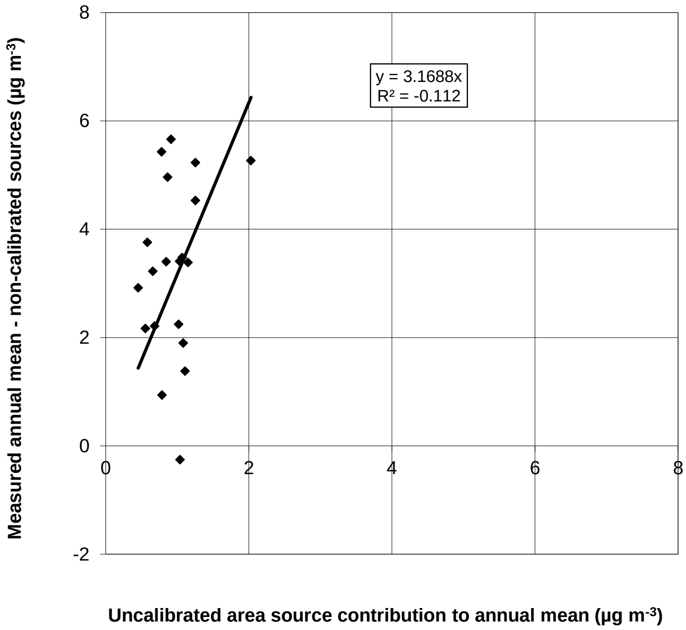


Table 6.2 - Emission caps applied to $PM_{2.5}$ sector grids

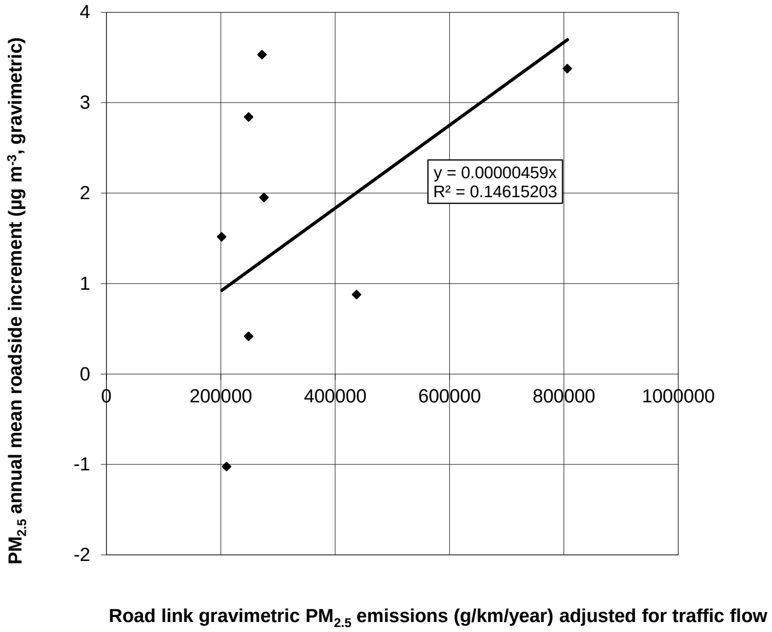
SNAP code	Description	Cap applied (t/a/km²)
SNAP 6 (Solvent use)	Industrial coatings - metal and plastic Metal and plastic coatings	6
SNAP 6 (Solvent use)	Industrial coatings - high performance High performance coatings	4
SNAP 6 (Solvent use)	Industrial coatings - marine Marine coatings	4
SNAP 6 (Solvent use)	Industrial coatings - commercial vehicles Commercial vehicle coatings	6
SNAP 6 (Solvent use)	Industrial coatings - aircraft Aircraft coatings	6
SNAP 6 (Solvent use)	Industrial coatings - agricultural and construction Ace coatings	6
SNAP 8 (Other Transport & mobile machinery)	Industrial off-road mobile machinery DERV	2
SNAP 8 (Other Transport & mobile machinery)	Industrial off-road mobile machinery Gas oil	2
SNAP 8 (Other Transport & mobile machinery)	Industrial off-road mobile machinery Petrol	2
SNAP10 (Agriculture forestry & land use change)	Agriculture livestock - pigs Housed livestock	4

SNAP code	Description	Cap applied (t/a/km^2)
SNAP10 (Agriculture forestry & land use change)	Agriculture livestock - laying hens Housed livestock	4
SNAP10 (Agriculture forestry & land use change)	Agriculture livestock - broilers Housed livestock	4
SNAP10 (Agriculture forestry & land use change)	Agriculture livestock - other poultry Housed livestock	4
SNAP 1 (Combustion in energy production & transformation)	Upstream oil and gas production - combustion at gas separation plant LPG	2
SNAP 1 (Combustion in energy production & transformation)	Upstream oil and gas production - combustion at gas separation plant OPG	2
SNAP 2 Combustion (commercial)	Public sector combustion Coal	6
SNAP 6 (Solvent use)	Industrial coatings - automotive Automotive coatings	6

6.3.4 Roadside concentrations

Figure 6.5 shows the calibration of the roadside increment model for annual mean $PM_{2.5}$ concentrations.

Figure 6.5 - Calibration of $PM_{2.5}$ roadside increment model 2013 (µg m^{-3}, gravimetric)



6.4 Results

6.4.1 Verification of mapped concentrations

Figure 6.6 and Figure 6.7 show comparisons of modelled and measured annual mean $PM_{2.5}$ concentrations in 2013 at background and roadside monitoring site locations. Lines representing y = x – 50 % and y = x + 50% are also shown because 50% is the AQD data quality objective for modelled annual mean $PM_{2.5}$ concentrations – see Section 1.5.

Summary statistics for the comparison between modelled and measured $PM_{2.5}$ concentrations are presented in Table 6.3 and Table 6.4.

There are a number of different categories of monitoring sites within these tables and graphs. This is because there are some sites in the national network at which only PM_{10} or $PM_{2.5}$, but not both are measured.

The agreement between the FDMS and gravimetric measurement data and the modelled values is generally good. The TEOM x 1.0 measurement data for verification sites are lower than the modelled estimates. This is as expected since TEOM x 1.0 is known to underestimate in comparison to the reference gravimetric monitoring method as a result of the loss of volatile components.

Figure 6.6 - Verification of background annual mean $PM_{2.5}$ model 2013

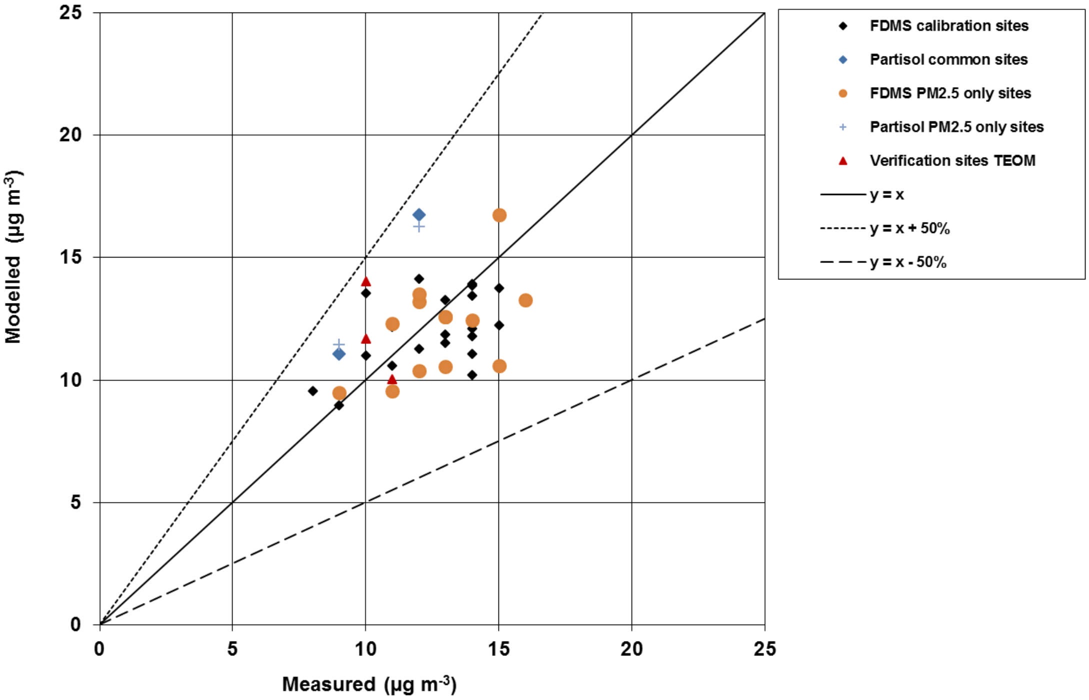


Figure 6.7 - Verification of roadside annual mean $PM_{2.5}$ model 2013

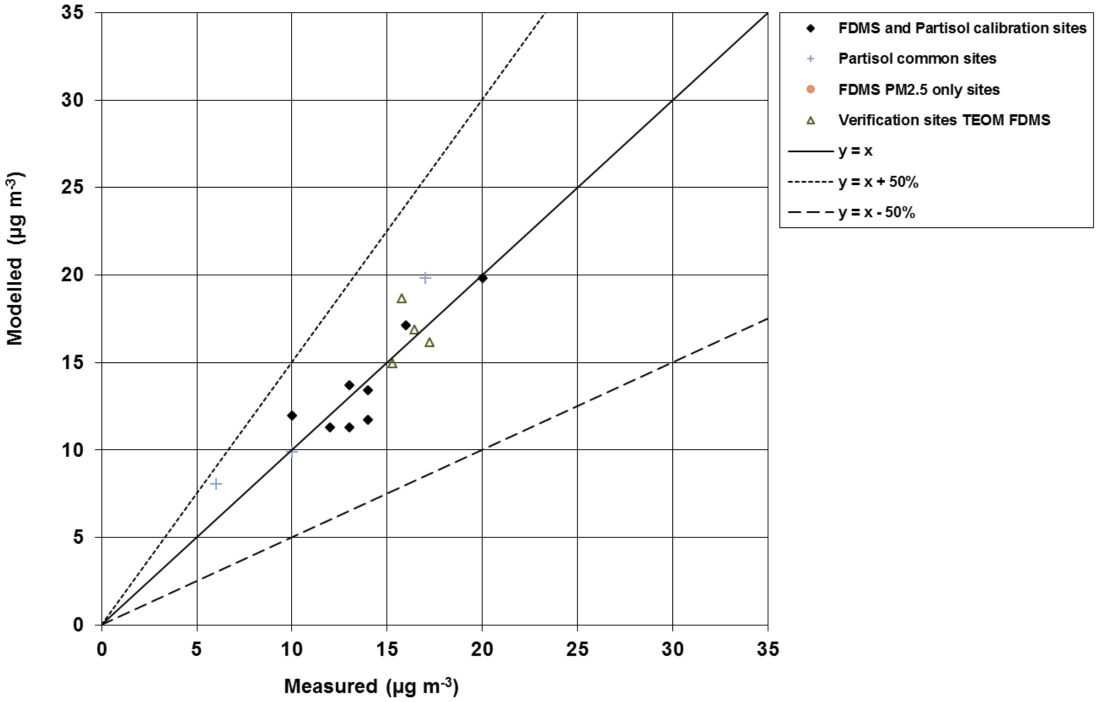


Table 6.3 - Summary statistics for comparison between gravimetric modelled and measured concentrations of $PM_{2.5}$ at background sites

	Mean of measurements (µg m^{-3}, grav)	Mean of model estimates (µg m^{-3}, grav)	R^2	% outside data quality objectives	Number of sites
National network FDMS (Calibration)	12.5	12.1	0.24	0	21
National network Partisol	10.5	13.9	1.00	0	2
National network FDMS PM2.5 only sites	12.8	12.1	0.28	0	13
National network Partisol PM2.5 only sites	8.3	11.5	-	33	3
Verification sites FDMS	-	-	-	-	-
Verification sites TEOM	10.3	11.9	0.66	0	3

Table 6.4 - Summary statistics for comparison between gravimetric modelled and measured concentrations of PM_{10} at roadside sites

	Mean of measurements (µg m^{-3}, grav)	Mean of model estimates (µg m^{-3}, grav)	R^2	% outside data quality objectives	Number of sites
National network FDMS (Calibration)	14.0	13.8	0.79	0	8
National network Partisol	11.0	12.6	0.95	0	4
National network FDMS PM2.5 only sites	-	-	-	-	-
National network Partisol PM2,5 only sites	-	-	-	-	-
Verification sites FDMS	16.2	16.7	0.09	0	4

6.4.2 $PM_{2.5}$ source apportionment at monitoring sites

Figure 6.8 and Figure 6.9 show the modelled annual mean $PM_{2.5}$ source apportionment for 2013 at national network background and roadside monitoring sites respectively. The measured concentration at each site is also shown for reference.

At background locations, the contributions from non-emissions inventory sources (i.e. regional background sources and urban dusts), which are shown in grey on the figures, dominate with a particularly large contribution from secondary aerosols. The smaller contribution from urban background emissions sources, shown in colour on the figures, are dominated in most locations by traffic, industry and off road mobile machinery.

At roadside locations the source apportionments follow a very similar pattern to background locations, except that there is an extra local road traffic component composed of local exhaust emissions, local brake and tyre wear emissions and local road abrasion emissions.

Overall regional secondary PM make a proportionally larger contribution to the total mass for $PM_{2.5}$ than for PM_{10}.

Figure 6.8 - Annual mean $PM_{2.5}$ source apportionment at background national network monitoring sites 2013

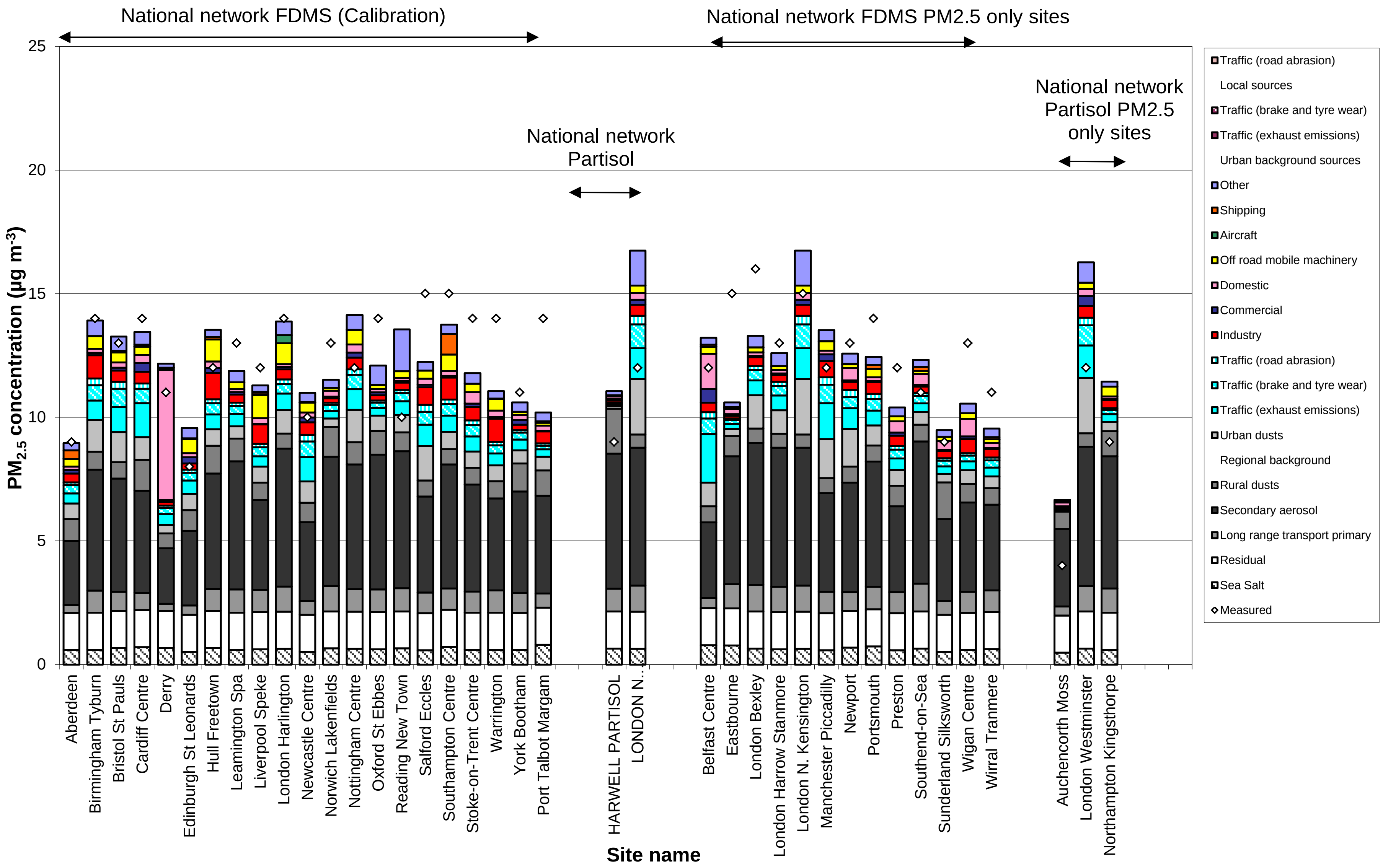
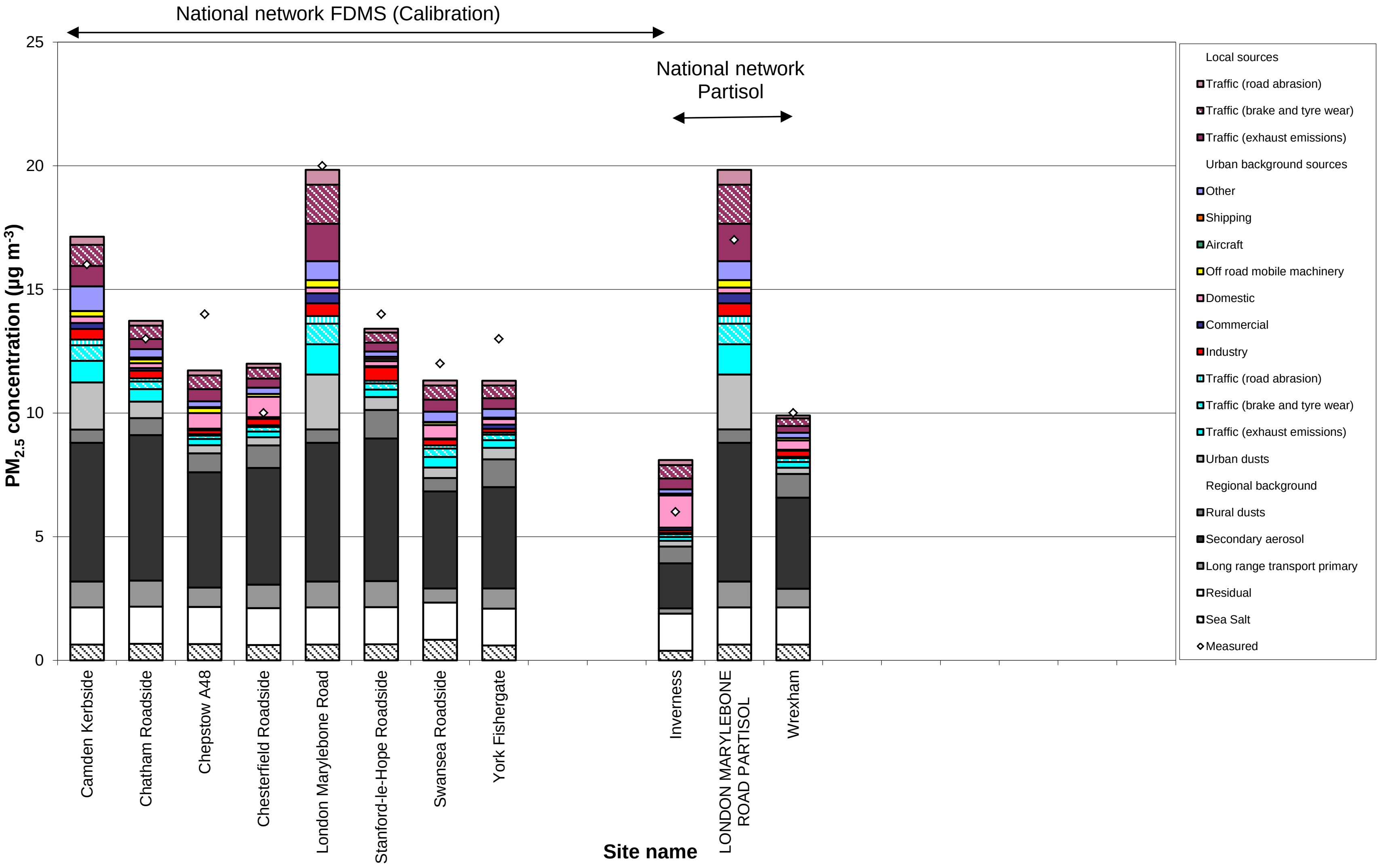


Figure 6.9 - Annual mean $PM_{2.5}$ source apportionment at roadside national network monitoring sites 2013



6.5 Subtraction of sea salt component

6.5.1 Introduction

The AQD (Article 20) requires member states to attribute exceedances of limit values due to natural sources when reporting the results of air quality assessments. The definition of natural sources in this directive includes sea spray. An assessment of concentrations with the contribution from natural sources subtracted is provided in e-reporting Data flow G (CDR, 2014) for locations with measured or modelled exceedances of the limit values. 2013 is the first year for which the contribution from natural sources has been subtracted for $PM_{2.5}$ for formal reporting within the framework of e-Reporting. Where exceedances are attributed to natural sources, subtraction is a requirement of the Directive.

6.5.2 Map of annual mean sea salt $PM_{2.5}$

The method used to estimate the sea salt contribution to annual mean $PM_{2.5}$ concentrations across the UK has been described in Section 5.3.6. The map of annual mean sea salt $PM_{2.5}$ can be used to subtract this contribution directly from measured or modelled annual mean concentrations. The uncertainties associated with estimating the sea salt contribution to annual mean $PM_{2.5}$ from measurements of particulate chloride have been discussed in Section 5.3.6. It is recognised that the interpolated map of sea salt concentrations will not capture the steep gradients in sea salt concentration very close to the coast. Thus the analysis presented may underestimate the sea salt contribution to exceedances in coastal areas.

6.5.3 Results

The results for annual mean $PM_{2.5}$ concentrations with the contribution from sea salt subtracted in zones with measured or modelled exceedances of the stage 2 indicative limit value of 20 µg m^{-3} are shown in Table 6.5. The modelled exceedance in the Greater London Urban Area remains after the subtraction of the contribution from sea salt. S8 in this table refers to natural sources, sea salt in this instance. Note that this indicative limit value is not currently in force.

There were no reported exceedances of the stage 1 annual mean limit value for $PM_{2.5}$ of 25 µg m^{-3} in 2013.

Table 6.5 - Exceedance of limit values of $PM_{2.5}$ due to natural events or natural contributions - Contribution of natural events to exceedance of the $PM_{2.5}$ limit value (annual mean stage 2)

Zone code	Zone	EoI station code	Annual mean (µg m^{-3})	Natural event code(s)	Estimated annual mean after subtraction of natural contribution (µg m^{-3})
UK0001	Greater London Urban Area	n/a	22	S8	21

6.6 Average Exposure Indicator

An exposure reduction target (ERT) and an exposure concentration obligation (ECO) for $PM_{2.5}$ have been set within the AQD. Both of these environmental objectives are based on the value calculated for the average exposure indicator (AEI). The AEI is calculated as the three-year average of annual mean measurements at urban background and suburban background monitoring sites (listed in Appendix 6) across a member state.

The AEI for the reference year 2013 has been calculated from measurements made during 2011, 2012 and 2013. The method used to calculate the AEI the 2013 reference year is the same as was used for the previous assessments (Brookes et al., 2012 and 2013). An assessment of compliance with the ECO is also presented in this section.

The AEI for the UK has been calculated using the method set out in guidance received for comment from the Commission on 3rd August 2012. This guidance was prepared by AQUILA and entitled “Procedures for Determining a National Average Exposure Indicator, for Assessment of a National Exposure Reduction Target, Requirements for Quality Assurance/Quality Control, and Requirements for the Estimation of their Measurement Uncertainties”. The guidance sets out recommended processes but recognises that Member States may adopt other procedures, and it confirms the order of the calculation method for this three-year average. An average is calculated across all of the sites for each year and the three-year average is then calculated from the values calculated for each year. The guidance also proposes a method for weighting the averages for each year according to the data capture achieved.

A total of 49 urban background and suburban background sites were included in the calculation. The calculation is based on the following excerpt from the AQUILA guidance.

$$AEI(p) = \frac{\sum_{i=1}^{n}(\overline{x}_i d_i)}{\sum_{i=1}^{n}(d_i)}$$

$$\overline{x}_i = \frac{\sum_{j=1}^{k}(x_{ij})}{k}$$

Where: d_i is the data capture at the i^{th} station, for all stations where $d_i \geq 75\%$,

$\overline{x_i}$ is the annual mean concentration in the year p at station j with the total of n stations,

X_{ij} is the daily or hourly average concentration measured at station j during every valid sampling day or hour j, and k is the number of valid sampling days or hours during the year at that site.

$$AEI = \frac{\sum_p AEI(p)}{3}$$

Three sites which only had a single valid year of data have been included in the calculation in order to provide a more representative calculation of average exposure. It is expected that there will be forced changes in site selection and equipment types between 2010 and 2020 which will impact on the uncertainty of the calculation.

Years 2011, 2012 and 2013 were used for the calculation, with means of 13.8, 12.4 and 12.2 µg m^{-3} respectively.

The mean of these three values (rounded to integer) is 13 µg m^{-3}. This is the AEI for the reference year of 2013. This value is compliant with the ECO of 20 µg m^{-3} to be achieved by 2015 set within the AQD.

The baseline AEI (based upon the years 2009, 2010, 2011) determined the National Exposure Reduction Target (NERT), to be achieved by 2020. With an AEI of value of 13 µg m^{-3} as the baseline, the AQD requires the UK to reduce the AEI by 15% from this value of 13 µg m^{-3} in the three-year average for the reference year 2020.

7 Benzene

7.1 Introduction

7.1.1 Limit values

A single limit value for ambient benzene concentrations is set out in the AQD. This limit value has been specified for the protection of human health and came into force on 01/01/2010. The limit value is an annual mean concentration of 5 µg m^{-3}.

Modelled and measured benzene concentrations for 2013 were below the limit value for all zones.

7.1.2 Annual mean model

Maps of annual mean benzene concentrations at background and roadside locations in 2013 are presented in Figure 7.1 and Figure 7.2 respectively.

Benzene concentrations have been calculated using a similar approach to that adopted for NO_X although a different approach has been adopted for the modelling of fugitive and process emissions from point sources.

It has been considered that annual mean background benzene concentrations are made up of contributions from:

- Distant sources (characterised by an estimate of rural background concentration)
- Combustion point sources
- Fugitive and process point sources
- Local area sources
- Point sources with emissions estimates for air quality pollutants based on reported carbon emissions (ETS points)

The area source model has been calibrated using measurements from the national monitoring networks. At locations close to urban roads an additional roadside contribution was added to account for contributions to total benzene from road traffic sources.

7.1.3 Chapter structure

This chapter describes modelling work carried out for 2013 to assess compliance with the benzene annual mean limit value described above. Emission estimates for benzene are described in Section 7.2, Section 7.3 describes the benzene modelling methods, and the modelling results in terms of verification and source apportionment are presented in Section 7.4.

Figure 7.1 - Annual mean background benzene concentration, 2013 (µg m^{-3})

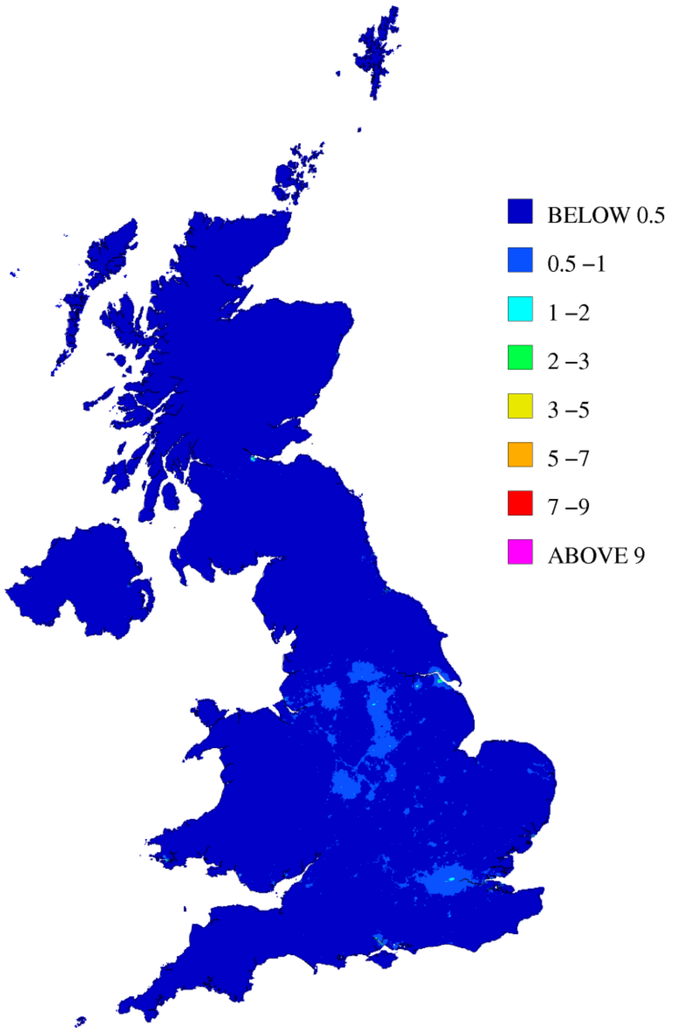
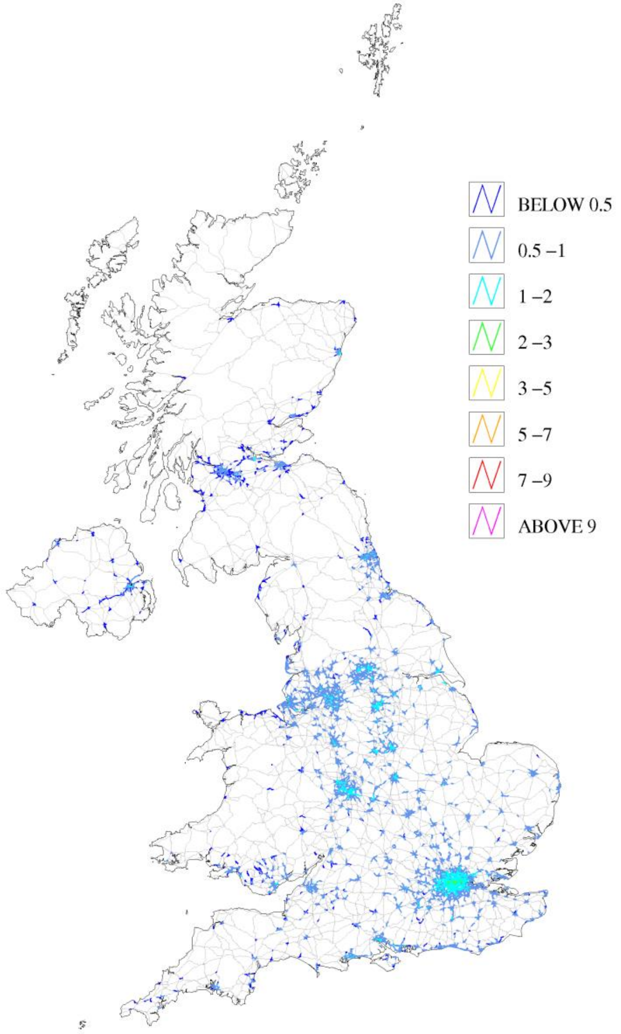


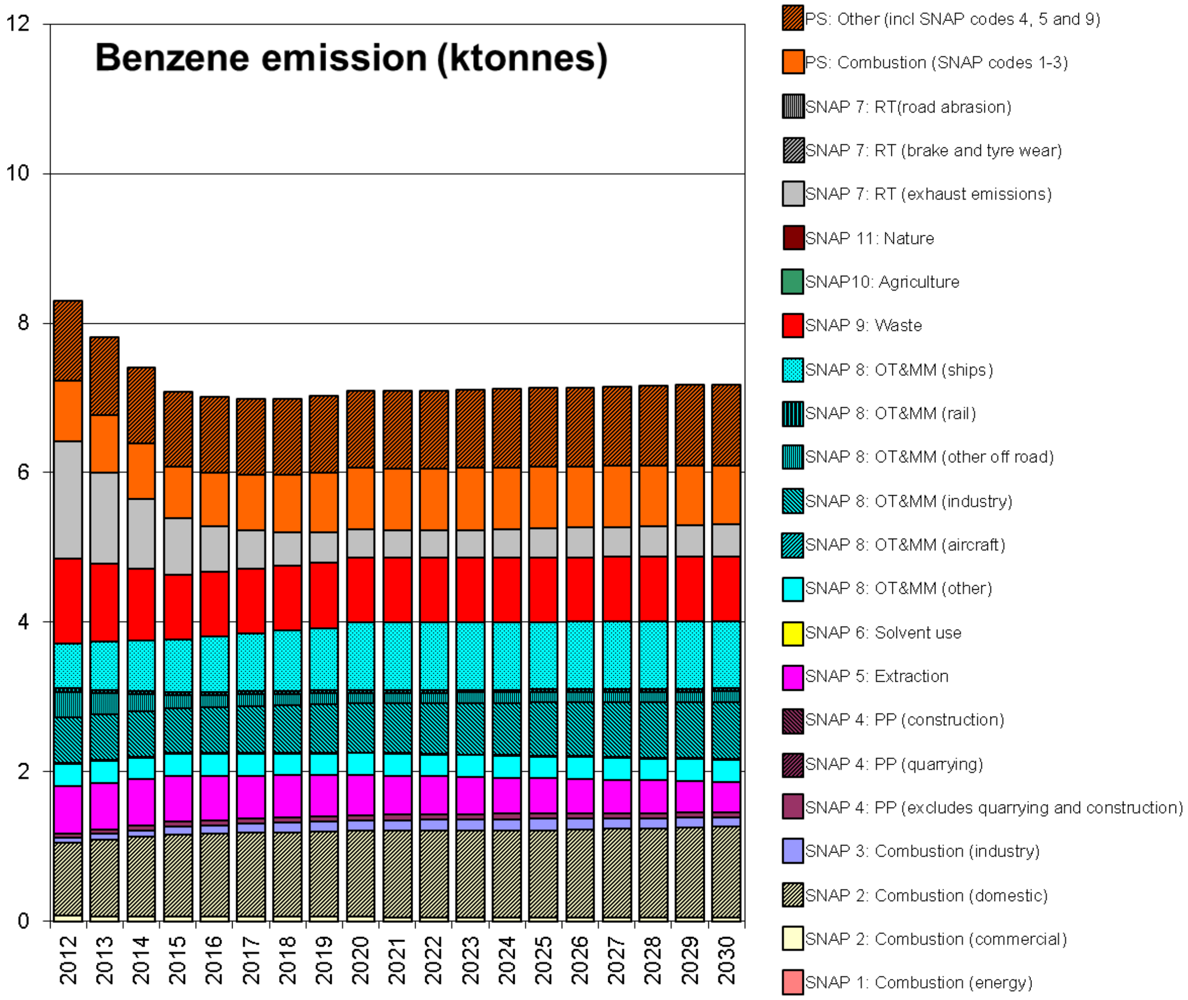
Figure 7.2 - Urban major roads, annual mean roadside benzene concentration, 2013 (µg m^{-3})



7.2 Benzene emissions

Estimates of the emissions of benzene from the UK National Atmospheric Emission Inventory 2012 (NAEI 2012) have been used in this study (Passant et al., 2014). Emissions projections have been provided by the NAEI (Passant pers. comm. 2014a) based on DECCs UEP48 energy and emissions projections (DECC, 2013). Figure 7.3 shows the UK total benzene emissions for 2012 and emissions projections for 2015, 2020, 2025 and 2030 split by SNAP code, with the coding described in Table 3.1. Values for intermediate years have been interpolated in this figure. The emissions include contributions from a variety of source sectors. Some of the largest contributions to the total in 2012 include domestic combustion, waste treatment and disposal, and off-road mobile machinery which are projected to remain relatively flat into the future from 2012. Decreases in emissions are largely related to road transport exhaust emissions which are projected to fall progressively until about 2020.

Figure 7.3 - Total UK benzene emissions for 2012 and emissions projections up to 2030 by SNAP code from NAEI 2012



7.3 Benzene modelling

7.3.1 Contributions from combustion point sources

Following a similar methodology as for NO_x, point sources in the NAEI 2012 have been classified as large if they fulfil either of the following criteria:

- Annual benzene emissions in the NAEI 2012 are greater than 5 tonnes for any given plant
- Stack parameters are already available for any given plant in the PCM stack parameters database (described in more detail in Section 3.3.1)

Contributions to ground level annual mean benzene concentrations from large combustion-related point sources in the NAEI 2012 were estimated by modelling each source explicitly using the atmospheric dispersion model ADMS 5.0 and sequential meteorological data for 2013 from Waddington. A total of 21 point sources were modelled as large point sources. Surface roughness was assumed to be 0.1 m at both the dispersion site and meteorological site. Concentrations were calculated for a 99 km x 99 km square composed of a regularly spaced 1 km x 1 km resolution receptor grid. Each receptor grid was centred on the point source. For each large point source information was retrieved from the PCM stack parameters database.

The NAEI emissions for combustion point sources are for the year 2012; however, the year 2013 has been modelled for the assessment. The NAEI emissions for point sources for 2012 were therefore scaled in order to provide values for 2013 as described in Section 3.3.1.

7.3.2 Contributions from fugitive and process point sources

The contributions to ambient concentrations from fugitive and process emission point sources were modelled using a small points model similar to the model described in Appendix 3, but adapted specifically for fugitive and process point sources of benzene. In line with the method applied for the large combustion point sources the NAEI 2012 emissions for fugitive and process emission point sources have been scaled to 2013 using the same source sector specific projection factors applied to the combustion point sources.

The emissions from these sources are not generally as well characterised in terms of exact location and release parameters as emissions from combustion sources. Separate models are used for the concentration in the 1 km x 1 km grid square that includes the source (the ‘in-square’ concentration) and the concentration in surrounding grid squares (the ‘out-square’ concentration). The ‘out-square’ concentration has been estimated using a dispersion kernel similar to the one used for area sources of benzene. The ‘in square’ concentration has been estimated by assuming a volume source of dimensions 200 m x 200 m x 30 m in the centre of the square with the concentration estimated as the average across receptors excluding those inside the central 800 m x 800 m of the 1000 m x 1000 m grid square. These parameters have been chosen to provide the best fit to the range and maximum of available monitoring data in the vicinity of refineries (Grice et al., 2009).

In common with the NAEI 2011 additional point source emissions data have been provided in the NAEI 2012. These emissions estimates have been derived from carbon emissions data reported under the EU-Emissions Trading Scheme (ETS), most recently described in Tsagatakis et al. (2014). These point sources are referred to as ETS points in this report. To model the contribution to background annual mean benzene concentrations from ETS points the emissions have been treated as an additional set of small point sources. As such they have been modelled using the benzene small points approach described above. These derived air quality pollutant emissions estimates are particularly uncertain, hence the emissions for particular sources have been capped at reporting thresholds given by the Scottish Pollutant Release Inventory (SPRI). Typically more than 90% of the ETS points do not exceed the SPRI reporting threshold, which for benzene is 1 tonne per year.

7.3.3 Contributions from rural background concentrations

Regional rural benzene concentrations were estimated from the map of rural NO_x concentration described in Section 3.3.4. The rural NO_x map was scaled using the ratio of measured annual mean benzene and NO_X concentrations at the rural Harwell monitoring site in 2013, a value of 0.026 for 2013.

7.3.4 Contributions from area sources

The 2013 area source benzene emissions maps have been calculated from the NAEI 2012 emissions maps following the method applied for NO_X, described in Section 3.3.5. An ADMS derived dispersion kernel has been used to calculate the contribution to ambient concentrations at a central receptor location from the area source emissions (excluding SNAP 3) within a 33 km x 33 km square surrounding each receptor. Hourly sequential meteorological data from Waddington in 2013 has been used to construct the dispersion kernels, as described in Appendix 4.

Revised methods introduced in the 2011 assessment (Brookes et al., 2012) for modelling the contributions to benzene from SNAP 2 (domestic and non-domestic combustion) and SNAP 3 (combustion in industry) area sources were used and have been described in Section 3.3.5.

For the area source model a cap has been applied to the emissions map for shipping, no other source sectors were capped for the benzene modelling. The reason for capping shipping emissions is due to uncertainty in the 1 km x 1 km resolution emissions maps at some dock areas. The method for deriving the shipping emissions maps and the cap applied is discussed in more detail in Appendix 5. The cap applied to shipping is given in Table 7.1.

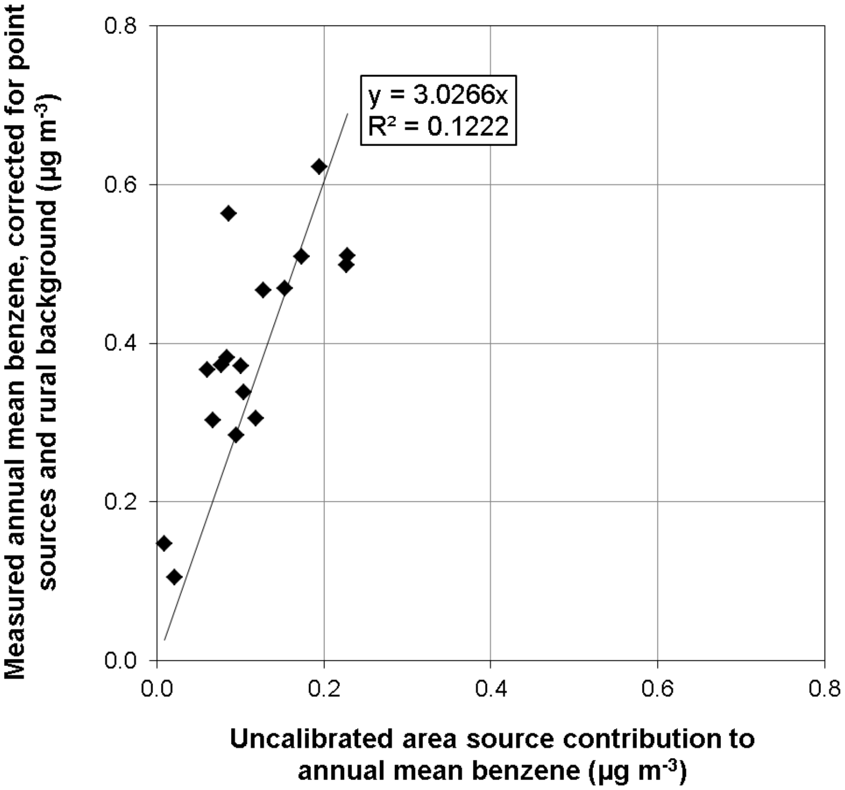
Table 7.1 - Emissions caps applied to benzene sector grids

SNAP code	Description	Cap applied (t/a)
SNAP 8 (shipping only)	Other Transport & Mobile Machinery	1.5

The calibration coefficient for the area source model is derived by linear regression of a corrected measured annual mean background benzene concentration versus the modelled uncalibrated area source contribution. The measurements were derived from three sites within the national automatic hydrocarbon network and fourteen non-automatic hydrocarbon sites. The corrected background concentration is derived by subtraction of the modelled contributions from SNAP 3 area sources, point sources and estimated rural benzene from the measured annual mean concentration at automatic and pumped tube background monitoring sites. Figure 7.4 shows the calibration of the area source model.

The modelled area source contribution (excluding SNAP 3) was multiplied by the background calibration coefficient to calculate the calibrated area source contribution for each grid square in the country. The SNAP 3 area source contribution, point source contributions and regional rural concentration were then added, resulting in a map of total background annual mean benzene concentrations.

Figure 7.4 - Calibration of area source benzene model, 2013 (µg m^{-3})

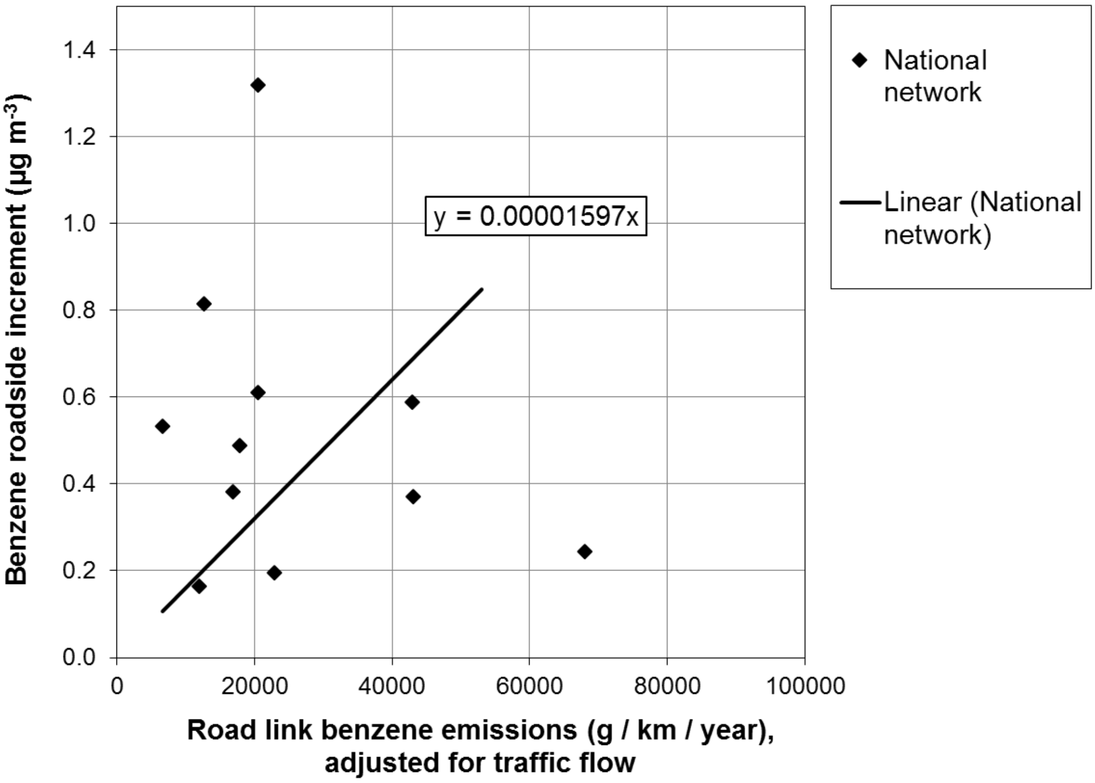


7.3.5 Roadside concentrations

Roadside annual mean concentrations of benzene for 2013 have been modelled using a similar method to the NO_X modelling described in Section 3.3.6. A roadside increment calibration coefficient has been derived from comparison of the measured roadside increment (the annual mean of measured benzene at roadside monitoring stations with point sources, SNAP 3 area sources, calibrated modelled background and rural contributions subtracted) to road link emissions adjusted for traffic flow.

Measurements from the national non-automatic hydrocarbon network, which employs benzene diffusion tubes, were used to calibrate the roadside model. A roadside calibration coefficient of 0.00001597 was used to estimate roadside annual mean concentrations of benzene for 2013.

Figure 7.5 - Calibration of benzene roadside increment model, 2013 (µg m-3)



7.4 Results

7.4.1 Verification of mapped values

Figure 7.6 and Figure 7.7 show comparisons of the modelled and measured annual mean benzene concentrations for background and roadside locations. Lines showing y = x – 50% and y = x + 50% are included in these charts (the data quality objective for modelled benzene concentrations specified by the AQD – see Section 1.5).

Summary statistics for the comparison between modelled and measured benzene concentrations are listed in Table 7.2 and Table 7.3. No monitoring sites[7] were available to provide an independent verification of the models (see Appendix 1) in Figure 7.6 and Figure 7.7.

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[7] Ineos kindly provided monitoring data for 10 sites in the vicinity of the Grangemouth site. These measurements have been used to verify the modelled concentrations resulting from fugitive emissions in close proximity to refineries.

Figure 7.6 - Verification of background annual mean benzene model 2013

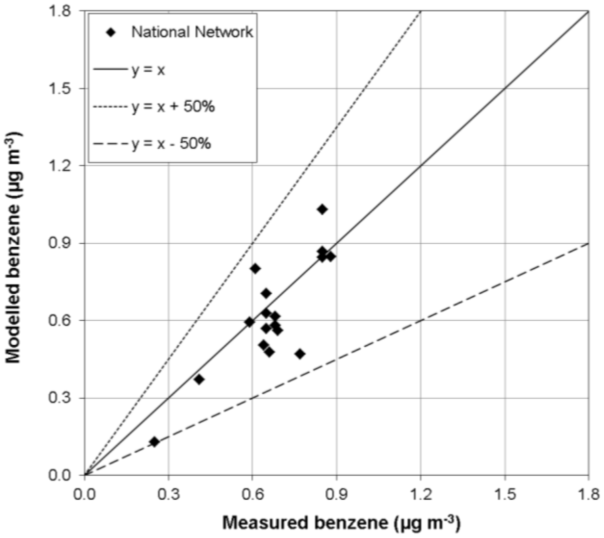


Figure 7.7 - Verification of roadside annual mean benzene model 2013

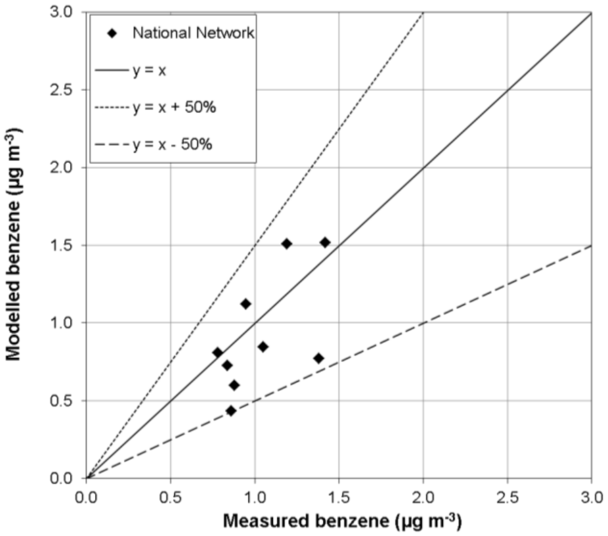


Table 7.2 - Summary statistics for comparison between modelled and measured benzene concentrations at background sites (µg m^{-3})

	Mean of measurements (µg m^{-3})	**Mean of modelled (µg m^{-3})**	**R^2**	**%outside data quality objectives**	**Number of sites**
National Network Sites	0.67	0.62	0.69	0	17

Table 7.3 - Summary statistics for comparison between modelled and measured benzene concentrations at roadside sites (µg m^{-3})

	Mean of measurements (µg m^{-3})	**Mean of modelled (µg m^{-3})**	**R^2**	**%outside data quality objectives**	**Number of sites**
National Network Sites	1.04	0.92	0.40	0	9

7.4.2 Benzene source apportionment at monitoring sites

Figure 7.8 and Figure 7.9 show the modelled annual mean benzene source apportionment for 2013 at AURN background and roadside monitoring sites, respectively. The measured concentration at each site is also shown for reference. The regional background is an important component in the source apportionment for the majority of background monitoring sites. The road traffic contribution dominates the source apportionment for those sites classified as urban and suburban background monitoring sites. The roadside source apportionment in Figure 7.9 shows that local traffic sources contribute up to 0.75 µg m^{-3} of benzene at these roadside sites.

Figure 7.8 - Annual mean benzene source apportionment at background AURN monitoring sites (the area type of each site is shown in parenthesis after its name)

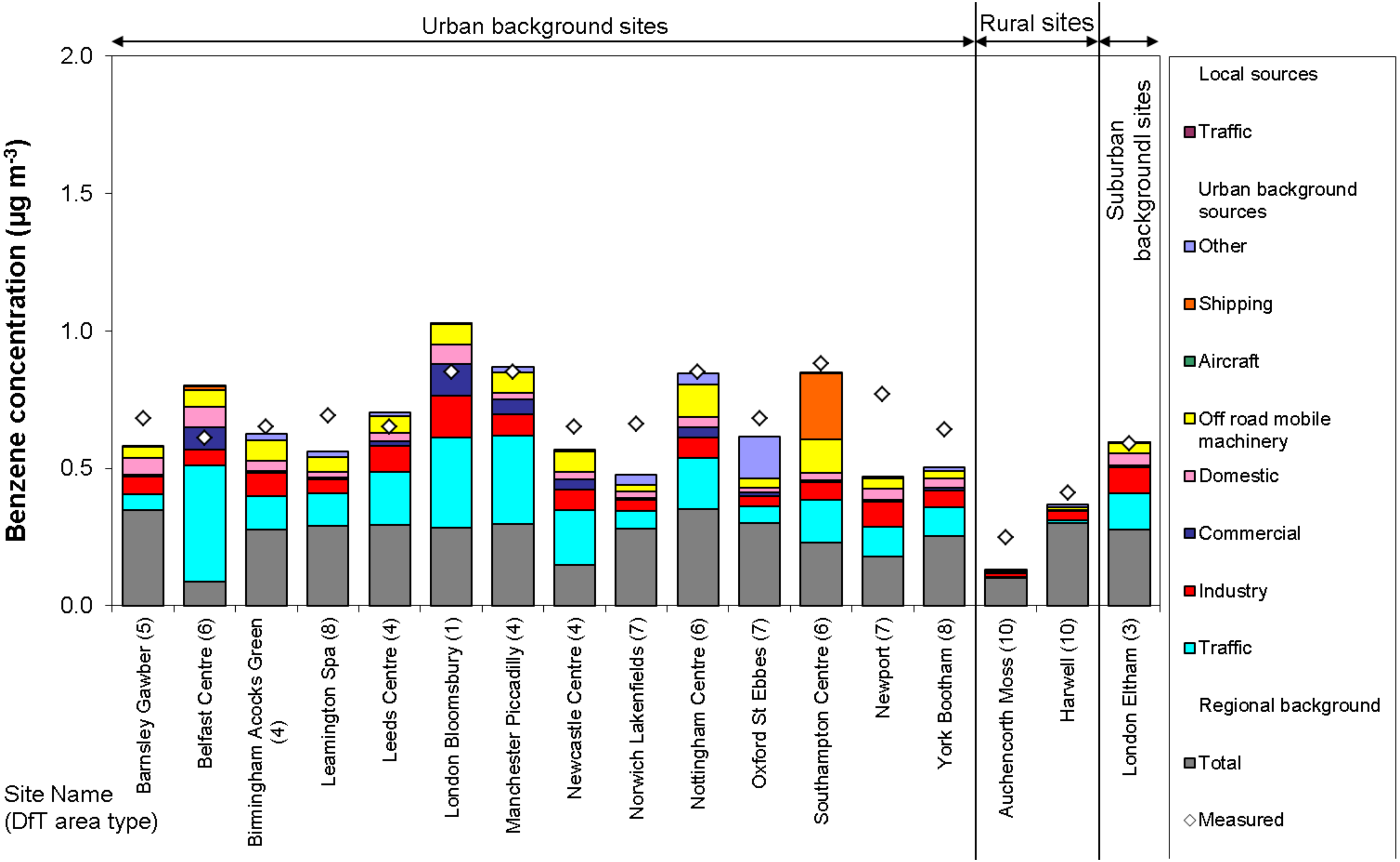
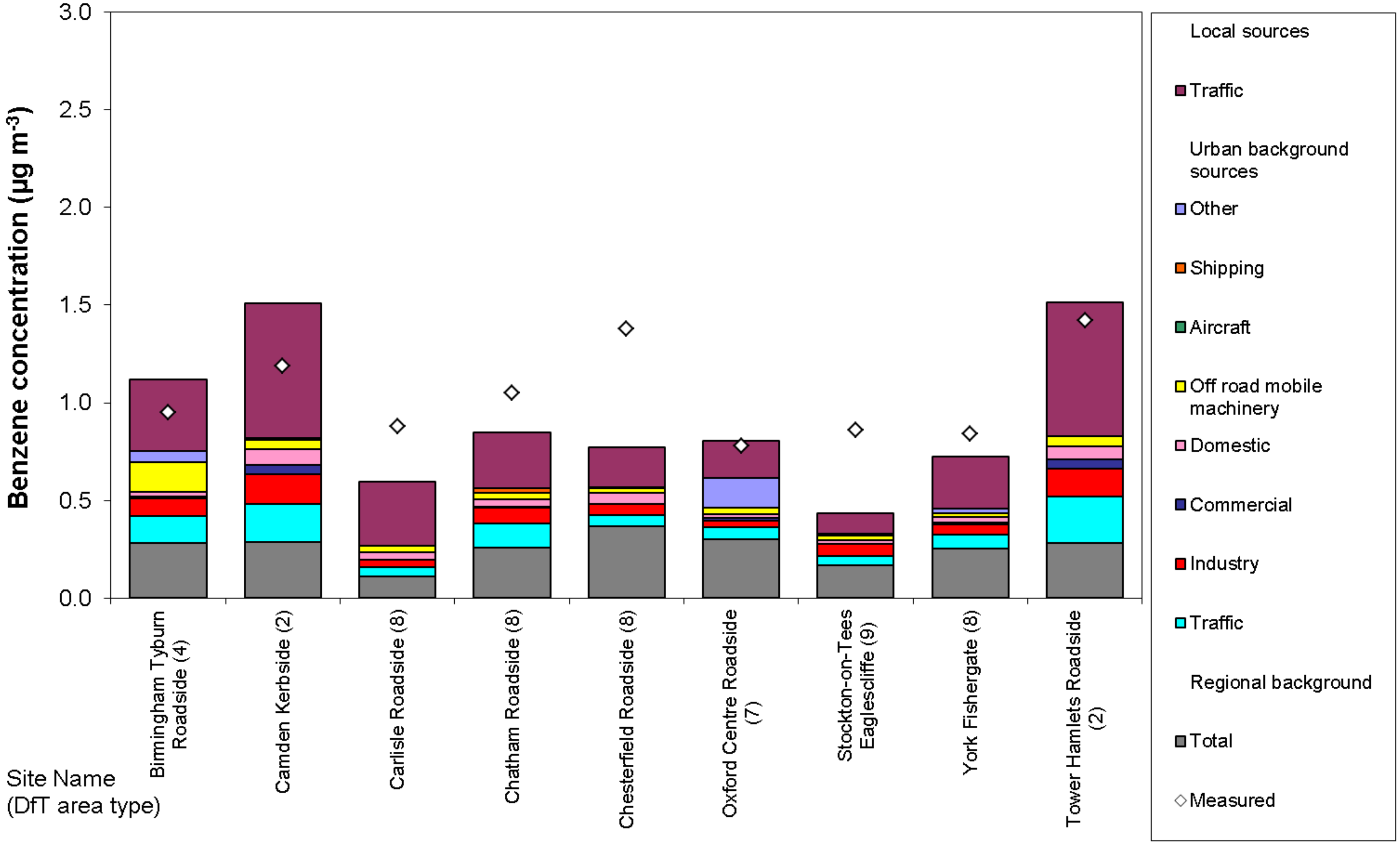


Figure 7.9 - Annual mean benzene source apportionment at roadside AURN monitoring sites (the area type of each site is shown in parenthesis after its name)



8 CO

8.1 Introduction

8.1.1 Limit values

A single limit value for ambient CO concentrations is set out in the AQD. This limit value has been specified for the protection of human health and came into force from 01/01/2005. The limit value is a maximum daily 8-hour mean concentration of 10 mg m^{-3}.

8.1.2 Objective Estimation

The maximum measured daily 8 hour running mean for 2013 are presented in Table 8.1, for sites where data capture was at least 82%. All values are below the lower assessment threshold of 5 mg m^{-3}.

Table 8.1 - Maximum daily 8-hour running mean (mg m^{-3}) in 2013[8]

EOI code	Site Name	Maximum daily 8-hour running mean (mg m^{-3})
GB0567A	Belfast Centre	1.1
GB0580A	Cardiff Centre	0.94
GB0839A	Edinburgh St Leonards	0.73
GB0584A	Leeds Centre	1.3
GB0682A	London Marylebone	2.4
GB0620A	London N. Kensington	1.8
GB0906A	Port Talbot Margam	2.2

The AQD states that objective estimation may be used to assess ambient air quality at levels below the lower assessment threshold (Article 6(4)). Objective estimation has been used to conclude that concentrations were likely to have been well below the limit value for CO in all zones during 2013. This assessment has been made on the basis of the low measured concentrations and the lack of any expected large increase in future CO emissions illustrated in the following section.

8.1.3 CO emissions

Estimates of the emissions from the UK National Atmospheric Emission Inventory 2012 (NAEI 2012) have been used in this assessment (Passant et al., 2014). Emissions projections have been provided by the NAEI (Passant pers. comm. 2014a) based on DECCs UEP48 energy and emissions projections (DECC, 2013). Figure 8.1 shows the UK total CO emissions for 2012 and emissions projections for 2015, 2020, 2025 and 2030 split by SNAP code, with the coding described in Table 3.1. Values for intermediate years have been interpolated in this figure.

Projected changes in combustion point sources (SNAP codes 1-3), area industry sources and road transport emissions dominate the overall trend in emissions over the period 2012 to 2030. The increases in combustion point sources (SNAP codes 1-3) and area industry sources are largely connected to increases in Renewable Heat Incentive (RHI) activity

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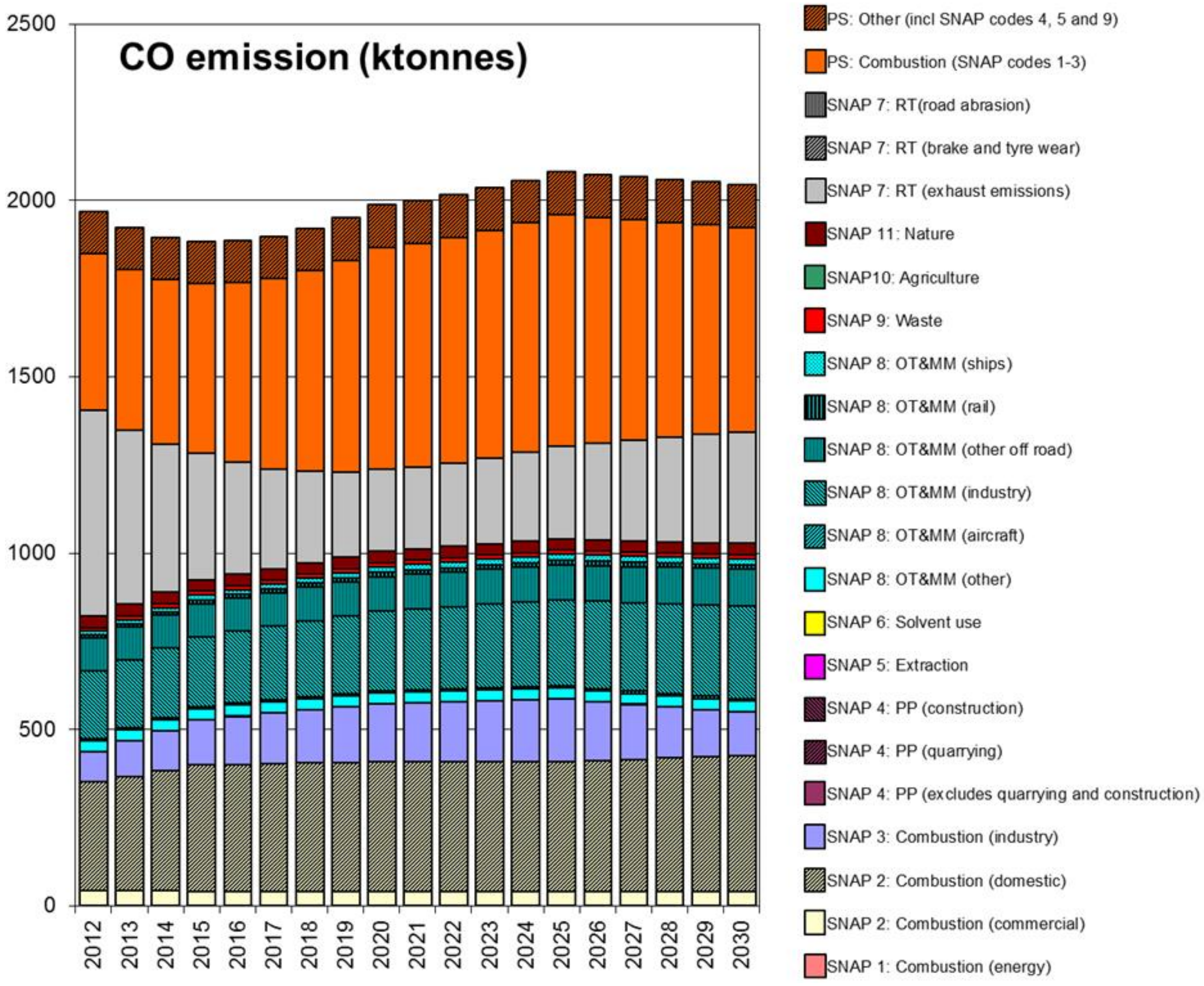
[8] Values have been presented to 2 significant figures to illustrate the dynamic range of the data.

become progressively more important as these emissions are projected to increase to 2025 and then remain relatively constant.

Road transport exhaust emissions continue to decrease to 2020, with relatively small increases in emissions beyond 2020.

Increases in emissions shown in Figure 8.1 are relatively small when viewed in the context of the significant decreases in CO emissions from road transport, domestic combustion and combustion point sources (SNAP codes 1-3) from 1980 to 2012 present in the NAEI 2012 (Passant et al., 2014), which lead to a reduction in total UK emissions of CO over this period of 76%.

Figure 8.1 - Total UK CO emissions for 2012 and emissions projections up to 2030 by SNAP code from NAEI 2012



9 Ozone

9.1 Introduction

9.1.1 Target values and long term objectives

Two target values (TV) for ambient ozone concentrations are set out in the AQD, these are:

- A maximum daily 8-hour mean concentration of 120 µg m^{-3}, not to be exceeded on more than 25 days per calendar year averaged over three years
- AOT40[9] (calculated from 1-h values) of 18000 µg m^{-3}.h May to July over five years

The TVs have been specified for the protection of human health and the protection of vegetation respectively, both came into force from 01/01/2010.

Two long term objectives (LTO) for ambient ozone concentrations are set out in the AQD, these are:

- A maximum daily 8-hour mean concentration of 120 µg m^{-3} within a calendar year
- AOT40 (calculated from 1-h values) of 6000 µg m^{-3}.h May to July

The LTOs have been specified for the protection of human health and the protection of vegetation respectively. The date for compliance with the LTOs has not been defined.

Results of the assessment in terms of comparisons of the modelled concentrations with the TV and LTO by zone have been reported in e-Reporting Data flow G (CDR, 2014).

9.1.2 Ozone modelling

Following recommendations made by a study comparing the relative performance of the available techniques for modelling ozone within the UK (Bush and Targa, 2005), an empirical mapping approach has been used for predicting ozone concentrations in 2013.

The empirical approach draws upon measurements from the 83 monitoring stations in the AURN during 2013 to produce functions describing ground-level ozone based on interpolated rural measurements of the ozone metrics corrected for local emissions of NO_X. These functions are capable of predicting ozone levels at a resolution of 1 km x 1 km and the methods are briefly described in the following sections. Full details can be sourced from the cited references.

The methods used here are based upon those presented by Coyle et al. (2002), NEGTAP (2001), PORG (1998) and Murrells et al. (2011). Murrells et al. (2011) have suggested that the observed dependence of the AOT40 metric on altitude, previously attributed to differences in surface deposition and reactions with local NO with altitude was largely explained by the proximity of monitoring stations to urban areas. In the 2013 assessment of the TV and LTO for AOT40 the altitude correction has therefore not been included in order to avoid double counting in terms of the NO_x urban decrement.

9.1.3 Chapter structure

This chapter describes modelling work carried out for 2013 to assess compliance with the ozone TVs and LTOs described above. Section 9.2 describes the modelling methods and

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[9] The definition of ATO40 has been given in Annex VII of the AQD

results in relation to the number of days exceeding 120 µg m^{-3} metrics. Section 9.3 describes the modelling methods and results in relation to the AOT40 metrics.

9.2 Modelling the number of days exceeding 120 µg m^{-3} metric

9.2.1 Days greater than 120 µg m^{-3} methodology

Maps of the modelled number of days with maximum daily 8-hour mean ozone concentrations greater than 120 µg m^{-3}, for comparison with the LTO (2013) and TV (averaged 2011 to 2013) are presented in Figure 9.1 and Figure 9.2 respectively.

At rural locations in the UK exceedances of 120 µg m^{-3} as a maximum daily 8-hour mean are broadly consistent over wide spatial scales. As a result, measured exceedances from rural monitoring stations have been interpolated by Kriging throughout the whole of the UK to represent the likely exceedances of this metric in the absence of any influence from local emissions of NO_x from combustion sources.

The resultant interpolated maps, however, will overestimate exceedances in urban areas, where nitric oxide emissions from combustion sources deplete ozone concentrations. This effect has been accounted for by adding an empirically derived urban ozone decrement, expressed as a percentage. The percentage decrement is defined as follows:

% decrement = 100((measured concentrations - rural interpolated concentration)/rural interpolated concentration)*

The derivation of a coefficient relating the percentage decrement to the modelled local NO_x concentration is shown in Figure 9.3 and Figure 9.4. The local NO_x component is calculated as the sum of contributions from local point and area sources of NO_x emissions, calculated as described in Section 3.3.

Figure 9.3 shows the decrement plot for days greater than 120 µg m^{-3} in 2013 (the LTO for human health metric) and Figure 9.4 shows the decrement plot for days greater than 120 µg m^{-3} between 2011 and 2013 (the TV for human health metric). For some monitoring sites the decrement is positive, indicating that the measured number of days exceeding 120 µg m^{-3} is higher than the corresponding estimated rural value i.e. that the urban influence for these sites is not properly represented in the model. The cluster of low values close to the origin of these plots largely consists of the rural and remote sites, at which there will be little difference between the rural estimated number of days exceeding 120 µg m^{-3} and the measured value. This helps to anchor the relationship to the origin. Percentage urban increments of -100% indicate that there were no measured exceedances of 120 µg m^{-3} at that monitoring site.

The calculated decrement is then used to correct the number of days where ozone concentrations are greater than 120 µg m^{-3} at rural sites, used for the interpolated maps:

Corrected days above 120 µg m^{-3} map = interpolated rural map + decrement

The decrement is a negative value and so reduces the concentration presented in the interpolated rural map to account for the reduction in ozone concentrations due to reaction with NO. Where the results of the expression predict a number of days less than 0.5, the predicted value is rounded to zero.

Figure 9.1 - Estimated number of days with an 8-hour mean ozone concentration above 120 µg m^{-3}, 2013

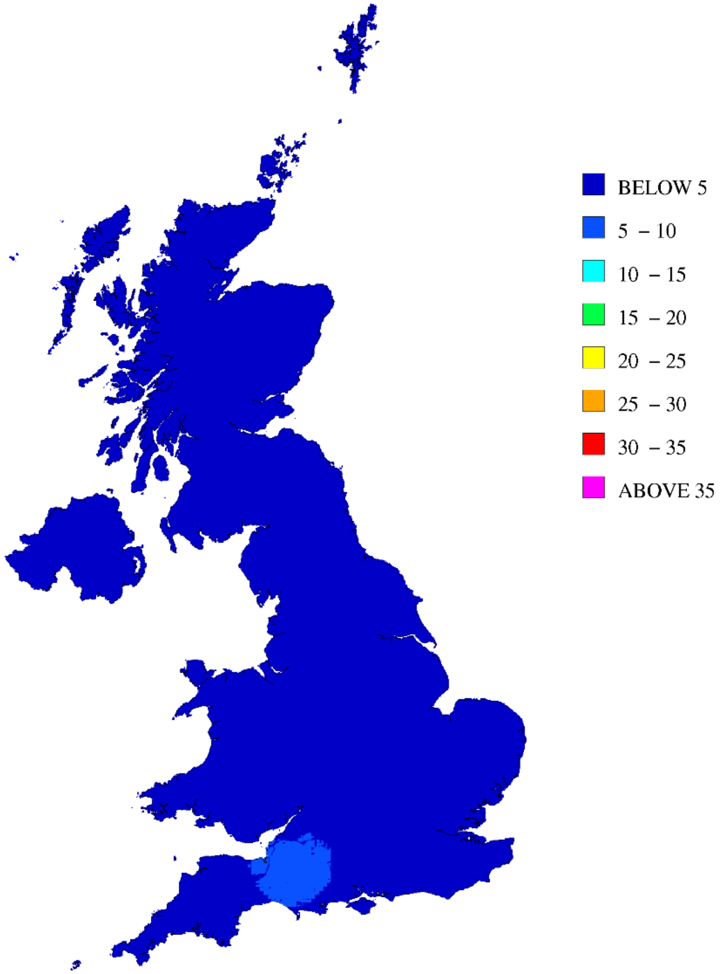


Figure 9.2 - Estimated average number of days with an 8-hour mean ozone concentration above 120 µg m^{-3}, 2011 to 2013

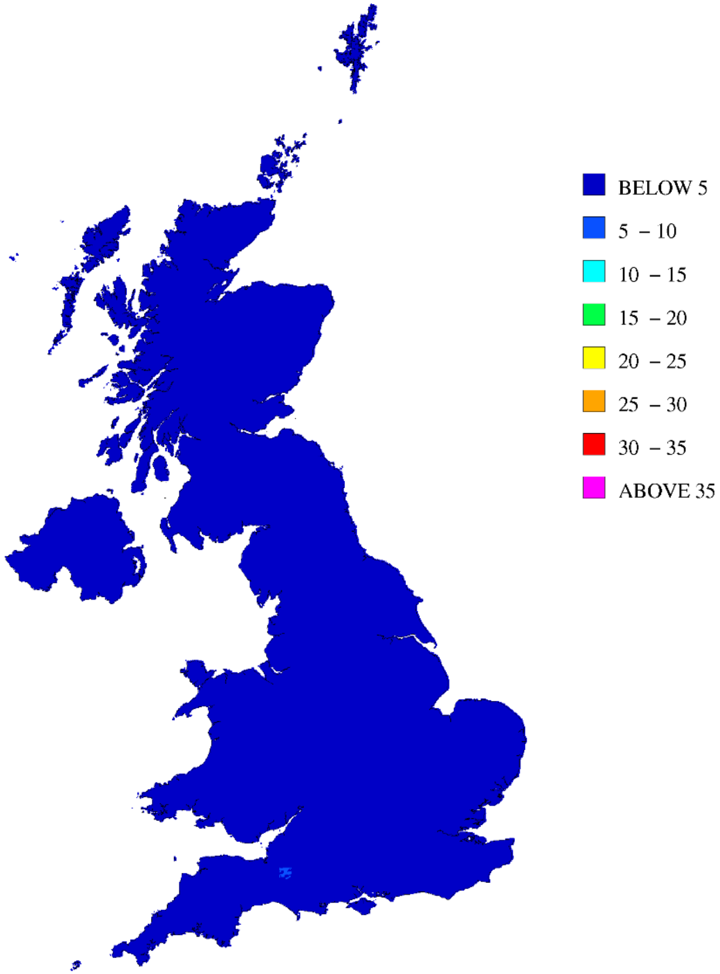


Figure 9.3 - Days greater than 120 µg m^{-3} percentage decrement in ozone concentrations, 2013

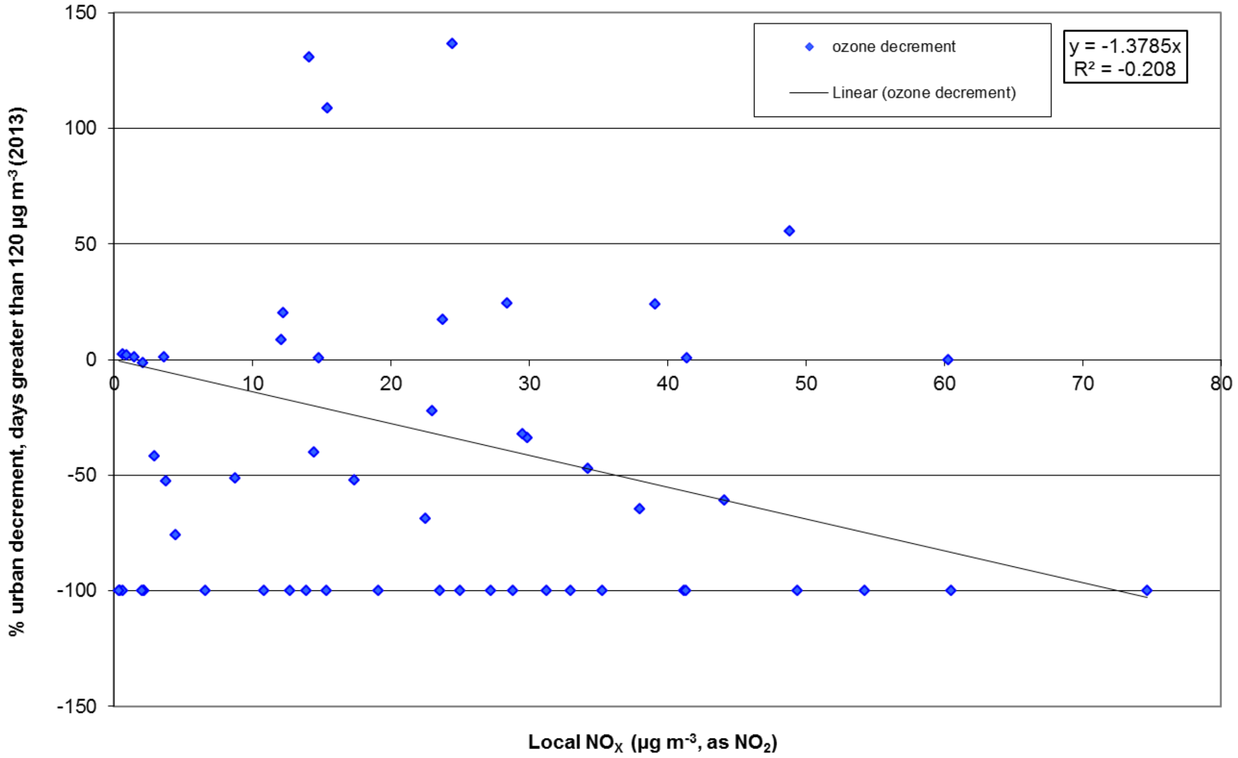
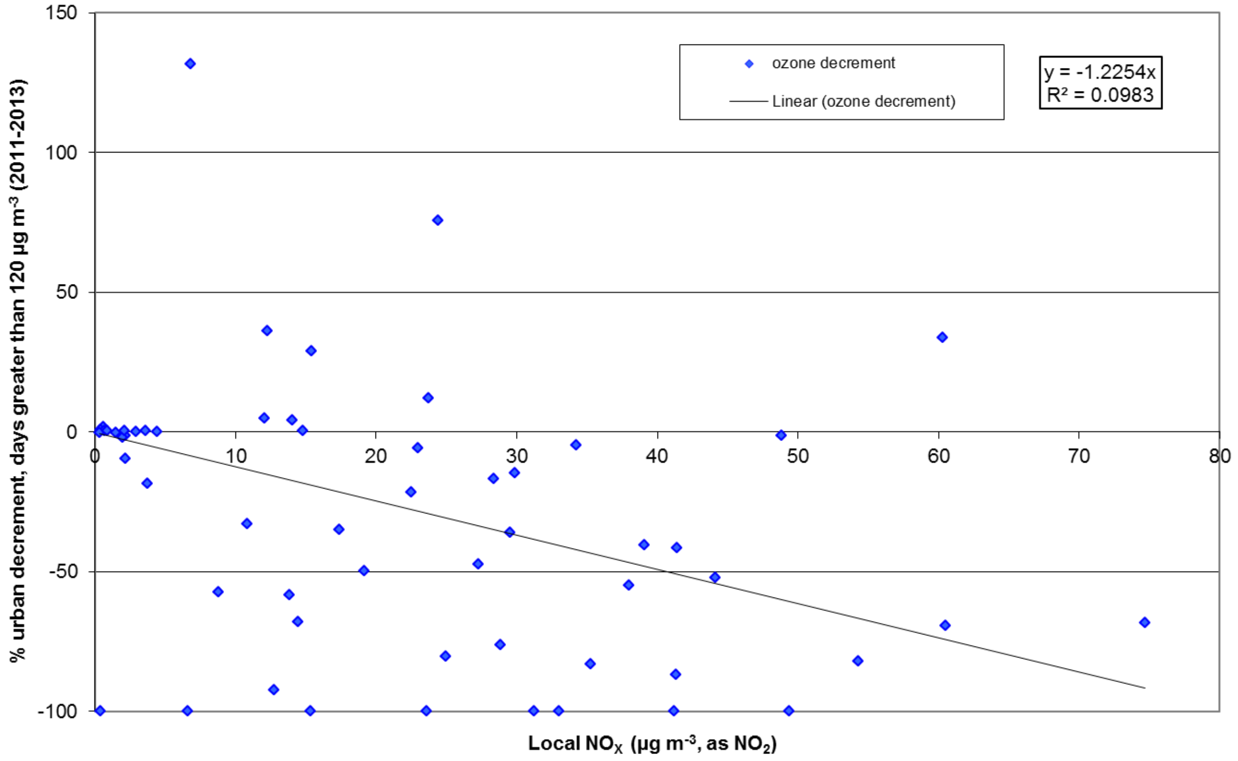


Figure 9.4 - Days greater than 120 µg m^{-3} percentage decrement in ozone concentrations, 2011-2013



9.2.2 Verification of the number of mapped days > 120 µg m^{-3} values

Figure 9.5 and Figure 9.6 compare the number of modelled and measured days with maximum daily 8-hour mean ozone concentrations greater than 120 µg m^{-3} in 2013 and averaged 2011-2013 at background locations, respectively. Both the national network sites used to calibrate the models and the verification sites are shown. Lines representing y = x + 50 % and y = x - 50% are also shown, as this is the AQD data quality objective for modelled ozone concentrations – see Section 1.5.

Figure 9.5 - Verification of background number of days > 120 µg m^{-3} model 2013

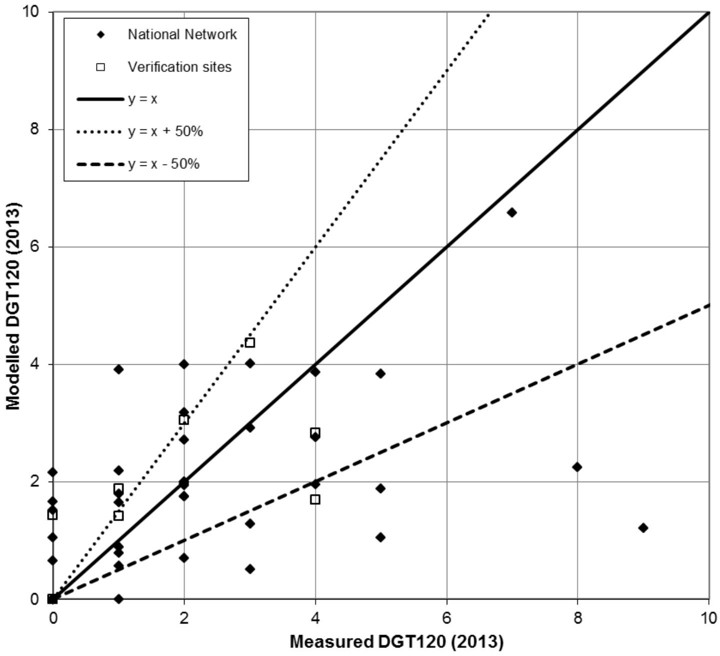


Figure 9.6 - Verification of background number of days > 120 µg m^{-3} model 2011-2013

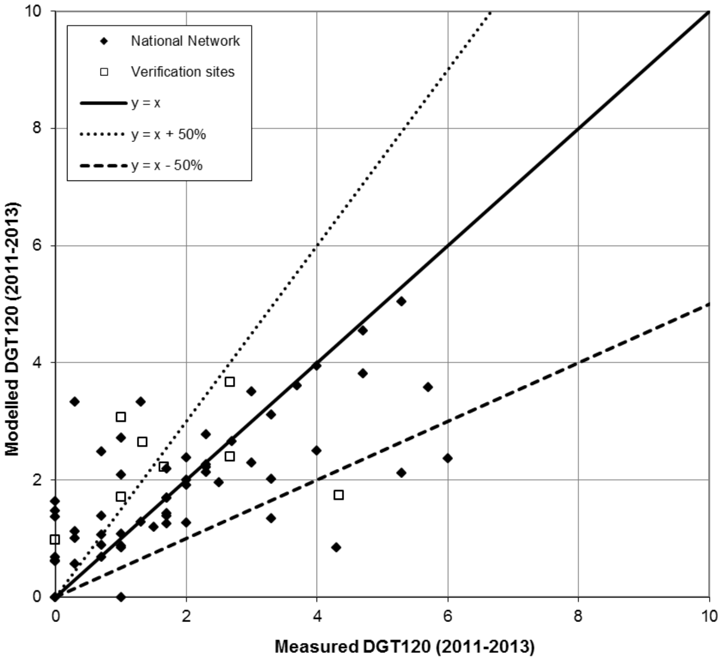


Figure 9.5 indicates that the verification sites were neither systematically over- or under-estimated for 2013. The R^2 value, shown in Table 9.1, of 0.38 for the verification sites is consistent with the R^2 value for the national network sites.

Figure 9.6 shows the model performance for the years 2011-2013. The model results for the national network sites are shown to more closely match the corresponding measured value than the verification sites as the national network sites were used to generate the relationships used in the model. In particular, the R^2 value for the verification sites for this multiple year metric is low at 0.06.

Table 9.1 - Summary statistics for comparison between modelled and measured number of days exceeding 120 µg m^{-3} as a maximum daily 8-hour mean

		Mean of measurements (days)	Mean of model estimates (days)	R^2	% outside DQO	No. sites
National network	2013	1.6	1.3	0.37	35%	57
Verification sites	2013	1.9	2.1	0.38	50%	8
National network	2011-2013	1.9	1.9	0.45	37%	57
Verification sites	2011-2013	1.8	2.3	0.06	63%	8

9.3 Modelling the AOT40 vegetation metric

9.3.1 AOT40 methodology

Maps of modelled AOT40 for comparison with the LTO (2013) and TV (averaged 2009 to 2013) are presented in Figure 9.7 and Figure 9.8 respectively.

The AOT40 vegetation metrics for 2013 and the averaged metric for 2009-2013 were calculated from measured data at rural monitoring stations in the AURN. These data were interpolated by Kriging to produce a rural map.

An urban decrement term was subsequently defined for those monitoring stations in the AURN and the rural map so as to correct for the depletion of ozone in areas close to sources of NO. As for the days above 120 µg m^{-3} metric, the decrement is closely related to the annual mean NO_x concentration, and has been defined in a similar fashion, using a percentage decrement in ozone concentrations associated with local NO_x concentrations.

Using the same methodology discussed in Section 9.2.1 for the days greater than 120 µg m^{-3} maps, the decrement was then used to correct the final AOT40 maps:

Corrected AOT40 map = interpolated rural map + decrement

The relationships between the decrement and modelled NO_X concentrations for 2013 and 2009-2013 averaged metrics are presented in Figure 9.9 and Figure 9.10 respectively.

Figure 9.7 - Estimated AOT40 vegetation metric, 2013 (µg m^{-3} hours)

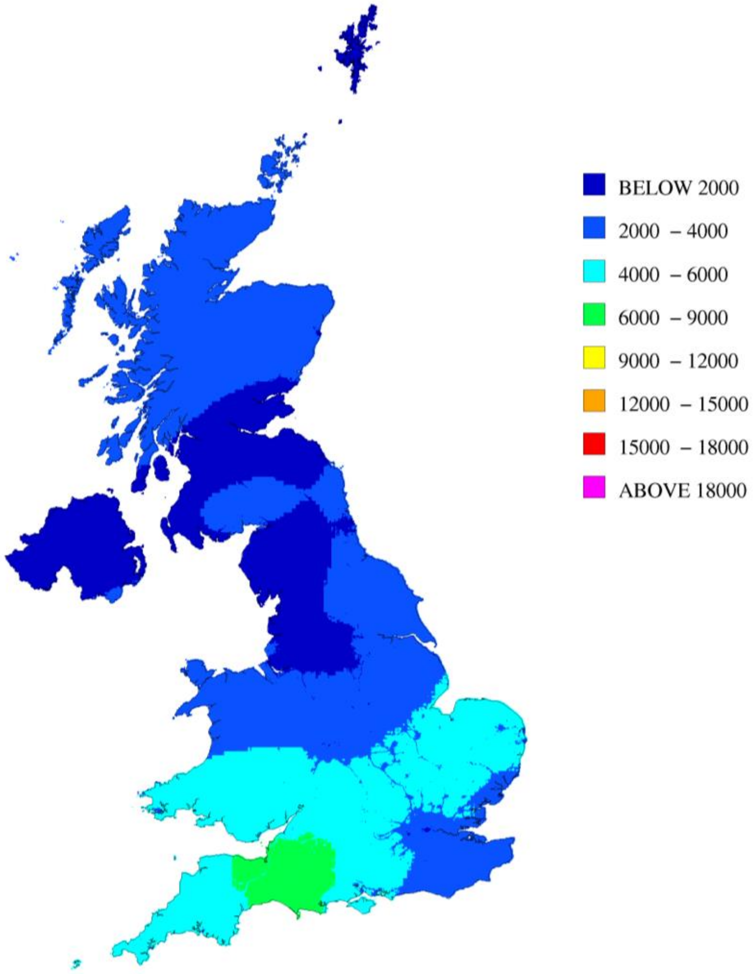


Figure 9.8 - Estimated AOT40 vegetation metric, averaged 2009-2013 (µg m^{-3} hours)

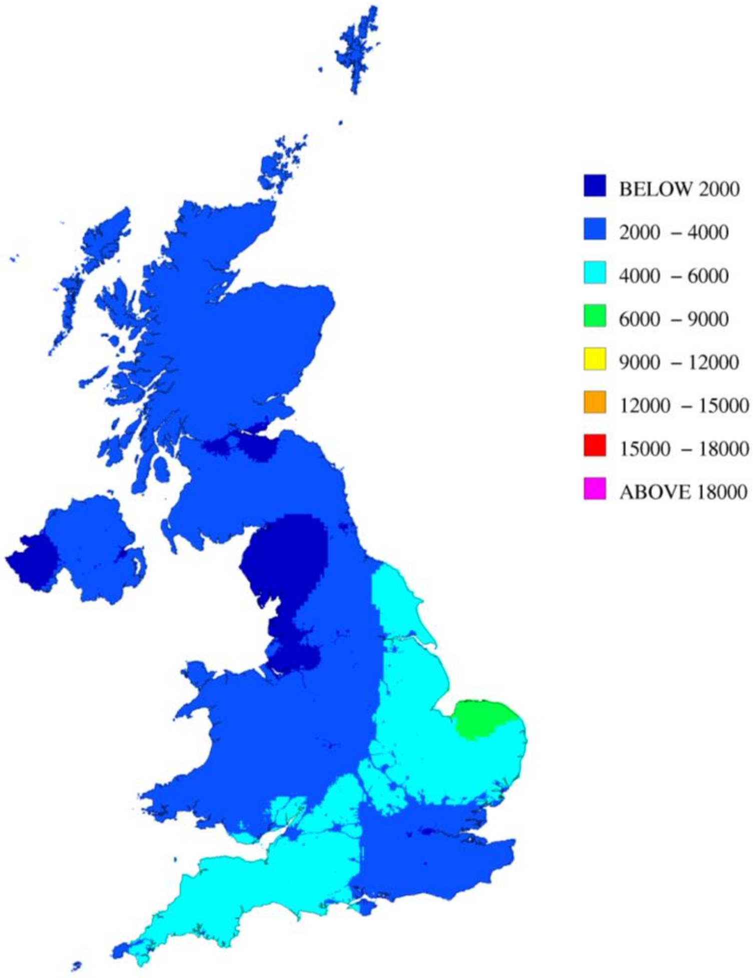


Figure 9.9 - AOT40 percentage decrement in ozone concentrations, 2013

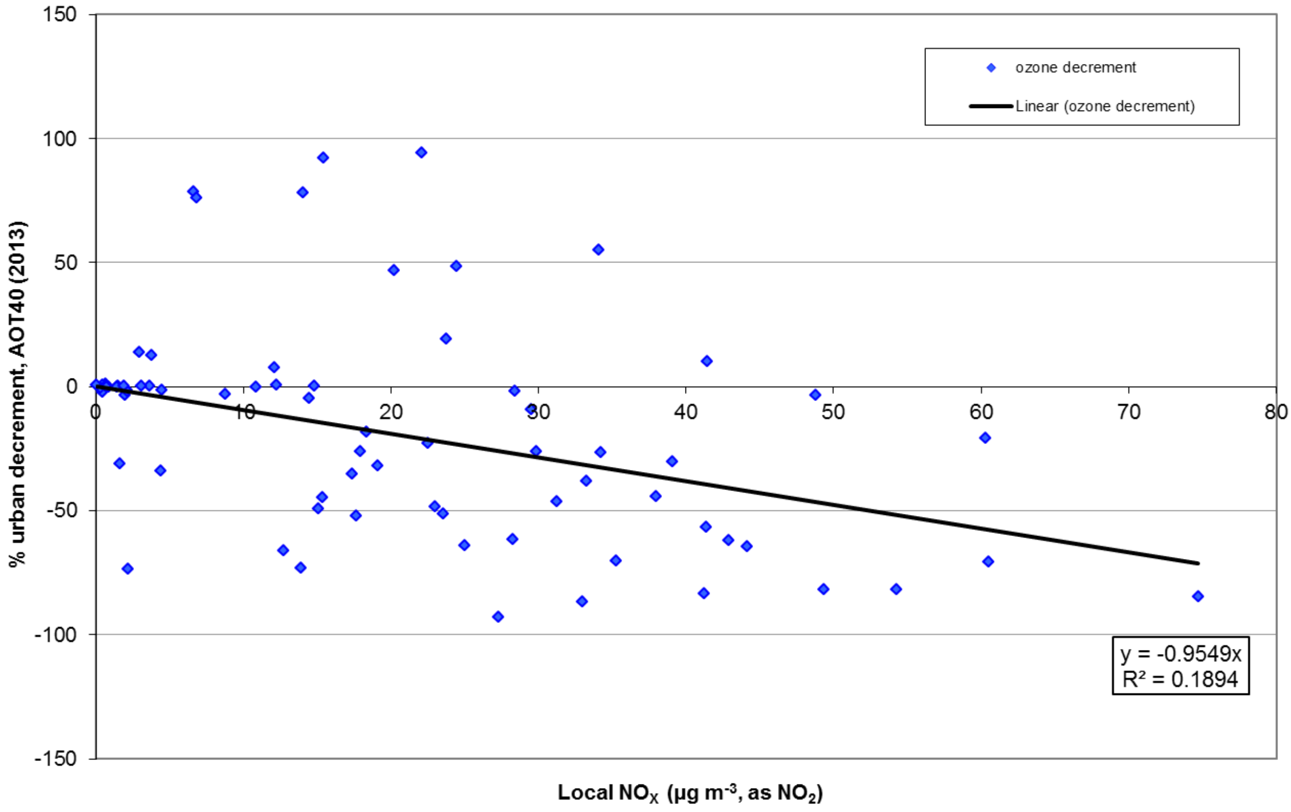
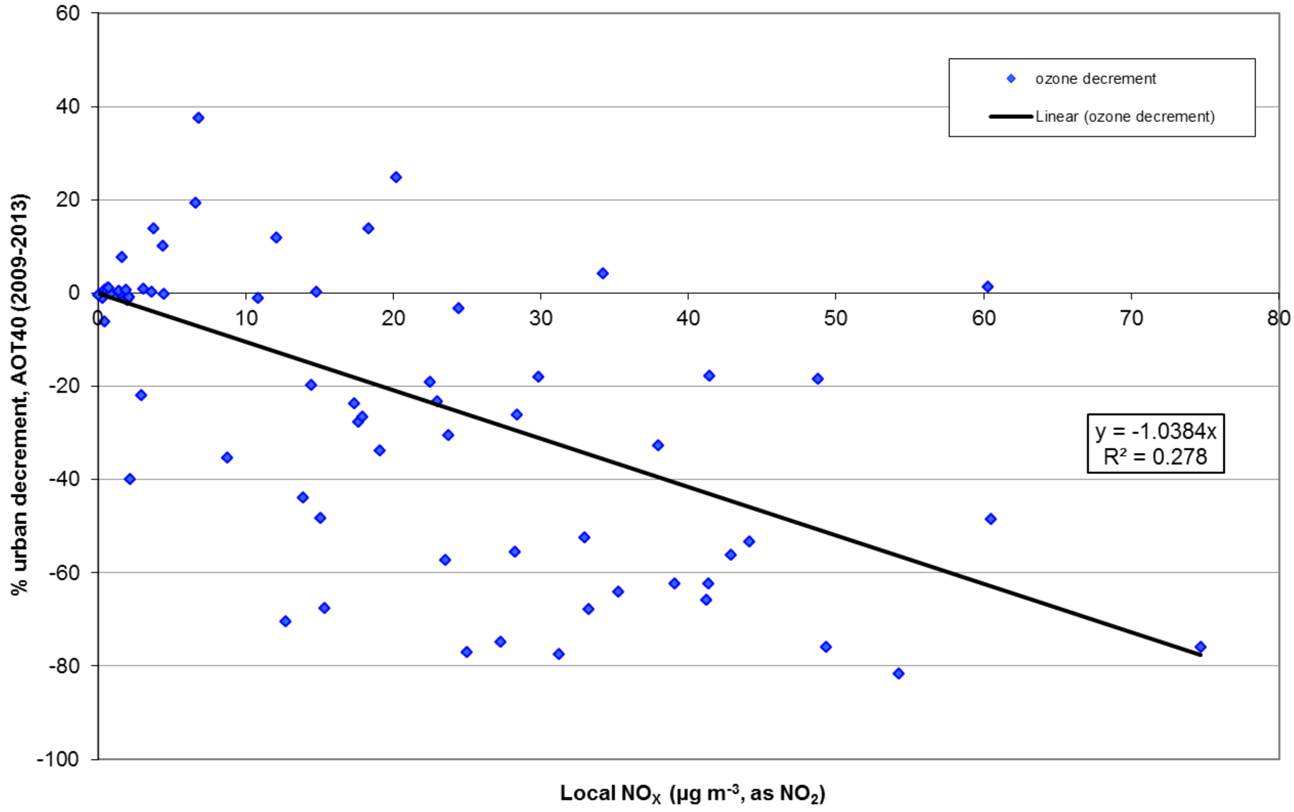


Figure 9.10 - AOT40 percentage decrement in ozone concentrations, 2009-2013



9.3.2 Verification of mapped AOT40 values

Figure 9.11 and Figure 9.12 show a comparison of modelled and measured AOT40 metrics in 2013 and averaged 2009-2013 at background locations. Both the national network sites used to calibrate the models and the verification sites are shown. Lines representing y = x + 50 % and y = x - 50% are also shown, as this is the AQD data quality objective for modelled ozone concentrations – see Section 1.5.

Figure 9.11 - Verification of background AOT40 vegetation model, 2013

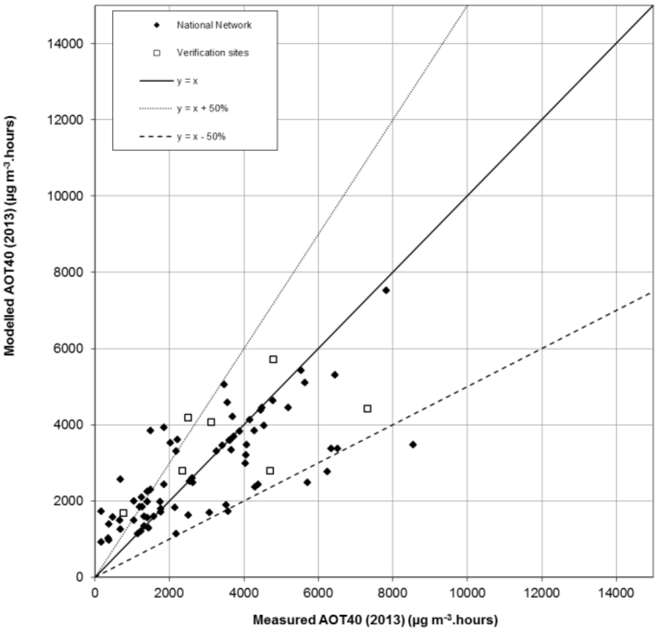
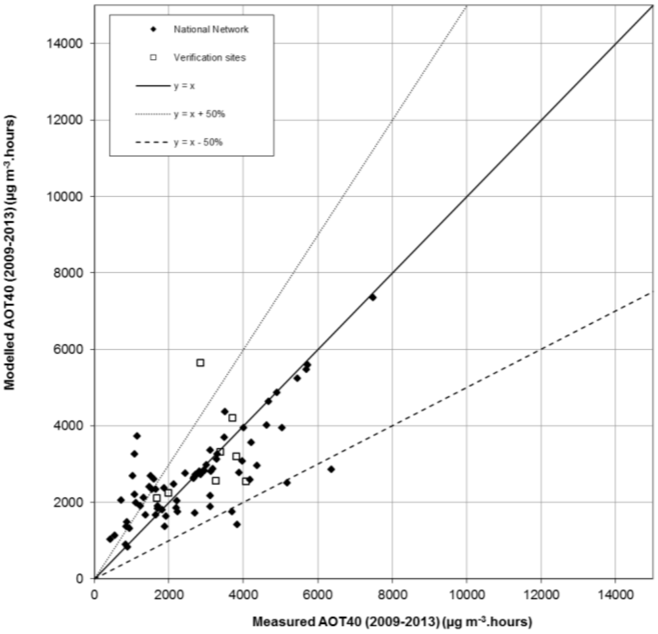


Figure 9.12 - Verification of background AOT40 vegetation model, 2009-2013



There is not a systematic over-estimation or under-estimation of the metric for 2013 apparent for the verification sites in Figure 9.11. This is also apparent in Table 9.2 which presents the summary statistics for the comparison between modelled and measured ozone concentrations. There are also fewer sites outside the ±50% DQO than for the number of days greater than 120 µg m^{-3} metric for both the national network and verification sites.

The multi-year metric (TV) for verification sites shows improved results relative to the ±50% DQO (i.e. lower percentage of sites outside the DQO range) but a poorer R^2 compared with the single year metric (LTO), as shown in Figure 9.12 and Table 9.2 below.

Table 9.2 - Summary statistics for comparison between modelled and measured AOT40 vegetation metric

		Mean of measurements (µg m^{-3} hours)	Mean of model estimates (µg m^{-3} hours)	R^2	% outside DQO	No. sites
National network	2013	2914	2791	0.54	32%	73
Verification sites	2013	3656	3627	0.36	29%	7
National network	2009-2013	2726	2702	0.59	30%	70
Verification sites	2009-2013	3106	3221	0.07	13%	8

10 Arsenic, Cadmium, Nickel, and Lead

10.1 Introduction

10.1.1 Target and Limit values

A single limit value for ambient lead (Pb) concentrations is set out in the AQD. This limit value has been specified for the protection of human health and came into force from 01/01/2005. The limit value is an annual mean concentration of 0.5 µg m^{-3}.

The target values (TV) for As, Cd and Ni included in the 4th Daughter Directive (AQDD4) are listed in Table 10.1. The Directive states that Member States should take all necessary measures not entailing disproportionate costs to ensure that the target values are not exceeded after the compliance date.2013 is the first year for which these TVs are in force.

Table 10.1 - Target values for As, Cd, and Ni

Pollutant	Averaging period	TV (ng m^3)	Date after which the TV is not to be exceeded
As	Calendar year	6	31 December 2012
Cd	Calendar year	5	31 December 2012
Ni	Calendar year	20	31 December 2012

10.1.2 Annual mean models

Maps of annual mean As, Cd, Ni and Pb concentrations in 2013 at background locations are shown in Figure 10.1, Figure 10.2, Figure 10.3 and Figure 10.4 respectively. These maps are presented in ng m^{-3}, where 1000 ng m^{-3} = 1 µg m^{-3}. The maps of background concentrations have been calculated by summing contributions from different sources:

- Large point source emissions
- Small point source emissions
- Fugitive point source emissions
- Point sources with emissions estimates for air quality pollutants based on reported carbon emissions (ETS points)
- Area sources related to domestic combustion
- Area sources related to road traffic
- Other area sources
- Regional concentration
- Re-suspension from bare soils
- Re-suspension as a result of vehicle movement

These components are aggregated to a single 1 km x 1 km background grid value for each pollutant.

Figure 10.1 - Annual mean background As concentration, 2013 (ng m^{-3})

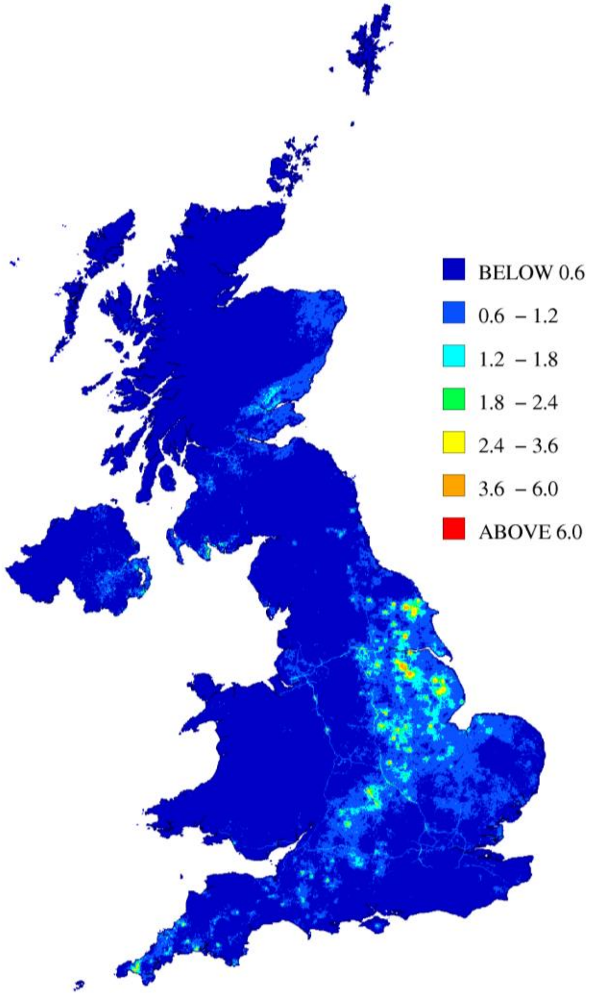


Figure 10.2 - Annual mean background Cd concentration, 2013 (ng m^{-3})

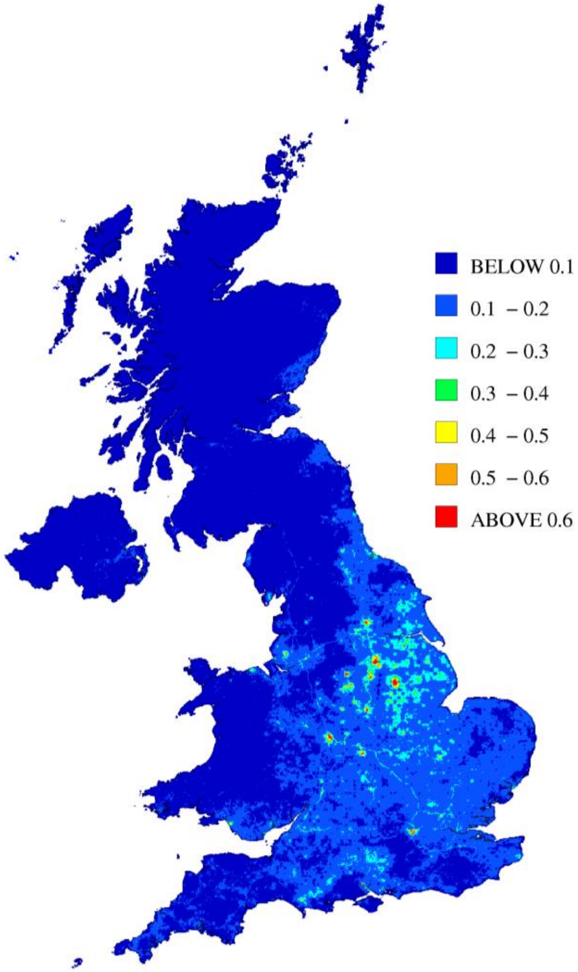


Figure 10.3 - Annual mean background Ni concentration, 2013 (ng m^{-3})

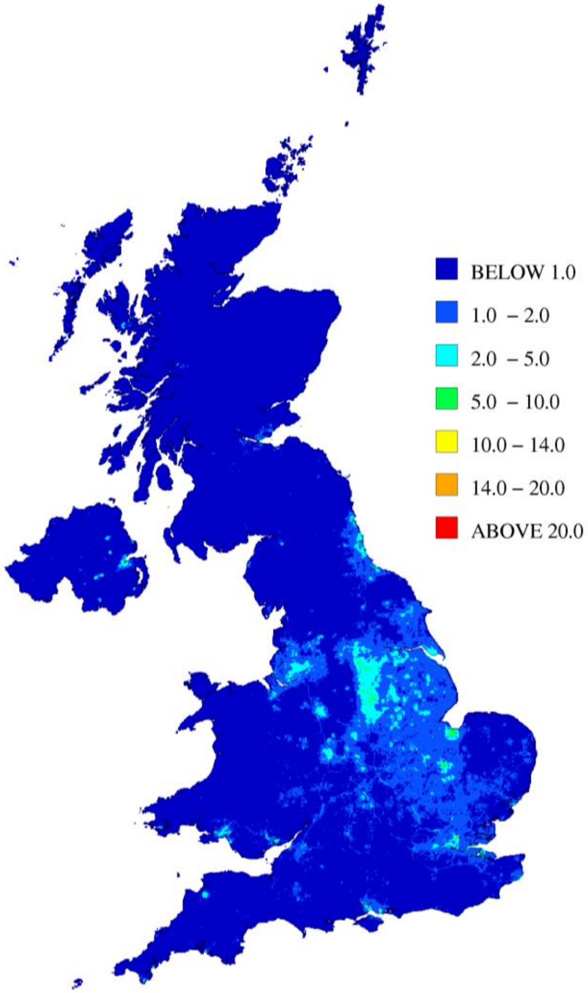
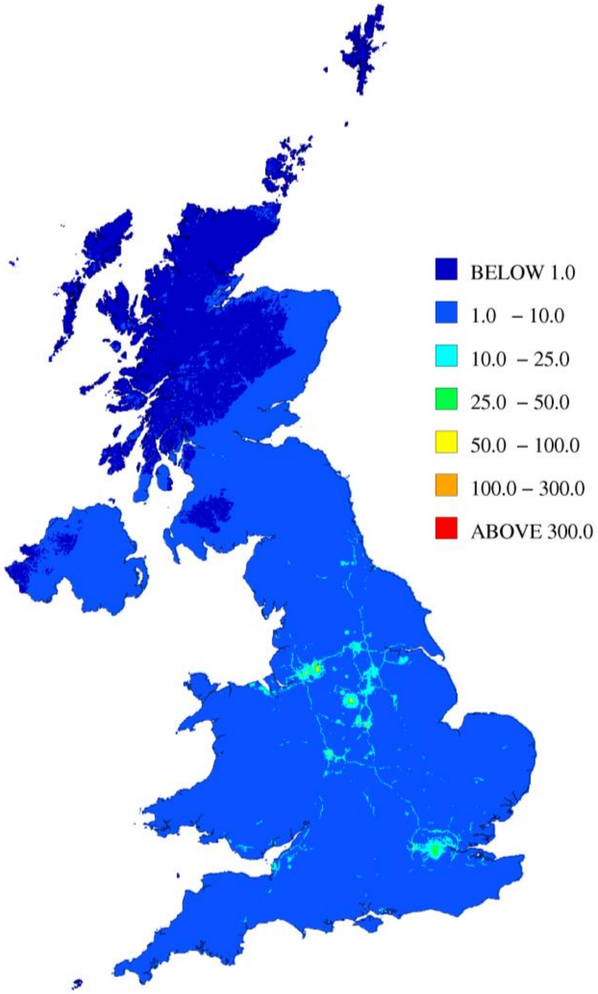


Figure 10.4 - Annual mean background Pb concentration, 2013 (ng m^{-3})



10.1.3 Chapter structure

This chapter describes modelling work carried out for 2013 to assess compliance with the Pb limit value and As, Cd, and Ni target values described above. Emission estimates are described in Section 10.2, Section 10.3 describes the modelling methods, and the modelling results are presented in Section 10.4 to 10.7. The source apportionment of ambient concentrations is discussed in each pollutant results section and is often very different from the split for total national emissions. Ambient concentrations are influenced by the location and release characteristics of the emissions and are also influenced by sources not included in the inventory, such as re-suspension.

10.2 Emissions

Estimates of the emissions of Heavy Metals from the UK National Atmospheric Emissions Inventory 2012 (NAEI 2012) have been used in this study (Passant et al., 2014). Emissions projections have been provided by the NAEI (Passant pers. comm. 2014a) based on DECCs UEP48 energy and emissions projections (DECC, 2013). UK total emissions for 2012 and emissions projections for 2015, 2020, 2025 and 2030 split by SNAP code for As, Cd, Ni and Pb are shown in Figure 10.5, Figure 10.6, Figure 10.7 and Figure 10.8 respectively, with the coding described in Table 3.1. Values for intermediate years have been interpolated in these figures.

Figure 10.5 shows that a small decrease in arsenic emission is forecast over the period 2012-2015. A small gradual increase expected between 2015 and 2025 and a subsequent small decrease in emissions up to 2030. In all years, combustion in industry accounts for over 60% of the total emissions. Emissions of arsenic are primarily from the combustion of solid fuel, and as such, the majority of emissions are estimated to be from the burning of wood treated with copper chromium arsenate. There are no reliable estimates of the extent of this activity, and since the emission factor for this source is also very uncertain, the total emission estimate for this source is highly uncertain. Point sources are also a significant source of arsenic emissions in the UK.

Point sources are the dominant source of cadmium across the time series, with road transport exhaust emissions also shown as a significant source. Figure 10.6 shows an increase in emissions from 2012 to 2025 due to an increase in activity in industries which are a dominant source of cadmium e.g. steel, iron, aluminium production. There is a small decrease in emissions from 2025 to 2030.

Figure 10.7 shows a small increase in nickel emissions between 2012 and 2015, and a decrease in total emissions to 2030. The figure indicates that point sources, shipping, domestic combustion and combustion in industry are the dominant emissions sources of nickel in the UK. Nickel emissions to the atmosphere arise primarily from the combustion of liquid fuels.

Figure 10.8 shows that overall lead emissions are dominated by point sources, from combustion in industry and production processes. Lead emissions are primarily from non-fuel related emissions. An increase in emissions is apparent in the years 2012 to 2020. Emissions remain roughly constant following 2020.

Figure 10.5 - Total UK As emissions for 2012 and emissions projections up to 2030 by SNAP code from NAEI 2012

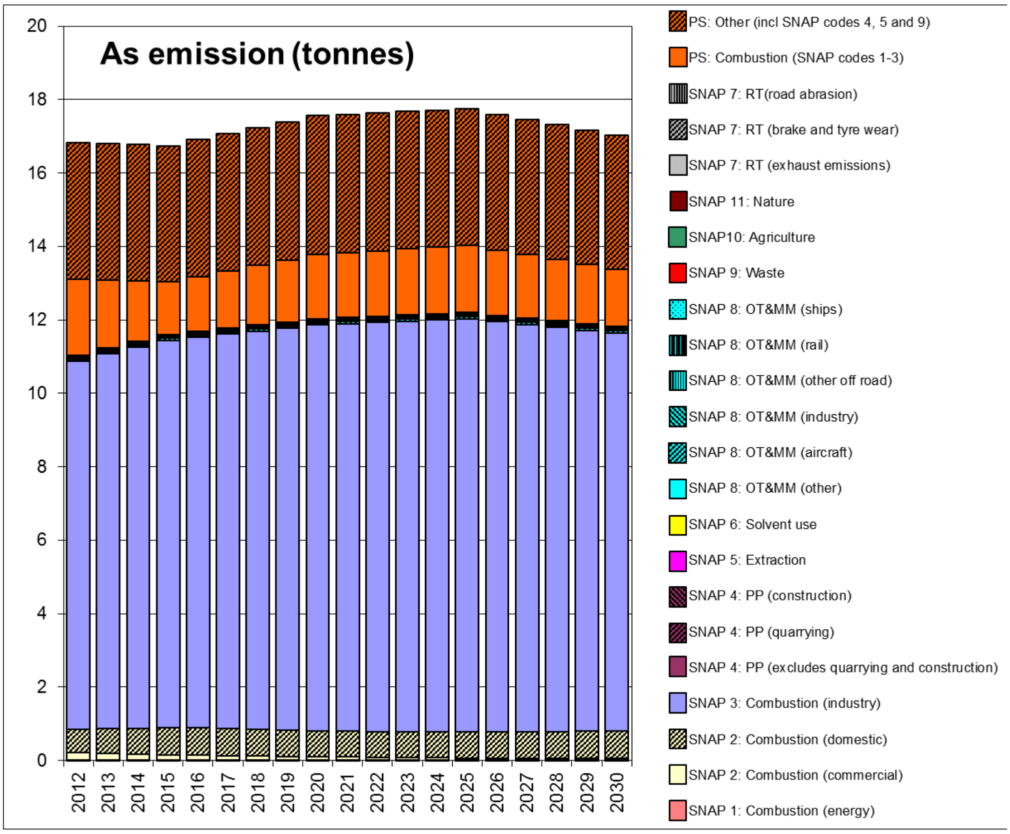


Figure 10.6 - Total UK Cd emissions for 2012 and emissions projections up to 2030 by SNAP code from NAEI 2012

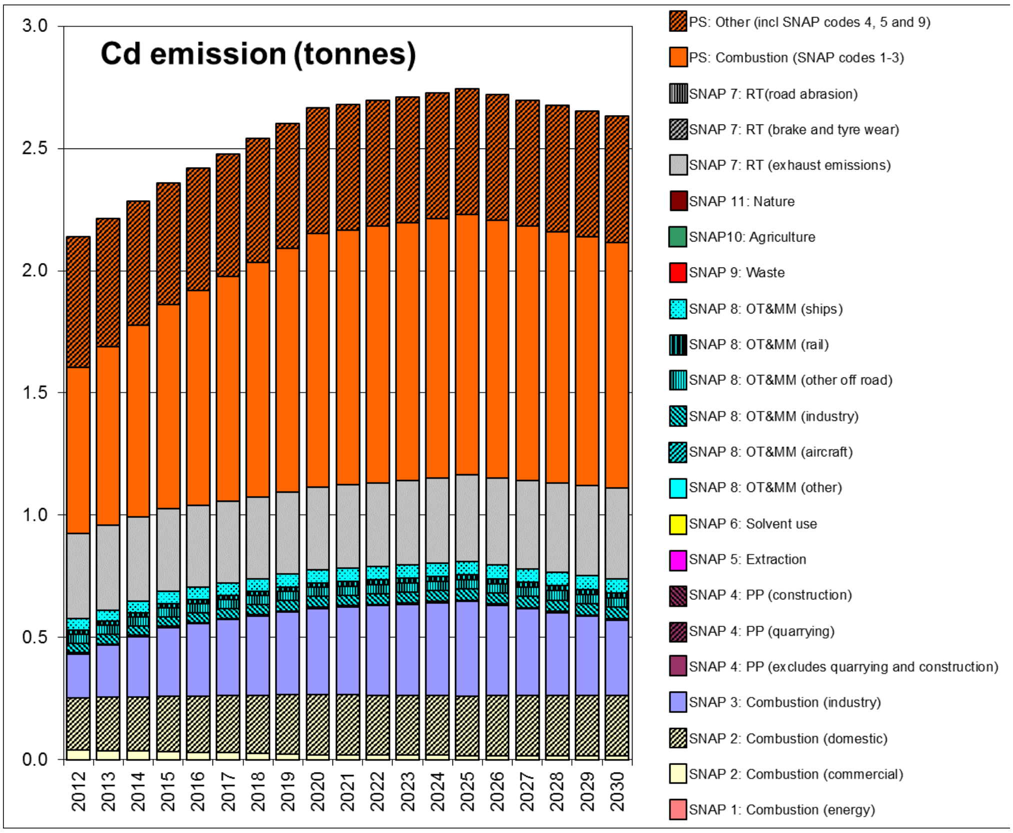


Figure 10.7 - Total UK Ni emissions for 2012 and emissions projections up to 2030 by SNAP code from NAEI 2012

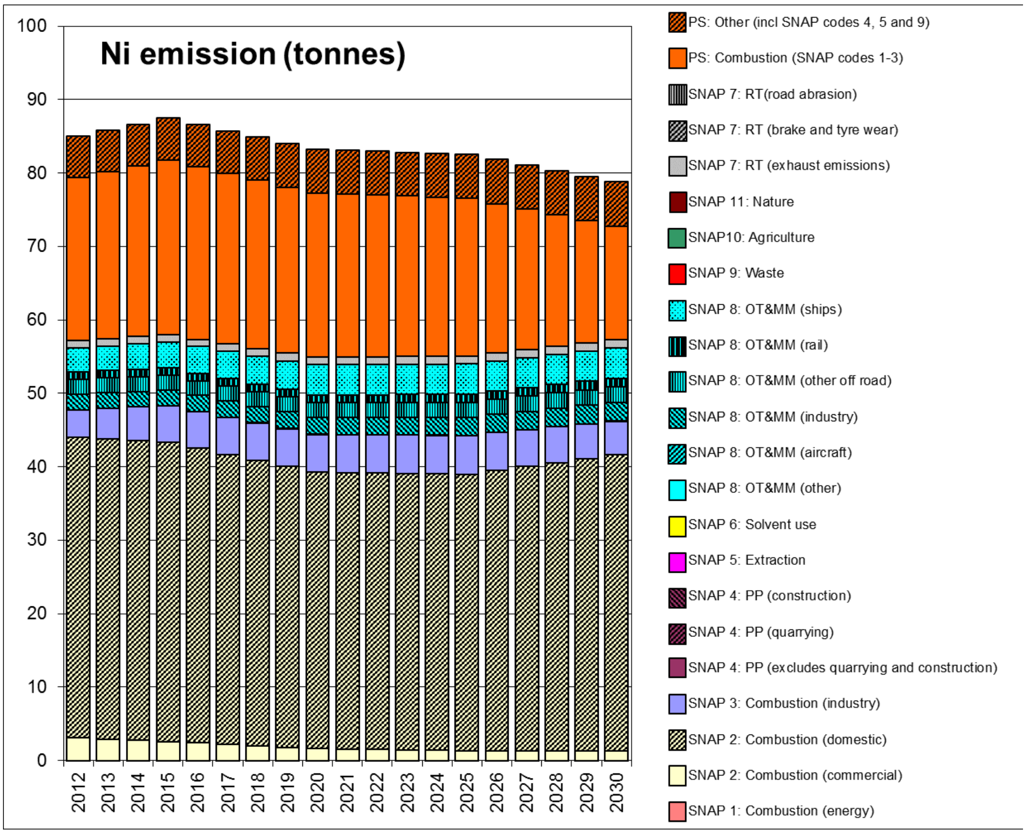
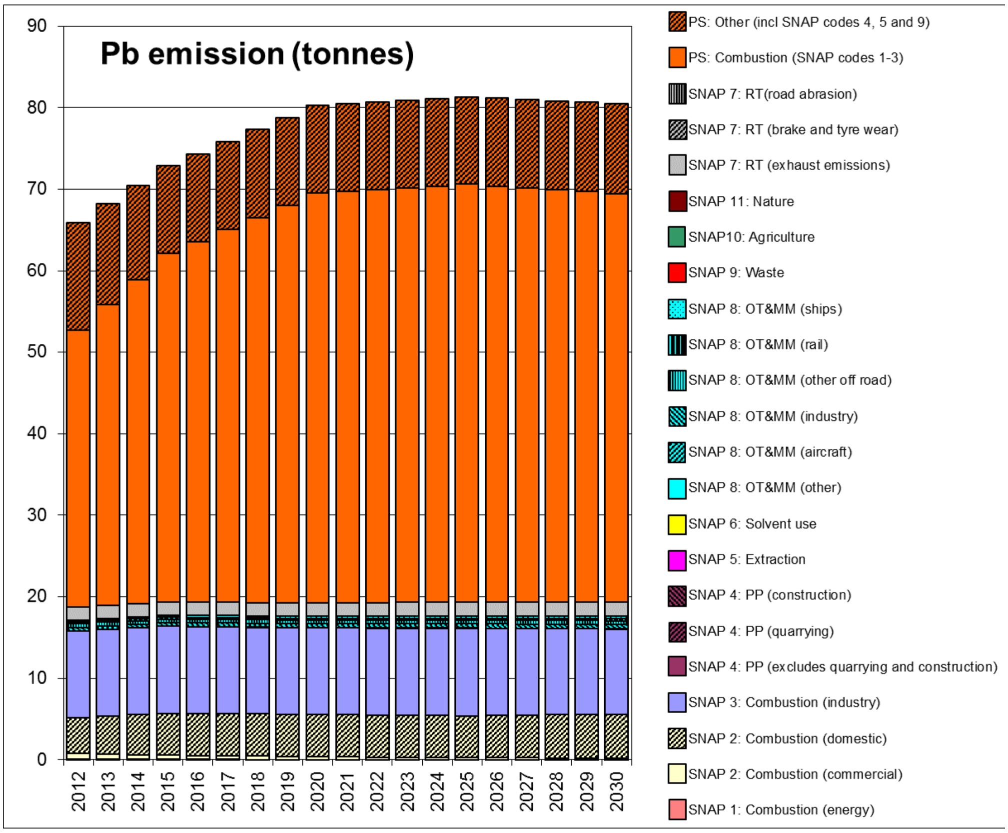


Figure 10.8 - Total UK Pb emissions for 2012 and emissions projections up to 2030 by SNAP code from NAEI 2012



10.3 The model

10.3.1 Contribution from large point sources

Contributions to ground level annual mean heavy metal concentrations from point sources (those with annual emissions of greater than the thresholds listed by pollutant in Table 10.2, or for which emission release characteristics are known) in the NAEI 2012 were estimated by modelling each source explicitly using the atmospheric dispersion model ADMS 5.0 and sequential meteorological data for 2013 from Waddington. Surface roughness was assumed to be 0.1 m at the dispersion site and 0.1 m at the meteorological site. Concentrations were calculated for a 99 km x 99 km square composed of a regularly spaced 1 km x 1 km resolution receptor grid. Each receptor grid was centred on the point source. The total number of point sources modelled explicitly is given in Table 10.2. For each large point source information was retrieved from the PCM stack parameters database (as described in Section 3.3.1). The NAEI emissions for point sources for 2012 were scaled in order to provide values for 2013 as described in Section 3.3.1.

A calibration coefficient of 0.3 has been applied to the modelled contribution of large point sources to As concentrations. Calibration coefficients of unity have been applied to the modelled contribution from large point sources to concentrations of Ni, Pb and Cd. Calibration coefficients were chosen to provide the best agreement of total model predictions with measured heavy metal concentrations. Activity levels for combustion of coal in industry were about 50% higher in the 2012 NAEI than in the previous year. Average measured concentrations of As across the UK showed a small decrease between 2011 and 2012, consequently a calibration factor of less than unity was required for industrial emissions of As.

10.3.2 Contributions from small point and fugitive sources

The contributions to ambient concentrations from fugitive and small point sources (those without stack parameters datasets and annual emissions less than or equal to values displayed in Table 10.2) in the NAEI 2012 were modelled using a small points model. The NAEI 2012 emissions for fugitive and small point sources have been scaled to 2013 using the same source sector specific projection factors applied to the large point sources.

The models consist of separate 'in-square' and 'out-of-square' components, in which concentrations are estimated using a point source dispersion kernel. The dispersion kernel has been calculated by using the dispersion model ADMS 5.0 to model the dispersion of unit emissions from a central source to a grid of receptors at a spatial resolution of 1 km x 1 km squares with the stack characteristics as presented in Table 10.3. Hourly sequential meteorological data from Waddington in 2013 has been used to construct the dispersion kernels. The greatest concentration would be expected close to the point of emission. The receptor for the central grid square within the dispersion kernel is, however, at exactly the same location as the point of release. The concentration at this location is therefore zero. The value for the central grid square within the dispersion kernel has therefore been assigned to be equal to the highest of the values for the adjacent grid squares.

A calibration coefficient of 0.3 has been applied to the modelled contribution of small point sources to As concentrations. Calibration coefficients of unity have been applied to the modelled contribution from small point sources to concentrations of Ni, Pb and Cd. Calibration coefficients were chosen to provide the best agreement of total model predictions with measured heavy metal concentrations.

Table 10.2 - Thresholds to determine modelling method, and number of large point sources for 2013

Pollutant	Tonnes per year	Number of large point sources
As	0.025	241
Cd	0.025	243
Ni	0.05	250
Pb	1.2	239

Table 10.3 - Stack release parameters used to characterise emissions from point sources with no available stack parameters

Variable	Parameters
Stack height	15 m
Diameter	1m
Temperature	15˚C
Emission rate as PM_{10}	1g/s
Surface roughness at dispersion site	0.5 m
Surface roughness at met site	0.02 m

In common with the NAEI 2011 additional point source emissions data have been provided in the NAEI 2012. These emissions estimates have been derived from carbon emissions data reported under the EU-Emissions Trading Scheme (ETS), most recently described in Tsagatakis et al. (2014). These point sources are referred to as ETS points in this report. To model the contribution to background annual mean As, Cd, Ni and Pb concentrations from ETS points the emissions have been treated as an additional set of small point sources. As such they have been modelled using the small points approach described above. These derived air quality pollutant emissions estimates are particularly uncertain, hence the emissions for particular sources have been capped at reporting thresholds given by the Scottish Pollutant Release Inventory (SPRI). Typically more than 90% of the ETS points do not exceed the SPRI reporting threshold, which for As, Cd, Ni and Pb is 1, 1, 10 and 100 kilogrammes per year respectively. As for small point sources, a calibration coefficient of 0.3 has been applied to the modelled contribution of ETS point sources to As concentrations. Calibration coefficients of unity have been applied to the modelled contribution from small point sources to concentrations of Ni, Pb and Cd.

Characterising the amount of fugitive heavy metal emission from industrial plant is notoriously difficult. For the modelling of Cd, Ni and Pb concentrations, assuming a fugitive emission of 0.05 times the reported emission was found to provide the best agreement with the available measurements. For the modelling of As, a fugitive emission 0.015 times the reported emission was assumed.

The emission release parameters are provided in Table 10.4. Once again, the value for the central grid square within the dispersion kernel has been set to the maximum of the values in the surrounding grid squares.

Table 10.4 - Stack release parameters used to characterise fugitive emission release

Variable	Parameters
Stack height	10m
Diameter	1m
Temperature	15˚C
Emission rate as PM_{10}	1g/s
Surface roughness at dispersion	0.5 m
Surface roughness at met site	0.02 m

10.3.3 Contributions from local area sources

The 2013 area source emissions maps for heavy metals have been calculated from the NAEI 2012 emissions maps following the method described in Section 3.3.5. ADMS derived dispersion kernels have been used to calculate the contribution to ambient concentrations on a 1 km x 1 km receptor grid, from the area source emissions within a 33 km x 33 km square surrounding each receptor. Hourly sequential meteorological data from Waddington in 2013 has been used to construct the dispersion kernels, as described in Appendix 4.

Revised methods introduced in the 2011 assessment (Brookes et al., 2012) for modelling the contributions to As, Cd, Ni and Pb from SNAP 2 (domestic and non-domestic combustion) and SNAP 3 (combustion in industry) area sources were used and have been described in Section 3.3.5.

A calibration coefficient of 0.3 has been applied to modelled contribution of Industrial area sources to As concentrations. Calibration coefficients of unity have been applied to the modelled contribution from area sources to concentrations of Ni, Pb and Cd, and to other area source types for As modelling. Calibration coefficients were chosen to provide the best agreement of total model predictions with measured heavy metal concentrations. For certain sectors (noted within each pollutant results section below) caps have been applied to emissions based on expert judgement of the model results in order to address known artefacts in the area source emissions grids and to reconcile the model results with the measured data at each monitoring site.

10.3.4 Contribution from long range transport of primary particulate matter

The contribution to ambient concentrations from long range transport of heavy metals was derived from estimates of regional primary particulate matter used in the 2013 PCM model for PM_{10} mass (Section 5.3.4). The contribution of long range transport sources to ambient heavy metal concentrations was derived by calculating a fraction of the PM mass for each heavy metal. This fraction was estimated as the ratio of the UK total emissions for each metal for each SNAP sector to the total PM_{10} emission for that sector. These ratios were also assumed to apply to the contribution from non-UK European sources.
A slightly different approach has been used for Pb in which the contribution calculated has been multiplied by scaling the relative emissions of Pb to those of PM_{10} by an additional factor of 5. Thus the regional contribution to ambient Pb concentration has been assumed to be greater than implied by the ratio of current emissions. This could be due to the previously significant emissions from road traffic from the use of leaded petrol, although the processes that would be involved in such a contribution are not fully understood at present. An alternative approach would have been to increase the scaling factors applied to the re-suspension contributions for Pb but the approach adopted was found to provide better agreement with available measurements.

10.3.5 Heavy metal contribution from re-suspension

The 2013 model for heavy metal concentrations includes a contribution to ambient concentrations from re-suspension calculated in the same way as in the 2011 models (Brookes et al., 2012). The contributions from two processes have been included:

- Regional PM dusts from re-suspension of soils and
- PM dusts from re-suspension due to vehicle activity.

The heavy metal contribution from re-suspension has been calculated by using the methods suggested by Abbott (2008). The methods used to estimate the total PM mass from these processes are detailed in Section 5.3.5.

Abbott (2008) also suggested a method for estimating the contributions to the ambient concentrations of heavy metals from soil and vehicle related re-suspension processes. The maps of PM mass from re-suspension of soils and re-suspension associated with vehicle movements can be used to estimate the contributions to the ambient concentration of heavy metals using a combination of information on the heavy metal content of soils and enhancement factors.

The National Soil Inventory (http://www.landis.org.uk/data/natmap.cfm) provides a data set of arsenic, cadmium, nickel and lead concentrations in topsoil at 5 km resolution throughout England and Wales. Measurement data on heavy metals concentration in topsoil for other areas of the UK is available from the Geochemical Atlas of Europe developed under the auspices of the Forum of European Geological Surveys (FOREGS) (http://www.gtk.fi/publ/foregsatlas/). These data were interpolated onto a 1 km x 1 km grid. The predicted annual PM emission rates and the contribution to atmospheric concentrations were multiplied by the topsoil concentrations to estimate the annual metal re-suspension rates and the contributions to atmospheric concentrations of the heavy metals.

There is some evidence that metal concentrations in the surface soils are higher than in the underlying topsoil. EMEP have suggested that there may be some enhancement of the metal content of the re-suspended dust because the metals may form complexes with humic matter (Abbott, 2008). Abbott (2008) carried out regression analyses of measured heavy metal concentrations against the combined model predictions for sites in the UK Rural Heavy Metal Network. This analysis suggested that there may be other mechanisms by which heavy metals are concentrated in the small particle fraction of soils. For example, much of the metal content may be present as the result of historical deposition of small particles or the application of sewage sludge and farmyard slurries. These materials may only be loosely bonded to the surface of the soil particles. The fine particles released by re-suspension mechanisms would therefore be likely to contain a much higher concentration of metals than the underlying topsoil. The enhancement factors listed in Table 10.5 have been chosen to provide the best agreement of total model predictions with measured heavy metal concentrations. The factors are broadly consistent with the regression coefficients determined by Abbott (2008).

Caps have been applied for the contribution generated from re-suspension of soil for some of the heavy metals. The values have been chosen as an estimate of the maximum likely concentration generated from this source and are also listed in Table 10.5.

Table 10.5 - Heavy metal enhancement factors used in the assessment

Pollutant	Enhancement factor	Maximum concentration (ng m^{-3})
As	35	3.5
Cd	35	-
Ni	7	7
Pb	35	5

10.4 Arsenic Results

10.4.1 Introduction

The map of modelled annual mean As concentrations is shown in Figure 10.1. There were no modelled or measured exceedances of the target value of 6 ng m^{-3} in 2013.

10.4.2 Verification of mapped concentrations

A comparison between modelled and measured annual mean As concentrations in 2013 at monitoring site locations is shown in Figure 10.9 to Figure 10.12. These figures include lines to represent the AQDD4 data quality objective for modelled annual mean As concentrations: y=x-60% and y=x+60% (see Section 1.5).

Summary statistics for modelled and measured As concentrations are listed in Table 10.6, including the percentage of sites at which modelled concentrations are outside of the data quality objectives (DQOs), and the total number of sites included in the analysis.

The mean of measured and modelled concentrations agree well for the urban background and roadside monitoring sites. However, the agreement between measured and modelled concentrations on a site-by-site basis (quantified using R^2) is poor for all monitoring sites, with the exception of rural monitoring locations.

It should be noted that non-emission inventory sources (such as fugitive, re-suspension and long range transport of primary PM) result in additional uncertainty when compared with a pollutant such as NO_X, for which the source apportionment is better known.

Figure 10.9 - Verification of annual mean As at Industrial sites

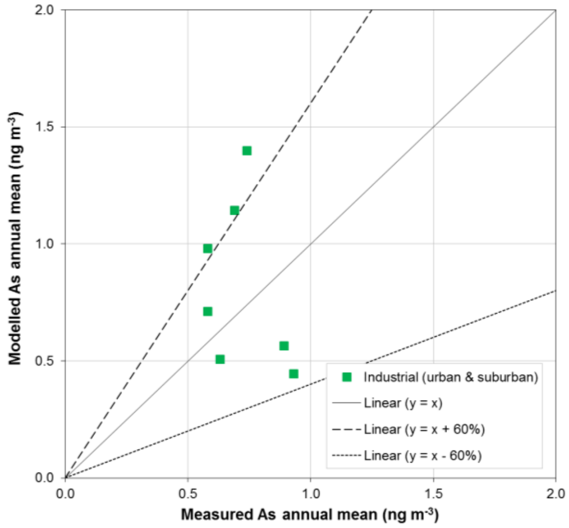


Figure 10.10 - Verification of annual mean As at urban background sites

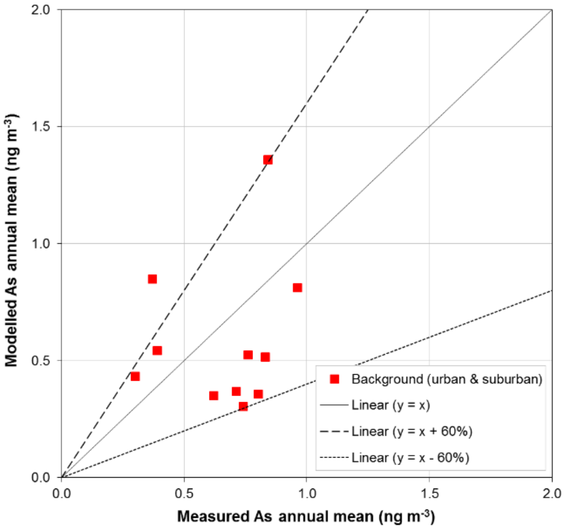


Figure 10.11 - Verification of annual mean As at roadside sites

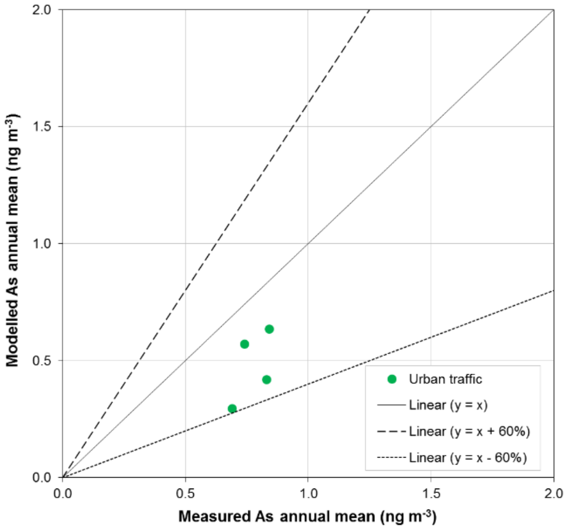


Figure 10.12 - Verification of annual mean As at rural sites

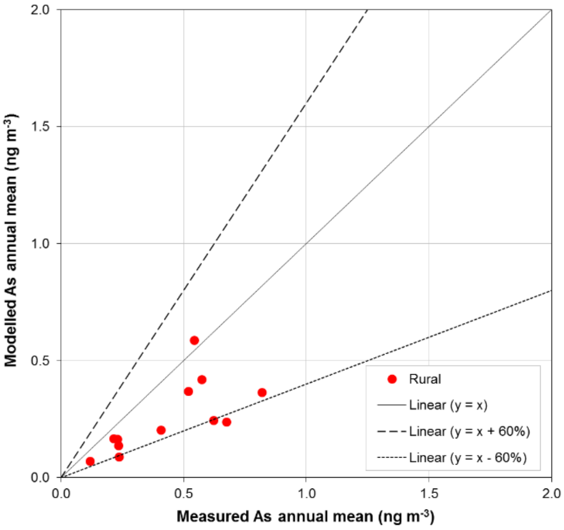


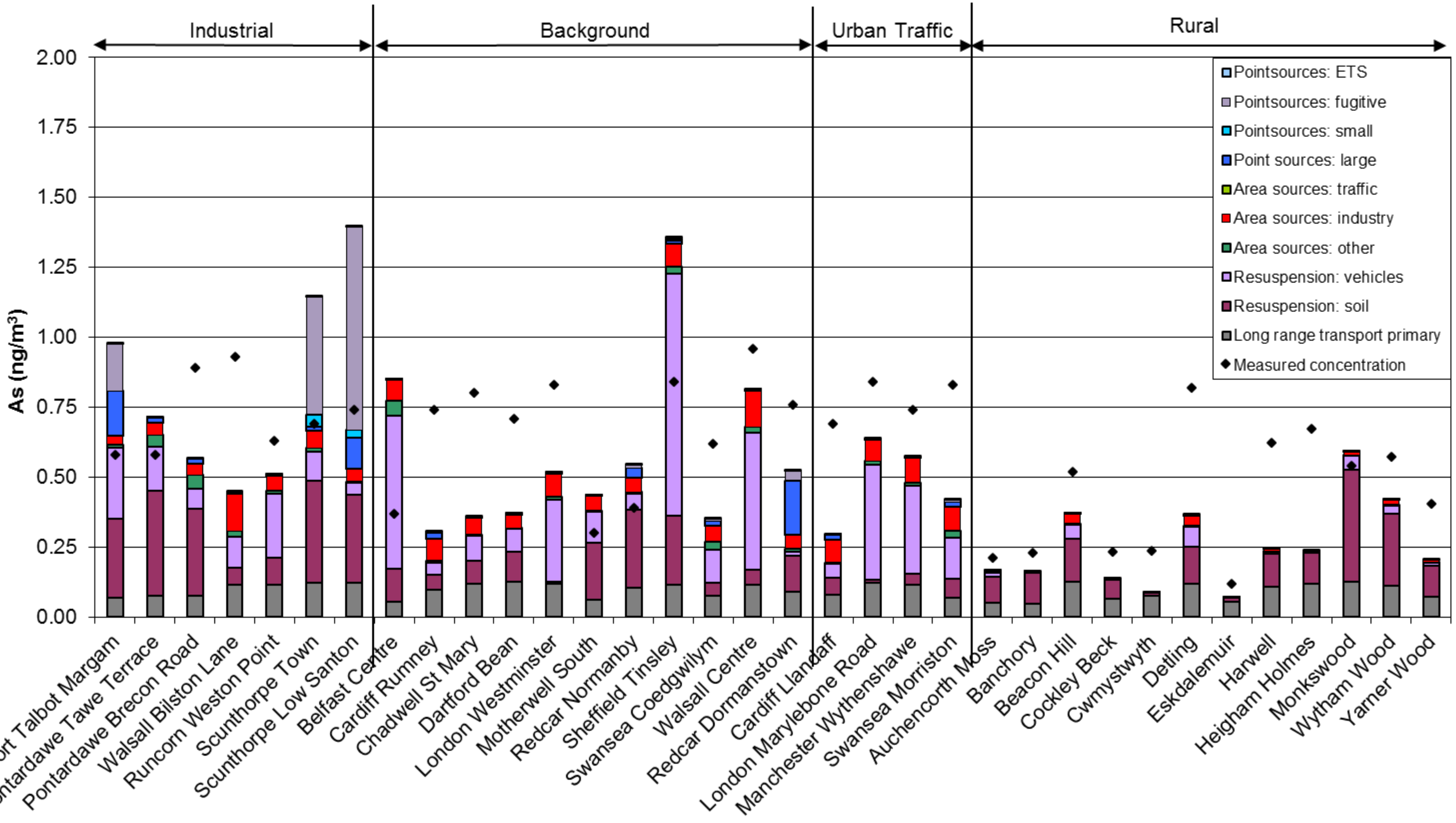
Table 10.6 - Summary statistics for comparison between modelled and measured annual mean As concentrations at different monitoring sites, 2013

	Mean of measurements (ng/m^3)	Mean of model estimates (ng/m^3)	R^2	% of sites outside DQO of ±60%	Number of sites in assessment
Industrial sites	0.72	0.82	0.10	43%	7
Urban background sites	0.67	0.58	0.03	18%	11
Roadside sites	0.78	0.48	0.33	0%	4
Rural sites	0.43	0.25	0.47	25%	12

10.4.3 Source apportionment

Figure 10.13 shows the modelled As contribution from different sources at monitoring site locations. Measured concentrations at the sites are also presented, giving an indication of the level of agreement between modelled and measured concentrations. This analysis suggests that the main sources of arsenic are emissions from point sources, non-road area sources and re-suspension processes.

Figure 10.13 - Annual mean As source apportionment at monitoring sites in 2013



10.5 Cadmium Results

10.5.1 Introduction

The map of modelled annual mean Cd concentrations is shown in Figure 10.2. There are no modelled or measured exceedances of the target value of 5 ng m^{-3} in 2013.

10.5.2 Verification of mapped concentrations

A comparison between modelled and measured annual mean Cd concentrations in 2013 at monitoring site locations is shown in Figure 10.14 to Figure 10.17. These figures include lines to represent the AQDD4 data quality objective for modelled annual mean Cd concentrations: y=x-60% and y=x+60% (see Section 1.5).

Summary statistics for modelled and measured Cd concentrations are listed in Table 10.7, including the percentage of sites at which modelled concentrations are outside of the DQOs and the total number of sites included in the analysis.

The agreement between measured and modelled concentrations on a site-by-site basis (quantified using R^2) is poor for roadside and industrial monitoring sites. The agreement is better at urban and rural monitoring locations.

It should be noted that non-emission inventory sources (such as fugitive, re-suspension and long range transport of primary PM) result in additional uncertainty when compared with a pollutant such as NO_X, for which the source apportionment is better known.

10.5.3 Source apportionment

Figure 10.18 shows the modelled Cd contribution from different sources at monitoring site locations. Measured concentrations at the sites are also presented, giving an indication of the level of agreement between modelled and measured concentrations. This analysis suggests that at those sites where the highest concentrations are measured, the main sources of cadmium are point source emissions (particularly fugitive industrial emissions) and re-suspension processes associated with vehicles.

Figure 10.14 - Verification of annual mean Cd at Industrial sites

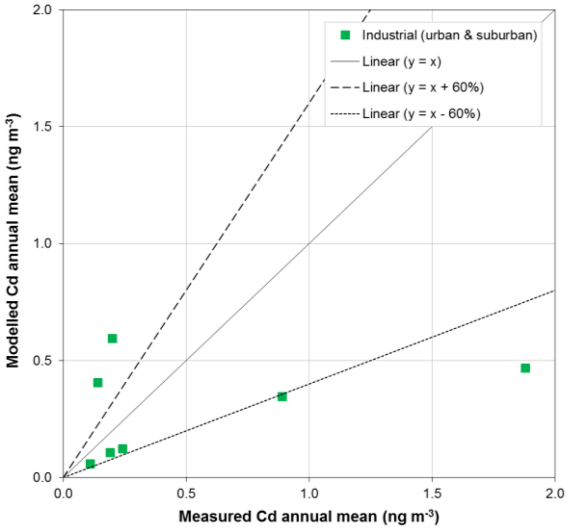


Figure 10.15 - Verification of annual mean Cd at urban background sites

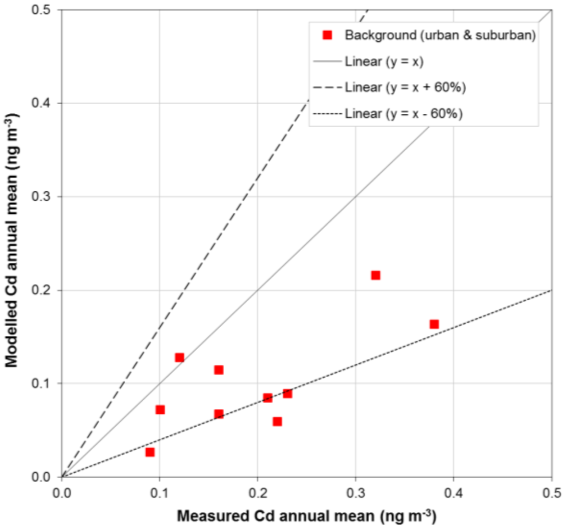


Figure 10.16 - Verification of annual mean Cd at roadside sites

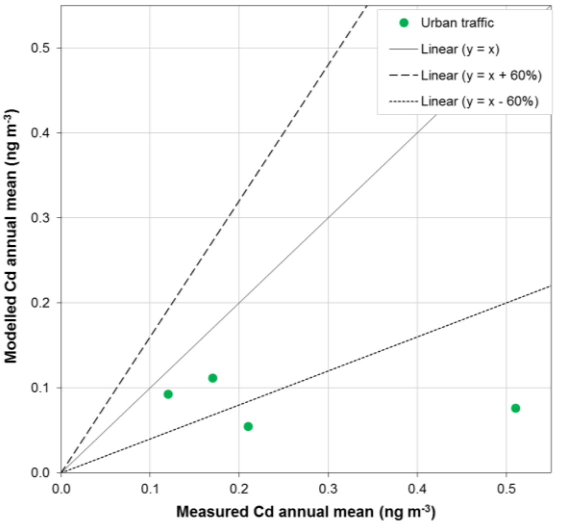


Figure 10.17 - Verification of annual mean Cd at rural sites

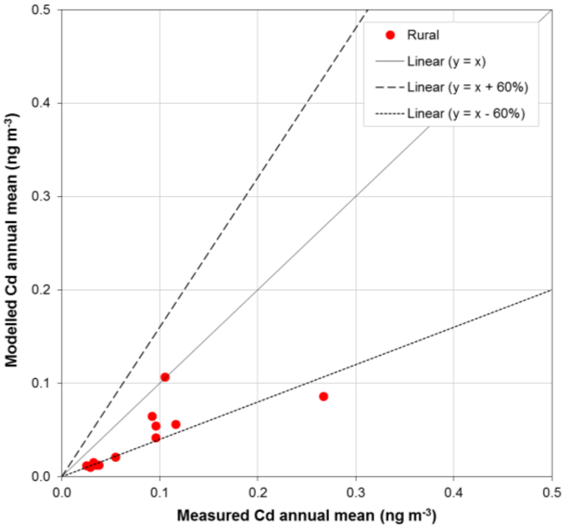
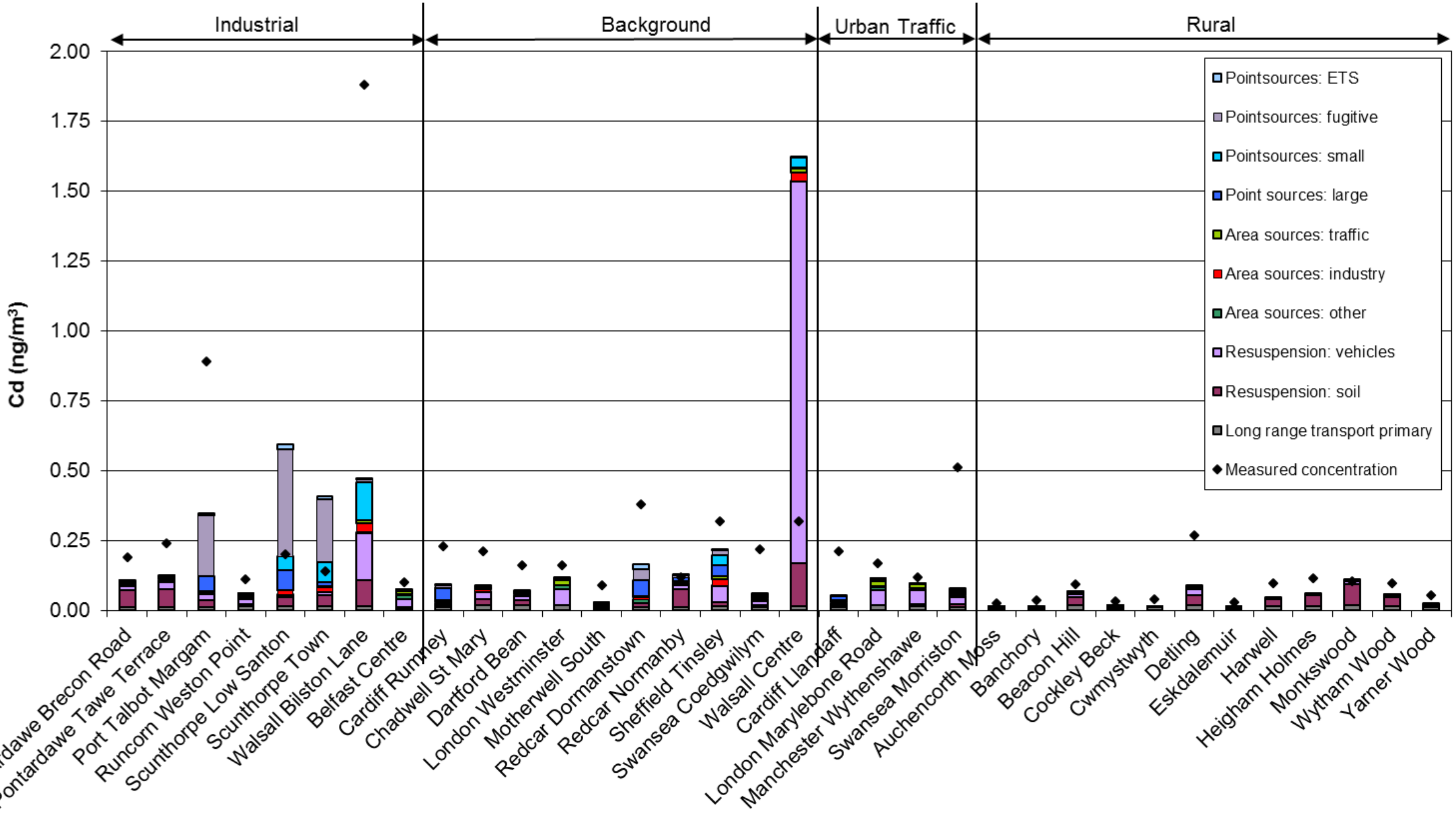


Table 10.7 - Summary statistics for comparison between modelled and measured annual mean Cd concentrations at different monitoring sites, 2013

	Mean of measurements (ng/m^3)	Mean of model estimates (ng/m^3)	R^2	% of sites outside DQO of ±60%	Number of sites in assessment
Industrial sites	0.52	0.30	0.16	57%	7
Urban background sites	0.21	0.24	0.20	36%	11
Roadside sites	0.25	0.08	0.11	50%	4
Rural sites	0.08	0.04	0.58	42%	12

Figure 10.18 - Annual mean Cd source apportionment at monitoring sites in 2013



10.6 Nickel Results

10.6.1 Introduction

The method used to estimate ambient Ni concentrations across the UK is described in Section 10.3 above.

A cap of 15 tonnes per km^2 was applied to area emissions from domestic combustion of petroleum coke. This was done in order to account for the uncertainty associated with the estimates of the spatial distribution of emissions from this source, which have been derived from a combination of several spatial datasets. A cap of 30 tonnes per km^2 was applied to emissions from Iron and Steel combustion plant fuel oil.

The map of modelled annual mean Ni concentrations is shown in Figure 10.3.

10.6.2 Verification of mapped concentrations

A comparison between modelled and measured annual mean Ni concentrations in 2013 at monitoring site locations is shown in Figure 10.19 to Figure 10.22. These figures include lines to represent the AQDD4 data quality objective for modelled annual mean Ni concentrations: y=x-60% and y=x+60% (see Section 1.5).

Summary statistics for modelled and measured Ni concentrations are listed in Table 10.8, including the percentage of sites for which the modelled values are outside of the DQOs as well as the total number of sites included in the analysis.

The mean measured and modelled concentrations agree reasonably well for the urban background and rural monitoring sites. The agreements between measured and modelled concentrations on a site-by-site basis (quantified using R^2) are poor for the urban background and roadside monitoring locations. The results for rural sites show slightly better agreement. The results for the Pontardawe Tawe Terrace site are discussed in Section 10.6.4.

It should be noted that non-emission inventory sources (such as fugitive, re-suspension and long range transport of primary PM) result in additional uncertainty when compared with a pollutant such as NO_X, whose source apportionment is better known.

10.6.3 Source apportionment

Figure 10.23 shows the modelled Ni contribution from different sources at monitoring site locations. Measured concentrations at the sites are also presented, giving an indication of the level of agreement between modelled and measured concentrations. This analysis suggests that the main sources of nickel are point sources including fugitive industrial emissions, non-road area sources and re-suspension processes. Emissions from a local industrial point source are important for Pontardawe Brecon Road and Pontardawe Tawe Terrace, and this is explored in detail in Section 10.6.4.

Figure 10.19 - Verification of annual mean Ni at Industrial sites

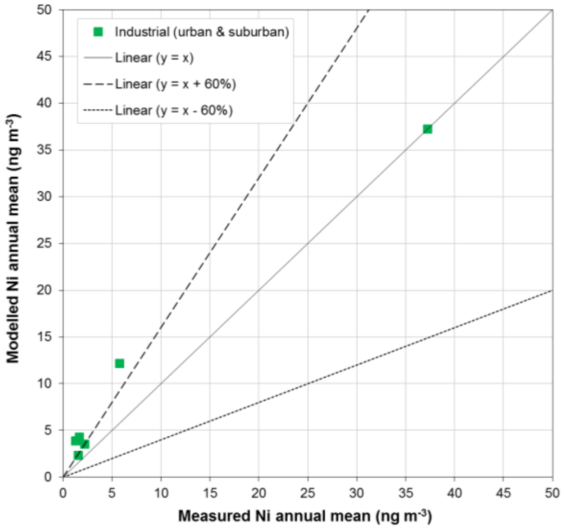


Figure 10.20 - Verification of annual mean Ni at urban background sites

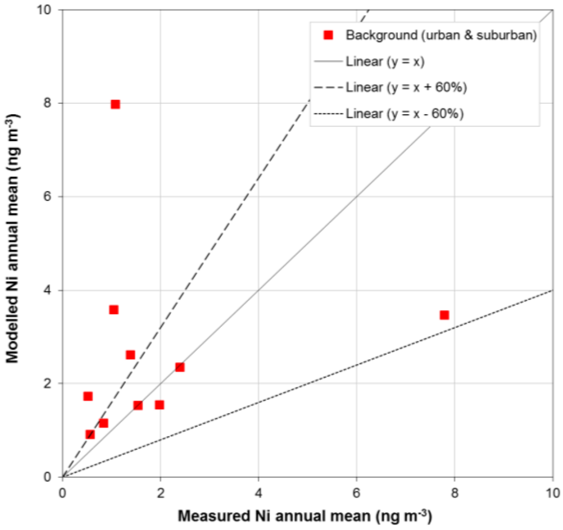


Figure 10.21 - Verification of annual mean Ni at roadside sites

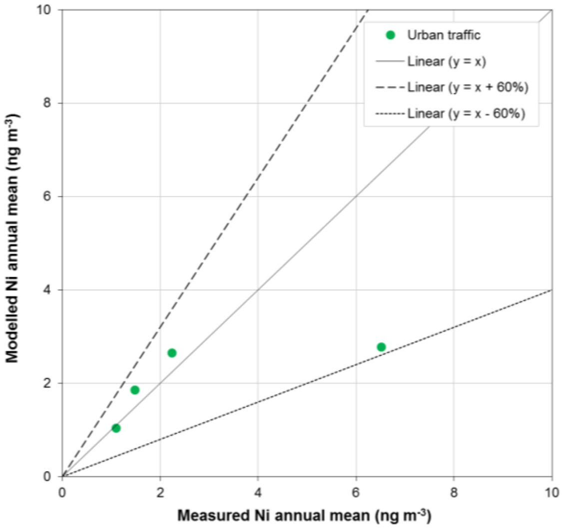


Figure 10.22 - Verification of annual mean Ni at rural sites

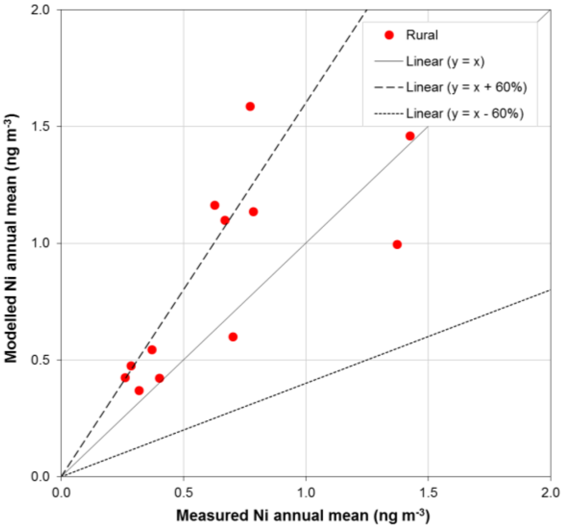
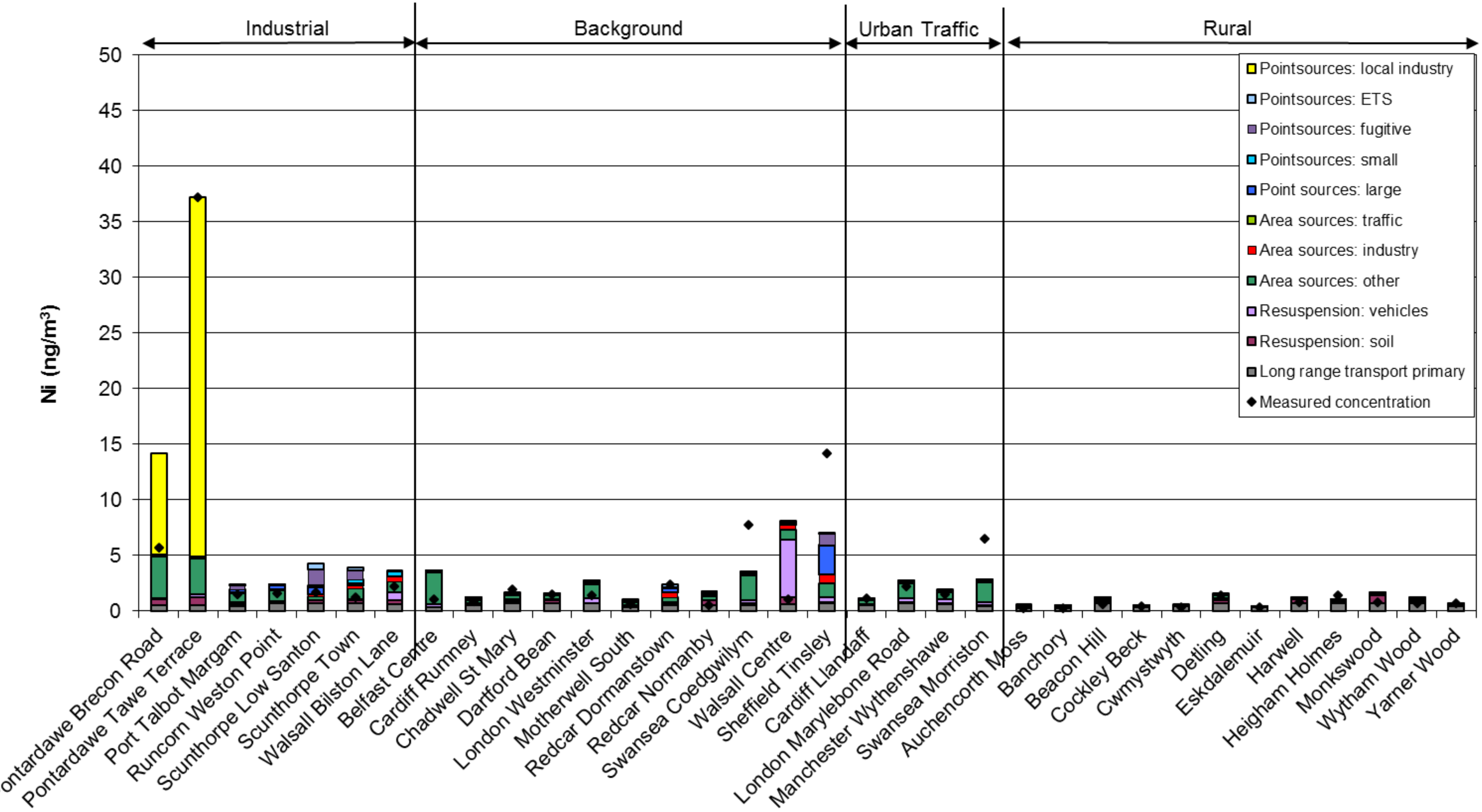


Table 10.8 - Summary statistics for comparison between modelled and measured annual mean Ni concentrations at different monitoring sites, 2013

	Mean of measurements (ng/m^3)	Mean of model estimates (ng/m^3)	R^2	% of sites outside DQO of ±60%	Number of sites in assessment
Industrial sites	7.30	9.42	0.97	57%	7
Urban background sites	3.02	3.08	0.28	45%	11
Roadside sites	2.83	2.09	0.52	0%	4
Rural sites	0.67	0.86	0.52	42%	12

Figure 10.23 - Annual mean Ni source apportionment at monitoring sites in 2013



10.6.4 Detailed comparison of modelled results with the target value

There was one measured exceedance of the Ni TV in 2013. The exceedance was measured at the Pontardawe Tawe Terrace site. Results of the assessment in terms of comparisons of the modelled concentrations with the TV have been reported in e-Reporting Data flow G (CDR, 2014). Exceedances of the TV for the Swansea Urban Area and South Wales zones were reported based upon the annual mean Ni concentration of 37 ng m^{-3} measured at Pontardawe Tawe Terrace. This monitoring site is within the Swansea Urban Area zone but is very near to the boundary of the South Wales zone. Detailed modelling of the principal source of local nickel emissions is described below.

Detailed dispersion modelling has been undertaken using ADMS 5.0 for the area in South Wales where exceedances of the annual mean TV of 20 ng m^{-3} have been measured. This small scale modelling has been used to assess the likely magnitude and spatial scale of the exceedance.

Information on the Ni emissions from the principal Ni point source were provided by the site operator. Ni emissions were taken to be 15.82 kg $year^{-1}$ for 2013, emitted from six emission points distributed across the site. This annual emission took into account recent abatement measures put in place on-site. Building effects were included in the model, and a 6 km x 6 km area was extracted OS Terrain 50 dataset to allow the effect of the topographical features of the valley to be included in the model. The height of the terrain was specified at the centre of each 50 m x 50 m grid square.

Further modelling was carried out to understand the impact fugitive emissions from the local industrial point source on Ni concentrations in the Swansea Valley. Fugitive emissions were modelled as a rectangular unit volume source emission of width 16 m, length 43 m and height 3 m and located at the site of the local industrial point source. Dispersion modelling of the volume source was carried out using ADMS 5.0 with the same methodology as described for the Ni point source emissions. The resulting calculated Ni concentrations were scaled so that the sum of contributions from the point source modelling and the fugitive emissions modelling matches the measured annual mean concentration of 37 ng m^{-3} at Pontadarwe Tawe Terrace. From this scaling the annual mean fugitive emissions can be estimated to be 5.41 kg $year^{-1}$ in 2013.

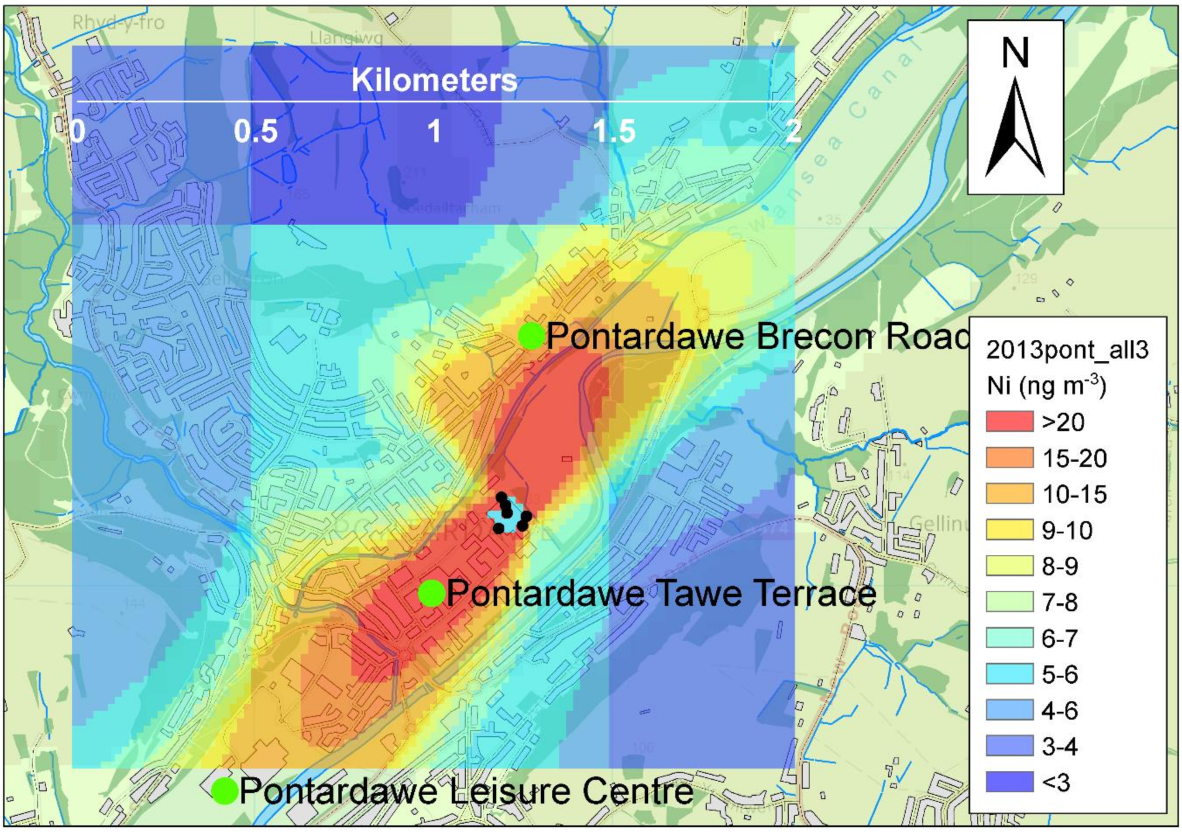
Figure 10.24 shows the modelled annual mean Ni concentration on a 20 m x 20 m grid resulting from the local industrial point source in Pontardawe and including fugitive source emissions. The Ni concentrations in Pontardawe were strongly influenced by the terrain in the area, as can be seen in Figure 10.24. The Swansea Valley runs south-west to north-east through the village of Pontardawe, where the point source is located. Figure 10.24 shows that the distribution of the Ni concentrations in the vicinity of Pontardawe corresponded with the local topography. This is believed to be due to channelling of the local wind flow by the Swansea Valley.

The conclusions from this dispersion modelling study are that there was an exceedance of the Ni TV in both the South Wales and Swansea urban area zones in 2013, as in previous years (2009, 2010, 2011 and 2012). This exceedance was likely to have extended over a spatial area of relevance to the directive (at least 250 m x 250 m for industrial locations).

Table 10.9 compares measured annual mean Ni concentrations with modelled concentrations with and without including the fugitive source emissions. Excellent agreement is obtained at Pontardawe Tawe Terrace, since this measurement was used to estimate the magnitude of fugitive emissions. Good agreement with measurements was also found for the Pontardawe Leisure Centre local authority monitoring site. Poor agreement was obtained at the Brecon Road site, where the combined model result is an over estimate.

The source apportionment plot (Figure 10.23) and scatter plots (Figure 10.19 to Figure 10.22) presented earlier in this Section include the contribution to ambient concentrations at the Pontardawe Tawe Terrace and Pontardawe Brecon Road sites from the local industrial point source.

Figure 10.24 - Modelled annual mean Ni concentration resulting from the local industrial point source in Pontardawe in 2013. (Black dots represent the locations of release points.)



Contains Ordnance Survey data © Crown copyright and database right [2014]

Table 10.9 – Comparison of annual mean measured and modelled Ni concentrations at Pontardawe Tawe Terrace, Pontardawe Leisure Centre and Pontardawe Brecon Road in 2013.

	Measured Ni (ng m^{-3})	Modelled Ni excl. fugitive emissions (ng m^{-3})	Modelled Ni inc. fugitive emissions (ng m^{-3})
Tawe Terrace	37	8	37
Leisure Centre	12	7	11
Brecon Road	6	6	14

10.7 Lead Results

10.7.1 Introduction

The method used to estimate the Pb ambient concentration across the UK is described in Section 10.3 above.

The map of modelled annual mean Pb concentrations is shown in Figure 10.4. There are no modelled or measured exceedances of the limit value of 0.5 µg/m^3 in 2013.

10.7.2 Verification of mapped concentrations

A comparison between modelled and measured annual mean annual mean Pb concentrations in 2013 at different monitoring site locations are shown in Figure 10.25 to Figure 10.28. These figures include lines to represent the AQD data quality objective for modelled annual mean Pb concentrations: y=x-50% and y=x+50% (see Section 1.5).

Summary statistics for modelled and measured Pb concentrations are listed in Table 10.10, including the percentage of sites at which modelled concentrations are outside of the data quality objectives (DQOs), and the total number of sites included in the analysis.

The mean of measured and modelled concentrations agree well for the monitoring sites, excluding industrial sites. However, the agreement between measured and modelled concentrations on a site-by-site basis (quantified using R^2) is poor for all monitoring sites, with the exception of rural monitoring locations.

It should be noted that non-emission inventory sources (such as fugitive, re-suspension and long range transport of primary PM) result in additional uncertainty when compared with a pollutant such as NO_X, for which the source apportionment is better known.

Figure 10.25 - Verification of annual mean Pb at Industrial sites

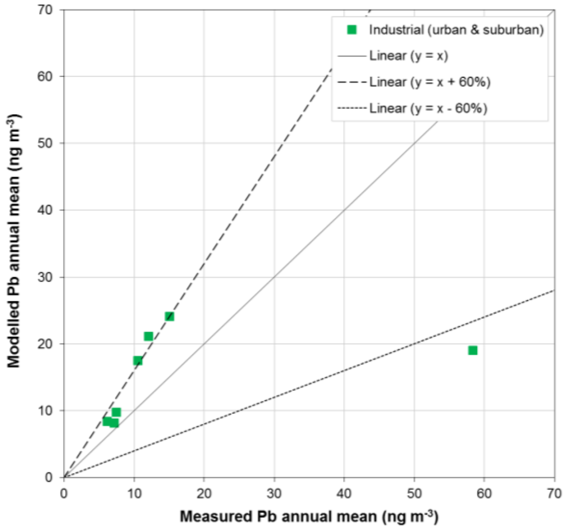


Figure 10.26 - Verification of annual mean Pb at urban background sites

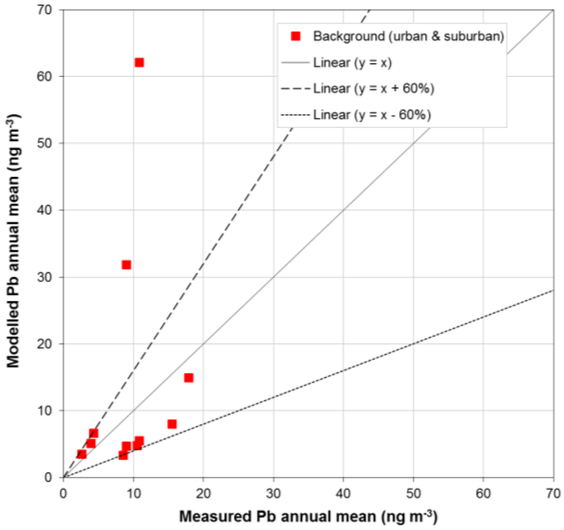


Figure 10.27 - Verification of annual mean Pb at roadside sites

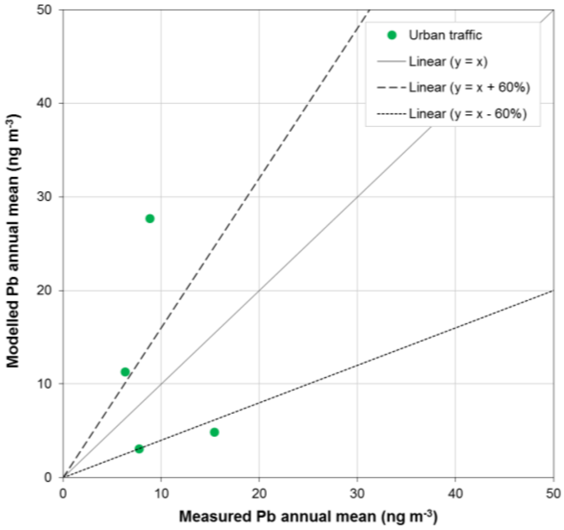


Figure 10.28 - Verification of annual mean Pb at rural sites

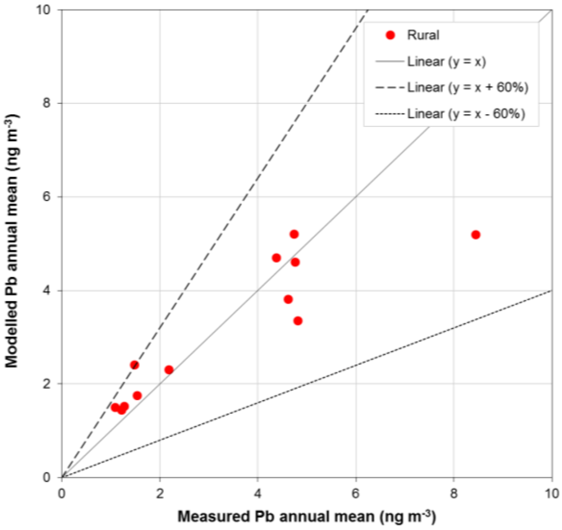


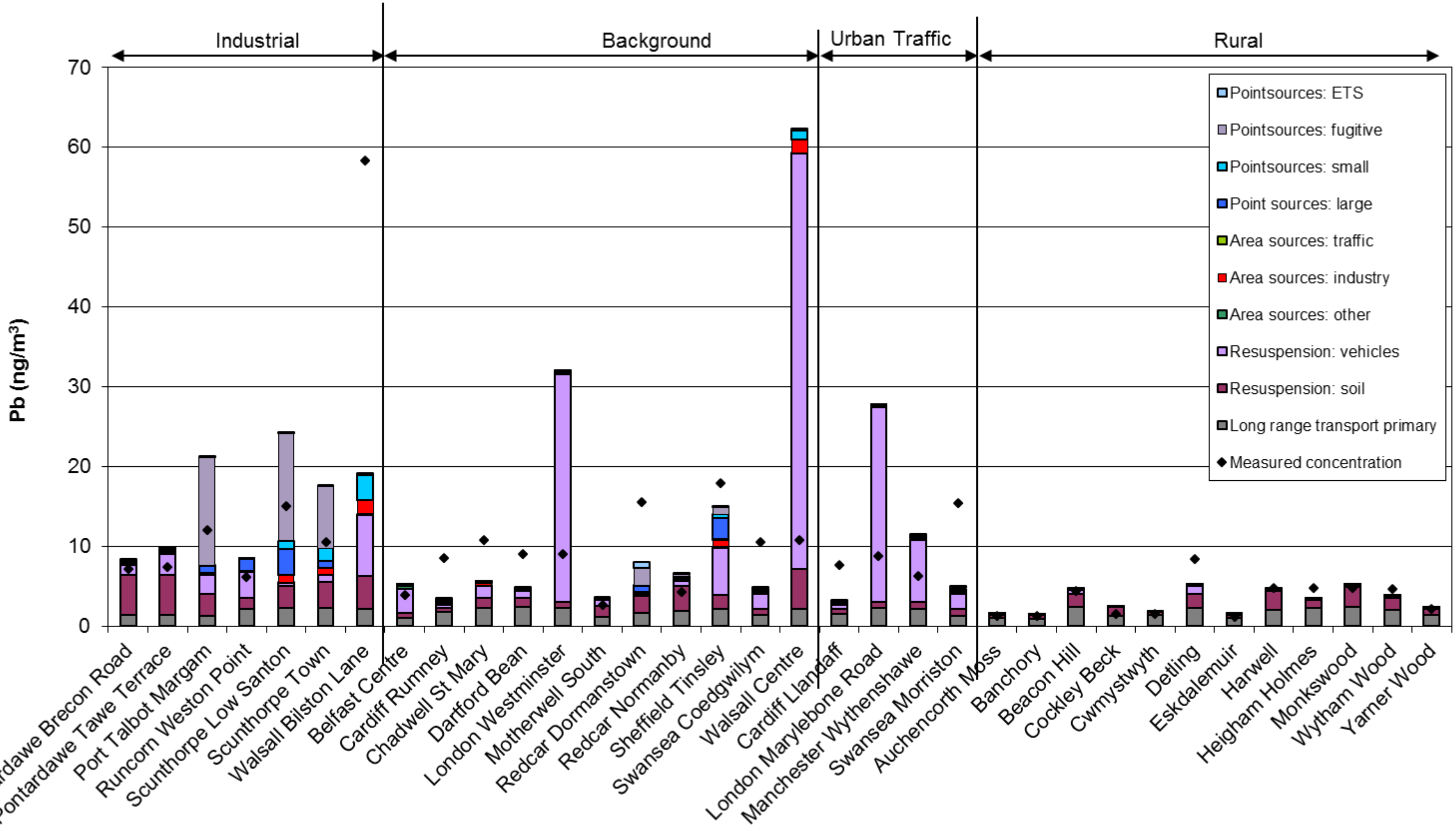
Table 10.10 - Summary statistics for comparison between modelled and measured annual mean Pb concentrations at different monitoring sites, 2013

	Mean of measurements (ng/m^3)	Mean of model estimates (ng/m^3)	R^2	% of sites outside DQO of ±60%	Number of sites in assessment
Industrial sites	16.63	15.48	0.16	57%	7
Urban background sites	9.35	13.71	0.05	27%	11
Roadside sites	9.55	11.74	0.07	75%	4
Rural sites	3.37	3.15	0.80	8%	12

10.7.3 Source apportionment

Figure 10.29 shows the modelled Pb contribution from different sources at monitoring locations. Measured concentrations at the sites are also presented, giving an indication of the level of agreement between modelled and measured concentrations. This analysis suggests that the main sources of lead are emissions from small point and fugitive industrial emissions but predominantly re-suspension processes.

Figure 10.29 - Annual mean Pb source apportionment at monitoring sites in 2013



11 Benzo(a)pyrene

11.1 Introduction

11.1.1 Target values

A single target value (TV) for ambient concentrations of benzo(a)pyrene (B(a)P) is set out in AQDD4. The Directive states that Member States should take all necessary measures not entailing disproportionate costs to ensure that the target value is not exceeded after 31 December 2012. The target value is an annual mean concentration of 1 ng m^{-3}. 2013 is the first year for which the TV is in force.

11.1.2 Annual mean modelling

A map of annual mean B(a)P in 2013 at background locations is shown in Figure 11.1. B(a)P concentrations were modelled for 2005 by Vincent et al. (2007) to inform the UK Preliminary Assessment for AQDD4 (Bush, 2007). 2013 is the sixth year for which a full air quality assessment is required and national modelling of B(a)P has been undertaken in order to assess compliance with the target value set out in the Directive.

The B(a)P annual mean model has been calibrated based on monitoring data from the national network since the 2008 assessment (Yap, 2009). This was a significant change to the modelling methodology over the 2005 assessment (Vincent et al., 2007), and the decision to follow this approach was made to ensure that the model result was representative of the measurements. Particular consideration was given to appropriate application of calibration factors to the model, and for this reason separate calibration factors are derived for the area and point source components of the model. The 2013 assessment follows a similar approach.

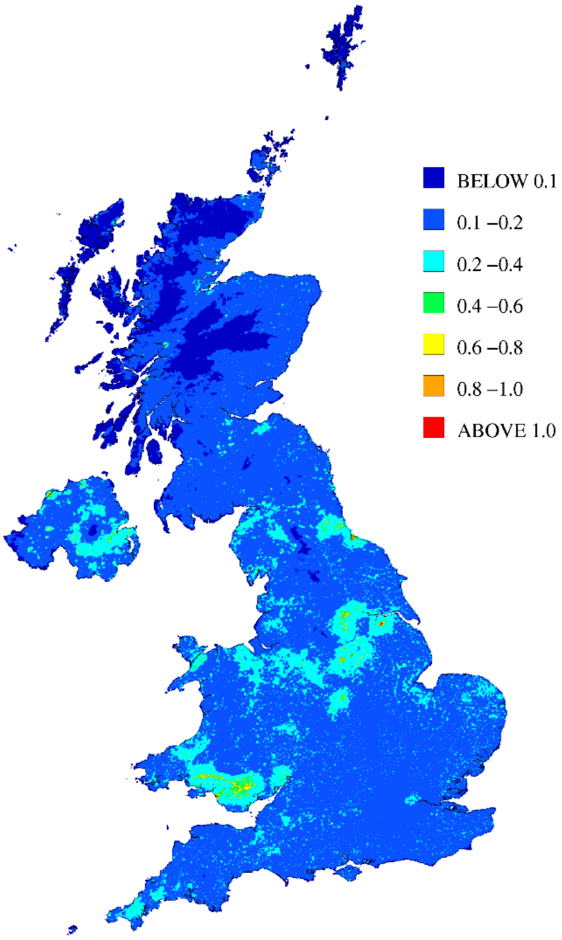
The 1 km x 1 km annual mean background B(a)P concentration map has been calculated by summing the contributions from:

- Large point sources
- Small point sources
- Local area sources
- Point sources with emissions estimates for air quality pollutants based on reported carbon emissions (ETS points)

11.1.3 Chapter structure

This chapter describes modelling work carried out for 2013 to assess compliance with the B(a)P target value described above. Emissions estimates for B(a)P are described in Section 11.2. Section 11.3 describes the B(a)P modelling methods for the annual mean. The modelling results are presented in Section 11.4.

Figure 11.1– Annual mean background B(a)P concentration, 2013 (ng m^{-3})



11.2 Emissions

Estimates of the emissions of B(a)P from the UK National Atmospheric Emissions Inventory 2012 (NAEI 2012) have been used in this study (Passant et al., 2014). Emissions projections have been provided by the NAEI (Passant pers. comm. 2014a) based on DECCs UEP48 energy and emissions projections (DECC, 2013). Figure 11.2 shows UK total B(a)P emissions for 2012 and emissions projections for 2015, 2020, 2025 and 2030 split by SNAP code, with the coding described in Table 3.1. Values for intermediate years have been interpolated in this figure.

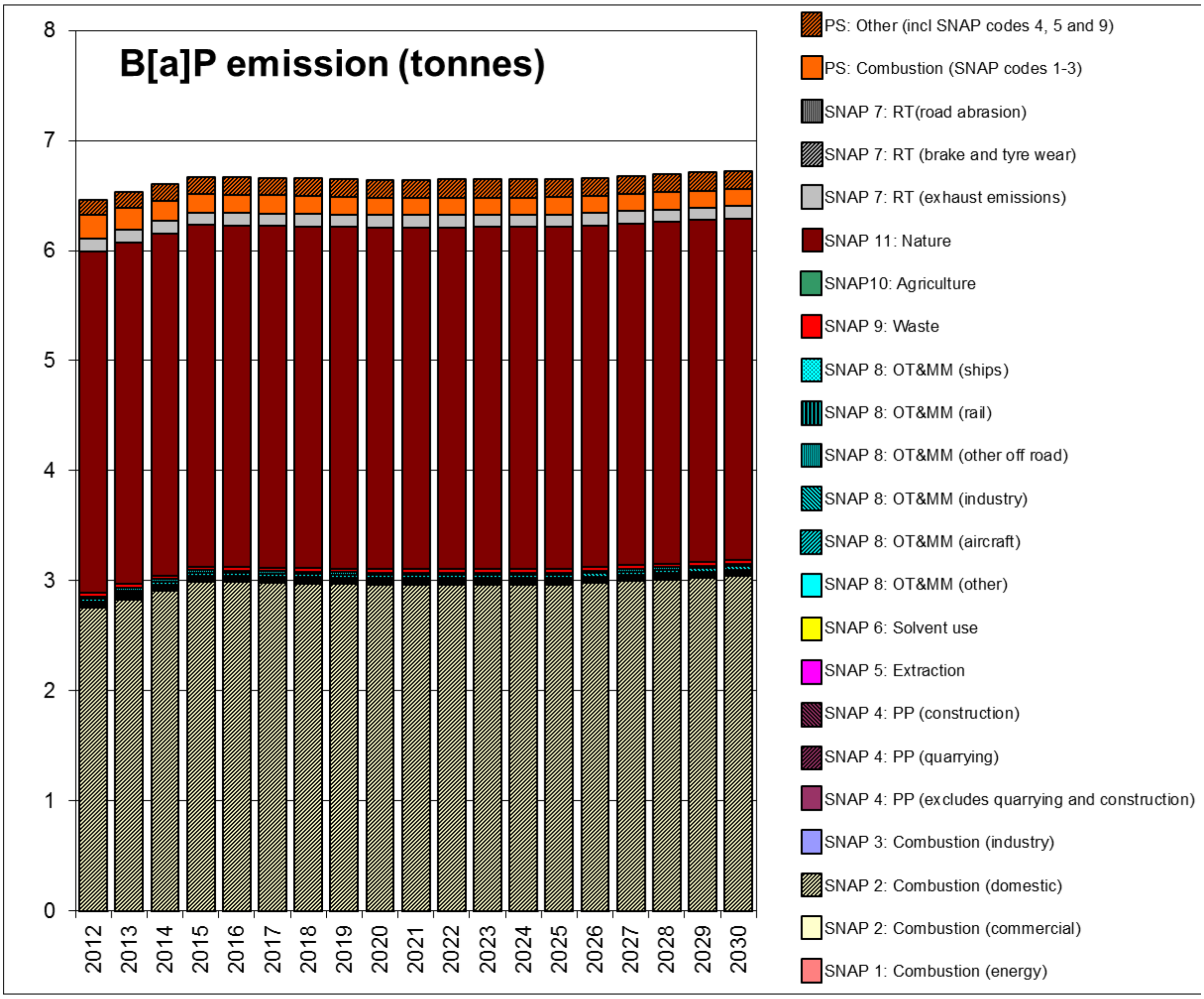
Figure 11.2 shows that emissions from B(a)P are projected to increase steadily from 2012 to 2015 and the remain relatively constant to 2030. The single largest source of B(a)P emissions is SNAP 11: ‘Nature’, which refers to B(a)P emissions from combustion in the natural environment such as forest fires. Despite the relatively high emissions contribution from this source sector, the method for distribution of these emissions used in the NAEI ensures that natural combustion is spread evenly across the UK and does not unduly affect the modelled ambient concentrations in any particular area. The emissions from this source are projected to remain constant through to 2030 and hence do not contribute the projected trend.

Figure 11.2 illustrates another significant source of emission is the combustion of solid fuels for domestic heating. The projected trend in B(a)P emissions to 2030 is largely being driven by the activity in this sector, and the rise in emissions to 2015 results from an increase in wood and coal combustion in the domestic sector in the UEP48 energy projections. The rise in activity is also accompanied by improvements to technology in response to the Renewable Heat Incentive (RHI). The emissions used in the 2013 assessment did not taken into account technological improvements from the RHI however this makes only a marginal difference in 2013; they have a greater impact on the trend in emissions beyond 2013 and the trend shown in the figure takes these improvements into account. Domestic combustion is a particularly important source in some more rural areas where there may be a heavy dependency on solid fuels instead of natural gas due to limitations of the gas supply infrastructure in more remote locations. It is a particularly important source in Northern Ireland where natural gas is less widely available in some areas.

The modelling for 2013 incorporates improvements to the spatial distribution of domestic emissions that have been introduced in the NAEI 2012 emissions maps (Tsagatakis et al., 2014). In previous years the allocation of solid fuel has been performed based upon urban boundaries and population criteria. The revised NAEI 2012 maps contain new information from the 2011 census which includes statistics of central heating fuel type. The inclusion of an additional question about fuel used for heating homes in the 2011 census has provided data previously unavailable to the NAEI and this has led to a more accurate spatial distribution of solid fuel. More information on the data used in the new maps is provided in the latest UK Emissions Methodology report (Tsagatakis et al., 2014).

The emissions inventory provides maps of emissions on a 1 km x 1 km grid, which is likely to be too coarse to incorporate very local variations in emissions from sources such as domestic heating, where there may be considerable in-square variation due to differences in fuel use as recently investigated by Vincent and Tsagatakis (2014).

Figure 11.2 - Total UK B(a)P emissions for 2012 and emissions projections up to 2030 by SNAP code from NAEI 2012



11.3 B(a)P modelling

11.3.1 Contributions from local area sources

11.3.1.1 Introduction

The 2013 area source B(a)P emissions maps have been calculated from the NAEI 2012 emissions maps following the method described in Section 3.3.5, including improved methods first introduced in the 2011 assessment (Brookes et al., 2012) for modelling the contributions to from SNAP 2 (domestic and non-domestic combustion). ADMS derived dispersion kernels have been used to calculate the contribution to ambient B(a)P concentrations on a 1 km x 1 km receptor grid, from the area source emissions within a 33 km x 33 km square surrounding each receptor. Hourly sequential meteorological data from Waddington in 2013 has been used to construct the dispersion kernels, as described in Appendix 4.

11.3.1.2 Area source model calibration

Figure 11.3 shows the calibration of the modelled annual mean area source B(a)P contribution. To compare the uncalibrated area source component from the model against measured concentrations the measured concentrations have been adjusted to represent background (non-industrial) concentrations only i.e. measured concentrations at background stations minus the uncalibrated modelled point source contributions at those locations. To reduce the interdependence of the area source and point source calibrations (see Section 11.3.2.2), those stations where the uncalibrated point source contribution was ≥ 5% were excluded from the area source calibration. To calculate the calibrated area source contribution for each grid square in the country the modelled area source contribution has been multiplied by the fit coefficient of 5.192593.

In contrast to the 2010 and 2011 assessments (Walker et al. (2011), Brookes et al. (2012)), the area source calibration for 2012 included the monitoring stations in Northern Ireland and the 2013 assessment continues this approach. In the 2010 and 2011 assessments the calibration excluded the Northern Ireland monitoring stations on the basis that the comparison of measured and modelled concentrations showed the Northern Ireland stations as outliers. The situation for 2010 and 2011 was attributed to the heavy influence of domestic fuel combustion emissions of B(a)P in Northern Ireland in comparison to the rest of the UK not captured by the emissions inventory – compounded in 2010 by a ‘double winter effect’, reduced in 2011 by the treatment of the time variation of domestic emissions but still present. A specific calibration was therefore applied for 2010 and 2011 to the domestic combustion sector for Northern Ireland. Figure 11.3 shows the Northern Ireland stations are not outliers for 2013, in common with the 2008, 2009 and 2012 assessments (Yap et al. (2009), Walker et al. (2010), Brookes et al. (2013)). Figure 11.4 shows that for 2013 the measured and uncalibrated modelled concentrations resulting from domestic combustion scale consistently with the B(a)P emissions from other sectors. Hence a specific calibration for the domestic sector has not been carried out for 2013.

As part of the calibration process emission caps have been applied to certain sectors; this is because the use of surrogate statistics for mapping area source emissions sometimes results in unrealistically large concentrations in some grid squares for a given sector. The emission caps applied are given in Table 11.1.

Table 11.1 - Emission caps applied to B(a)P sector grids

SNAP code	Description	Cap applied (kg/a/km^2)
SNAP 2 (domestic combustion, coal)	Combustion in Commercial, Institutional & residential & agriculture (domestic only)	0.33
SNAP 2 (domestic combustion, wood)	Combustion in Commercial, Institutional & residential & agriculture (domestic only)	0.33
SNAP 2 (domestic combustion, SSF)	Combustion in Commercial, Institutional & residential & agriculture (domestic only)	0.33

Figure 11.3 - Calibration of area source model for B(a)P

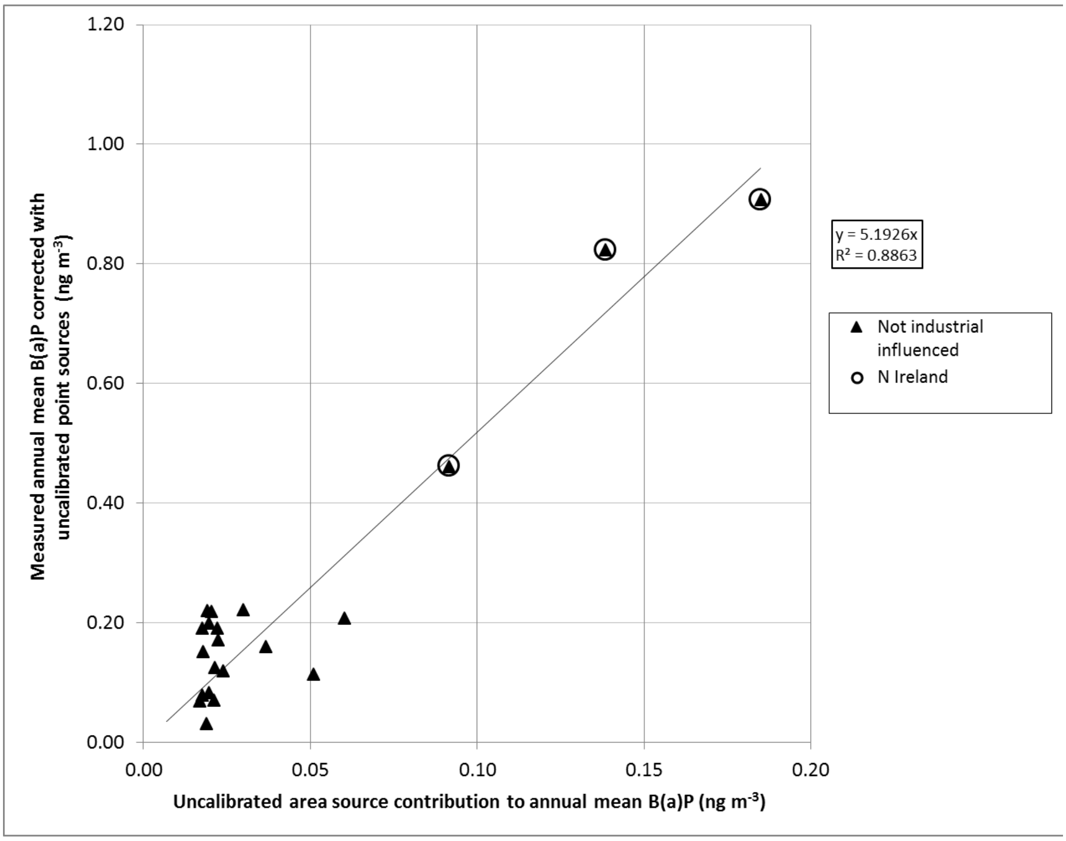
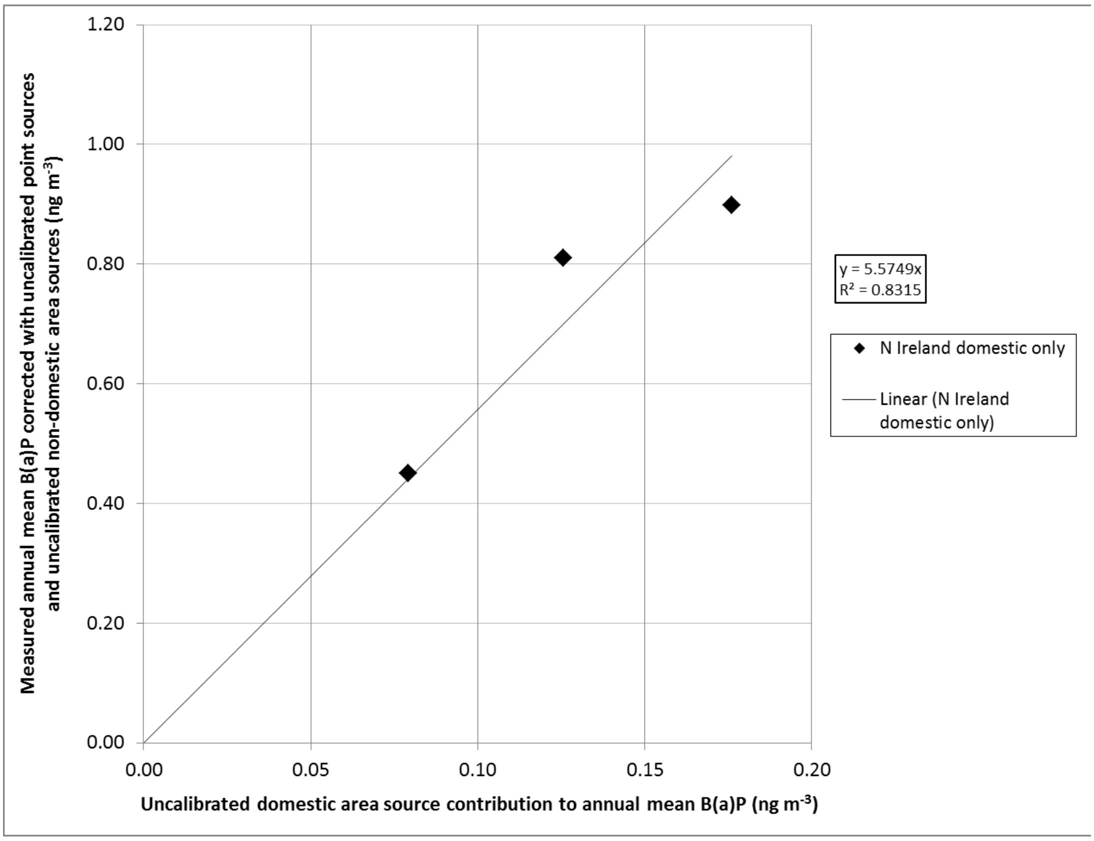


Figure 11.4 - Comparison of area source model for B(a)P domestic emissions in Northern Ireland



11.3.2 Contributions from large and small point sources

11.3.2.1 Introduction

Contributions to ground level annual mean B(a)P concentrations from large point sources (those with annual emissions greater than 0.001 tonnes, or for which emission release characteristics are known) in the NAEI 2012 have been estimated by modelling each source explicitly using the atmospheric dispersion model ADMS 5.0 and sequential meteorological data for 2013 from Waddington. Surface roughness was assumed to be 0.1 m at the dispersion site and 0.1 m at the meteorological site. Concentrations were calculated for a 99 km x 99 km square composed of a regularly spaced 1 km x 1 km resolution receptor grid. Each receptor grid was centred on the point source.

Industrial point sources of B(a)P are either fugitive (as from coking plants) or from clearly defined stacks for other sources. The emission amount is derived either from direct measurement or by emission factors. A total of 122 large points sources were modelled for B(a)P of which 7 were modelled using specifically tailored modelling parameters to accommodate non-standard stack arrangements. These included coke works at Barnsley, Teesside, Port Talbot and Scunthorpe which were all modelled as line sources. The NAEI 2012 emissions for the coking plants were used and where there are multiple coke ovens at a plant, the split in emissions was estimated from data provided by Peter Coleman (personal communication, 2009). For the remaining 115 point sources emissions release information was retrieved from the PCM stack parameters database (described in more detail in Section 3.3.1).

The NAEI emissions for point sources for 2012 were scaled in order to provide values for 2013 as described in Section 3.3.1. Contributions from B(a)P point sources with less than 0.001 tonnes per year emissions and without stack parameters were modelled using an area source approach. In line with the method applied to large point sources the NAEI 2012 emissions for small point sources were scaled to 2013 emissions using the same source sector specific projection factors applied to the large point sources. These emissions were aggregated onto a 1 km x 1 km grid before applying an ADMS 5.0 derived dispersion kernel (for non-domestic, non-road transport) to calculate the contribution to ambient concentrations at a central receptor location from small point source emissions within a 33 km x 33 km square surrounding each receptor. The method used to generate area source dispersion kernels is described in Appendix 4.

In common with the NAEI 2011 additional point source emissions data have been provided in the NAEI 2012. These emissions estimates have been derived from carbon emissions data reported under the EU-Emissions Trading Scheme (ETS), most recently described in Tsagatakis et al. (2014). These point sources are referred to as ETS points in this report. To model the contribution to background annual mean B(a)P concentrations from ETS points the emissions have been treated as an additional set of small point sources. As such they have been modelled using the B(a)P small points approach described above. These derived air quality pollutant emissions estimates are particularly uncertain, hence the emissions for particular sources have been capped at reporting thresholds given by the Scottish Pollutant Release Inventory (SPRI). Typically more than 90% of the ETS points do not exceed the SPRI reporting threshold, which for B(a)P is also 0.001 tonnes per year.

11.3.2.2 Point source model calibration

In order to obtain a model result that was consistent with measured concentrations, the modelled point source contribution (the sum of large, small and ETS point source contributions) was calibrated using monitoring data from the national network. Industrial sites only were used to calibrate the point source contribution (Figure 11.5). In the calibration measured industrial concentrations have been adjusted by subtracting the calibrated modelled area source contribution so that the measured value represented the industrial component only. The uncalibrated modelled point source contribution was multiplied by the fit coefficient (6.903363) to calculate the calibrated point source contribution.

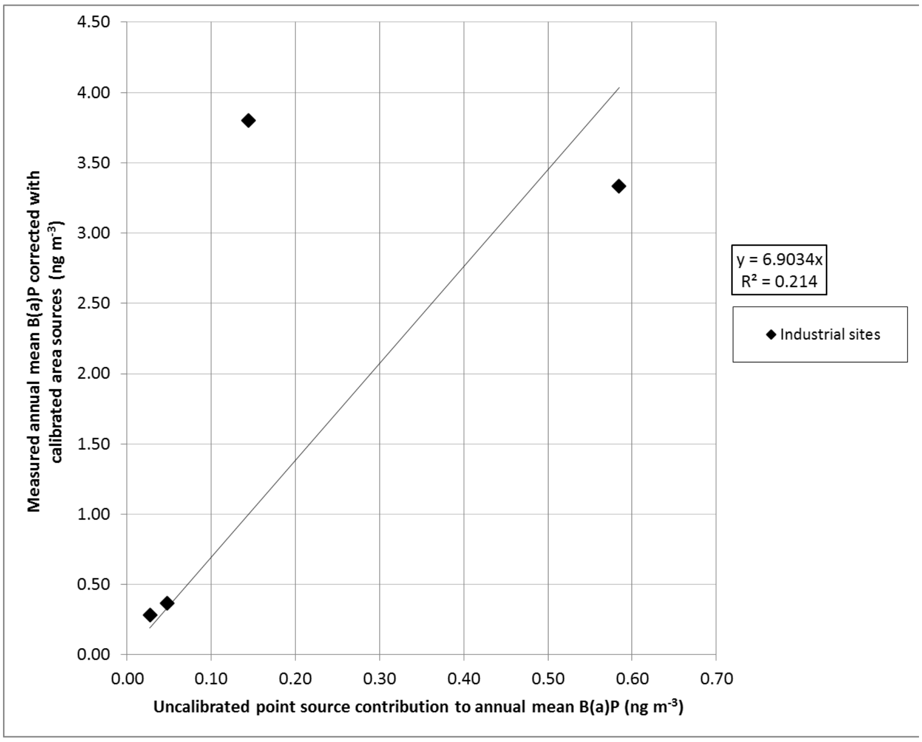
There is an element of circularity involved in the calibration of both area and point sources because the calibration process for each requires the subtraction of the other in order to isolate the component being calibrated. A new approach was introduced to minimise interdependence of the calibrations in the 2012 assessment and this has been carried forward into the 2013 assessment as summarised here:

- The area source component is calibrated first and as discussed in Section 11.3.1.2 only monitoring stations where the uncalibrated point source contribution is < 5%, are included in the area source calibration. This minimises influencing the area source calibration with the point source signal, since the contribution from point sources at non-industrial monitoring sites is typically very small and is guaranteed to be < 5% by the new approach (Brookes et al., 2013).
- In addition monitoring stations where the uncalibrated point source contribution is ≥ 5%, but still relatively low (< 50%) are excluded from the model calibration completely. Data for these stations are still included in the model verification.
- Given the 2 conditions above only monitoring stations where the uncalibrated point source contribution is ≥ 50% of the uncalibrated modelled concentration (area sources plus point sources) are included in the calibration of the point sources.

A multiple regression analysis for all monitoring sites has previously been considered but has been rejected because it tends to over fit to the data and not provide realistic coefficients.

An outlier is visible to the top left of Figure 11.5. This monitoring station (Scunthorpe Town) appears as an outlier in the calibration plot for 2013 as the result of combination of a period of unusual North Easterly winds in March and the location of the site meaning that it was strongly influenced by industrial emissions from nearby steel works to the North East during this period. This station is upwind of these sources for the prevailing wind direction. This period skews the annual mean concentration measured for the site compared to that modelled. The unusual concentrations observed at this monitoring station and the causes have been confirmed with the monitoring network operator (NPL, 2014).

Figure 11.5 - Calibration of point source model for B(a)P



11.4 Results

11.4.1 Verification of mapped values

Figure 11.6, Figure 11.7 and Figure 11.8 present comparisons of modelled and measured annual mean B(a)P concentrations in 2013 at monitoring station locations. These figures include lines to represent the AQDD4 data quality objective for modelled annual mean B(a)P concentrations: y=x-60% and y=x+60% (see Section 1.5).

Figure 11.6 - Verification of annual mean B(a)P at industrial sites

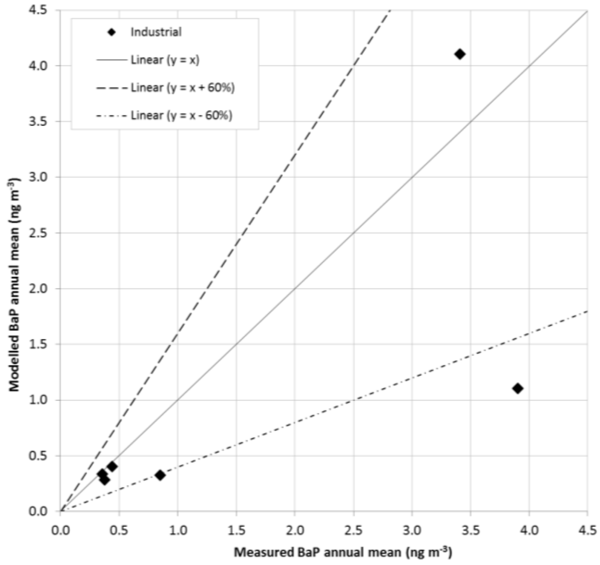


Figure 11.7 - Verification of annual mean B(a)P at urban background sites

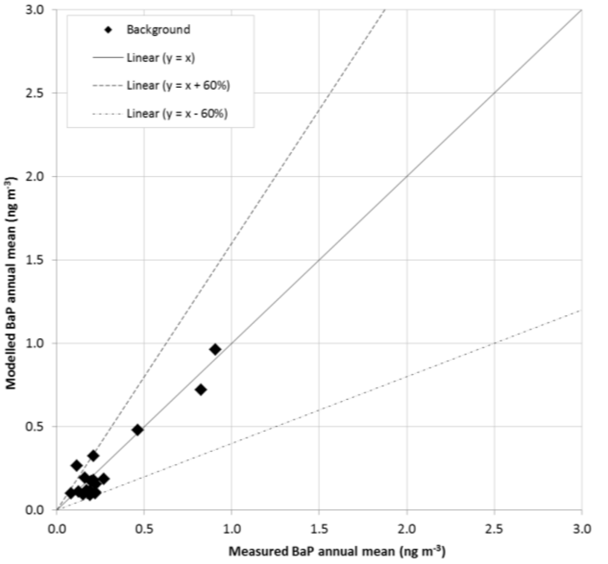
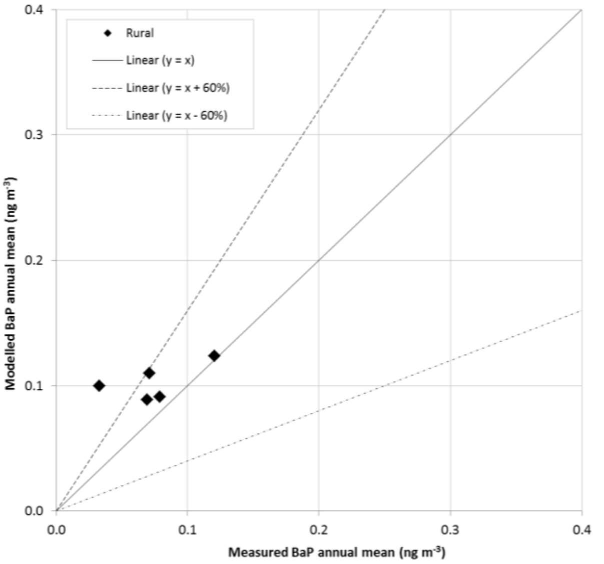


Figure 11.8 - Verification of annual mean B(a)P at rural sites



Summary statistics for modelled and measured B(a)P concentrations are listed in Table 11.2, including the percentage of sites at which modelled concentrations are outside of the data quality objectives (DQOs), and the total number of sites included in the analysis.

The calculated means of measured compared with modelled concentrations are in reasonable agreement for all monitoring stations. The agreement between measured and modelled concentrations at industrial sites is less close than indicated by the agreement in the mean. It is likely that variation of B(a)P concentrations in close proximity to these major sources is not as well represented at the resolution of the model. The R^2 values are high for industrial and urban background sites but poor for rural sites. This is because the model results are principally driven by the calibration process in which industrial and urban background sites are prominent in defining the relationship.

Table 11.2 - Summary statistics for comparison between modelled and measured annual mean B(a)P concentrations at different monitoring sites, 2013

	Mean of measurements (ng/m^3)	Mean of model estimates (ng/m^3)	R^2	% of sites outside DQO of ±60%	Number of sites in assessment
Industrial sites	1.56	1.09	0.50	33%	6
Urban background sites	0.27	0.24	0.89	5%	19
Rural sites	0.07	0.10	0.36	20%	5

11.4.2 Source apportionment

A source apportionment graph has been plotted in Figure 11.9 to present the B(a)P contribution from different sources at monitoring station locations. Measured concentrations at the sites are also presented, giving an indication of the level of agreement between modelled and measured concentrations. Domestic combustion is a significant component of the background at urban non-industrial stations and particularly for those in Northern Ireland. Industry is a significant driver of the background at industrial sites.

11.4.3 Detailed comparison of modelling results with the target value

Results of the assessment in terms of comparisons of the modelled concentrations with the TV have been reported in e-Reporting Data flow G (CDR, 2014).

Exceedances of the 1 ng m^{-3} target value have been modelled for six zones.

Exceedances in the South Wales zone have been associated with domestic combustion in 3 km^2 and with industrial emissions from the steel plant at Port Talbot in 4 km^2. Industrial emissions from the steel plant at Port Talbot are also associated with the 3 km^2 of exceedances in Swansea Urban Area.

There were no zones in exceedance in Northern Ireland during 2013.

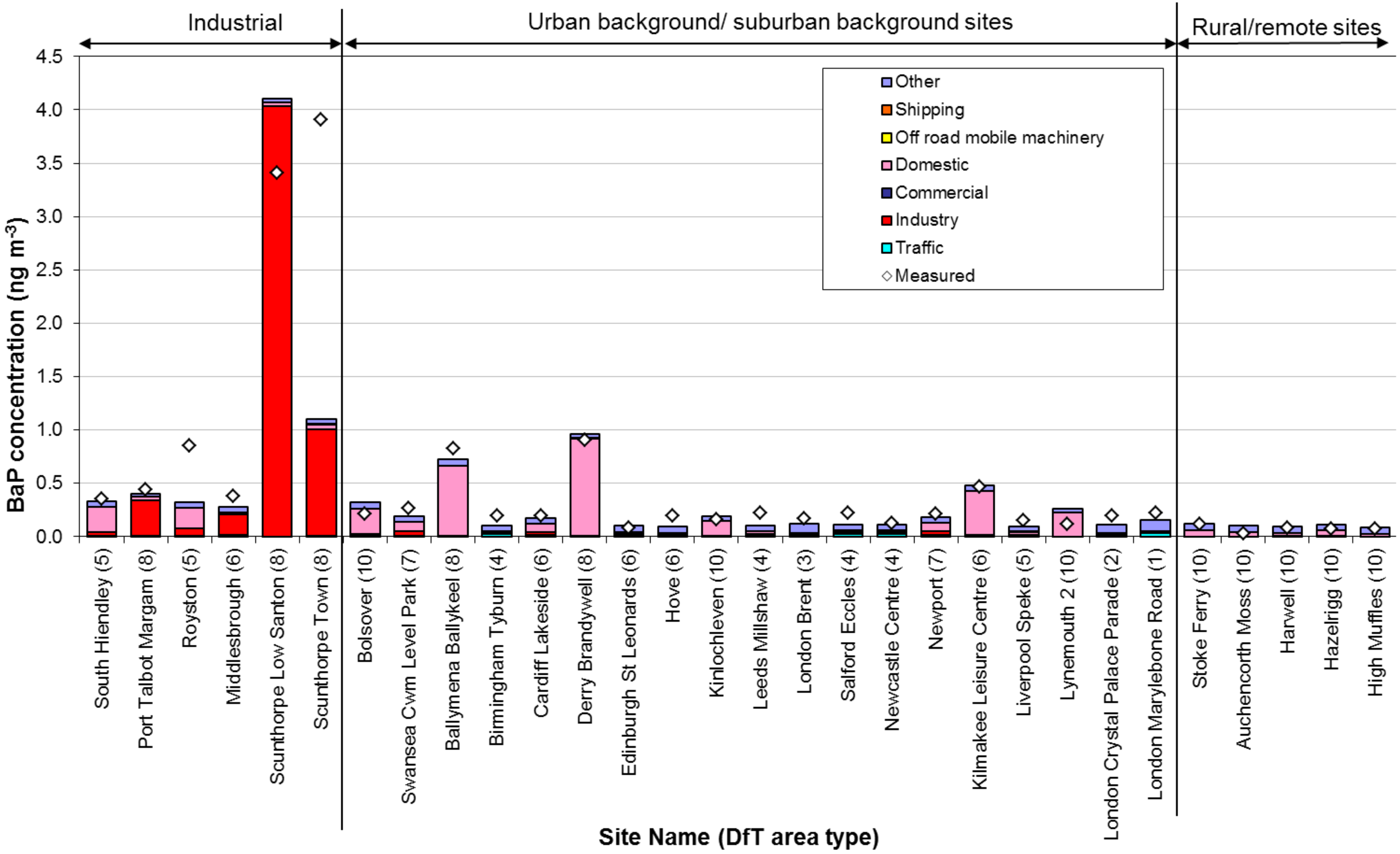
Exceedances in 9 km^2 in the Yorkshire & Humberside zone have been associated with coking operations at Scunthorpe. Exceedance in 1 km^2 has been associated with domestic solid fuel use.

Exceedances in the Teesside Urban Area (4 km^2) and North East zone (4 km^2) have been associated with coking operations at Southbank and Redcar.

Exceedances (2 km^2) in the East Midlands zone have been associated with domestic combustion.

Measured concentrations also exceeded the target value in the Yorkshire & Humberside zone and therefore measured exceedances have been reported for this zone in the air quality assessment.

Figure 11.9 - Annual mean B(a)P source apportionment at background national network monitoring stations in 2013 (the area type of each station is shown in parenthesis after its name)



12 Acknowledgements

This work was funded by the UK Department for Environment, Food and Rural Affairs, Welsh Government, the Scottish Government and the Department of the Environment for Northern Ireland. Permission to include air quality monitoring and site meta data for the verification sites was kindly provided by the Local Authorities whose air quality monitoring stations are listed in Table A1.1 in Appendix 1.

The authors would also like to thank: JEP and AES Northern Ireland for providing SO_2 measurements and emissions information for power stations; Hanson Building Products Limited for providing SO_2 measurements; ERG for providing measurements from the LAQN and other regional monitoring networks and INEOS for providing benzene measurements.

Detailed information and measurements for the monitoring Pontardawe Leisure Centre site was kindly provided by Neath Port Talbot County Borough Council. This monitoring site was included in the analysis for verification of the local scale modelling of Ni concentrations in Pontardawe. The authors would also like to thank the Environment Agency, local authorities and plant operators for helping with the nickel emission data and release characteristics for specific plants.

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Appendices

Appendix 1 – Monitoring sites used to verify the mapped estimates

Table A1.1. Monitoring sites available for verification of the mapped estimates (PM_{10} measurements by gravimetric, TEOM and FDMS instruments were used in the verification)

Sitename	Site type	Network	NO_X, NO_2	PM_{10}	$PM_{2.5}$	SO_2	O_3	Bz
Aylesbury Friarage Road 2	Roadside	AQE	Y					
Aylesbury Stoke Road A413	Roadside	AQE	Y					
Barnsley A628 Pogmoor Roadside	Roadside	AQE	Y					
Barnsley A635 Kendray Roadside	Roadside	AQE	Y					
Barnsley Royston	Urban Industrial	AQE		Y				
Birmingham Airport 2	Airport	AQE	Y	Y		Y	Y	
Cambridge Gonville Place	Roadside	AQE	Y	Y	Y			
Cambridge Montague Road	Roadside	AQE	Y	Y				
Cambridge Parker Street	Roadside	AQE	Y	Y				
Canterbury PM10	Roadside	AQE		Y				
Durham Crossgate	Roadside	AQE	Y					
Gatwick LGW3	Airport	AQE	Y					
Heathrow Green Gates	Airport	AQE	Y	Y	Y			
Heathrow LHR2	Airport	AQE	Y	Y	Y			
Heathrow Oaks Road	Airport	AQE	Y	Y	Y			
Henley	Kerbside	AQE	Y					
Hillingdon 1 - South Ruislip	Roadside	AQE	Y	Y				

Sitename	Site type	Network	NO_X, NO_2	PM_{10}	$PM_{2.5}$	SO_2	O_3	Bz
Hounslow Brentford	Roadside	AQE		Y				
London Hillingdon Harmondsworth	Urban Background	AQE	Y					
London Hillingdon Hayes	Roadside	AQE	Y	Y				
London Hillingdon Oxford Avenue	Urban Centre	AQE	Y	Y				
Manchester Oxford Road	Kerbside	AQE	Y	Y				
Manchester Piccadilly LA	Urban Centre	AQE		Y				
Manchester South SO2	Suburban	AQE				Y		
Oxford High St	Roadside	AQE	Y	Y				
Oxford St Ebbes (Cal Club)	Urban Background	AQE					Y	
S Cambs Impington	Roadside	AQE	Y					
S Cambs Orchard Park School	Urban Background	AQE	Y	Y				
Salford M60	Roadside	AQE	Y	Y				
Sipson	Urban Background	AQE	Y					
Slough Chalvey	Roadside	AQE	Y					
Slough Colnbrook	Urban Background	AQE	Y	Y				
Slough Colnbrook Osiris	Urban Background	AQE		Y	Y			
Slough Lakeside 1 Osiris	Urban Background	AQE		Y	Y			
Slough Lakeside 2	Urban Background	AQE	Y					
Slough Town Centre A4	Urban Background	AQE	Y	Y				
South Bucks Gerrards Cross	Roadside	AQE	Y	Y				
South Holland Westmere School	Rural	AQE	Y	Y			Y	

Sitename	Site type	Network	NO_X, NO_2	PM_{10}	$PM_{2.5}$	SO_2	O_3	Bz
Spalding Monkhouse School	Urban Background	AQE	Y					
Stansted 3	Airport	AQE	Y					
Stansted 4	Airport	AQE	Y					
Stockport Hazel Grove	Roadside	AQE	Y	Y			Y	
Tally Ho	Kerbside	AQE	Y	Y				
Tameside Two Trees School	Urban Background	AQE		Y				
Trafford	Urban Background	AQE	Y	Y				
Trafford A56	Roadside	AQE		Y				
Waltham Forest Leyton	Roadside	AQE	Y					
Warrington Chester Rd	Roadside	AQE	Y					
Warrington Parker St	Roadside	AQE	Y					
Leicester - Abbey Lane	Roadside	ERG	Y					
Leicester - Ely	Roadside	ERG	Y					
Leicester - Glenhills Way	Roadside	ERG	Y					
Leicester - Melton Road	Roadside	ERG	Y					
Leicester - St Matthews Way	Roadside	ERG	Y					
Leicester - Vaughan Way	Roadside	ERG	Y					
New Forest - Fawley	Industrial	Hants network				Y		
New Forest - Holbury	Industrial	Hants network		Y		Y		
New Forest - Lyndhurst	Roadside	Hants network	Y					
New Forest - Totton	Roadside	Hants network	Y	Y				
Southampton - Bitterne	Urban Background	Hants network	Y	Y				

Sitename	Site type	Network	NO_X, NO_2	PM_{10}	$PM_{2.5}$	SO_2	O_3	Bz
Southampton - Onslow Road	Roadside	Hants network	Y					
Southampton - Redbridge	Roadside	Hants network		Y				
Southampton - Victoria Road	Roadside	Hants network	Y					
Hounslow 2 - Cranford	Suburban	Heathrow Airwatch					Y	
Hounslow 4 - Chiswick High Road	Roadside	Heathrow Airwatch	Y	Y				
Hounslow Heston Road	Roadside	Heathrow Airwatch	Y	Y				
Canterbury Military Road	Roadside	Kent & Medway Network	Y					
Canterbury Roadside	Roadside	Kent & Medway Network	Y					
Canterbury St. Peters Place	Roadside	Kent & Medway Network	Y					
Chatham Luton Background	Urban Background	Kent & Medway Network	Y	Y		Y	Y	
Dartford Bean Interchange Roadside	Roadside	Kent & Medway Network	Y	Y				
Dartford St Clements Roadside	Kerbside	Kent & Medway Network	Y	Y				
Dartford Town Centre Roadside	Roadside	Kent & Medway Network	Y	Y				
Dover Centre Roadside	Roadside	Kent & Medway Network		Y				
Gravesham A2 Roadside	Roadside	Kent & Medway Network	Y	Y				

Sitename	Site type	Network	NO_X, NO_2	PM_{10}	$PM_{2.5}$	SO_2	O_3	Bz
Gravesham Industrial Background	Urban Background	Kent & Medway Network	Y	Y				
Maidstone A229 Kerbside	Kerbside	Kent & Medway Network	Y	Y				
Maidstone Rural	Rural	Kent & Medway Network	Y	Y				
Swale Canterbury Road	Roadside	Kent & Medway Network	Y					
Swale Newington 3	Roadside	Kent & Medway Network	Y					
Swale Ospringe Roadside 2	Roadside	Kent & Medway Network	Y	Y				
Swale St Pauls Street	Urban	Kent & Medway Network	Y					
Thanet Airport	Urban Background	Kent & Medway Network	Y					
Thanet Birchington Roadside	Roadside	Kent & Medway Network	Y	Y				
Thanet Ramsgate Roadside	Roadside	Kent & Medway Network	Y					
Tonbridge Roadside 2	Roadside	Kent & Medway Network	Y					
Tunbridge Wells A26 Roadside	Roadside	Kent & Medway Network	Y	Y				
Barking and Dagenham - Rush Green	Suburban	LAQN	Y			Y		
Bexley - Belvedere	Suburban	LAQN	Y	Y				
Bexley - Belvedere FDMS	Suburban	LAQN		Y				

Sitename	Site type	Network	NO_X, NO_2	PM_{10}	$PM_{2.5}$	SO_2	O_3	Bz
Bexley - Belvedere West	Urban Background	LAQN	Y	Y			Y	
Bexley - Belvedere West FDMS	Urban Background	LAQN		Y				
Bexley - Erith	Industrial	LAQN	Y	Y	Y			
Bexley - Manor Road East Gravimetric	Industrial	LAQN		Y				
Bexley - Manor Road West Gravimetric	Industrial	LAQN		Y				
Brent - Ikea	Roadside	LAQN		Y				
Brent - John Keble Primary School	Roadside	LAQN		Y				
Brent - Neasden Lane	Industrial	LAQN	Y	Y				
Brentwood - Brentwood Town Hall	Urban Background	LAQN	Y					
Camden - Euston Road	Roadside	LAQN	Y					
Camden - Shaftesbury Avenue	Roadside	LAQN	Y	Y				
Castle Point - Hadleigh	Roadside	LAQN	Y			Y		
City of London - Beech Street	Roadside	LAQN	Y	Y				
City of London - Sir John Cass School	Urban Background	LAQN	Y	Y				
City of London - Upper Thames Street	Roadside	LAQN		Y				
City of London - Walbrook Wharf	Roadside	LAQN	Y					
Crawley - Gatwick Airport	Urban Background	LAQN	Y					
Croydon - George Street	Roadside	LAQN	Y	Y				
Croydon - Norbury	Kerbside	LAQN	Y					

Sitename	Site type	Network	NO_X, NO_2	PM_{10}	$PM_{2.5}$	SO_2	O_3	Bz
Croydon - Purley Way A23	Roadside	LAQN	Y					
Dacorum - High Street Northchurch	Roadside	LAQN	Y					
Ealing - Hanger Lane Gyratory	Roadside	LAQN	Y	Y				
Ealing - Horn Lane	Industrial	LAQN	Y					
Ealing - Horn Lane TEOM	Industrial	LAQN		Y				
Ealing - Southall	Urban Background	LAQN	Y	Y			Y	
Ealing - Southall Railway	Roadside	LAQN	Y	Y				
Ealing - Western Avenue	Roadside	LAQN	Y	Y				
Eastbourne - Devonshire Park	Urban Background	LAQN	Y				Y	
Enfield - Bush Hill Park	Suburban	LAQN	Y					
Enfield - Derby Road	Roadside	LAQN	Y	Y		Y		
Enfield - Prince of Wales School	Urban Background	LAQN	Y					
Greenwich - A206 Burrage Grove	Roadside	LAQN	Y					
Greenwich - Blackheath	Roadside	LAQN	Y	Y				
Greenwich - Fiveways Sidcup Rd A20	Roadside	LAQN	Y					
Greenwich - Millennium Village	Industrial	LAQN	Y	Y	Y			
Greenwich - Plumstead High Street	Roadside	LAQN	Y		Y		Y	
Greenwich - Trafalgar Road	Roadside	LAQN	Y	Y				
Greenwich - Westhorne Avenue	Roadside	LAQN	Y	Y	Y		Y	

Sitename	Site type	Network	NO_X, NO_2	PM_{10}	$PM_{2.5}$	SO_2	O_3	Bz
Greenwich - Woolwich Flyover	Roadside	LAQN	Y	Y			Y	
Greenwich and Bexley - Falconwood	Roadside	LAQN	Y				Y	
Greenwich and Bexley - Falconwood FDMS	Roadside	LAQN			Y			
Hackney - Old Street	Roadside	LAQN	Y	Y			Y	
Harrow - Pinner Road	Roadside	LAQN	Y	Y				
Havering - Rainham	Roadside	LAQN	Y					
Havering - Romford	Roadside	LAQN	Y	Y				
Hounslow and Ealing - Gunnersbury Avenue	Roadside	LAQN	Y	Y				
Islington - Arsenal	Urban Background	LAQN	Y	Y				
Islington - Holloway Road	Roadside	LAQN	Y					
Kensington and Chelsea - Cromwell Road	Roadside	LAQN		Y	Y			
Kensington and Chelsea - Earls Court Rd	Kerbside	LAQN	Y	Y				
Kensington and Chelsea - Kings Road	Roadside	LAQN	Y					
Kensington and Chelsea - Knightsbridge	Roadside	LAQN	Y					
Lewisham - Catford	Urban Background	LAQN	Y			Y	Y	
Lewisham - Loampit Vale	Roadside	LAQN	Y	Y				
Lewisham - Mercury Way	Industrial	LAQN		Y				

Sitename	Site type	Network	NO_X, NO_2	PM_{10}	$PM_{2.5}$	SO_2	O_3	Bz
Lewisham - New Cross	Roadside	LAQN	Y			Y		
Merton - Merton Road	Roadside	LAQN		Y				
Merton - Morden Civic Centre	Roadside	LAQN	Y					
Mole Valley - Dorking	Urban Background	LAQN	Y	Y				
Redbridge - Gardner Close	Roadside	LAQN	Y	Y				
Redbridge - Perth Terrace	Urban Background	LAQN	Y	Y			Y	
Richmond Upon Thames - Barnes Wetlands	Suburban	LAQN	Y	Y			Y	
Richmond Upon Thames - Castlenau	Roadside	LAQN	Y	Y				
Richmond Upon Thames - Hanworth Road	Kerbside	LAQN	Y	Y			Y	
Rother - De La Warr Road	Roadside	LAQN	Y	Y				
Sevenoaks - Bat and Ball	Roadside	LAQN	Y	Y				
Sevenoaks - Greatness Park	Urban Background	LAQN	Y	Y			Y	
Southwark - Elephant and Castle	Urban Background	LAQN	Y	Y			Y	
Sutton - Beddington Lane	Industrial	LAQN	Y	Y				
Sutton - Carshalton	Suburban	LAQN	Y				Y	
Sutton - Worcester Park	Kerbside	LAQN	Y					
Thurrock - Calcutta Road Tilbury	Roadside	LAQN	Y			Y		
Thurrock - London Road (Purfleet)	Roadside	LAQN	Y	Y				
Tower Hamlets - Blackwall	Roadside	LAQN	Y				Y	

Sitename	Site type	Network	NO_X, NO_2	PM_{10}	$PM_{2.5}$	SO_2	O_3	Bz
Tower Hamlets - Victoria Park	Urban Background	LAQN	Y	Y		Y		
Wandsworth - Battersea	Roadside	LAQN	Y	Y				
Wandsworth - Putney	Urban Background	LAQN	Y					
Wandsworth - Putney High Street	Kerbside	LAQN	Y					
Wandsworth - Putney High Street Facade	Roadside	LAQN	Y					
Wandsworth - Wandsworth Town Hall	Urban Background	LAQN	Y			Y	Y	
Westminster - Oxford Street	Kerbside	LAQN	Y	Y				
Windsor and Maidenhead - Clarence Road	Roadside	LAQN	Y					
Windsor and Maidenhead - Frascati Way	Roadside	LAQN	Y					
Worthing - Grove Lodge	Roadside	LAQN	Y					
Ballymena North Road	Roadside	NIAUN	Y					
Belfast Newtownards Road	Roadside	NIAUN	Y					
Belfast Stockmans Lane	Roadside	NIAUN	Y	Y				
Belfast Westlink Roden Street	Roadside	NIAUN	Y	Y				
Castlereagh Dundonald	Roadside	NIAUN	Y					
Derry Marlborough Street	Kerbside	NIAUN	Y					
Downpatrick Roadside	Roadside	NIAUN	Y					
Lisburn Dunmurry Seymour Hill	Urban Background	NIAUN				Y		

Sitename	Site type	Network	NO_X, NO_2	PM_{10}	$PM_{2.5}$	SO_2	O_3	Bz
Londonderry Dales Corner	Roadside	NIAUN	Y					
Newry Canal Street	Roadside	NIAUN	Y	Y				
Newry Monaghan Row	Urban Background	NIAUN		Y				
Newry Trevor Hill	Roadside	NIAUN		Y				
Newtownabbey Antrim Road	Roadside	NIAUN	Y					
North Down Holywood A2	Roadside	NIAUN	Y	Y				
Strabane Springhill Park	Urban Background	NIAUN		Y		Y		
Glasgow Waulkmillglen Reservoir	Rural	SARN	Y	Y			Y	
Aberdeen Anderson Dr	Roadside	SAUN	Y	Y				
Aberdeen King Street	Roadside	SAUN	Y	Y				
Aberdeen Market Street 2	Roadside	SAUN	Y	Y				
Aberdeen Wellington Road	Roadside	SAUN	Y	Y				
Alloa	Roadside	SAUN		Y				
Dundee Broughty Ferry Road	Urban Industrial	SAUN		Y		Y		
Dundee Lochee Road	Kerbside	SAUN	Y	Y				
Dundee Mains Loan	Urban Background	SAUN		Y				
Dundee Meadowside	Roadside	SAUN	Y	Y				
Dundee Seagate	Kerbside	SAUN	Y	Y				
Dundee Union Street	Roadside	SAUN	Y	Y				
Dundee Whitehall Street	Roadside	SAUN	Y					
East Ayrshire Kilmarnock John Finnie St	Roadside	SAUN	Y					

Sitename	Site type	Network	NO_X, NO_2	PM_{10}	$PM_{2.5}$	SO_2	O_3	Bz
East Dunbartonshire Bearsden	Roadside	SAUN	Y					
East Dunbartonshire Bishopbriggs	Roadside	SAUN	Y					
East Dunbartonshire Kirkintilloch	Roadside	SAUN	Y	Y				
East Dunbartonshire Milngavie	Roadside	SAUN	Y	Y				
East Lothian Musselburgh N High St	Roadside	SAUN	Y	Y				
East Renfrewshire Sheddens	Roadside	SAUN		Y				
Edinburgh Currie	Suburban	SAUN	Y					
Edinburgh Glasgow Road	Roadside	SAUN	Y	Y				
Edinburgh Gorgie Road	Roadside	SAUN	Y					
Edinburgh Queen Street	Roadside	SAUN	Y	Y				
Edinburgh Queensferry Road	Roadside	SAUN		Y				
Edinburgh Salamander St	Roadside	SAUN	Y	Y				
Edinburgh St Johns Road	Kerbside	SAUN	Y					
Falkirk Banknock	Roadside	SAUN		Y				
Falkirk Grangemouth MC	Urban Background	SAUN	Y	Y		Y		
Falkirk Haggs	Roadside	SAUN	Y	Y				
Falkirk Hope St	Roadside	SAUN	Y			Y		
Falkirk Park St	Roadside	SAUN	Y	Y		Y		
Falkirk West Bridge Street	Roadside	SAUN	Y	Y				
Fife Cupar	Roadside	SAUN	Y					
Fife Dunfermline	Roadside	SAUN	Y	Y				

Sitename	Site type	Network	NO_X, NO_2	PM_{10}	$PM_{2.5}$	SO_2	O_3	Bz
Fife Kirkcaldy	Roadside	SAUN	Y	Y				
Fife Rosyth	Roadside	SAUN	Y	Y				
Glasgow Abercromby Street	Roadside	SAUN		Y				
Glasgow Anderston	Urban Background	SAUN	Y	Y		Y		
Glasgow Burgher St.	Roadside	SAUN	Y	Y				
Glasgow Byres Road	Roadside	SAUN	Y					
Glasgow Dumbarton Road	Roadside	SAUN	Y	Y				
Inverclyde Greenock Dunlop Street	Roadside	SAUN	Y					
N Lanarkshire Chapelhall	Roadside	SAUN	Y	Y				
N Lanarkshire Coatbridge Whifflet	Urban Background	SAUN		Y				
N Lanarkshire Croy	Roadside	SAUN	Y	Y		Y		
N Lanarkshire Moodiesburn	Roadside	SAUN	Y	Y				
N Lanarkshire Motherwell	Roadside	SAUN		Y				
N Lanarkshire Shawhead Coatbridge	Roadside	SAUN	Y	Y				
North Ayrshire Irvine High St	Kerbside	SAUN	Y					
North Lanarkshire Cumbernauld	Roadside	SAUN	Y	Y		Y		
Paisley Central Road	Roadside	SAUN	Y					
Paisley Glasgow Airport	Airport	SAUN	Y					
Paisley St James St	Roadside	SAUN		Y				
Perth Atholl Street	Roadside	SAUN	Y	Y				
Perth Crieff	Roadside	SAUN	Y	Y				

Sitename	Site type	Network	NO_X, NO_2	PM_{10}	$PM_{2.5}$	SO_2	O_3	Bz
Perth High Street	Roadside	SAUN	Y	Y				
Perth Muirton	Urban Background	SAUN		Y				
South Ayrshire Ayr Harbour	Roadside	SAUN	Y					
South Ayrshire Ayr High St	Roadside	SAUN	Y	Y				
South Lanarkshire East Kilbride	Roadside	SAUN		Y				
South Lanarkshire Hamilton	Roadside	SAUN	Y					
South Lanarkshire Lanark	Roadside	SAUN	Y					
South Lanarkshire Raith Interchange	Roadside	SAUN	Y					
South Lanarkshire Rutherglen	Roadside	SAUN	Y	Y				
South Lanarkshire Uddingston	Roadside	SAUN	Y					
Stirling Craigs Roundabout	Roadside	SAUN	Y	Y				
West Dunbartonshire Clydebank	Roadside	SAUN	Y					
West Lothian Broxburn	Roadside	SAUN	Y	Y				
West Lothian Linlithgow High Street	Roadside	SAUN	Y					
West Lothian Newton	Roadside	SAUN	Y					
Chichester - A27 Chichester Bypass	Roadside	Sussex network	Y	Y				
Chichester - Orchard Street	Roadside	Sussex network	Y					
Horsham - Cowfold	Roadside	Sussex network	Y					
Horsham - Park Way	Roadside	Sussex network	Y	Y				

Sitename	Site type	Network	NO_X, NO_2	PM_{10}	$PM_{2.5}$	SO_2	O_3	Bz
Lewes - West Street	Roadside	Sussex network	Y	Y				
Reigate and Banstead - Horley South	Suburban	Sussex network	Y					
Reigate and Banstead - Poles Lane	Rural	Sussex network	Y				Y	
Caerphilly Blackwood High Street	Roadside	WAQN	Y	Y				
Caerphilly White Street	Urban Centre	WAQN	Y	Y				
Cimla Road / Victoria Gardens	Roadside	WAQN	Y					
Hafodyrynys	Kerbside	WAQN	Y					
Marchlyn Mawr	Remote	WAQN	Y					
Nantgarw Road	Roadside	WAQN	Y	Y				
Newport M4 Junction 25	Roadside	WAQN	Y				Y	
Pontardawe Swansea Road	Roadside	WAQN	Y					
Port Talbot Docks	Urban Background	WAQN		Y				
Port Talbot Dyffryn School	Urban Background	WAQN		Y				
Port Talbot Little Warren	Urban Industrial	WAQN		Y				
Port Talbot Prince Street	Urban Industrial	WAQN		Y				
Port Talbot Prince Street (FDMS only)	Urban Industrial	WAQN		Y				
Port Talbot Talbot Road	Roadside	WAQN		Y				
Port Talbot Theodore Road	Roadside	WAQN		Y				
Port Talbot Twll-yn-y-Wal Park	Roadside	WAQN		Y				

Sitename	Site type	Network	NO_X, NO_2	PM_{10}	$PM_{2.5}$	SO_2	O_3	Bz
Rhondda Pontypridd Gelliwastad Rd	Roadside	WAQN	Y					
Rhondda-Cynon-Taf Broadway	Roadside	WAQN	Y					
Swansea Cwm Level Park	Urban Background	WAQN	Y				Y	
Swansea Hafod DOAS	Roadside	WAQN	Y				Y	
Swansea Morriston Roadside	Roadside	WAQN	Y				Y	
Swansea St Thomas DOAS	Roadside	WAQN	Y			Y	Y	
Twynyrodyn	Urban Industrial	WAQN		Y	Y			
V Glamorgan Dinas Powys Roadside	Roadside	WAQN	Y					
V Glamorgan Fonmon	Rural	WAQN	Y	Y		Y	Y	
Wrexham Isycoed	Urban Industrial	WAQN	Y			Y		

Table A1.2 lists the air quality monitoring network name, including URL, containing the sites used to verify the 2013 model output of the pollutants given in Table A1.2. Table A1.3 lists the additional monitoring sites, operated by JEP (RWE-NPOWER) and Hanson Building Products Ltd., which are used to verify the SO_2 models.

Table A1.2 Air quality monitoring network and URL

Air quality monitoring network/data provider	Abbreviation	URL
AQE	AQE	http://www.airqualityengland.co.uk/
Kent & Medway Network		http://www.kentair.org.uk/index.php
Welsh Air Quality Network	WAQN	http://www.welshairquality.co.uk/index.php
Heathrow Airwatch		http://www.heathrowairwatch.org.uk/
London Air Quality Network	LAQN	http://www.londonair.org.uk/LondonAir/Default.aspx
Northern Ireland Automatic Urban Network	NIAUN	http://www.airqualityni.co.uk/index.php?site_id=ND1&t_action=info
Scottish Automatic Rural	SARN	http://www.scottishairquality.co.uk/
Scottish Automatic Urban	SAUN	http://www.scottishairquality.co.uk/
Sussex Network		http://www.sussex-air.net/
Hants Network		http://www.hantsair.org.uk/
ERG		*

***** Data provided by King's College London Environmental Research Group (ERG) (Green, 2014)

Table A1.3 Additional monitoring sites used to verify the SO_2 models

Site	Data supplier
Bentley Hall Farm	JEP (RWE-NPOWER)
Bexleyheath	JEP (RWE-NPOWER)
Blair Mains	JEP (RWE-NPOWER)
Bottesford	JEP (RWE-NPOWER)
Carr Lane	JEP (RWE-NPOWER)
Font-y-Gary	JEP (RWE-NPOWER)
Northfleet	JEP (RWE-NPOWER)
Park Farm	JEP (RWE-NPOWER)
Ruddington	JEP (RWE-NPOWER)
Stile Cop Cemetery	JEP (RWE-NPOWER)
Thorney	JEP (RWE-NPOWER)
West Bank	JEP (RWE-NPOWER)
West Thurrock	JEP (RWE-NPOWER)
Bradley Fen	Hanson Building Products Limited
Whittlesey	Hanson Building Products Limited

Appendix 2 – Monitoring sites for As, Cd, Ni, Pb and B(a)P

The monitoring stations operating during 2013 for the purpose of AQD and AQDD4 reporting have been listed within e-Reporting Data flow C (Assessment Regimes), which can be found on the CDR (CDR, 2014). A summary of the annual mean As, Cd, Ni, Pb and B(a)P measurements used for calibrating and verifying the modelling used in the assessment are provided here.

Heavy Metal Monitoring sites

2013 annual mean concentrations of As, Cd, Ni and Pb are presented in Table A2.1 for rural and urban heavy metal monitoring sites where data capture was at least 75%. The mass concentrations presented are rounded to two significant figures.

Table A2.1 Summary of urban and rural heavy metal mass concentrations, 2013

EoI code	Site name	Site type*	Annual mean (ng m^{-3})				%dc
			As	Cd	Ni	Pb	
GB0048R	Auchencorth Moss	RB	0.21	0.025	0.29	1.3	90.4
GB0091R	Banchory	RB	0.23	0.035	0.26	1.2	97.5
GB0855A	Beacon Hill	RB	0.52	0.092	0.63	4.4	93.6
GB0567A	Belfast Centre	UB	0.37	0.10	1.0	3.9	94.5
GB0369A	Cardiff Llandaff	UT	0.69	0.21	1.1	7.7	100
GB0984A	Cardiff Rumney	UB	0.74	0.23	0.83	8.5	100
GB0985A	Chadwell St Mary	UB	0.80	0.21	2.0	11	100
GB0853A	Cockley Beck	RB	0.23	0.032	0.40	1.5	97.7
GB0854A	Cwmystwyth	RB	0.24	0.038	0.37	1.5	79.9
GB0986A	Dartford Bean	UB	0.71	0.16	1.5	9.0	98.6
GB0886A	Detling	RB	0.82	0.27	1.4	8.4	98.5
GB0002R	Eskdalemuir	RB	0.12	0.029	0.32	1.1	98.3
GB0036R	Harwell	RB	0.62	0.096	0.79	4.8	100
GB0017R	Heigham Holmes	RB	0.67	0.12	1.4	4.8	89.3
GB0682A	London Marylebone	UT	0.84	0.17	2.2	8.8	98.1
GB0743A	London Westminster	UB	0.83	0.16	1.4	9.0	100
GB0370A	Manchester	UT	0.74	0.12	1.5	6.3	96.2
GB0856A	Monkswood	RB	0.54	0.11	0.77	4.7	93
GB1003A	Motherwell South	UB	0.30	0.090	0.56	2.6	100
GB1015A	Pontardawe Brecon	SI	0.89	0.19	5.7	7.1	97.6
GB1016A	Pontardawe Tawe	UI	0.58	0.24	37	7.4	98.1
GB0906A	Port Talbot Margam	UI	0.58	0.89	1.5	12	100
GB1021A	Redcar Dormanstown	SB	0.76	0.38	2.4	16	100
GB0980A	Redcar Normanby	UB	0.39	0.12	0.51	4.3	98.1
GB0877A	Runcorn Weston Point	UI	0.63	0.11	1.6	6.1	97.8
GB1004A	Scunthorpe Low Santon	UI	0.74	0.20	1.7	15	90.4
GB0841A	Scunthorpe Town	UI	0.69	0.14	1.26	11	96.2
GB0538A	Sheffield Tinsley	UB	0.84	0.32	14.14	18	81.5

EoI code	Site name	Site type*	Annual mean (ng m^{-3})				%dc
			As	Cd	Ni	Pb	
GB0981A	Swansea Coedgwilym	UB	0.62	0.22	7.78	11	100
GB0979A	Swansea Morriston	UT	0.83	0.51	6.51	15	100
GB0983A	Walsall Bilston Lane	UI	0.93	1.9	2.18	58	99.6
GB0382A	Walsall Centre	UB	0.96	0.32	1.07	11	90.7
GB0858A	Wytham Wood	RB	0.57	0.096	0.67	4.6	100
GB0013R	Yarner Wood	RB	0.41	0.055	0.70	2.2	97.7

*RB = Rural Background, UB = Urban Background, UT = Urban Traffic, UI = Urban Industrial, SB = Suburban Background.

B(a)P Monitoring sites

2013 annual B(a)P mean concentrations are presented in Table A2.2 for those sites where data capture was at least 75%. The mass concentrations presented are rounded to two significant figures. All measurements were obtained using Digitel DHA-80 samplers.

Table A2.2 Summary of B(a)P mass concentrations, 2013

EoI code	Site name	Site type*	Annual mean B(a)P, ng/m^3	%dc
GB0048R	Auchencorth Moss	RB	0.033	91.5
GB0934A	Ballymena Ballykeel	UB	0.82	100
GB0851A	Birmingham Tyburn	UB	0.20	97.8
GB0700A	Bolsover	UB	0.21	100
GB0869A	Cardiff Lakeside	UB	0.20	100
GB0944A	Derry Brandywell	UB	0.91	97
GB0839A	Edinburgh St Leonards	UB	0.084	100
GB0036R	Harwell	RB	0.079	100
GB0702A	Hazelrigg	RB	0.071	100
GB0014R	High Muffles	RB	0.069	87.1
GB0850A	Hove	UB	0.19	91.5
GB1023A	Kilmakee Leisure Centre	UB	0.46	96.2
GB0705A	Kinlochleven	UB	0.16	100
GB0867A	Leeds Millshaw	UB	0.22	86.3
GB0777A	Liverpool Speke	UI	0.15	99.7
GB0849A	London Brent	UB	0.17	100
GB0847A	London Crystal Palace Parade	UT	0.19	86.9
GB0682A	London Marylebone Road	UT	0.22	100
GB1010A	Lynemouth 2	SI	0.11	97.5
GB0583A	Middlesbrough	UI	0.38	100
GB0568A	Newcastle Centre	UB	0.13	100
GB0962A	Newport	UB	0.21	97
GB0906A	Port Talbot Margam	UI	0.44	92.9
GB0940A	Royston	UI	0.85	100
GB0660A	Salford Eccles	UB	0.22	100
GB1004A	Scunthorpe Low Santon	UI	3.4	100
GB0841A	Scunthorpe Town	UI	3.9	98.1
GB0942A	South Hiendley	UI	0.35	90.7
GB0004R	Stoke Ferry	RB	0.12	91.5
GB0943A	Swansea Cwm Level Park	UB	0.27	92.3

*RB = Rural Background, UB = Urban Background, UT = Urban Traffic, UI = Urban Industrial, SI = Suburban Industrial.

Appendix 3 – Small point source model

Introduction

Small industrial sources have generally been represented in earlier maps (Stedman et al., 2002) as 1 km square volume sources. However, this approach has in some cases lead to unreasonably high concentrations close to the source. The overestimation arises because the release height, buoyancy and momentum of discharges from industrial chimneys are not taken into account. A revised small point source model has been developed which uses dispersion kernels that will take these factors into account.

The dispersion model ADMS 3.0 was used to prepare the dispersion kernels.

Discharge Conditions

The National Atmospheric Emission Inventory contains limited information concerning the discharge characteristics of individual emission sources. In many cases the information is limited to data on the total annual emission of individual pollutants. It is therefore necessary to make some general assumptions concerning the discharge height, the discharge temperature, the volumetric flow rate of the discharge and the discharge velocity. The approach adopted has been to make reasonable, but generally conservative assumptions corresponding to industrial practice.

Sulphur dioxide

For sulphur dioxide, it was assumed that the plant operates continuously throughout the year. The stack height was estimated using the following equations taken from the 3rd edition of the Chimney Heights Memorandum:

If the sulphur dioxide emission rate, R_A kg/h, is less than 10 kg/h, the chimney height, U m, is given by:

$$U = 6R_A^{0.5},$$

If R_A is in the range 10-100 kg/h:

$$U = 12R_A^{0.2},$$

Emission rates in excess of 100 kg/h were not considered in this study.

No account was taken of the effects of buildings: it was assumed that the increase in chimney height to take account of building effects provided by the Memorandum would compensate for the building effects.

It was then assumed that the sulphur dioxide concentration in the discharge would be at the limit for indigenous coal and liquid fuel for new and existing plant provided by Secretary of States Guidance-Boilers and Furnaces, 20-50 MW net rated thermal input PG1/3(95). The limit is 3000 mg m^{-3} at reference conditions of 273 K, 101.3 kPa, 6% oxygen for solid fuel firing and 3% oxygen for liquid firing and dry gas. It was assumed that the oxygen content in the discharge corresponds with the reference condition. The moisture content of the discharge was ignored. It was assumed that the temperature of discharge was 373 K: higher temperatures would lead to improved buoyancy and hence lower ground level concentrations while lower temperatures usually result in unacceptable water condensation. A discharge velocity of 10 m/s was selected to be representative of most combustion source discharges. The discharge diameter d m was calculated from;

$$d = \sqrt{\frac{4qT}{273\pi cv}},$$

where: q is the sulphur dioxide emission rate, g s^{-1}

T is the discharge temperature, 373 K

c is the emission concentration at reference conditions, 3 g m^{-3}

v is the discharge velocity, 10 m s^{-1}

Table A3.1 shows the modelled stack heights and diameters.

Table A3.1. Modelled stack heights and diameters for sulphur dioxide

Emission rate			Stack height, m	Stack diameter, m
g s^{-1}	kg h^{-1}	t a^{-1}		
0.1	0.36	3.2	3.60	0.08
0.2	0.72	6.3	5.09	0.11
0.5	1.8	15.8	8.05	0.17
1	3.6	31.5	11.38	0.24
2	7.2	63.1	16.10	0.34
5	18	157.7	21.39	0.54
10	36	315.4	24.57	0.76
20	72	630.7	28.23	1.08

Oxides of nitrogen

For nitrogen dioxide, it was assumed that the plant operates continuously throughout the year. The stack height was estimated using the following equation taken from the 3rd edition of the Chimney Heights Memorandum for very low sulphur fuels:

$$U = 1.36Q^{0.6}(1 - 4.7\times10^{-5}Q^{1.69}),$$

where: Q is the gross heat input in MW.

This relationship applies for heat inputs up to 150 MW. For larger heat inputs a fixed height of 30 m was used corresponding to an approximate lower limit derived from available data on stack heights for large sources.

The gross heat input used in the above equation was calculated from the oxides of nitrogen emission rate using an emission factor of 10600 kg/MTh (0.100 g/MJ) for oxides of nitrogen emitted from natural gas combustion in non-domestic non-power station sources taken from the NAEI.

For fuels containing significant sulphur, the actual stack height will be greater to allow for the dispersion of sulphur dioxide so that the approach taken is expected to lead to an overestimate of ground level concentrations.

The emission limits for oxides of nitrogen provided by Secretary of States Guidance-Boilers and Furnaces, 20-50 MW net rated thermal input PG1/3(95) depend on the type of fuel and are in the range 140-650 mg m^{-3} at reference conditions. A value of 300 mg m^{-3} was used in the calculation of the stack discharge diameter. Other assumptions concerning discharge conditions followed those made for sulphur dioxide above. Table A3.2 shows the modelled stack heights and diameters.

Table A3.2. Modelled stack heights and diameters for oxides of nitrogen

Emission rate		Height, m	Diameter, m
g s^{-1}	t a^{-1}		
0.1	3.2	1.36	0.24
0.2	6.3	2.06	0.34
0.5	15.8	3.57	0.54
1	31.5	5.40	0.76
2	63.1	8.15	1.08
5	157.7	13.72	1.70
10	315.4	19.12	2.41
20	630.7	21.34	3.41
50	1576.8	30.00	5.38
100	3153.6	30.00	7.61

Particulate matter, PM_{10}

The stack heights and diameters used for oxides of nitrogen were also used to provide the kernels for particulate matter PM_{10}. This will provide a conservative assessment of PM_{10} concentrations for the following reasons. The emission limits for total particulate matter provided by Secretary of States Guidance-Boilers and Furnaces, 20-50 MW net rated thermal input PG1/3(95) depend on the type of fuel and are in the range 5-300 mg m^{-3} at reference conditions. The emission limit for total particulate matter includes but is not limited to the contribution from PM_{10}.

Dispersion Modelling

The dispersion model ADMS 3.0 was used to predict ground level concentrations on two receptor grids:

- an “in-square” grid covering an area 1 km x 1 km with the source at the centre and with receptors at 33.3 m intervals;
- an “outer-grid” covering an area 30 km x 30 km with the source at the centre and with receptors at 1 km intervals.

A surface roughness value of 0.5 m was used, corresponding to areas of open suburbia. Meteorological data for Heathrow for the years 1993-2002 was used in the assessment, with most model runs using the 2000 data.

Results

Sulphur dioxide

Table A3.3 shows the predicted "in-square average" concentration for the 1 km square centred on the emission source for 2000 meteorological data.

Table A3.3. Predicted in-square concentration, for sulphur dioxide

Emission rate, g s^{-1}	Average in square concentration, $\mu g\ m^{-3}$
0.1	0.599
0.2	0.934
0.5	1.555
1	2.19
2	2.92
5	4.57
10	6.56
20	8.86

The results shown in Table A3.3 may be approximated by the relationship

$$C = Aq^{0.5} ,$$

where: C is the in-square concentration, $\mu g\ m^{-3}$ and q is the emission rate, g s^{-1}. A is a proportionality factor (2.07 in 2000).

Table A3.4 shows the predicted in-square concentration for an emission rate of 10 g s^{-1} for meteorological years 1993-2002. Table A3.4 also shows the inter-annual variation in the factor *A*.

Table A3.4. In-square concentrations for 10 g/s emissions

Year	In-square concentration, $\mu g\ m^{-3}$	Factor *A*
1993	6.21	1.96
1994	6.01	1.90
1995	6.12	1.94
1996	6.23	1.97
1997	6.10	1.93
1998	6.18	1.95
1999	6.49	2.05
2000	6.56	2.07
2001	6.32	2.00
2002	6.51	2.06

Figure A3.1 shows the predicted "outer-grid" concentration along the east-west axis through the source for 2000 meteorological data for a range of rates of emission (in g/s). Figure A3.1 does not include results for the 1 km source square.

Figure A3.1. Sulphur dioxide concentration on east-west axis, 2000 meteorological data

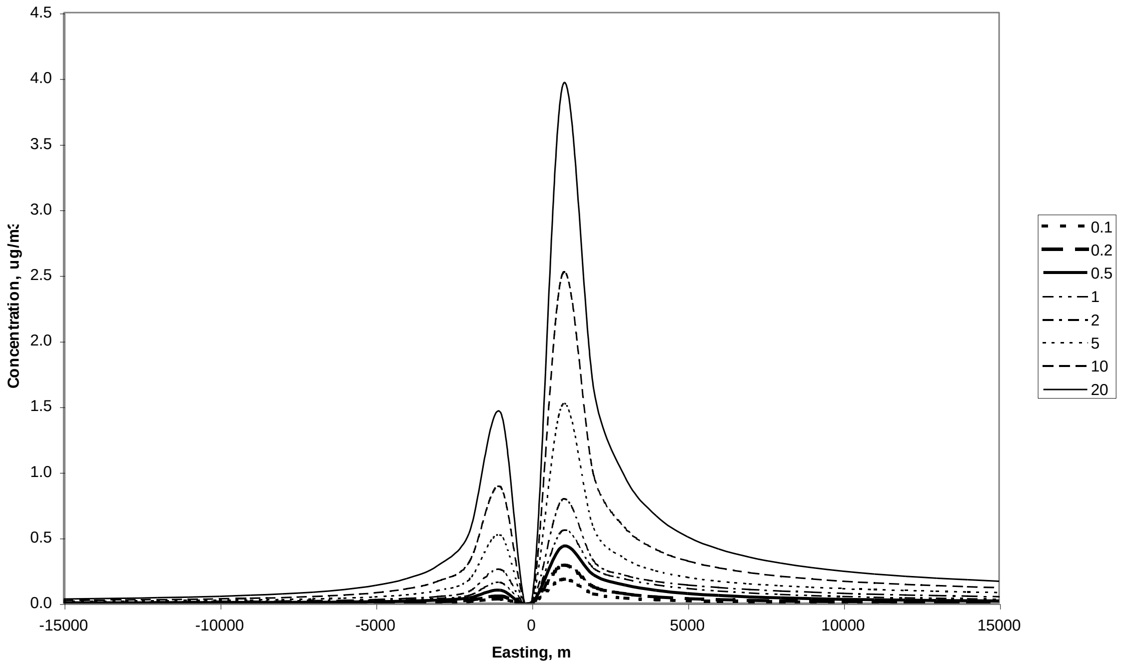
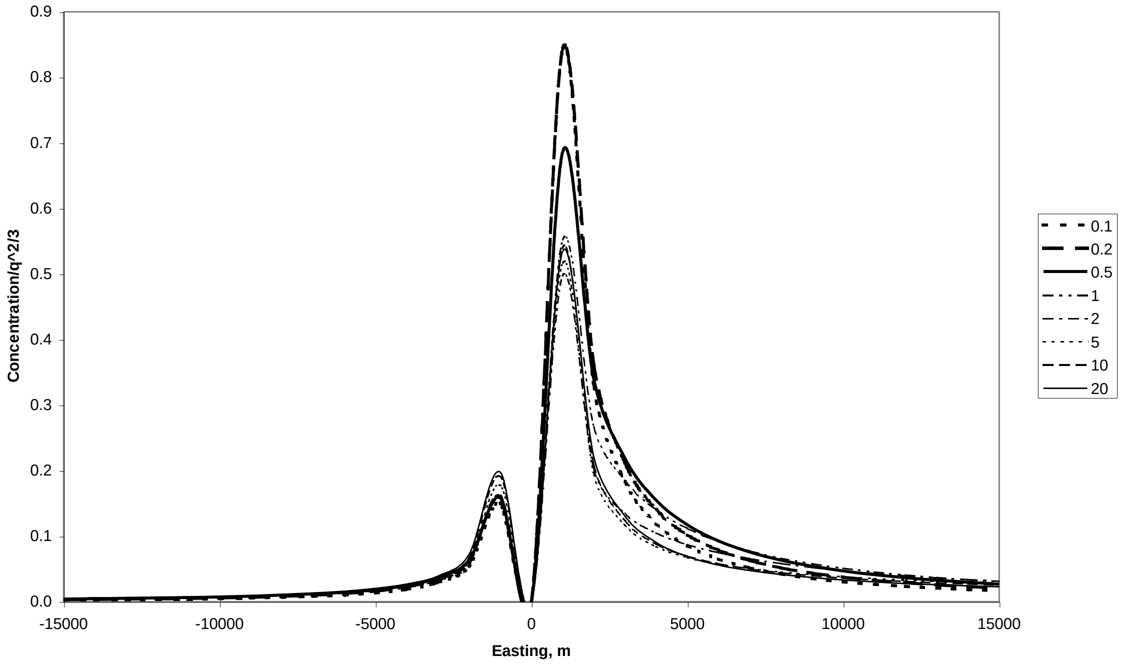


Figure A3.2 shows the same model results plotted as $C/q^{2/3}$. The spread of the model results is greatly reduced so that as a reasonable approximation all the model results may be reduced to a single line.

Figure A3.2. Reduced sulphur dioxide concentrations on the east-west axis, 2000 meteorological data



Thus it is proposed to use the results for an emission rate of 10 g/s for all emission rates in the range 0.1-20 g/s in the preparation of dispersion kernels for industrial sulphur dioxide emissions. The dispersion kernel will be multiplied by $10.(q/10)^{2/3}$ to provide estimates of the impact of emission q (g s^{-1}) at each receptor location. Separate kernels have been created from each meteorological data year 1993-2002.

Oxides of nitrogen

Table A3.5 shows the predicted "in-square average" concentration for the 1 km square centred on the emission source for 2000 meteorological data.

Table A3.5. In-square oxides of nitrogen concentrations, 2000

Emission rate, g s^{-1}	In square concentration, $\mu g\ m^{-3}$
0.1	0.464
0.2	0.764
0.5	1.37
1	1.97
2	2.6
5	3.31
10	3.58
20	4.34
50	3.745
100	4.3

The results shown in Table A3.5 may be approximated in the range 0.1-20 g s^{-1} by the relationship

$$C = B \log_{10}(10q)+0.464,$$

where: C is the in-square concentration, $\mu g\ m^{-3}$ and q is the emission rate, g s^{-1}. and B is a numerical constant, 1.68 in 2000.

For emission rates in the range 20-100 g s^{-1}, the in-square concentration is approximately 4 $\mu g\ m^{-3}$.

Table A3.6 shows the predicted in-square concentration for an emission rate of 20 g s^{-1} for meteorological years 1993-2002. Table A3.6 also shows the inter-annual variation in the factor B.

Table A3.6. Inter annual variation in in-square oxides of nitrogen concentration

Year	In-square concentration, $\mu g\ m^{-3}$	Factor B
1993	3.62	1.37
1994	3.88	1.48
1995	3.74	1.42
1996	4.3	1.67
1997	3.66	1.39
1998	3.64	1.38
1999	4.14	1.60
2000	4.34	1.68
2001	4.02	1.55
2002	4.68	1.83

Figure A3.3 shows the predicted “outer-grid” oxides of nitrogen concentration along the east-west axis through the source for a range of rates of emission (in g s^{-1}).

Figure A3.3. Oxides of nitrogen concentration on east-west axis, 2000 meteorological data

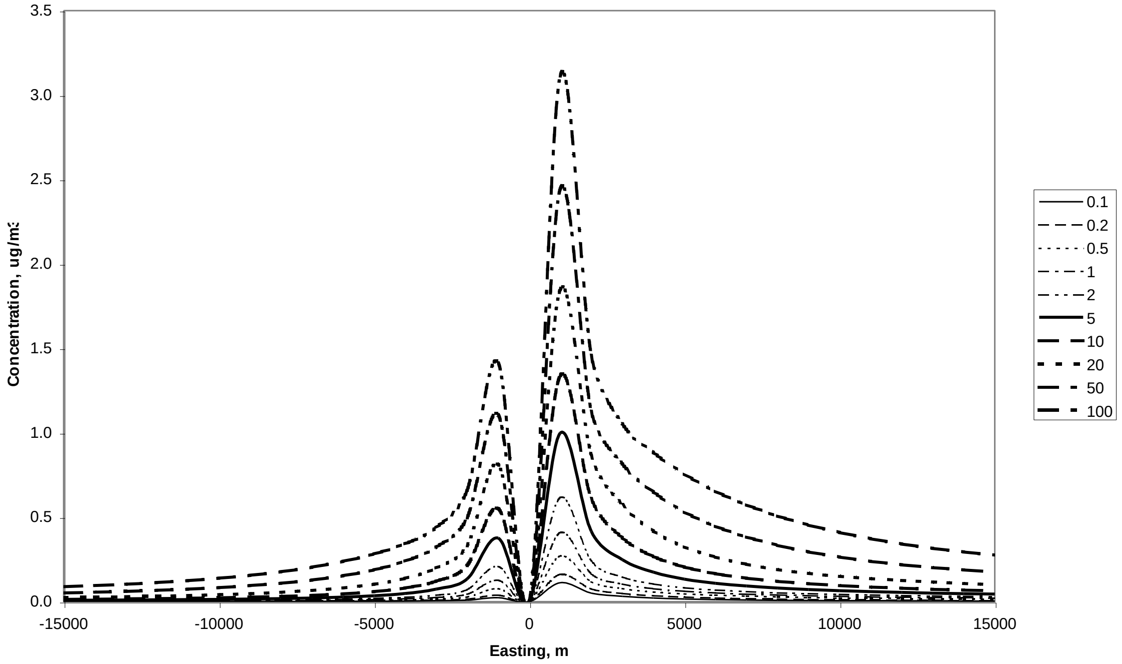
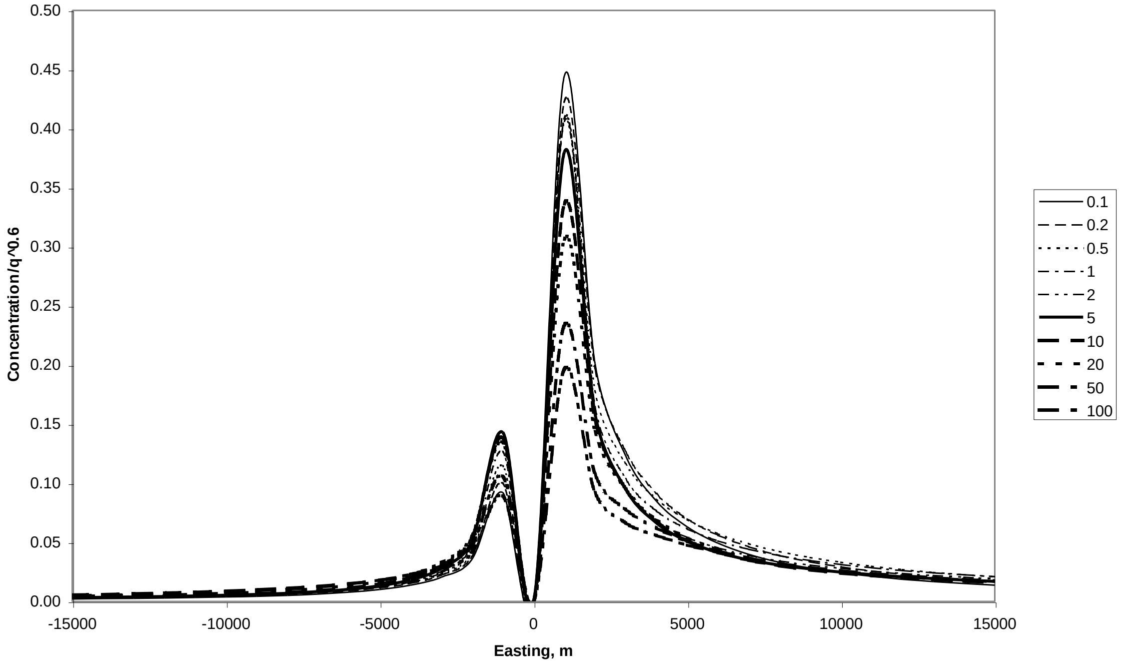


Figure A3.4 shows the same model results plotted as $C/q^{0.6}$. The spread of the model results is greatly reduced so that as a reasonable approximation all the model results may be reduced to a single line.

Figure A3.4. Reduced oxides of nitrogen concentrations on the east-west axis, 2000 meteorological data



Thus it is proposed to use the results for an emission rate of 20 g s^{-1} for all emission rates in the range 0.1-100 g s^{-1} in the preparation of dispersion kernels for oxides of nitrogen emissions. The dispersion kernel will be multiplied by $20.(q/20)^{0.6}$ to provide estimates of the impact of emission q g s^{-1} at each receptor location. Separate kernels have been created for each meteorological data year 1993-2002.

Method

Sulphur dioxide

Point sources with emissions greater than or equal to 500 tonnes per year (15.85 g s^{-1}) have been modelled explicitly using ADMS. Point sources with emissions less than 500 tonnes per year have been modelled using the small points model. This model has two components.

The in-square concentration for each source has been calculated using the following function:

$$C = 1.98.q^{0.5}$$

where C is the in-square concentration, μg m^{-3} and q is the emission rate, g s^{-1} and 1.98 is a numerical constant, calculated as the average value over the years 1993-2002 for met data at Heathrow.

The outer-grid concentration has been calculated by adjusting the emissions for each source using the function:

$$Q = 10.(q/10)^{0.667} ,$$

where: q is the emission rate, g s^{-1} and Q is the adjusted emissions. The sum of the adjusted emission was then calculated for each grid square and the outer-grid concentration calculated using a small points dispersion kernel (which was calculated as the average over the years 1993-2002 for met data at Heathrow).

The in-square and outer-grid concentrations were then summed to calculate the total contribution to ambient annual mean concentrations from these small point sources.

Oxides of nitrogen

Point sources with emissions greater than or equal to 500 tonnes per year (15.85 g s^{-1}) have been modelled explicitly using ADMS. Point sources with emissions less than 500 tonnes per year have been modelled using the small points model. This model has two components.

The in-square concentration for each source has been calculated using the following function:

$$C = 1.54. \log_{10}(10q)+0.464,$$

where: C is the in-square concentration, μg m^{-3} and q is the emission rate, g s^{-1} and 1.54 is a numerical constant, calculated as the average value over the years 1993-2002 for met data at Heathrow.

The outer-grid concentration has been calculated by adjusting the emissions for each source using the function:

$$Q = 20. (q/20)^{0.6} ,$$

where: q is the emission rate, g s^{-1} and Q is the adjusted emissions. The sum of the adjusted emission was then calculated for each grid square and the outer-grid concentration calculated using a small points dispersion kernel (which was calculated as the average over the years 1993-2002 for met data at Heathrow).

The in-square and outer-grid concentrations were then summed to calculate the total contribution to ambient annual mean concentrations from these small point sources.

PM_{10} and $PM_{2.5}$

The method for PM_{10} and $PM_{2.5}$ was the same as for NO_x, except that point sources with emissions greater than or equal to 200 tonnes per year (6.34 g s^{-1}) have been modelled explicitly using ADMS. Point sources with emissions less than 200 tonnes per year have been modelled using the small points model.

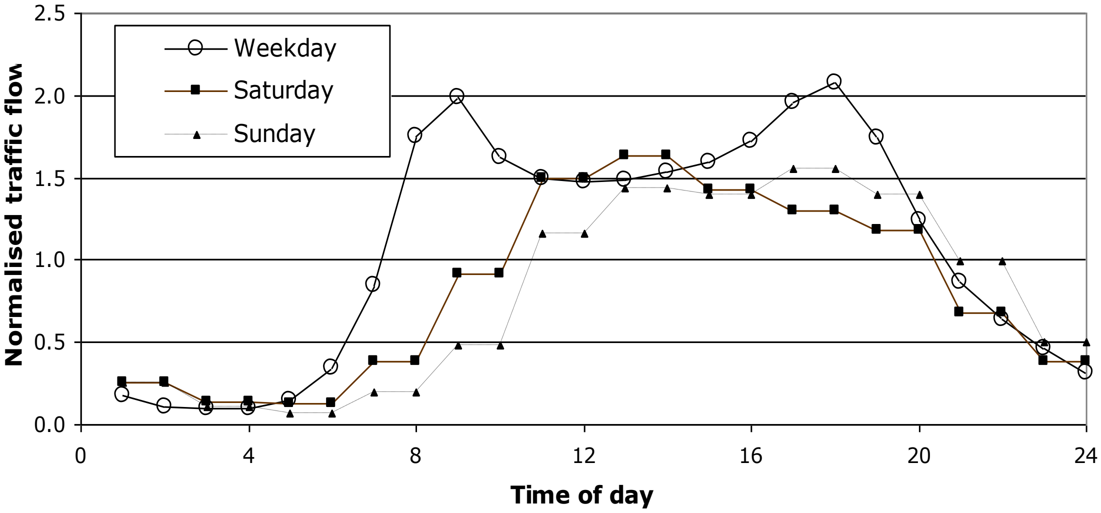
Benzene

The method for benzene was the different. Point sources with combustions emissions greater than or equal to 5 tonnes per year (0.16 g s^{-1}) have been modelled explicitly using ADMS. Fugitive and process point sources have been modelled using a different small points model, as described in Section 7.3.2.

Appendix 4 – Dispersion kernels for the area source model

Dispersion kernels for calculating the annual mean contribution of emissions from area sources to ambient annual mean concentrations were calculated using ADMS 5.0. Separate kernels were calculated for traffic, domestic and other area sources (which were assumed to have a constant temporal profile of emissions). Kernels were generated for the assessment year using sequential meteorological data from Waddington. The dispersion parameters used to calculate the kernels are listed in Table A4.1. The emission profile used to represent traffic emissions for the traffic kernels is shown in Figure A4.1. This was obtained from a distribution of all traffic in the United Kingdom by time of day (DETR, 2000).

Figure A4.1. Temporal profile of traffic emissions



A time varying emissions profile was applied for domestic sources the first time in the 2011 assessment in order to better represent emissions related to domestic combustion. Both seasonal and diurnal profiles have been used to weight domestic emissions. These weightings have been developed and applied following a similar method to Coleman et al. (2001). In this work a normalised diurnal profile has been superimposed onto a seasonal profile based on degree days calculated from temperature data for the Waddington meteorological station and the assessment year. The diurnal profile applied has been estimated from Coleman et al. (2001), see Figure A4.2. Degree days provide a simple but effective tool to relate energy use and emissions from buildings to the weather (Day et al, 2006). A degree day is unit used to determine the heating requirements of buildings, representing a fall of one degree below a specified average outdoor temperature (15.5 C, in this case). Degree days for Waddington have been calculated from the equation:

$$D_d = \frac{\sum_{i=1}^{N} \theta_b - \theta_{o,i_{(\theta_b - \theta_{o,i} \geq 0)}}}{N}$$

Where D_d is the daily degree days for one day, θ_b is the base temperature, $\theta_{o,i}$ is the ambient (or outdoor) air temperature and N is the number of hours of available data in a given day. Figure A4.3 shows the seasonal profile of degree days calculated for the year 2013. The seasonal profile of degree days has been verified versus National Grid, National Transmission System gas demand data.

Figure A4.2. Diurnal profile of domestic emissions estimated from Coleman et al. (2001)

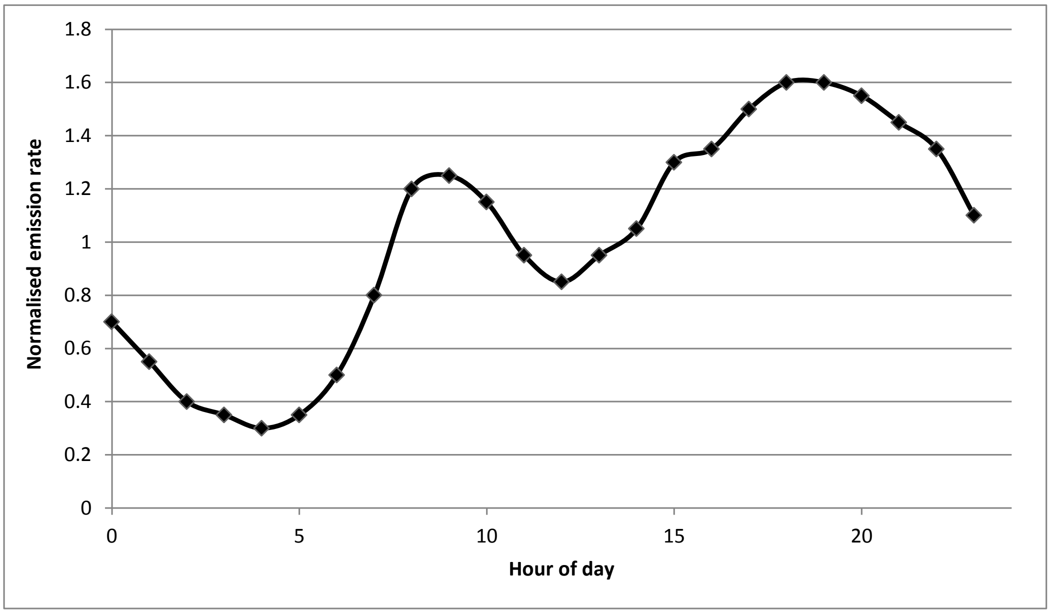
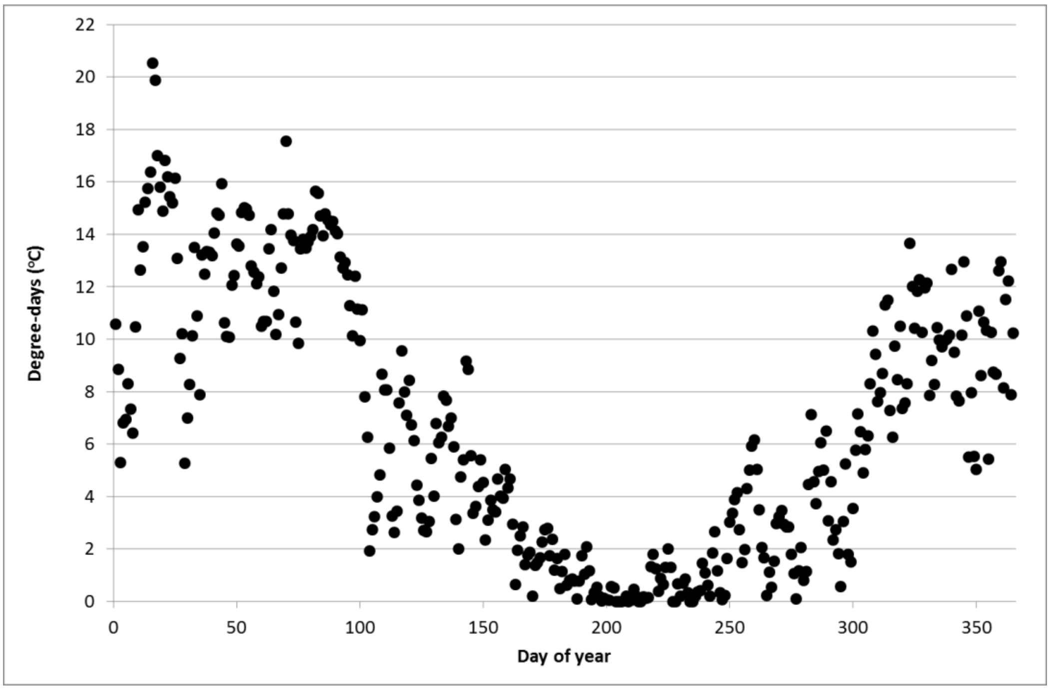


Figure A4.3. Seasonal profile of degree days calculated for the Waddington meteorological station in 2013 (base temperature of 15.5°C)



For SO_2, NO_x, NO_2, PM_{10}, $PM_{2.5}$, C_6H_6, heavy metals (Pb, As, Cd, Ni) and B(a)P the area source dispersion kernels are on a 1 km x 1 km resolution matrix and are made using ADMS 5.0. The centre squares have been scaled to remove the impact of sources within 50 m of the receptor location in that square on the basis that background sites are not located very close to specific sources such as major roads. Different kernels have been made for different area types, to take into account different dispersion conditions in urban areas of different sizes. The kernels have been made specific to different types of location by varying minimum

Monin Obukhov Length (LMO) and surface roughness due to different land use. The location of the different area types are shown in Figure A4.4.

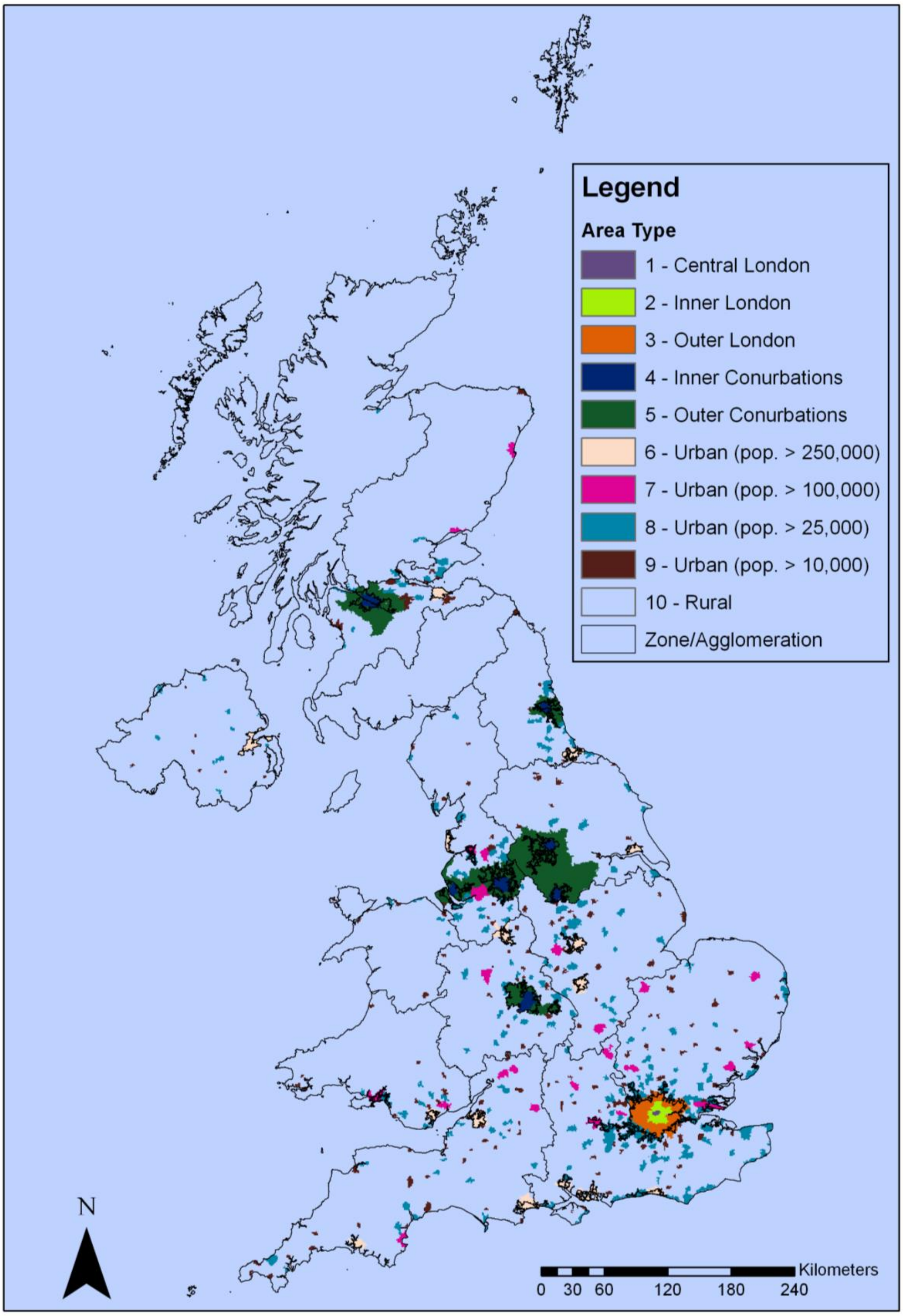
Table A4.1. Summary of inverted dispersion kernel parameters

Kernel name	**Area types**	**Type of location**	**LMO (m)**	**Surface roughness**		**Height (m) of volume source**	**Variable emission profile?**	**Emission rate ($g\ m^{-3}\ s^{-1}$)**
				Disp. site	Met. site			
Non road transport	1,2,4	Conurbation	25	0.5	0.1	30	N	3.33E-08
Non road transport	3,4,5,6, 7,8	Smaller urban	20	0.5	0.1	30	N	3.33E-08
Non road transport	9,10	Rural	10	0.5	0.1	30	N	3.33E-08
Domestic	1,2,4	Conurbation	25	0.5	0.1	20	Y	5.0E-08
Domestic	3,4,5,6, 7,8	Smaller urban	20	0.5	0.1	20	Y	5.0E-08
Domestic	9,10	Rural	10	0.5	0.1	20	Y	5.0E-08
Road transport	1,2,4	Conurbation	25	0.5	0.1	10	Y	1.0E-7
Road transport	3,4,5,6, 7,8	Smaller urban	20	0.5	0.1	10	Y	1.0E-7
Road transport	9,10	Rural	10	0.5	0.1	10	Y	1.0E-7

ADMS 4.2 recommended using a minimum Monin Obukhov Length (LMO) of 30 m for an urban area. However, sensitivity testing showed 20 m worked better in ADMS 4.2. The same settings have been applied in ADMS 5.0 after sensitivity tests indicated only marginal differences between the outputs for the area source kernels, between the different versions of ADMS.

The dispersion kernels used for fugitive and process point sources of benzene are the same as the non-road transport kernels but with the values for the central receptor location calculated as described in Section 7.3.2.

Figure A4.4. Map of UK area types



Appendix 5 – Method for calculating and mapping emissions from aircraft and shipping

Aircraft

Aircraft emissions were calculated using data obtained from the NAEI (Passant et al., 2014) for emissions from planes in various phases of flying (e.g. take off, landing, taxiing). The NAEI provides estimates of total emissions for aircraft, which include emissions up to a height of 1000 m. Ground level emissions for use in PCM modelling were calculated on the basis of:

Ground level emissions = Taxi out + Hold + Taxi in + APU arrival + APU departure + (0.5 x Take off) + (0.5 x Landing) + (0.5 x Reverse thrust).

The factor of 0.5 has been chosen on the basis of findings from detailed studies (Underwood, 2009). Initial climb, climb-out and approach are included in the emission inventory but excluded from ground level emissions used for the PCM model.

Figures A5.1 and A5.2 show good agreement between the measured and modelled annual mean ground-level NO_X concentrations at monitoring sites in the vicinity of Heathrow and Gatwick airports for 2008, respectively, based on this approach.

Figure A5.1. Comparison of the measured and modelled annual mean NO_X at Heathrow Airport for 2008

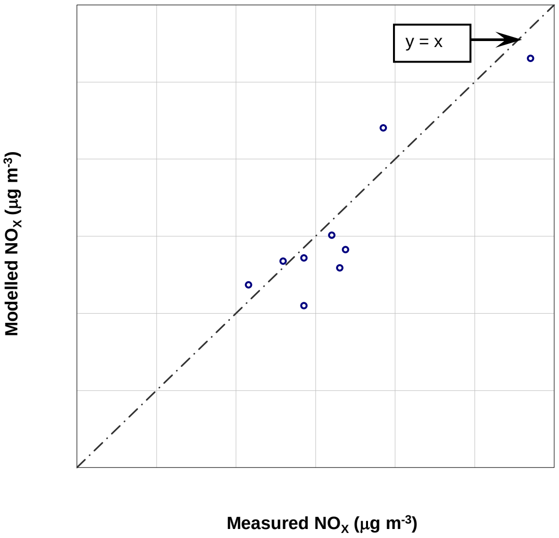
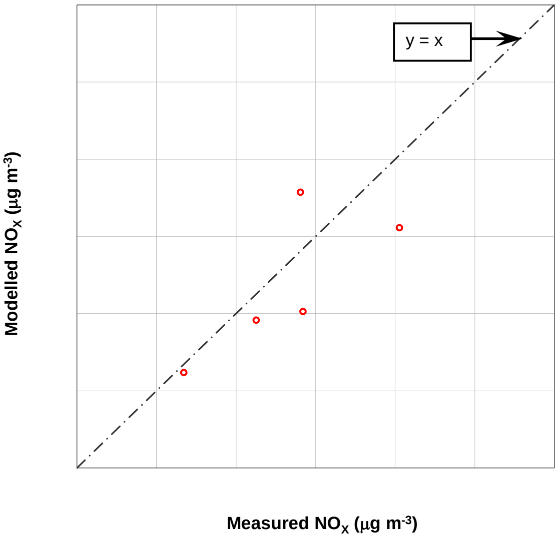


Figure A5.2. Comparison of the measured and modelled annual mean NO_X at Gatwick Airport for 2008



Shipping

Entec developed a detailed gridded ship emissions inventory for UK waters using recent information on ship movements, vessel engine characteristics and emission factors to quantify atmospheric emissions from shipping sources (Entec, 2010). The methodology developed was based on guidance from the EMEP/CORINAIR Atmospheric Emission Inventory Guidebook (2006) and relies on the following information, which largely dictates the emissions from a vessel:

- Installed engine power
- Type of fuel consumed
- Vessel speed and the distance travelled (or the time spent travelling at sea)
- Time spent in port
- Installed emission abatement technologies

Emissions and fuel consumption estimates were calculated at a 5 km x 5 km grid resolution (based on the EMEP grid) for an emissions domain extending 200 miles from the UK coastline. The emissions were re-mapped to a 1 km x 1 km grid based on the OSGB grid system. Subsequently, emissions within UK territorial waters (within 12 nautical miles of the coastline) have been mapped as total UK emissions. A detailed distribution of emissions by historical NAEI shipping sectors (coastal shipping, international shipping and naval shipping) is not currently available.

The 1x1 km emission maps generated from the 5 km x 5km grid resolution were found to provide better agreement with measurement data than previously used distribution grids. However, concentrations have been overestimated by the model close to some ports. This is thought to be caused by the uncertainties associated with disaggregating the 5x5 km gridded emissions estimates based upon the EMEP grid, to the 1 km x 1 km grid squares for the NAEI maps. This is particularly the case in port areas where the 5 km x 5 km grid may include a large proportion of land. The spatial distributions at major ports have been revised for the 2012 NAEI so that the ‘Berth’ and ‘Manoeuvring’ emissions have been constrained to be within the exact location of the 1km grid squares of these ports. This revision was made on the following major ports: Southampton; Immingham; Liverpool; Middlesbrough; Pembroke; Bristol; Aberdeen; Felixstowe; Canvey Island. Furthermore, the ‘Sea’ emissions have been excluded from the 1x1km grids where land covers 50% and above of the grid area. Some uncertainties remain, however for the exact location of shipping emissions. The following method, which has been used in previous assessments, was therefore retained.

A review of 2007 monitoring data recorded at sites close to UK ports was used to inform where, if any, emission caps should be applied:

- The 2007 measured annual mean NO_X concentration recorded at Dover Docks, a site located within the dock area, very close to shipping emission sources (within ~100m), was 135 µg m^{-3} (as NO_2);
- The 2007 measured annual mean NO_X concentration recorded at Castle Point 1 Town Centre, approximately 3km from significant shipping emissions, was 34 µg m^{-3} (as NO_2);
- The 2007 measured annual mean NO_X concentration recorded at Southampton Centre AURN site, approximately 2 km from significant shipping emissions, was 67 µg m^{-3} (as NO_2).

As the high concentrations recorded at Dover Docks are so close to the source of emissions, while Castle Point 1 Town Centre and Southampton Centre are away from the emissions source, the monitoring results suggest that a contribution of up to ~30 µg m^{-3} (as NO_2) is a reasonable concentration to be modelled for a grid square average with significant emissions.

The NO_X shipping emission maps were therefore capped to ensure that the modelled contribution from this source was not greater than 30 µg m^{-3}. Caps for other air pollutants covered in this report were calculated using the ratio of total UK shipping emissions for each pollutant to the total UK NO_X shipping emissions.

Appendix 6 – Monitoring stations used in $PM_{2.5}$ AEI calculation

Table A6.1. List of urban and suburban background monitoring station used in AEI calculation

EoI code	Station name	Station classification	Instrument type
GB0729A	Aberdeen	Urban Background	TEOM FDMS
GB0567A	Belfast Centre	Urban Background	TEOM FDMS
GB1013A	Birmingham Acocks Green	Urban Background	TEOM FDMS
GB0851A	Birmingham Tyburn	Urban Background	TEOM FDMS
GB0882A	Blackpool Marton	Urban Background	TEOM FDMS
GB0741A	Bournemouth	Urban Background	GRAV EMFAB
GB0860A	Brighton Preston Park	Urban Background	GRAV EMFAB
GB0884A	Bristol St Paul's	Urban Background	TEOM FDMS
GB0580A	Cardiff Centre	Urban Background	TEOM FDMS
GB0929A	Chesterfield	Urban Background	TEOM FDMS
GB0739A	Coventry Memorial Park	Urban Background	TEOM FDMS
GB1005A	Eastbourne	Urban Background	TEOM FDMS
GB0839A	Edinburgh St Leonards	Urban Background	TEOM FDMS
GB0641A	Glasgow Centre *	Urban Background	TEOM FDMS
GB1028A	Glasgow Townhead	Urban Background	TEOM FDMS
GB0776A	Hull Freetown	Urban Background	TEOM FDMS
GB0643A	Leamington Spa	Urban Background	TEOM FDMS
GB0584A	Leeds Centre	Urban Background	TEOM FDMS
GB1026A	Leicester University	Urban Background	TEOM FDMS
GB0777A	Liverpool Speke	Urban Background	TEOM FDMS
GB0608A	London Bexley	Suburban Background	TEOM FDMS
GB0566A	London Bloomsbury	Urban Background	TEOM FDMS
GB0586A	London Eltham	Suburban Background	TEOM FDMS
GB0959A	London Harrow Stanmore	Urban Background	TEOM FDMS
GB0620A	London N. Kensington	Urban Background	TEOM FDMS
GB0644A	London Teddington	Urban Background	TEOM FDMS
GB1025A	London Teddington Bushy Park	Urban Background	TEOM FDMS
GB0743A	London Westminster	Urban Background	GRAV EMFAB
GB0613A	Manchester Piccadilly	Urban Background	TEOM FDMS
GB0583A	Middlesbrough	Urban Background	TEOM FDMS
GB0568A	Newcastle Centre	Urban Background	TEOM FDMS
GB0962A	Newport	Urban Background	TEOM FDMS
GB0738A	Northampton *	Urban Background	GRAV EMFAB

EoI code	Station name	Station classification	Instrument type
GB1019A	Northampton Kingsthorpe	Urban Background	GRAV EMFAB
GB0995A	Norwich Lakenfields	Urban Background	TEOM FDMS
GB0646A	Nottingham Centre	Urban Background	TEOM FDMS
GB0920A	Oxford St Ebbes	Urban Background	TEOM FDMS
GB0687A	Plymouth Centre	Urban Background	TEOM FDMS
GB0733A	Portsmouth	Urban Background	TEOM FDMS
GB0731A	Preston	Urban Background	TEOM FDMS
GB0840A	Reading New Town	Urban Background	TEOM FDMS
GB0615A	Sheffield Centre	Urban Background	TEOM FDMS
GB1027A	Sheffield Devonshire Green	Urban Background	TEOM FDMS
GB0598A	Southampton Centre	Urban Background	TEOM FDMS
GB0728A	Southend-on-Sea	Urban Background	TEOM FDMS
GB0658A	Stoke-on-Trent Centre	Urban Background	TEOM FDMS
GB0863A	Sunderland Silksworth	Urban Background	TEOM FDMS
GB0958A	Warrington	Urban Background	TEOM FDMS
GB0864A	Wigan Centre	Urban Background	TEOM FDMS
GB0730A	Wirral Tranmere	Urban Background	TEOM FDMS
GB0918A	York Bootham	Urban Background	TEOM FDMS

* No longer operational. Not used in calculation of AEI for 2013.

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