

UK modelling under the Air Quality Framework Directive (96/62/EC) and Fourth Daughter Directive (2004/107/EC) for 2010 covering As, Cd, Ni and B(a)P



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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. Historically this has been performed 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.

In 2010 the UK undertook the annual air quality assessment in accordance with the requirements of the AQD and the AQDD4. The assessment presented in this report takes the form of comparisons of measured and modelled air pollutant concentrations with the target values set out in the AQDD4. Air quality modelling has been carried out to supplement the information available from the UK national air quality monitoring networks. The results were submitted to the European Commission in the form of a standard questionnaire (the 'questionnaire') which each member state must complete and upload onto the Central Data Repository of the European Environment Agency:

<http://cdr.eionet.europa.eu/gb/eu/annualair>.

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 results from the questionnaire for the AQDD4 pollutants and additional technical information on the modelling methods that have been used. Full details of the assessment carried out under the AQD are included in the accompanying report (Brookes et al., 2011).

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, target values and long term objectives have been assessed. The results of the assessment against the target values are presented in Table E1.

Table E1. Summary results of AQDD4 air quality assessment for 2010: comparison with target values

Pollutant	Averaging time	Number of zones exceeding target value
As	Annual	None
Cd	Annual	None
Ni	Annual	2 zones modelled (Swansea, S Wales)
B(a)P	Annual	8 zones, (2 zones measured: N Ireland, Yorkshire & Humberside + 6 zones modelled: Teesside UA, Belfast Metropolitan UA, West Midlands UA, NE England Zone, S Wales Zone, N Wales Zone)

Table of contents

1	Introduction	1
1.1	The EU ambient air quality directives	1
1.2	This report.....	2
1.3	Preliminary assessments and definition of zones.....	2
1.4	Monitoring sites.....	5
1.5	Target values	5
1.6	Data quality objectives for modelling results and model verification	5
1.7	Air quality in Gibraltar in 2010.....	6
2	Heavy metals	7
2.1	Introduction	7
2.2	Monitoring sites.....	7
2.3	Emissions.....	10
2.4	The model.....	14
2.5	Arsenic	19
2.6	Cadmium.....	24
2.7	Nickel	29
3	Benzo(a)pyrene	37
3.1	Introduction	37
3.2	Monitoring sites.....	37
3.3	Emissions.....	38
3.4	The model.....	40
3.5	Results	43
4	Results of the air quality assessments	49
5	Acknowledgements.....	51
6	References	52
	Appendices	
Appendix 1	Dispersion kernels for area source model	

1 Introduction

1.1 The EU ambient air quality directives

European Union directives on ambient air quality require 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 has been under:

- 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, which covers the pollutants presented in this report, remains in force.

In 2010 the UK undertook the annual air quality assessment in accordance with the requirements of the AQD and the AQDD4. This assessment takes the form of comparisons of measured and modelled air pollutant concentrations with the limit values, target values and long term objectives set out in the air quality directives. The results were submitted to the European Commission in the form of a standard reporting questionnaire (the 'questionnaire') which each member state must complete and upload onto the Central Data Repository of the European Environment Agency: <http://cdr.eionet.europa.eu/gb/eu/annualair> (CDR, 2011).

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

- sulphur dioxide (SO₂)
- nitrogen dioxide (NO₂) and oxides of nitrogen (NO_x)
- particles (PM₁₀)
- lead (Pb)
- benzene (C₆H₆)
- carbon monoxide (CO)

The AQD also includes:

- 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 (O₃)

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 is defined within the air quality directives and is significantly reduced if other means of assessment, in addition to fixed monitoring sites, are also 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 provides detailed information on the modelling methods that have been used to assess concentrations of As, Cd, Ni and B(a)P in 2010 throughout the UK and a summary of the key results of the air quality assessment for AQDD4. Full details of the assessment carried out for SO₂, NO₂/NO_x, PM₁₀, PM_{2.5}, lead, benzene, CO and ozone (all covered by the AQD) are included in the accompanying report (Brookes et al., 2011). A report summarising the UK's 2010 submission on air quality to the European Commission and presenting air quality modelling data and measurements from the UK national air quality monitoring networks has also been uploaded onto the CDR (Air Pollution in the UK, 2010, Compliance Assessment Summary).

Sections 2 and 3 of this report describe the Pollution Climate Mapping (PCM) modelling methods used to calculate concentrations of heavy metals (As, Cd, Ni) and B(a)P. These include:

- Details of the modelling methods
- Information on the verification of the models used and comparisons with data quality objectives (DQO)
- Detailed modelling results

The status of zones in relation to the target values for the AQDD4 pollutants have been reported to the EU in the questionnaire (CDR, 2011) and a summary of the results of the assessments are included in Section 4. The status has been determined from a combination of monitoring data and model results.

2010 is the third year for which an annual air quality assessment for these pollutants has been carried out. The results of the air quality assessment for 2009 and a description of the modelling methods used have been presented by Walker et al. (2010).

1.3 Preliminary assessments and definition of zones

The Framework Directive includes 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. A report describing the preliminary assessment for the UK for AQDD4 has been prepared (Bush, 2007) which includes the definition of a set of zones to be used for air quality assessment in the UK. Table 1.1 contains details of area, population (from 2001 census) and urban road length contained in each zone and agglomeration. The zones and agglomerations map for the UK is presented in Figure 1.1.

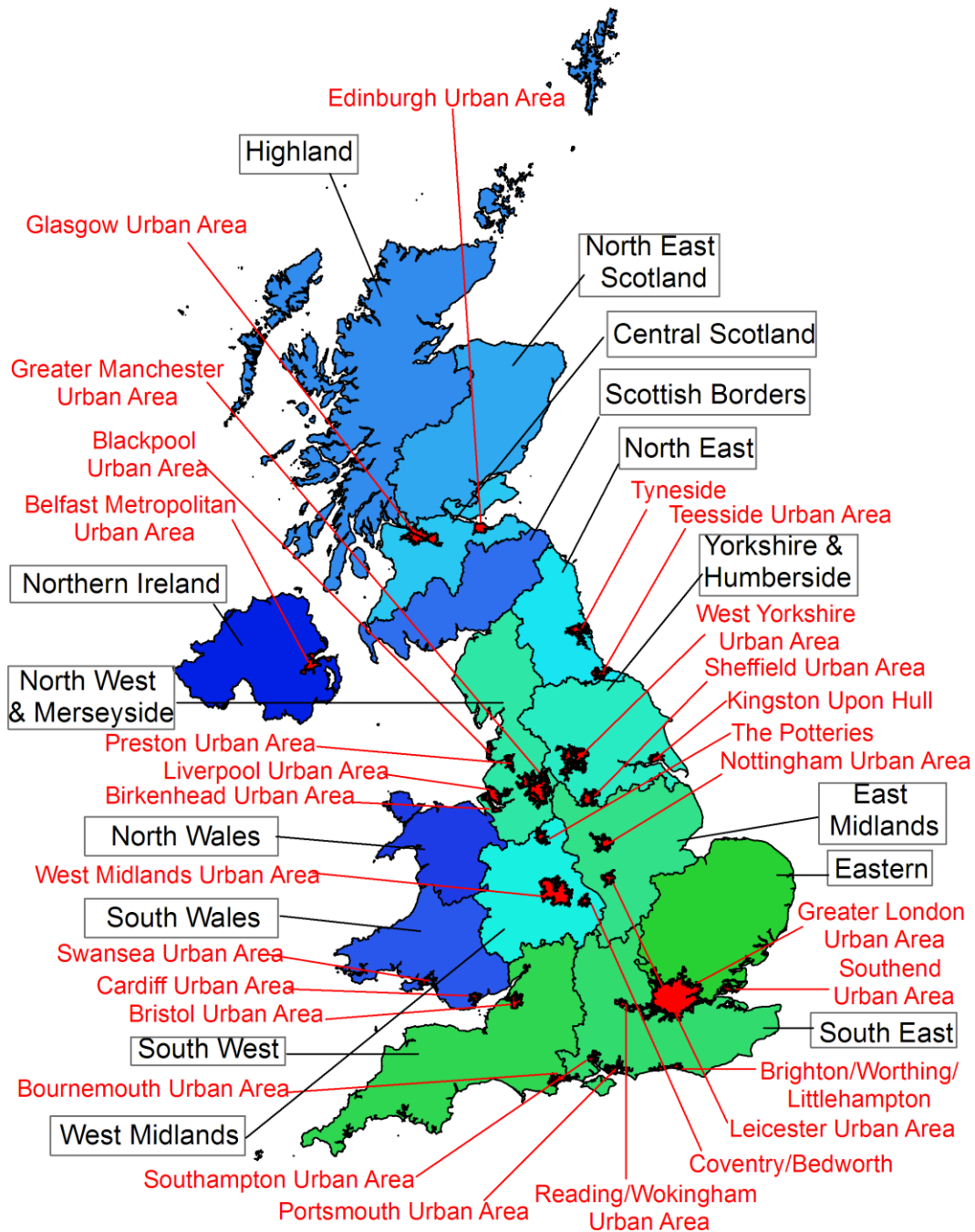
Table 1.1: Zones for Ambient Air Quality Directive reporting

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	8278251	1629.9	1881	1896
West Midlands Urban Area	UK0002	ag	2284093	599.7	385	545
Greater Manchester Urban Area	UK0003	ag	2244931	556.5	554	671
West Yorkshire Urban Area	UK0004	ag	1499465	370.0	275	423
Tyneside	UK0005	ag	879996	210.7	164	202
Liverpool Urban Area	UK0006	ag	816216	186.1	250	214
Sheffield Urban Area	UK0007	ag	640720	162.2	106	160
Nottingham Urban Area	UK0008	ag	666358	158.4	124	134
Bristol Urban Area	UK0009	ag	551066	139.8	112	116
Brighton/Worthing/Littlehampton	UK0010	ag	461181	94.1	59	91
Leicester Urban Area	UK0011	ag	441213	101.6	66	81
Portsmouth Urban Area	UK0012	ag	442252	94.4	56	78
Teesside Urban Area	UK0013	ag	365323	114.3	62	72
The Potteries	UK0014	ag	362403	96.6	113	129
Bournemouth Urban Area	UK0015	ag	383713	108.1	48	72
Reading/Wokingham Urban Area	UK0016	ag	369804	93.2	65	76
Coventry/Bedworth	UK0017	ag	336452	75.5	29	40
Kingston upon Hull	UK0018	ag	301416	80.4	38	60
Southampton Urban Area	UK0019	ag	304400	72.8	61	78
Birkenhead Urban Area	UK0020	ag	319675	89.1	64	72
Southend Urban Area	UK0021	ag	269415	66.8	31	51
Blackpool Urban Area	UK0022	ag	261088	65.8	48	67
Preston Urban Area	UK0023	ag	264601	60.4	35	47
Glasgow Urban Area	UK0024	ag	1168270	368.7	219	326
Edinburgh Urban Area	UK0025	ag	452194	120.1	60	102
Cardiff Urban Area	UK0026	ag	327706	75.6	39	61
Swansea Urban Area	UK0027	ag	270506	79.7	30	71
Belfast Metropolitan Urban Area	UK0028	ag	515484	198.1	42	204
Eastern	UK0029	non-ag	4909880	19133.7	574	807
South West	UK0030	non-ag	4039460	23562.6	422	646
South East	UK0031	non-ag	6160630	18672.6	793	1280
East Midlands	UK0032	non-ag	3261330	15495.9	397	654
North West & Merseyside	UK0033	non-ag	3470620	13722.9	508	822
Yorkshire & Humberside	UK0034	non-ag	3003870	14796.6	316	568
West Midlands	UK0035	non-ag	2624020	12186.3	334	512
North East	UK0036	non-ag	1443910	8291.4	181	273
Central Scotland	UK0037	non-ag	1883010	9347.6	208	338
North East Scotland	UK0038	non-ag	976022	18631.4	133	234
Highland	UK0039	non-ag	341329	39134.5	10	35
Scottish Borders	UK0040	non-ag	250529	11184.1	35	47
South Wales	UK0041	non-ag	1698080	12228.4	159	306
North Wales	UK0042	non-ag	702506	8382.6	83	155
Northern Ireland	UK0043	non-ag	1149150	13974.1	90	274

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

Figure 1.1: UK zones and agglomerations for 2010

UK Agglomerations (red) and Non-Agglomeration Zones



Agglomeration zones (red)

Non-agglomeration zones (blue/green)

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1.4 Monitoring sites

The monitoring stations operating during 2010 for the purpose of AQDD4 reporting are listed in Form 3 of the questionnaire, which can be found on the CDR (2011). Not all sites had sufficient data capture during 2010 for data to be reported. The data quality objective (DQO) for AQDD4 measurements is 90% data capture.

All measurements with at least 75% data capture for the entire year have been included in the analysis to ensure that maximum use is made of data from the monitoring sites operational for the whole of 2010 for reporting purposes. Data capture statistics for sites operational during 2010 are also presented in Form 3 of the reporting questionnaire.

The monitoring data for the sites used in this assessment are shown in Table 2.1 (heavy metals) and Table 3.1 (B(a)P).

1.5 Target values

The target values (TV) included in AQDD4 are listed in Table 1.2. The Directive states that Member States should take all necessary measures not entailing disproportionate costs to ensure that the target values are met by the compliance date.

Table 1.2: Target values for As, Cd, Ni and B(a)P

Pollutant	Averaging period	TV (ng/m ³)	Date by which TV is to be met
As	Calendar year	6	31 December 2012
Cd	Calendar year	5	31 December 2012
Ni	Calendar year	20	31 December 2012
B(a)P	Calendar year	1	31 December 2012

1.6 Data quality objectives for modelling results and model verification

AQDD4 sets data quality objectives (DQOs) in terms of accuracy, which acts as a guide for quality assurance programmes when identifying an acceptable level of accuracy for assessment methods appropriate for supplementary assessment. Accuracy is defined in the Directive as the maximum deviation of the measured and calculated concentration levels, over the period considered by the target value, without taking into account the timing of events. DQOs have been set at 60% for annual averages of As, Cd, Ni and B(a)P.

Model accuracy has been defined in more detail 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 TV and a highly detailed assessment of the spatial representativity of the sites has not been carried out.

The models used to calculate the air pollution maps presented in this report have been verified using national network monitoring data for those sites that are listed in Form 3 of the reporting questionnaire. Model verification results are listed in the following sections for each pollutant.

1.7 Air quality in Gibraltar in 2010

Air quality monitoring data collected in Gibraltar are submitted to the Commission each year via a separate questionnaire from that compiled for the UK (CDR, 2011). Further information on air quality monitoring in Gibraltar can be found at <http://www.gibraltairquality.gi/>.

2 Heavy metals

2.1 Introduction

Heavy metals are dangerous to both human health and to the environment. Scientific evidence shows that heavy metals are human genotoxic carcinogens and that there is no identifiable threshold below which these substances do not pose a risk to human health. Impact on human health and the environment occurs via concentrations in ambient air and via deposition. TVs were set in the 4th Daughter Directive (AQDD4) for As, Cd, Ni with the aim of minimising the harmful effects on human health of airborne heavy metals, paying particular attention to sensitive populations and the environment as a whole.

An assessment to determine the concentration of each of the heavy metals listed above in ambient air has been undertaken. The annual mean background concentration of each of the pollutants is calculated by summing the contributions from:

- Area sources
- Point sources
- The heavy metal component of regional primary PM mass resulting from long range transport
- Re-suspension of heavy metals from bare soils and re-suspension associated vehicle activity

Modelling work was previously undertaken by Vincent and Passant (2008) to predict ambient concentrations of As, Cd and Ni in preparation for the implementation of AQDD4. Measured concentrations were under-predicted by the model which suggested that the source apportionment of ambient concentrations was poorly understood. Only area and point sources were considered as sources of ambient concentrations – the re-suspension of heavy metals from bare soils and vehicles was not included in the previous modelling assessment, which used only reported emissions inventories.

Abbott (2008) recommended methods for estimating the contribution of soil and vehicle related re-suspension processes to ambient heavy metal concentrations. These methods were applied for the first time in the modelling carried out for the 2008 air quality assessment (Yap et al., 2009), and subsequently in the 2009 air quality assessment (Walker et al., 2010). The methods used to estimate PM mass and the heavy metal concentrations from re-suspension processes are described below.

2.2 Monitoring sites

Annual mean concentrations of As, Cd and Ni are presented in Table 2.1 for those sites where data capture was at least 75%.

Table 2.1: Measured annual mean heavy metal concentrations and data capture (DC) recorded in 2010 where data capture >75%

Eol code	Site Name	Site Type	Annual Mean As		Annual Mean Cd		Annual Mean Ni	
			ng/m ³	DC %	ng/m ³	DC %	ng/m ³	DC %
GB0048R	Auchencorth Moss	Rural Background	0.29	100	0.05	100	0.52	100
GB0091R	Banchory	Rural Background	0.31	100	0.06	100	0.49	100
GB0855A	Beacon Hill	Rural Background	0.67	98	0.12	98	0.79	98
GB0567A	Belfast Centre	Urban Background	0.51	100	0.13	100	0.71	100
GB0878A	Bristol Avonmouth	Urban Industrial	0.69	100	0.35	100	1.10	100
GB0789A	Bristol Hallen	Urban Industrial	0.67	100	0.26	100	0.58	100
GB0369A	Cardiff Llandaff	Urban traffic	0.80	96	0.18	96	1.01	96
GB0984A	Cardiff Rumney	Urban Background	0.78	98	0.19	98	0.83	98
GB0985A	Chadwell St Mary	Urban Background	0.78	100	0.25	100	1.80	100
GB0853A	Cockley Beck	Rural Background	0.38	95	0.05	95	0.42	95
GB0986A	Dartford Bean	Urban Background	0.81	93	0.18	93	1.37	93
GB0886A	Detling	Rural Background	0.87	94	0.15	94	1.22	94
GB0002R	Eskdalemuir	Rural Background	0.14	97	0.02	97	0.15	97
GB0036R	Harwell	Rural Background	0.47	94	0.08	94	0.82	94
GB0017R	Heigham Holmes	Rural Background	0.50	94	0.10	94	1.11	94
GB0695A	London Cromwell Road 2	Urban traffic	0.77	96	0.16	96	1.63	96
GB0682A	London Marylebone Road	Urban traffic	0.60	77	0.14	77	2.84	77
GB0743A	London Westminster	Urban Background	0.69	98	0.15	98	1.45	98
GB0370A	Manchester Wythenshawe	Urban traffic	0.99	96	0.18	96	1.63	96
GB0856A	Monkswood	Rural Background	0.62	95	0.10	95	0.80	95
GB1003A	Motherwell South	Urban Background	0.76	90	0.24	90	0.32	90
GB0906A	Port Talbot Margam	Urban Industrial	0.72	100	0.33	100	1.51	100
GB0977A	Redcar	Suburban Background	0.62	96	0.15	96	2.22	96
GB0980A	Redcar Normanby	Urban Background	0.44	100	0.08	100	0.39	100
GB0877A	Runcorn Weston Point	Urban Industrial	0.84	93	0.17	93	1.03	93
GB1004A	Scunthorpe Low Santon	Urban Industrial	0.80	100	0.15	100	1.01	100
GB0841A	Scunthorpe Town	Urban Industrial	0.78	98	0.14	98	0.82	98
GB0792A	Sheffield Brinsworth	Urban Industrial	1.16	98	0.40	98	14.69	98

Eol code	Site Name	Site Type	Annual Mean As		Annual Mean Cd		Annual Mean Ni	
			ng/m ³	DC %	ng/m ³	DC %	ng/m ³	DC %
GB0615A	Sheffield Centre	Urban Background	0.69	98	0.18	98	2.49	98
GB0981A	Swansea Coedgwilym	Urban Background	0.76	98	0.19	98	10.48	98
GB0979A	Swansea Morrision	Urban traffic	0.88	98	0.30	98	15.28	98
GB0983A	Walsall Bilston Lane	Urban Background	1.16	94	1.87	94	1.67	94
GB0382A	Walsall Centre	Urban Industrial	0.92	92	0.38	92	1.10	92
GB0858A	Wytham Wood	Rural Background	0.59	98	0.09	98	0.63	98
GB0013R	Yarner Wood	Rural Background	0.51	100	0.06	100	0.68	100

2.3 Emissions

Emissions estimates for heavy metals are published annually in the National Atmospheric Emissions Inventory (NAEI). The latest available inventory year is 2009, details of which are given in Murrells et al., 2011. To calculate area source emission grids for 2010, emissions projections from the NAEI (Wagner pers. comm. 2011) have been used for each source code-activity code combination to scale 2009 emissions forwards to 2010. The emissions projections are based on DECC's UEP38 energy projections (DECC, 2009). The 2010 area source emissions have then been mapped using the same distribution grids as for the 2009 maps (Tsgatakis et al., 2011).

Emissions estimates for 2009, 2010, 2015, 2020 and 2025 by SNAP code are shown in Figure 2.1, Figure 2.2 and Figure 2.3 for As, Cd and Ni respectively. Values for intermediate years have been interpolated in these figures.

Point source emissions (the top two categories in Figure 2.1 to Figure 2.3) are emissions of a known quantity from a known location, such as power stations. Area source emissions (the remaining categories in Figure 2.1 to Figure 2.3) are 'diffuse emissions' from many unspecified locations, such as the emissions from domestic heating.

Figure 2.1 shows that a small, gradual reduction in As emissions is forecast over the period 2009-2025. In all years, SNAP code 3: Combustion in Industry, accounts for over 70% of 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 As emissions in the UK.

Point sources are the dominant source of Cd across the time series, with road transport exhaust emissions, SNAP Code 7, also shown as a significant source. Figure 2.2 shows a decrease in emissions from 2009 to 2010 due to a reduction in activity in industries which are a dominant source of cadmium e.g. steel, iron, aluminium production. A steady rise in emissions is apparent in the years 2010 to 2015, which results from the interpolation of the emissions between these projection years.

Figure 2.3 shows an 11% decrease in Ni emissions in 2010, relative to 2009, and a further decrease in total emissions throughout the time series. The Figure indicates that point sources, shipping (SNAP code 8), domestic combustion and Combustion in Industry (SNAP code 3) are the dominant emissions sources of Ni in the UK. Ni emissions to the atmosphere arise primarily from the combustion of liquid fuels.

Ambient concentrations of the heavy metals are influenced by the relative location and release characteristics of emissions. They are also influenced by sources which are not explicitly included in the emissions inventory, such as re-suspension.

Figure 2.1: UK total As emissions for 2009 and emission projections up to 2025 by SNAP code (NAEI 2009)

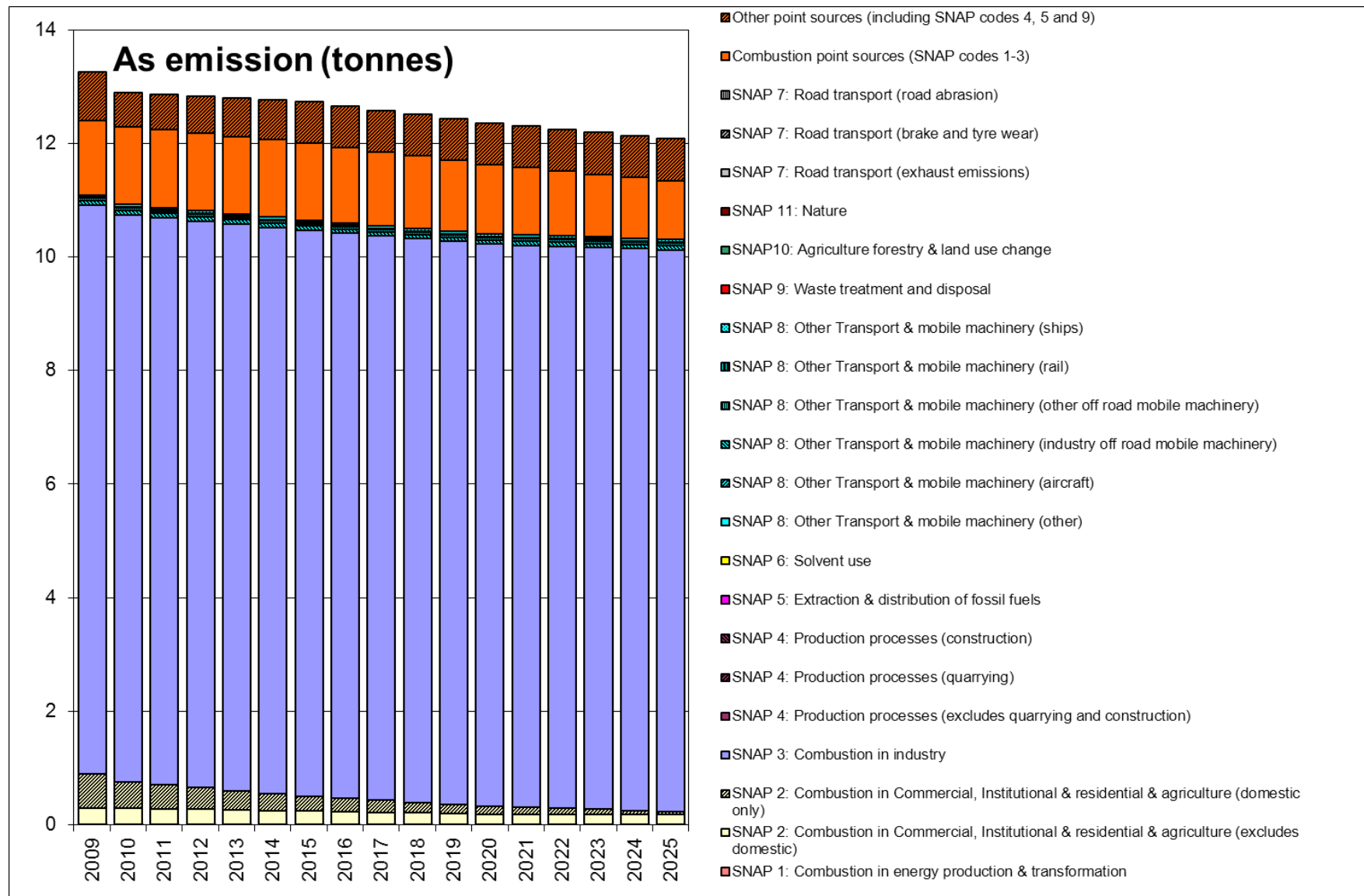


Figure 2.2: UK total Cd emissions for 2009 and emissions projections up to 2025 by SNAP code (NAEI 2009)

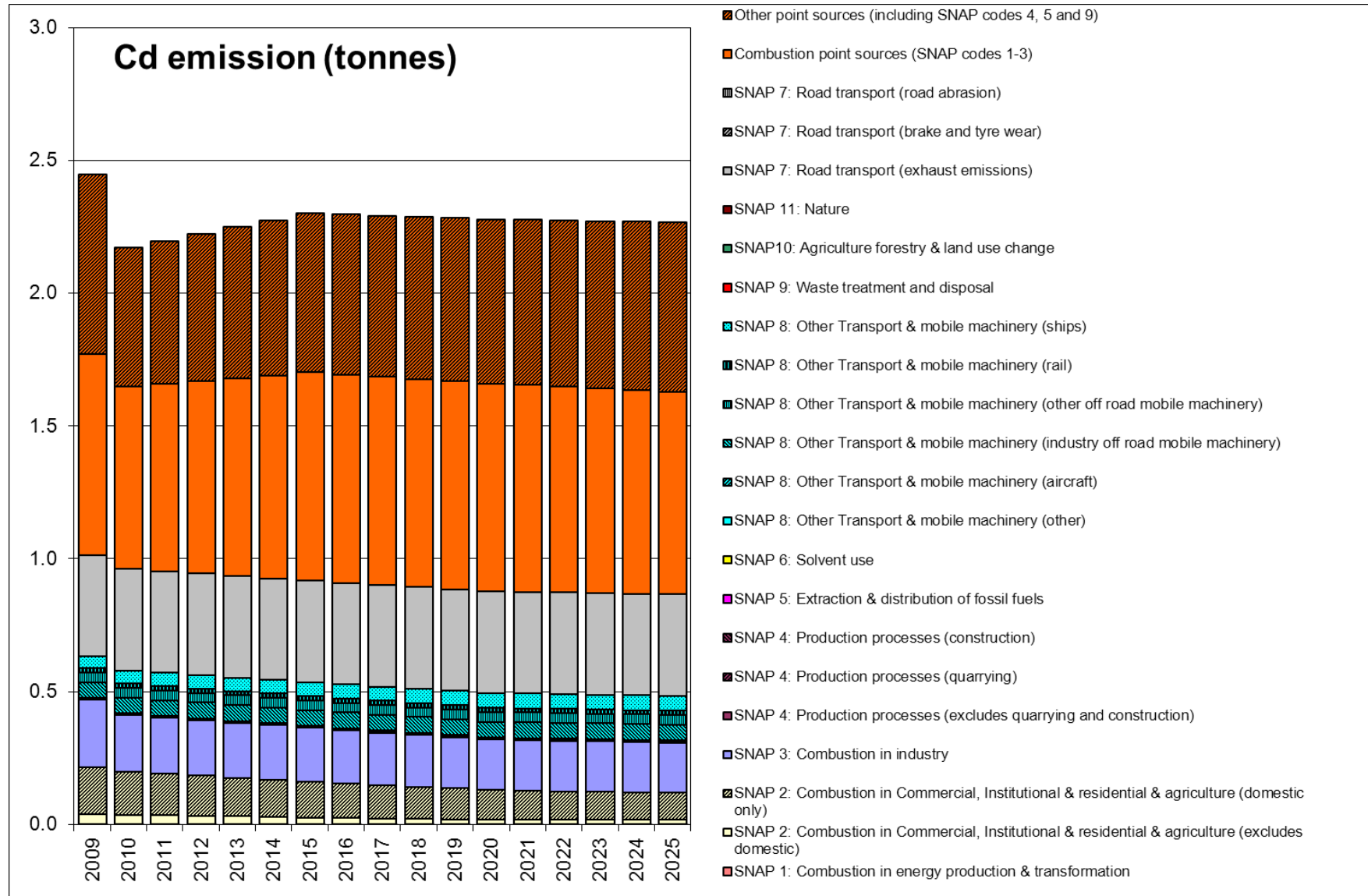
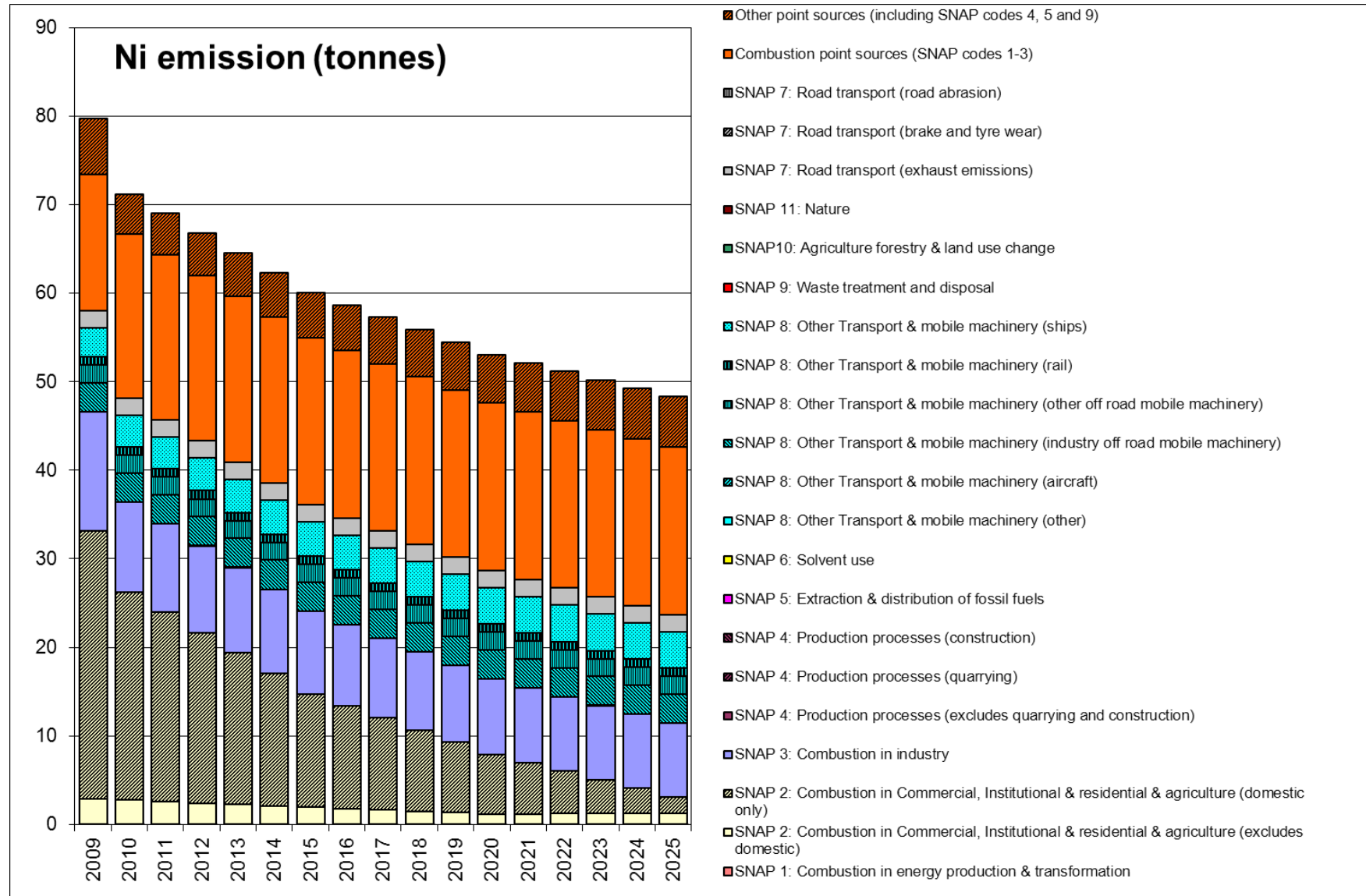


Figure 2.3: UK total Ni emissions for 2009 and emissions projections up to 2025 by SNAP code (NAEI 2009)



2.4 The model

2.4.1 Heavy metal contribution from large point sources

The contribution to ground level annual mean heavy metal concentrations from emissions from large point sources (those with annual emissions of greater than 1.2 tonnes per year or with stack parameters datasets in the PCM database) in the 2009 NAEI was estimated by modelling each source explicitly using an atmospheric dispersion model (ADMS 4.2) and sequential meteorological data for 2010 from Waddington, UK. A total of 238 large point sources were modelled for As, Cd and 246 for Ni. 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. 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 UKAAQA 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 SO₂ 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 were applied.

The NAEI emissions for large point sources are available for the year 2009, however, the year 2010 has been modelled for the assessment. There are also some point sources in the 2009 NAEI which closed before the start or early on in the year 2010. The modelled concentrations for 2009 have been scaled to 2010 using projection factors calculated from NAEI source sector total emissions for point sources for 2009 and NAEI emissions projections for 2010. Closure of particular plant or activities has been 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 2009. The point sources in the 2009 NAEI which closed before the start or early on in the year 2010 have been removed from the 2010 modelling, based on recommendations from the NAEI team (Passant, personal communication, 2011).

2.4.2 Heavy metal contribution from small point and fugitive sources

The contribution of emissions from small point sources (those without stack parameters datasets) and fugitive sources in the 2009 NAEI was modelled using the small point model. The model consists of separate 'in-square' and 'out-of-square' components, in which concentrations are estimated using a point source dispersion kernel. The dispersion kernel was calculated by using the dispersion model ADMS 4.2 to model the dispersion of unit emissions from a central source to a 31km x 31km grid of receptors at a spatial resolution of 1km x 1km, using the stack characteristics presented in Table 2.2. Hourly sequential meteorological data from Waddington in 2010 was used to construct the dispersion kernels.

The greatest concentrations would be expected close to the point of emission. The value for the central square within the dispersion kernel has therefore been assigned to be equal to the highest of the values modelled for the adjacent grid squares. The receptor for the central

grid square within the dispersion kernel is at exactly the same location as the point of release, and the modelled concentration at this location would otherwise have been zero.

Table 2.2: Stack release parameters used to characterise emissions from point sources with no available stack parameters

Variable	Parameters
Stack height	15m
Diameter	1m
Temperature	15°C
Surface roughness at dispersion site	0.5m
Surface roughness at met site	0.02m

Characterising the fugitive heavy metal emissions from an industrial plant is notoriously difficult. The emission release parameters used in the model for fugitive emissions are provided in Table 2.3. Once again, the value for the central square within the dispersion kernel has been set to the maximum of the values in the surrounding grid squares. Assuming a fugitive emission of 0.05 times the reported emission was found to provide the best agreement with available measurement data.

Table 2.3: Stack release parameters used to characterise fugitive emission release

Variable	Parameters
Stack height	10m
Diameter	1m
Temperature	15°C
Surface roughness at dispersion site	0.5m
Surface roughness at met site	0.02m

2.4.3 Heavy metal contribution from local area sources

The uncalibrated modelled area source contribution was calculated by applying an ADMS 4.2 derived dispersion kernel to calculate the contribution to ambient concentrations at a central receptor location from area source emissions within a 33km x 33km square surrounding each receptor. Hourly sequential meteorological data from Waddington in 2010 was used to construct the dispersion kernels, as described in Appendix 1.

Previously, the area source calibration coefficient derived for NO_x within the PCM model has been used to calculate the calibrated heavy metal area source contribution for each grid square in the country e.g. Grice at al., 2011. However for 2010, the area source calibration coefficient derived for NO_x was almost double that reported last year (Grice et al., 2011) although the fit remains similarly robust. Several factors are thought to drive the under-prediction by the uncalibrated model:

- It is now understood that current emissions inventories over predict the decline in NO_x emissions from road transport over approximately the last five years (Carslaw et al., 2011);
- The extended periods of cold weather experienced by the UK in both early and late 2010 meant that combustion emissions associated with space heating may have been higher than projected. These factors would combine to produce higher ambient concentrations than calculated by the uncalibrated model.

These factors are not considered to significantly influence ambient concentrations of As, Cd or Ni, and application of the NO_x calibration coefficient would have lead to over prediction of modelled concentrations when compared to monitoring data. Therefore an area source calibration coefficient of unity was applied to the heavy metal modelling. This gave good

agreement between modelled and monitored concentrations. A B(a)P-specific calibration coefficient was applied for this pollutant (see Section 3).

For certain sectors (noted within each pollutant section described 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. The application of these caps is annually reported back to the NAEI as part of the quality checking process to ensure that continual improvements are made in the emissions grids.

2.4.4 Heavy metal contribution from regional PM mass as a result of long-range transport

The contribution to ambient concentrations from long range transport of heavy metals was derived from estimates of regional primary particulate matter used in the 2010 PCM model for PM₁₀ mass (Brookes et al., 2011). Contributions from the long range transport of PM particles on a 20km x 20km grid were 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, with all sources within 10km of the receptor point excluded from the TRACK model. This allowed the area source and the point source models to be nested within the long-range transport model without duplicating any source contributions.

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 PM₁₀ emission for that sector. These ratios were also assumed to apply to the contribution from non-UK European sources.

2.4.5 Heavy metal contribution from re-suspension

The 2010 model for heavy metal concentrations includes a contribution to ambient concentrations from re-suspension. The contributions from two processes have been included:

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

The heavy metal contribution from re-suspension was calculated using the methodology suggested by Abbott (2008). The methods used to estimate the total PM mass from these processes were revised by Grice et al (2009) to provide estimates suitable for inclusion in the PCM model.

PM₁₀ mass from re-suspension of soils

The contribution to PM mass from re-suspension of soils is calculated using the proportions of bare soils, root crops and cereal crops in 1km x 1km grid squares across the UK, within the Land Cover Map 2000 (Land Cover Map 2000, 2009). The concentration of PM mass cannot be calculated using the standard approach, which is by use of 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 dependent upon 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 upon hourly sequential meteorological data from twelve sites throughout the UK for 1999. This year was selected because the data were readily available.

This methodology has been adapted for use within the PCM model 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.

PM₁₀ mass re-suspension due to vehicle activity

Abbott (2008) also developed a method for estimating the contribution to PM mass from re-suspension due to vehicle activity. This method takes vehicle km statistics for heavy-duty vehicles (heavy goods vehicles and buses) as its starting point. These estimates are likely to be subject to greater uncertainty than the estimates for re-suspension from rural 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 twelve meteorological stations for 1999; one to represent rural, and one to represent urban conditions. The estimated re-suspension rate was considerably higher for rural conditions due to the higher vehicle speeds assumed. These two sets of kernels were then used to calculate the contribution to PM₁₀ concentrations according to the proportion of urban and rural land cover within each 1km x 1km grid square. A detailed examination of the results from this assessment showed that the concentrations in urban areas were largely driven by the small proportion of rural land cover in the urban areas. The urban kernel was hence applied to all roads within the PCM model.

Estimating heavy metal concentrations

The maps of PM mass from the re-suspension of soils and re-suspension associated with vehicle movements are used to estimate contributions to the ambient concentration of heavy metals (Abbott, 2008). This is undertaken 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 and nickel concentrations in topsoil at 5km resolution throughout England and Wales. Measurements of heavy metals in topsoil for other areas of the UK can be obtained from the Geochemical Atlas of Europe, developed under the auspices of the Forum of European Geological Surveys (FOREGS) [www.gtk.fi/publ/foregsatlas]. These data were interpolated to a 1km x 1km 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 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 2.4 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).

Table 2.4: Heavy metal enhancement factors used in the assessment

Pollutant	Enhancement factor
As	35
Cd	35
Ni	7

2.5 Arsenic

2.5.1 Introduction

The method used to estimate the As ambient concentration across the UK is described in Section 2.4 above.

A cap of 3.5 ng/m^3 was applied to the contribution generated from the re-suspension of bare soils. This value was chosen as an estimate of the maximum likely concentration generated from this source.

2.5.2 Maps of annual mean concentrations

Figure 2.4 shows the modelled annual mean As concentrations. There are no modelled exceedances of the target value of 6 ng/m^3 in 2010. The maximum estimated As annual mean concentration across the UK was 5.05 ng/m^3 .

2.5.3 Source apportionment

Figure 2.5 shows the modelled As contribution from different sources at 36 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 arsenic are emissions from point sources, non-road area sources and re-suspension processes.

2.5.4 Verification of mapped concentrations

An alternative presentation of the comparison between modelled and measured annual mean As concentrations in 2010 at different monitoring site locations are shown in Figure 2.6 to Figure 2.9. 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 1.6).

Summary statistics for modelled and measured As concentrations are listed in Table 2.5, 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 industrial, 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. The agreement between the measured and modelled annual mean heavy metal concentrations in this current assessment is much better than the assessment presented by Vincent and Passant (2008). This is because the current assessment includes contributions from re-suspension processes in addition to emission sources included within the emissions inventory. The agreement is much better at the rural sites in particular, where the previous assessment predicted much lower concentrations.

2.5.5 Comparison of modelling and measurement results with the target value

There were no modelled or measured exceedances of the target value for As in 2010.

Figure 2.4: Annual mean map of As concentrations for comparison with the As target value of 6ng/m^3 , 2010 (ng/m^3)

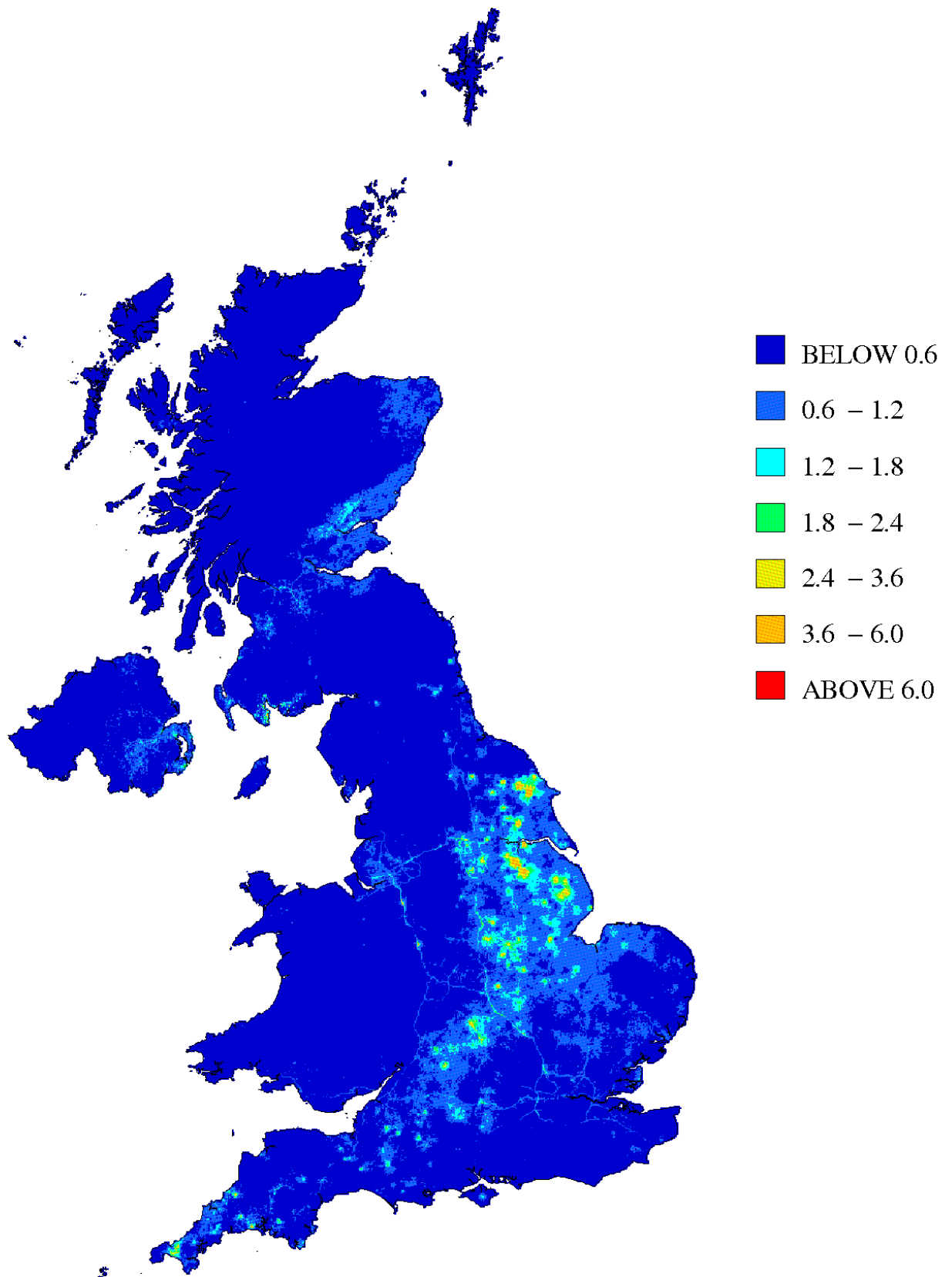


Figure 2.5: Source apportionment for As, 2010

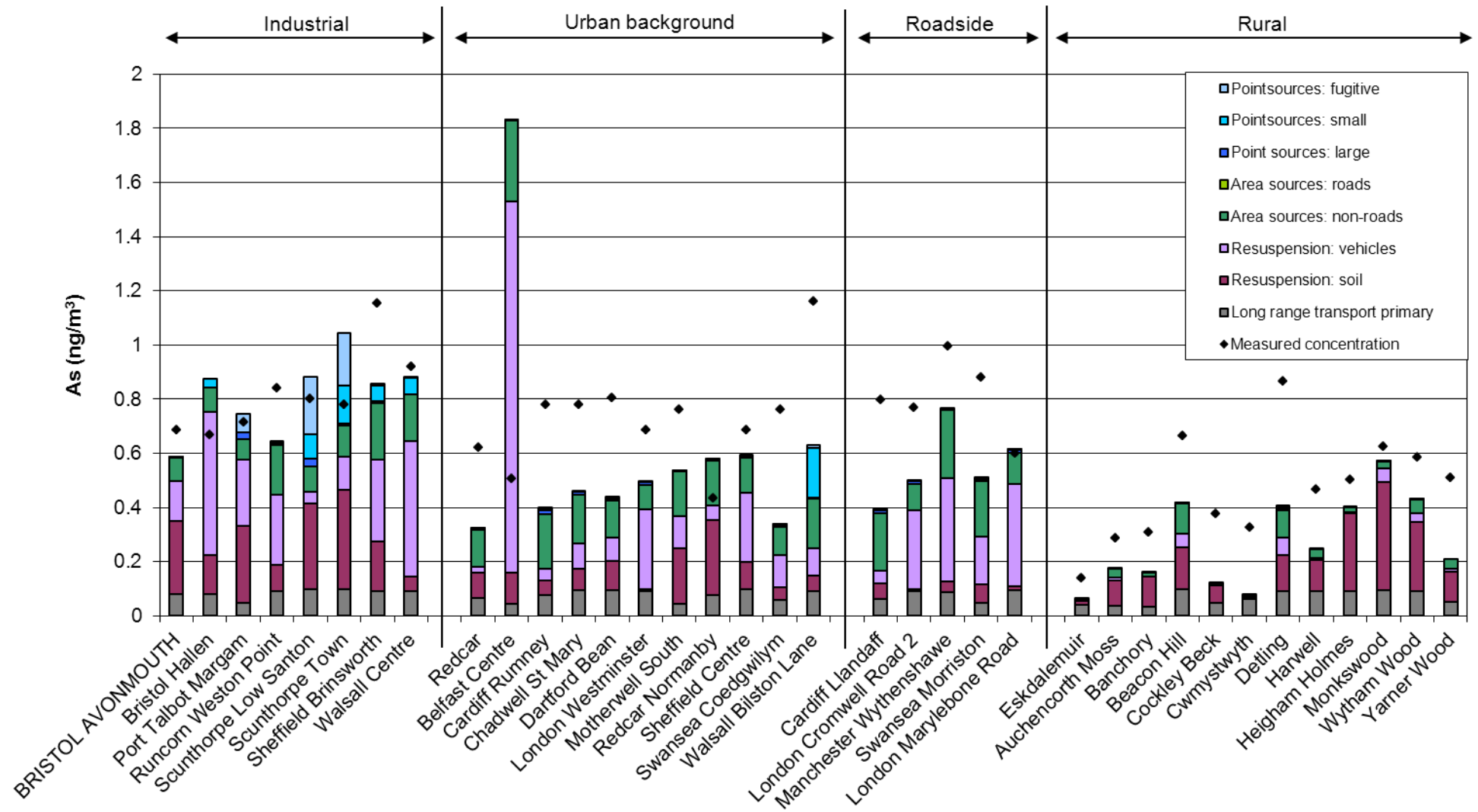


Figure 2.6: Verification of annual mean As at Industrial sites

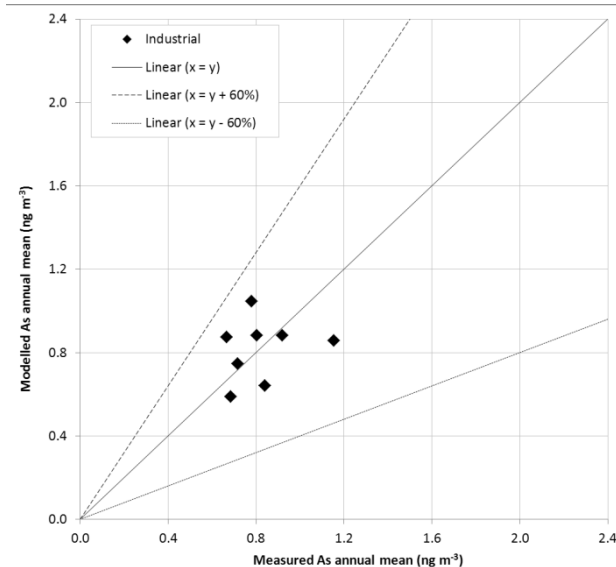


Figure 2.7: Verification of annual mean As at urban background sites

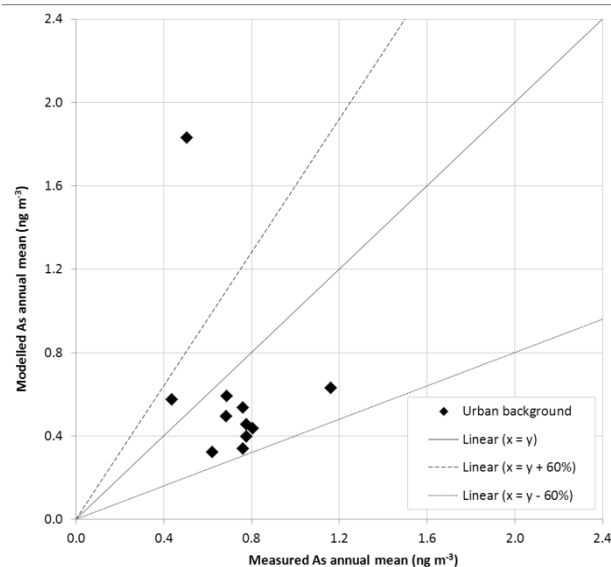


Figure 2.8: Verification of annual mean As at roadside sites

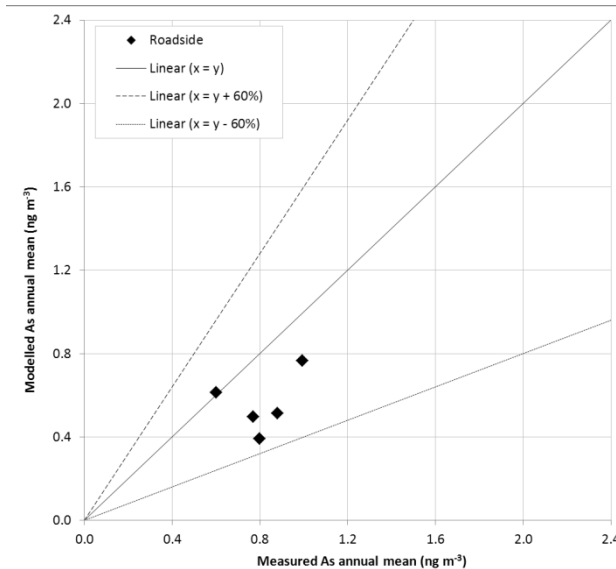


Figure 2.9: Verification of annual mean As at rural sites

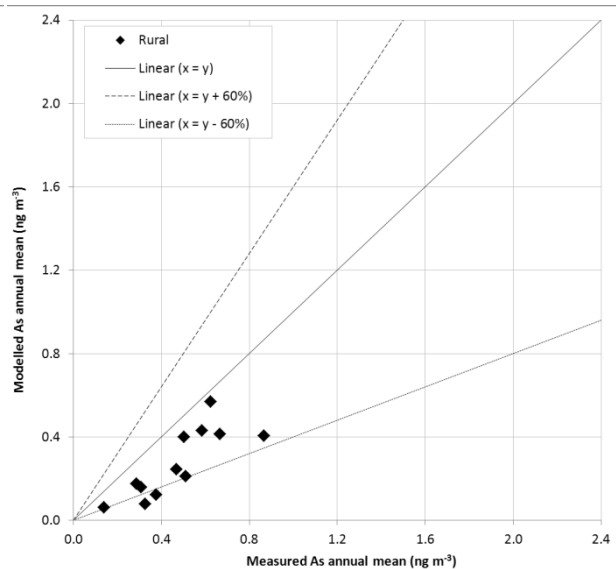


Table 2.5: Summary statistics for comparison between modelled and measured annual mean As concentrations at different monitoring sites, 2010

	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	0.82	0.81	0.05	0.0	8
Urban background sites	0.73	0.60	0.11	9.1	11
Roadside sites	0.81	0.56	0.11	0.0	5
Rural sites	0.47	0.27	0.67	16.7	12

2.6 Cadmium

2.6.1 Introduction

The method used to estimate the Cd ambient concentration across the UK is described in Section 2.4.

2.6.2 Maps of annual mean concentrations

Figure 2.10 shows the modelled annual mean Cd concentrations. There are no modelled exceedances of the target value of 5 ng/m³ in 2009. The maximum estimated Cd annual mean concentration was 2.50 ng/m³.

2.6.3 Source apportionment

Figure 2.11 shows the modelled Cd contribution from different sources at 36 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.

2.6.4 Verification of mapped concentrations

An alternative presentation of the comparisons of modelled and measured annual mean Cd concentrations in 2010 at different monitoring site locations are shown in Figure 2.12 to Figure 2.15. 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 1.6).

Summary statistics for modelled and measured Cd concentrations are listed in Table 2.6, 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 urban and industrial monitoring sites. The agreement is better at roadside 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. The agreement between the measured and modelled annual mean heavy metal concentrations in this current assessment is much better than the assessment presented by Vincent and Passant (2008). This is because the current assessment includes contributions from re-suspension processes in addition to emission sources included within the emissions inventory. The agreement is much better at the rural sites in particular, where the previous assessment predicted much lower concentrations.

2.6.5 Comparison of modelling and measurement results with the target value

There were no modelled or measured exceedances of the target value for Cd in 2010.

Figure 2.10: Annual mean map of Cd concentrations for comparison with the Cd target value of 5ng/m^3 , 2010 (ng/m^3)

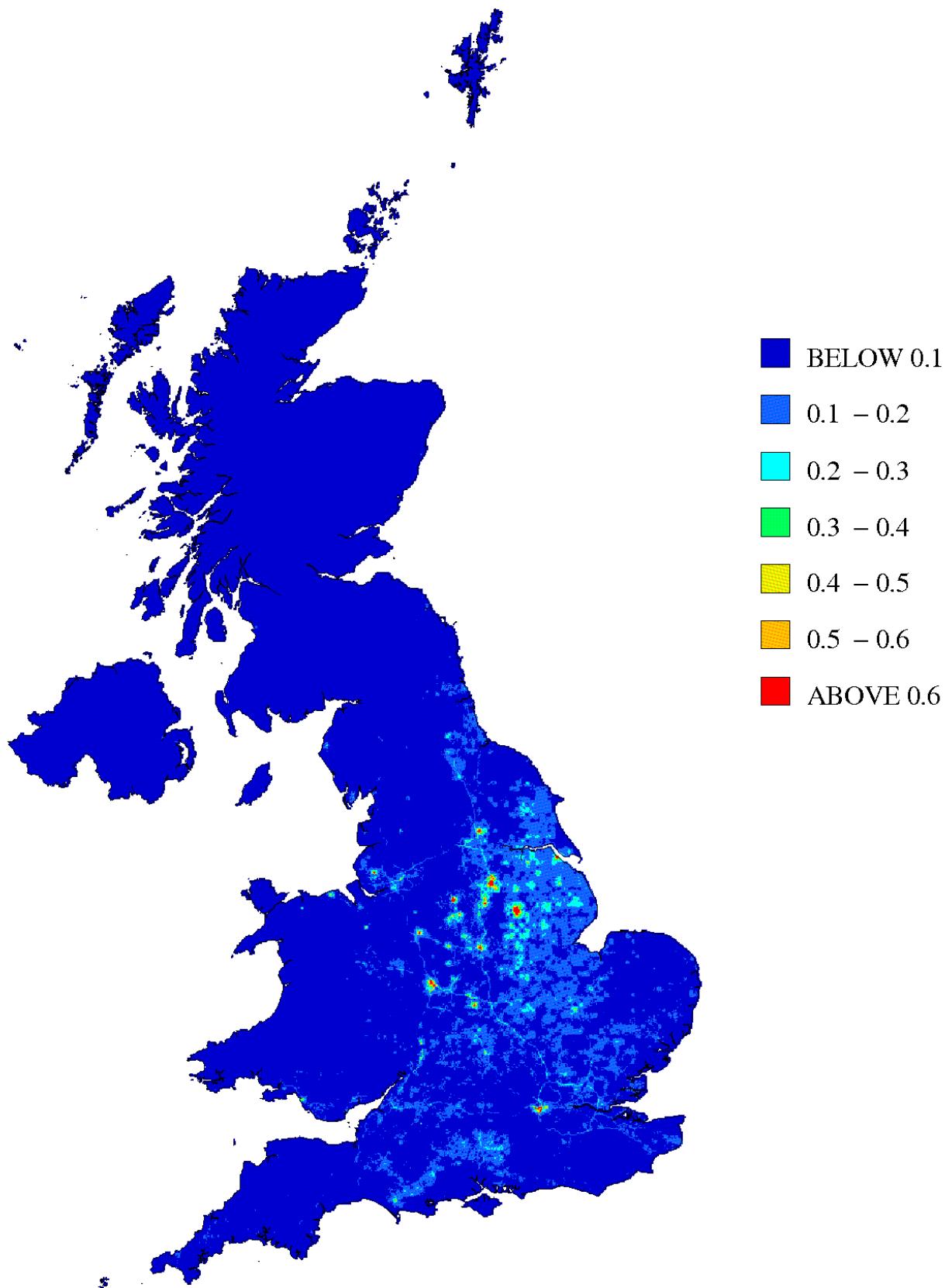


Figure 2.11: Source apportionment for Cd, 2010

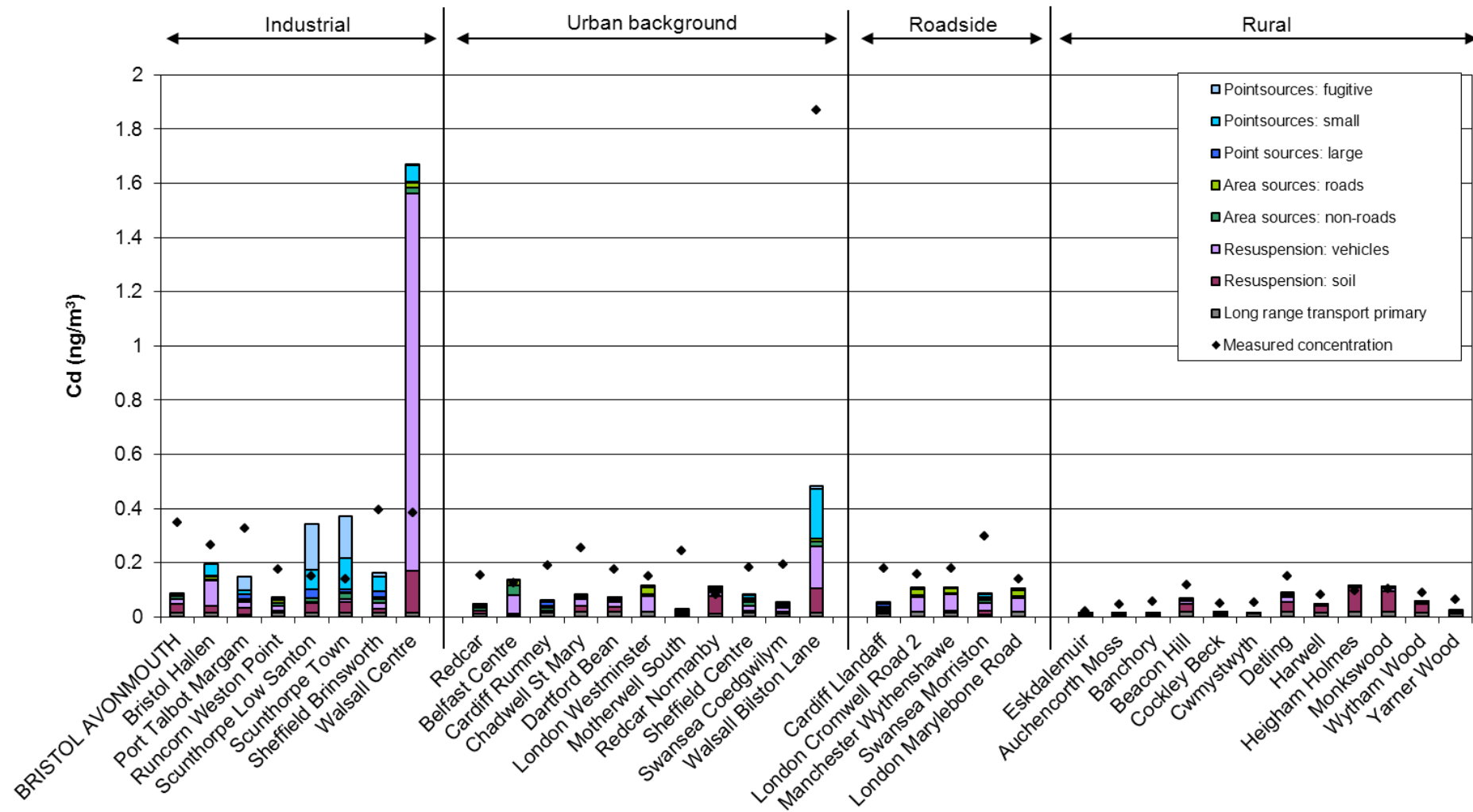


Figure 2.12: Verification of annual mean Cd at Industrial sites

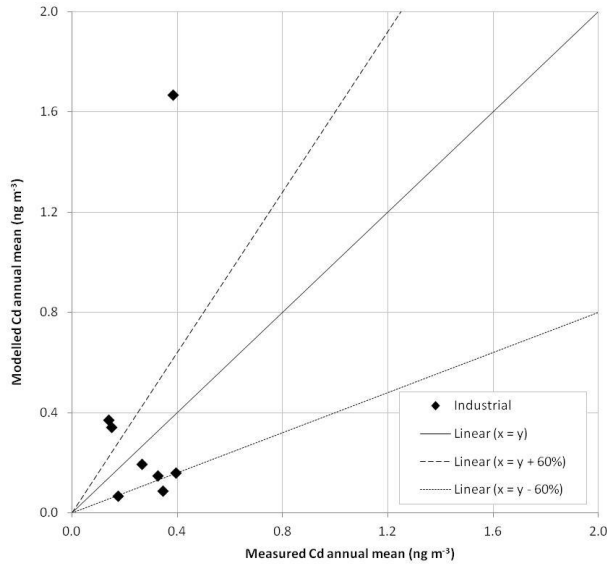


Figure 2.13: Verification of annual mean Cd at urban background sites

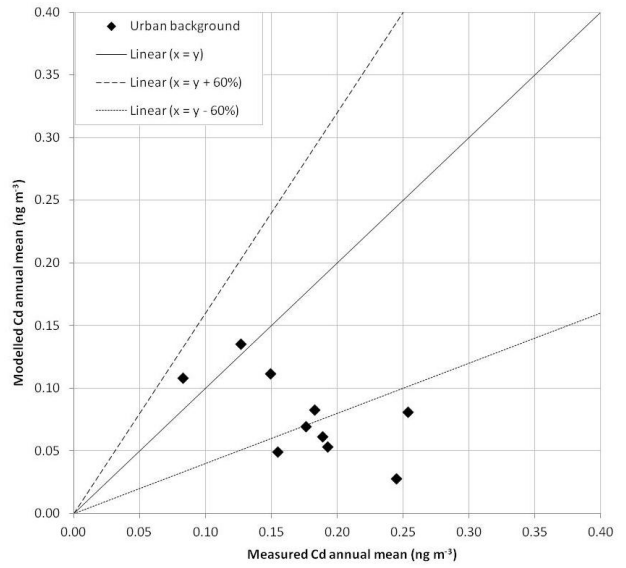


Figure 2.14: Verification of annual mean Cd at roadside sites

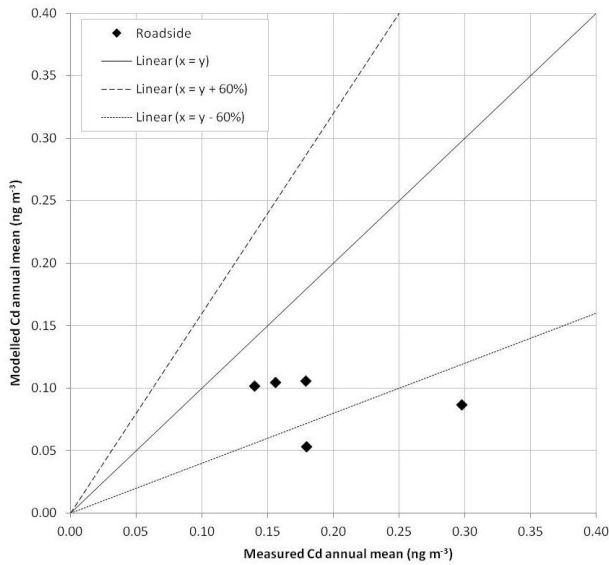


Figure 2.15: Verification of annual mean Cd at rural sites

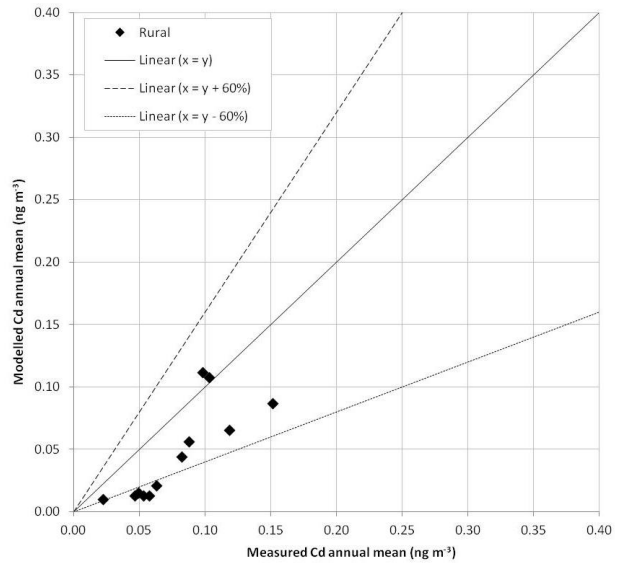


Table 2.6: Summary statistics for comparison between modelled and measured annual mean Cd concentrations at different monitoring sites, 2010

	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	0.27	0.38	0.09	62.5	8
Urban background sites	0.33	0.11	0.90	63.6	11
Roadside sites	0.19	0.09	0.05	40.0	5
Rural sites	0.08	0.05	0.67	41.7	12

2.7 Nickel

2.7.1 Introduction

The method used to estimate ambient Ni concentrations across the UK is described in Section 2.4.

A cap of 15 tonnes per km² 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 7 ng/m³ was applied to the contribution generated from the re-suspension of bare soils. This value was chosen as an estimate of the maximum likely concentration generated from this source.

2.7.2 Maps of annual mean concentrations

Figure 2.16 shows the modelled annual mean Ni concentrations. The maximum estimated Ni annual mean concentration was 16.87 ng/m³.

2.7.3 Source apportionment

Figure 2.17 shows the modelled Ni contribution from different sources at 36 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.

2.7.4 Verification of mapped concentrations

An alternative presentation of the comparisons of modelled and measured annual mean Ni concentrations in 2010 at different monitoring site locations are shown in Figure 2.18 to Figure 2.21. 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 1.6).

Summary statistics for modelled and measured Ni concentrations are listed in Table 2.7, 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 roadside monitoring sites. The agreements between measured and modelled concentrations on a site-by-site basis (quantified using R²) are poor for the urban background and industrial monitoring locations. The results for rural sites show slightly better agreement.

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. The agreement between the measured and modelled annual mean heavy metal concentrations in this current assessment is much better than the assessment presented by Vincent and Passant (2008). This is because the current assessment includes contributions from re-suspension processes in addition to emission sources included within the emissions inventory. The agreement is much better at the rural sites in particular, where the previous assessment predicted much lower concentrations.

Table 2.7: Summary statistics for comparison between modelled and measured annual mean Ni concentrations at different monitoring sites, 2010

	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	2.73	3.13	0.01	75.0	8
Urban background sites	2.16	1.95	0.02	45.5	11
Roadside sites	4.48	1.46	0.18	20.0	5
Rural sites	0.68	0.81	0.66	25.0	12

Figure 2.16: Annual mean map of Ni concentrations for comparison with the Ni target value of 20ng/m³, 2010 (ng/m³)

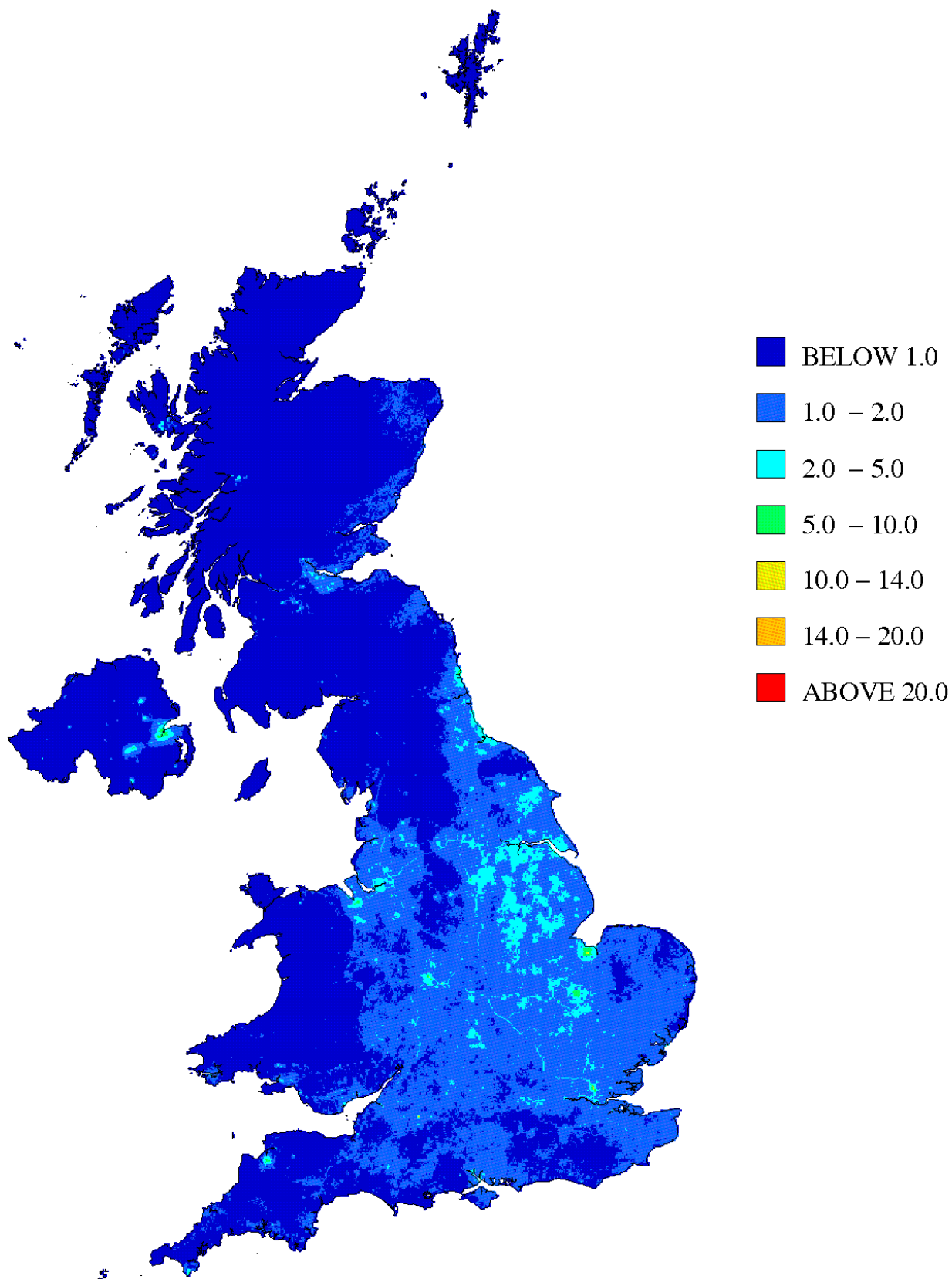


Figure 2.17: Source apportionment for Ni, 2010

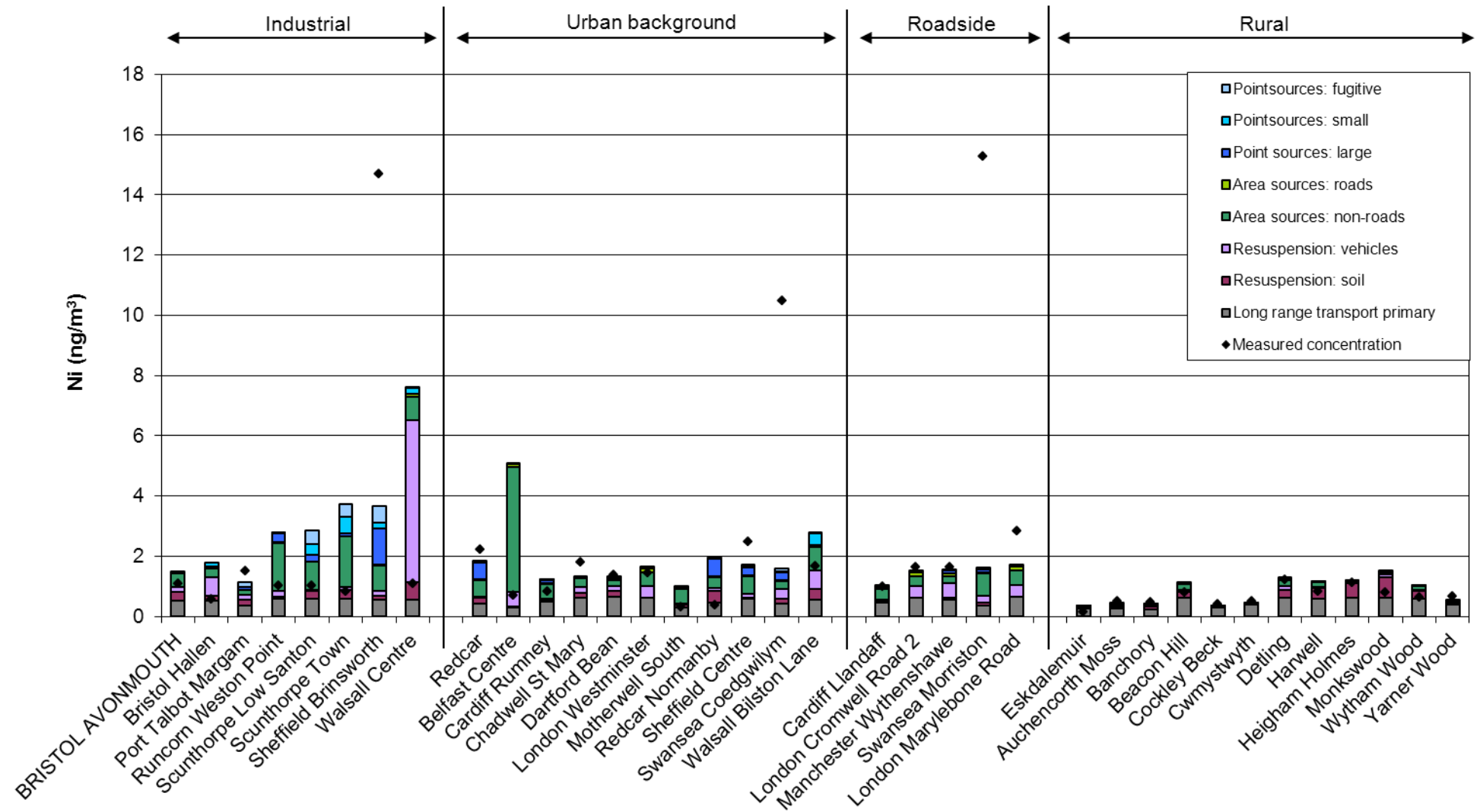


Figure 2.18: Verification of annual mean Ni at Industrial sites

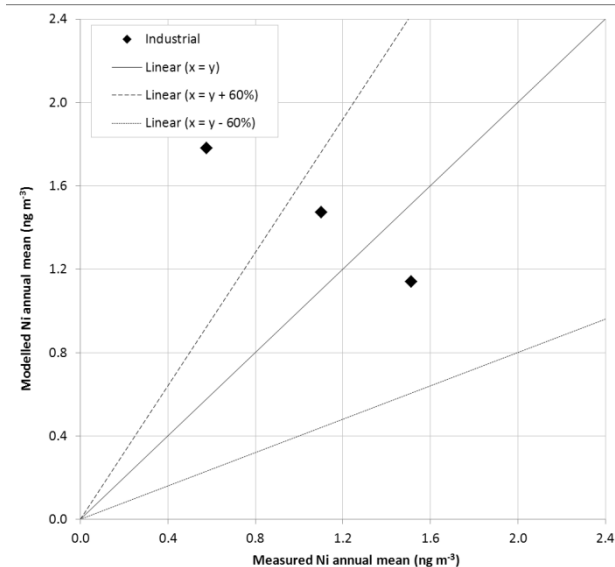


Figure 2.19: Verification of annual mean Ni at urban background sites

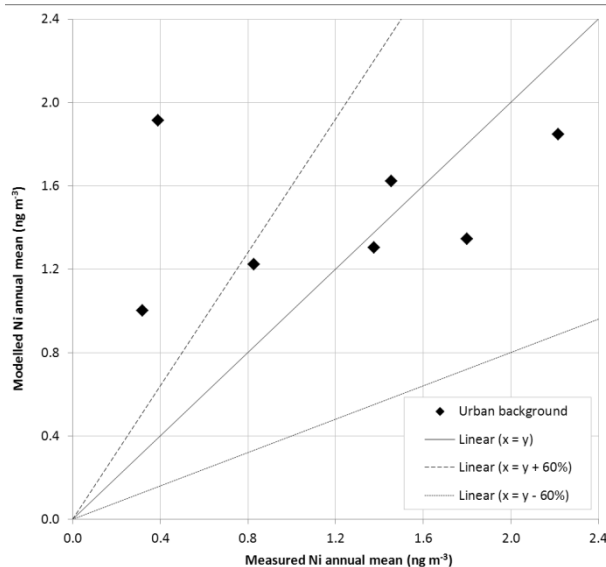


Figure 2.20: Verification of annual mean Ni at roadside sites

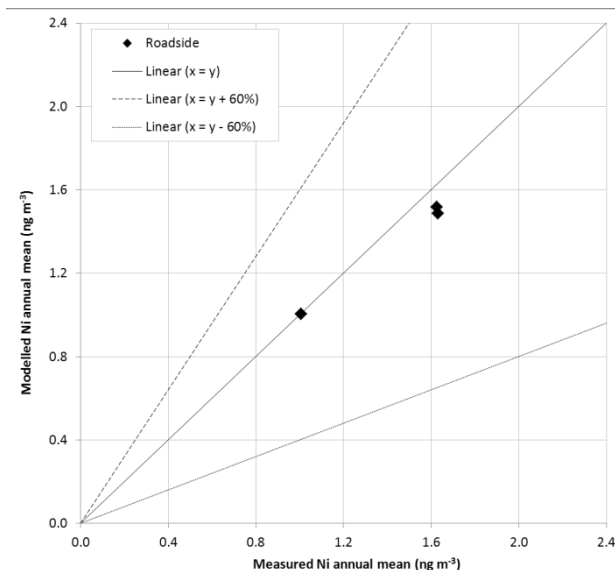
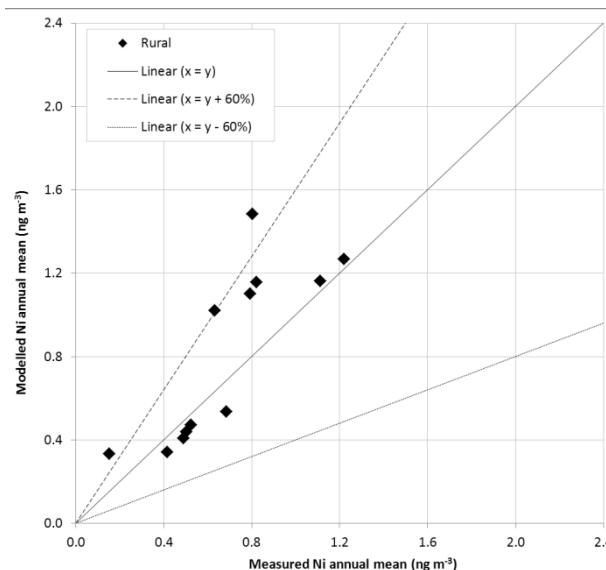


Figure 2.21: Verification of annual mean Ni at rural sites



2.7.5 Detailed comparison of modelled results with the target value

There were no measured exceedances of the TV at any of the monitoring sites within the National Monitoring Network. The tabular results for the supplementary assessment for Ni are presented in Table 2.8, taken from Form 19j of the questionnaire. Exceedances of the TV for the Swansea Urban Area and South Wales zones have been reported based upon the annual mean concentration of 50 ng/m³ measured at Pontardawe Tawe Terrace (a site which became part of the National Network in January 2011) and the detailed local modelling analysis described below. This monitoring site is within the Swansea Urban Area zone but is very near to the boundary of the South Wales zone.

Since the 2008 (Yap et al., 2009) and 2009 (Walker et al., 2011) assessments, detailed dispersion modelling has been undertaken using ADMS 4.2 for the area in South Wales where exceedances of the annual mean target value of 20 ng/m³ have been measured. This small scale modelling has been used to assess the likely magnitude and spatial scale of the exceedance.

The emission of nickel from the relevant industrial point source was taken as 89.93 kg/year for 2010, emitted from seven locations across the complex (data provided by industrial operator). This annual emission took into account recent abatement measures put in place at the industrial point source. Building effects were included in the model, and a 6km x 6km area was extracted from a single 20km x 20km Land-Form PANORAMA® tile to model the topographical effects of the valley. The height of the terrain was specified at the centre of each 50m x 50m grid square.

Figure 2.22 shows the modelled ambient concentration estimates on a 20m x 20m grid resulting from the point source emissions. The distribution of Ni concentrations from the point source are strongly influenced by the terrain in the area, as can be seen in Figure 2.22 – the Swansea Valley runs south-west to north-east through the village of Pontardawe, where the point source is located.

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

The source apportionment and scatter graphs in the sections above do not include the contribution to ambient concentrations at the Pontardawe Tawe Terrace site from the identified local industrial source. The addition of this contribution brings the total modelled concentration up to 60.42 ng/m³, which is reasonably good agreement with the measured annual mean concentration of 50 ng/m³.

Further emission abatement at the relevant plant is in place (2011) in order to reduce the impact of these emissions on local ambient air quality. Further modelling work will be undertaken following the completion of the installation of the improved abatement and subsequent emission measurements.

The Pontardawe Tawe Terrace monitoring site is located south-west of the point source, and a new monitoring location, which will be located downwind of the site under a prevailing south-westerly wind (north-east of the point source), is currently being finalised.

Table 2.8: Tabular results of and methods used for supplementary assessment for Ni

Zone	Zone code	Above TV for health (annual mean)			
		Area		Population exposed	
		km ²	Method	Number	Method
Greater London Urban Area	UK0001	0	B	0	B
West Midlands Urban Area	UK0002	0	B	0	B
Greater Manchester Urban Area	UK0003	0	B	0	B
West Yorkshire Urban Area	UK0004	0	B	0	B
Tyneside	UK0005	0	B	0	B
Liverpool Urban Area	UK0006	0	B	0	B
Sheffield Urban Area	UK0007	0	B	0	B
Nottingham Urban Area	UK0008	0	B	0	B
Bristol Urban Area	UK0009	0	B	0	B
Brighton/Worthing/Littlehampton	UK0010	0	B	0	B
Leicester Urban Area	UK0011	0	B	0	B
Portsmouth Urban Area	UK0012	0	B	0	B
Teesside Urban Area	UK0013	0	B	0	B
The Potteries	UK0014	0	B	0	B
Bournemouth Urban Area	UK0015	0	B	0	B
Reading/Wokingham Urban Area	UK0016	0	B	0	B
Coventry/Bedworth	UK0017	0	B	0	B
Kingston upon Hull	UK0018	0	B	0	B
Southampton Urban Area	UK0019	0	B	0	B
Birkenhead Urban Area	UK0020	0	B	0	B
Southend Urban Area	UK0021	0	B	0	B
Blackpool Urban Area	UK0022	0	B	0	B
Preston Urban Area	UK0023	0	B	0	B
Glasgow Urban Area	UK0024	0	B	0	B
Edinburgh Urban Area	UK0025	0	B	0	B
Cardiff Urban Area	UK0026	0	B	0	B
Swansea Urban Area	UK0027	1	B	1674	B
Belfast Metropolitan Urban Area	UK0028	0	B	0	B
Eastern	UK0029	0	B	0	B
South West	UK0030	0	B	0	B
South East	UK0031	0	B	0	B
East Midlands	UK0032	0	B	0	B
North West & Merseyside	UK0033	0	B	0	B
Yorkshire & Humberside	UK0034	0	B	0	B
West Midlands	UK0035	0	B	0	B
North East	UK0036	0	B	0	B
Central Scotland	UK0037	0	B	0	B
North East Scotland	UK0038	0	B	0	B
Highland	UK0039	0	B	0	B
Scottish Borders	UK0040	0	B	0	B
South Wales	UK0041	1	B	1577	B
North Wales	UK0042	0	B	0	B
Northern Ireland	UK0043	0	B	0	B
Total		2		3250	

Method 'B' is the modelling methodology described in this report.

3 Benzo(a)pyrene

3.1 Introduction

Benzo(a)pyrene, (B(a)P) concentrations were modelled for 2005 by Vincent et al. (2007) to inform the UK Preliminary Assessment for AQDD4 (Bush, 2007). 2010 is the third 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 of 1 ng/m^{-3} set out in the Directive.

3.2 Monitoring sites

The monitoring sites operational during 2010 for the purposes of AQDD4 reporting are listed in Form 3 of the questionnaire (CDR 2011). In previous years a combination of two different monitoring instruments has been used (Andersen and Digital instruments). In 2010, only Digital instruments were used. A summary of the monitoring data for 2010 is presented in Table 3.1.

Table 3.1: Summary of B(a)P monitoring data for 2010

Eol code	Site name	Site type	Annual Mean B(a)P	
			ng/m ³	DC %
GB0048R	Auchencorth Moss	Rural Background	0.03	84%
GB0934A	Ballymena	Urban Background	2.01	98%
GB0851A	Birmingham Tyburn	Urban Background	0.29	89%
GB0700A	Bolsover	Urban Industrial	0.50	85%
GB0869A	CARDIFF LAKESIDE	Urban Background	0.22	93%
GB0944A	Derry Brandywell	Urban Background	1.93	98%
GB0839A	Edinburgh St Leonards	Urban Background	0.12	79%
GB0641A	Glasgow Centre	Urban Background	0.23	97%
GB0036R	Harwell	Rural Background	0.13	81%
GB0702A	Hazelrigg	Rural Background	0.08	82%
GB0014R	High Muffles	Rural Background	0.07	94%
GB0850A	Hove	Urban Background	0.20	91%
GB0705A	Kinlochleven	Urban Background	0.27	96%
GB0867A	Leeds Millshaw	Urban Background	0.37	84%
GB0706A	Lisburn Dunmurry High School	Suburban Background	1.44	68%
GB0777A	Liverpool Speke	Urban Background	0.26	85%
GB0849A	London Brent	Urban Background	0.18	83%
GB0847A	London Crystal Palace Parade	Urban traffic	0.27	89%
GB0682A	London Marylebone Road	Urban traffic	0.25	82%
GB0583A	Middlesbrough	Urban Background	0.44	99%
GB0568A	Newcastle Centre	Urban Background	0.16	88%
GB0962A	Newport	Urban Background	0.25	84%
GB0906A	Port Talbot Margam	Urban Industrial	0.38	88%
GB0940A	ROYSTON	Urban Industrial	1.13	84%
GB0660A	Salford Eccles	Urban Industrial	0.37	94%
GB1004A	Scunthorpe Low Santon	Urban Industrial	1.80	94%

Eol code	Site name	Site type	Annual Mean B(a)P	
			ng/m ³	DC %
GB0841A	Scunthorpe Town	Urban Industrial	1.30	80%
GB0942A	SOUTH HIENDLEY	Urban Industrial	0.63	91%
GB0004R	Stoke Ferry	Rural Background	0.13	87%
GB0943A	SWANSEA CWM LEVEL PARK	Urban Background	0.29	84%

3.3 Emissions

Emissions estimates for B(a)P are published annually in the National Atmospheric Emissions Inventory (NAEI). The latest available inventory year is 2009, details of which are given in Murrells et al., 2011. To calculate area source emission grids for 2010, emissions projections from the NAEI (Wagner pers. comm. 2011) have been used for each source code-activity code combination to scale 2009 emissions forwards to 2010. The emissions projections are based on DECC's UEP38 energy projections (DECC, 2009). The 2010 area source emissions have then been mapped using the same distribution grids as for the 2009 maps (Tsagatakis et al., 2011).

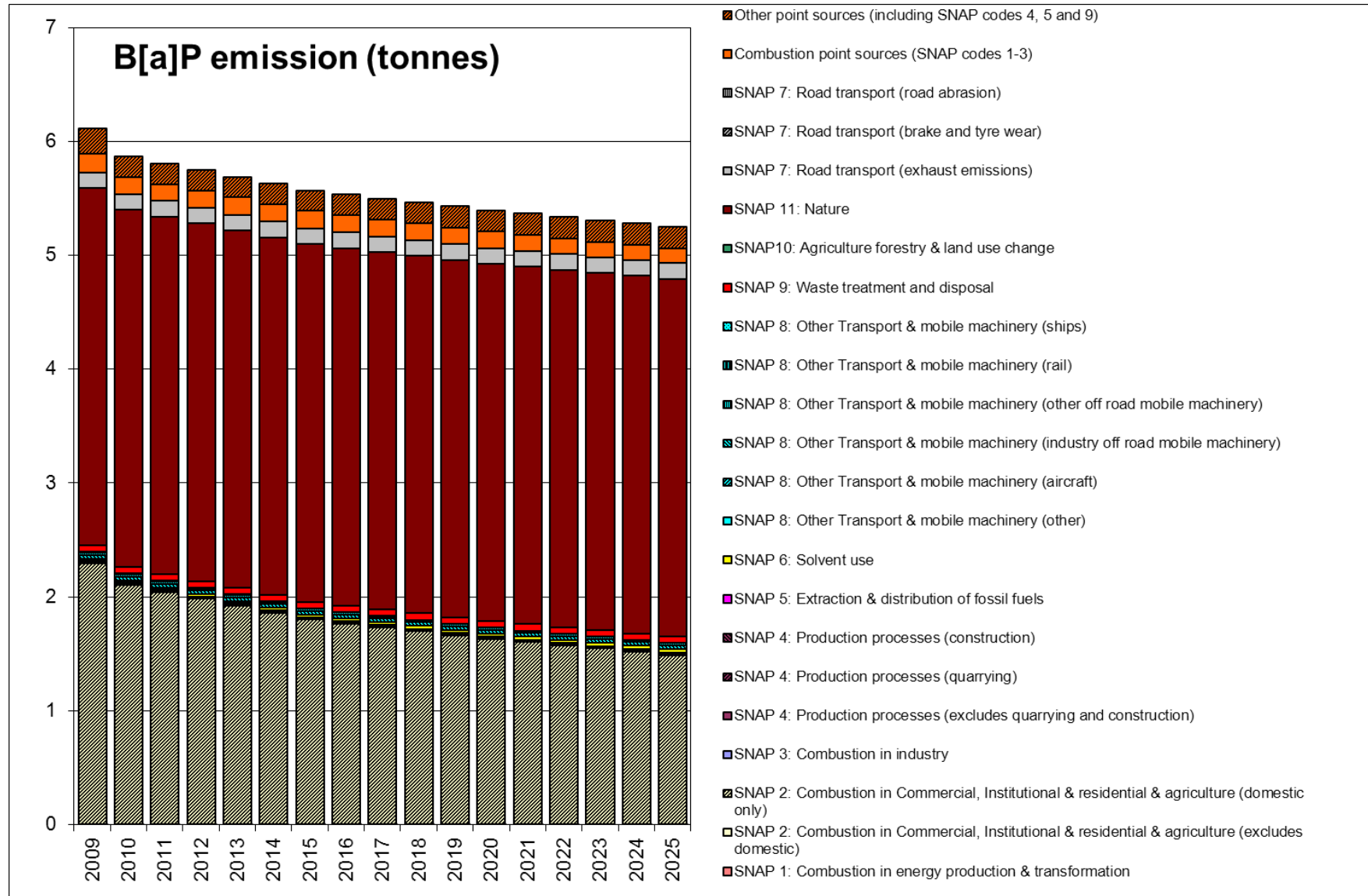
Emissions estimates for 2009, 2010, 2015, 2020 and 2025 by SNAP code are shown in Figure 3.1. Values for intermediate years have been interpolated in this figure.

Point source emissions are emissions of a known quantity from a known location, such as power stations. Area source emissions are 'diffuse emissions' from many unspecified locations, such as the emissions from domestic heating.

Figure 3.1 shows that emissions from B(a)P are expected to decline from 2009 to 2015 with the sharpest decline until 2010. From 2010 onwards the projected decline in emissions is anticipated to be steady but less significant. A contributory factor for this more gradual decline is that some of the most significant sources of B(a)P emissions are outside of regulatory controls. For example, the single largest source 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.

Another significant source of emission is the combustion of solid fuels for domestic heating as shown in Figure 3.1. This is a particularly important source in rural areas (particularly in Northern Ireland and, to a lesser extent Scotland) 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. The emissions inventory provides maps of emissions in a 1km x 1km 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. Updates to the mapped NAEI emissions inventory for 2009 used in this modelling included new information on the spatial distribution of domestic gas use across the UK. This revision is particularly significant for Northern Ireland which was last updated for the 2004 inventory having been omitted from the NAEI 2008 revision to this sector due to a lack of appropriate data.

Figure 3.1: UK total B(a)P emissions for 2009 and emissions projections up to 2025 by SNAP code (NAEI 2009)



3.4 The model

Ground level annual mean concentrations of B(a)P are considered to consist of:

- Point sources from industrial processes
- Area source emissions

A significant change to the modelling methodology since the 2005 assessment (Vincent et al., 2007) has been the decision to implement a calibration based on monitoring data from the national network. This decision was made to ensure that the model result was realistically consistent with the measurements. Particular consideration was given to appropriate application of calibration factors to the model, and for this reason separate calibration factors were derived for the area and point source components of the model.

3.4.1 Area sources

The modelled uncalibrated area source contribution has been calculated by applying an ADMS 4.2 derived dispersion kernel to calculate the contribution to ambient concentrations at a central receptor location from area source emissions within a 33km x 33km square surrounding each receptor. Hourly sequential meteorological data from Waddington in 2010 has been used to construct the dispersion kernels, as described in Appendix 1.

A calibration has been applied to the modelled B(a)P area source component (Figure 3.2). This has been calculated by plotting the uncalibrated area source component from the model against measured concentrations that have been adjusted to represent background (non-industrial) concentrations only (i.e. measured concentrations at background sites minus modelled point source contributions at those locations). The modelled area source contribution was multiplied by the coefficient (8.3563) to calculate the calibrated area source contribution for each grid square in the country.

Figure 3.2a shows that sites in Northern Ireland do not conform to the relationship established for other monitoring sites in the national network. BaP emissions in Northern Ireland are heavily influenced by domestic fuel combustion to a much greater extent than the mainland UK – this explains the higher concentrations measured at these sites relative to the uncalibrated model component. It is likely this was further compounded in 2010 by a ‘double-winter effect’ caused by sharp winter conditions in the early part of the year and again towards the end of 2010 and associated increases in domestic combustion for heating. In order to realistically represent this in the model, the domestic emissions sector for Northern Ireland has been subjected to a specific calibration, shown in Figure 3.2b. The remaining sectors in Northern Ireland have been calibrated using the standard relationship shown (i.e. a calibration factor of 8.3563) on the assumption that these sectors are consistent with those on the UK mainland.

As part of the calibration process concentration 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.

A cap of 0.33 tonnes per km² was applied to area emissions from domestic combustion of coal and wood. These caps have been applied 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. The application of these caps is annually reported back to the NAEI as part of the quality checking process to ensure that continual improvements are made in the emissions grids.

Figure 3.2a: Calibration of area source model for B(a)P

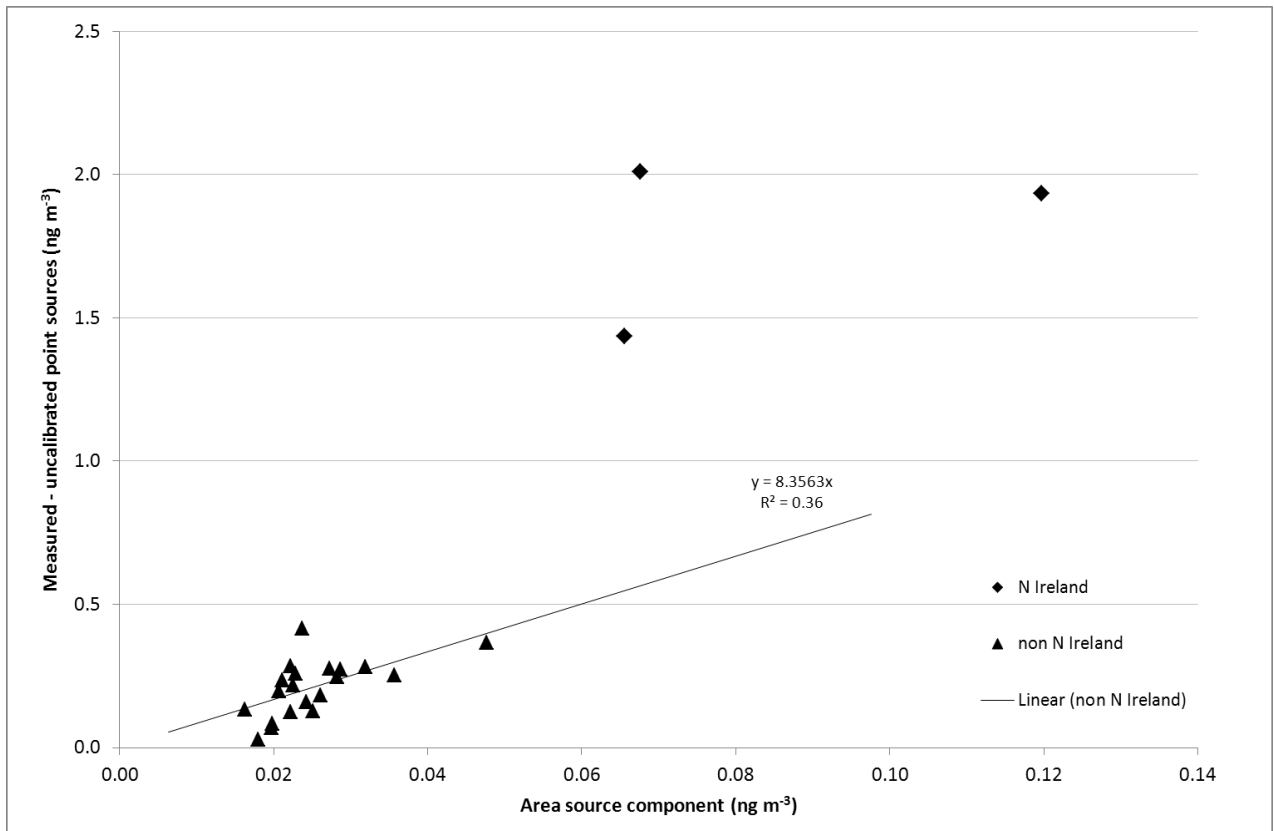
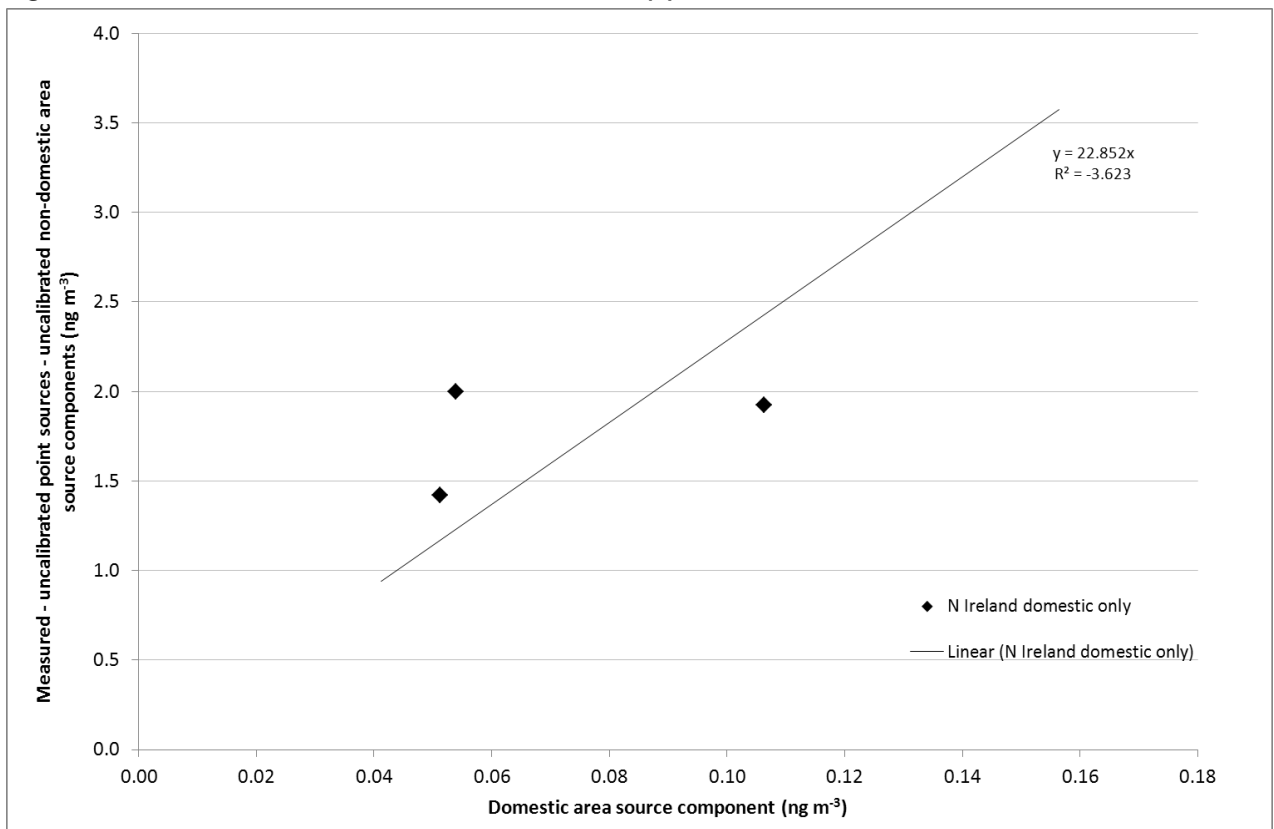


Figure 3.3b: Calibration of area source model for B(a)P domestic emissions in Northern Ireland



3.4.2 Point sources

Contributions to ground level annual mean B(a)P concentrations from point sources in 2010 were estimated by scaling the emissions from NAEI 2009 according to projections for 2010 and modelling each source explicitly using an atmospheric dispersion model (ADMS 4.2) and sequential meteorological data for 2010 from Waddington.

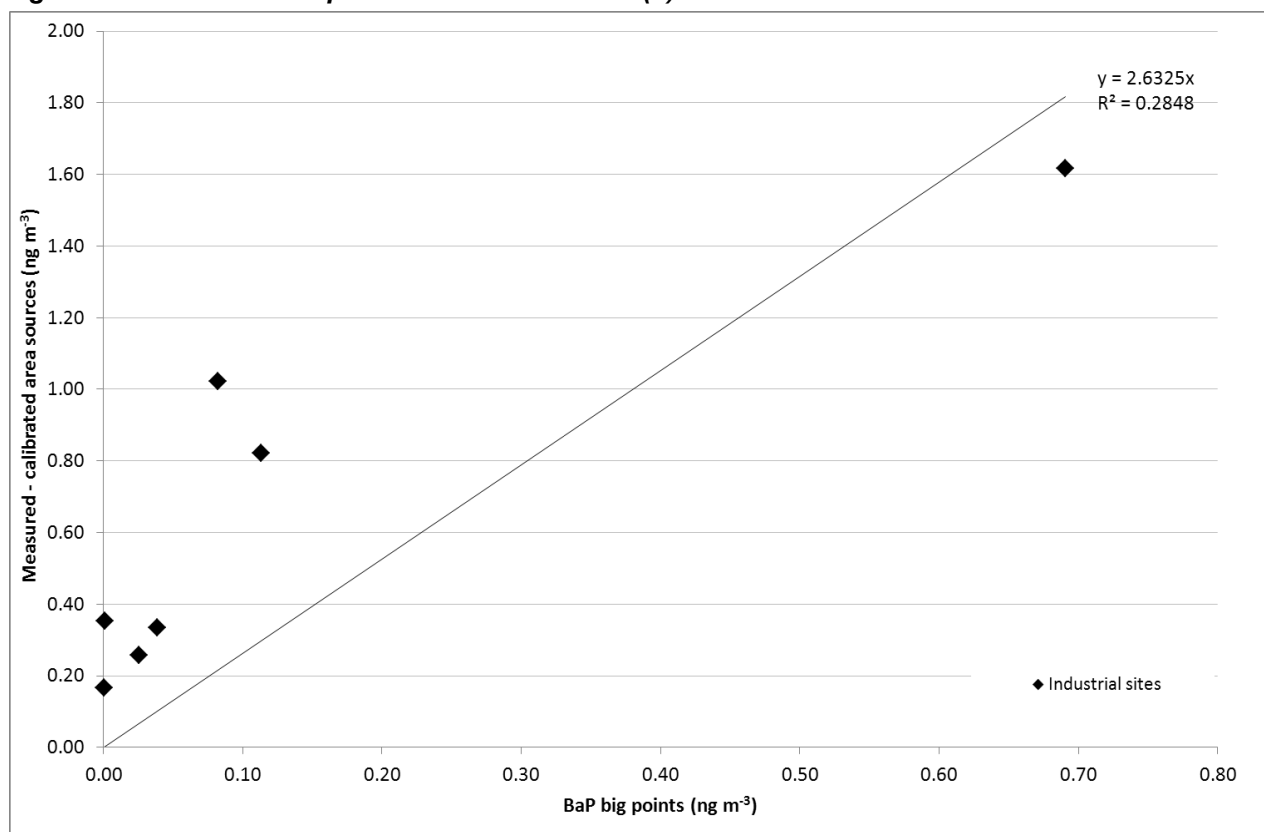
Industrial point sources of B(a)P are either fugitive (as from coking plants) or from clearly defined stacks for other sources. The emission amount is derived either from direct measurement or by emission factors. Release characteristics were obtained from the NAEI point sources database and included parameters such as:

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

A total of 154 large point 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. Specific emission information for coking plants was provided by Peter Coleman (personal communication, 2009) and covered Barnsley (Monkton coke oven), Teesside (Redcar and South Bank coke ovens and sinter plant), Port Talbot (Morfa coke works and sinter plant) and Scunthorpe (Dawes Lane and Appleby coke ovens and sinter plant).

In order to obtain a model result that was consistent with measured concentrations, the model was calibrated using monitoring data from the national network. Industrial sites only were used to calibrate the point source contribution (Figure 3.4). Measured industrial concentrations were adjusted by subtracting the calibrated modelled area source concentration so that the measured value represented the industrial component only. 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 decision was made to calibrate the area source component first using the uncalibrated modelled point source component and then to use the calibrated area source component to subtract from the measured industrial concentrations in the calibration of the point sources. This is reasonable since the contribution from point sources at non-industrial monitoring sites is very small. A multiple regression analysis for all monitoring sites was considered but was rejected because it would be likely to over fit to the data and not provide realistic coefficients.

Figure 3.4: Calibration of point source model for B(a)P



The modelled point source contribution was multiplied by the coefficient (2.6325) to calculate the calibrated point source contribution.

3.5 Results

3.5.1 Map of annual mean concentrations

Figure 3.5 shows the modelled annual mean B(a)P concentrations. The maximum estimated B(a)P annual mean concentration was 6.3 ng/m³.

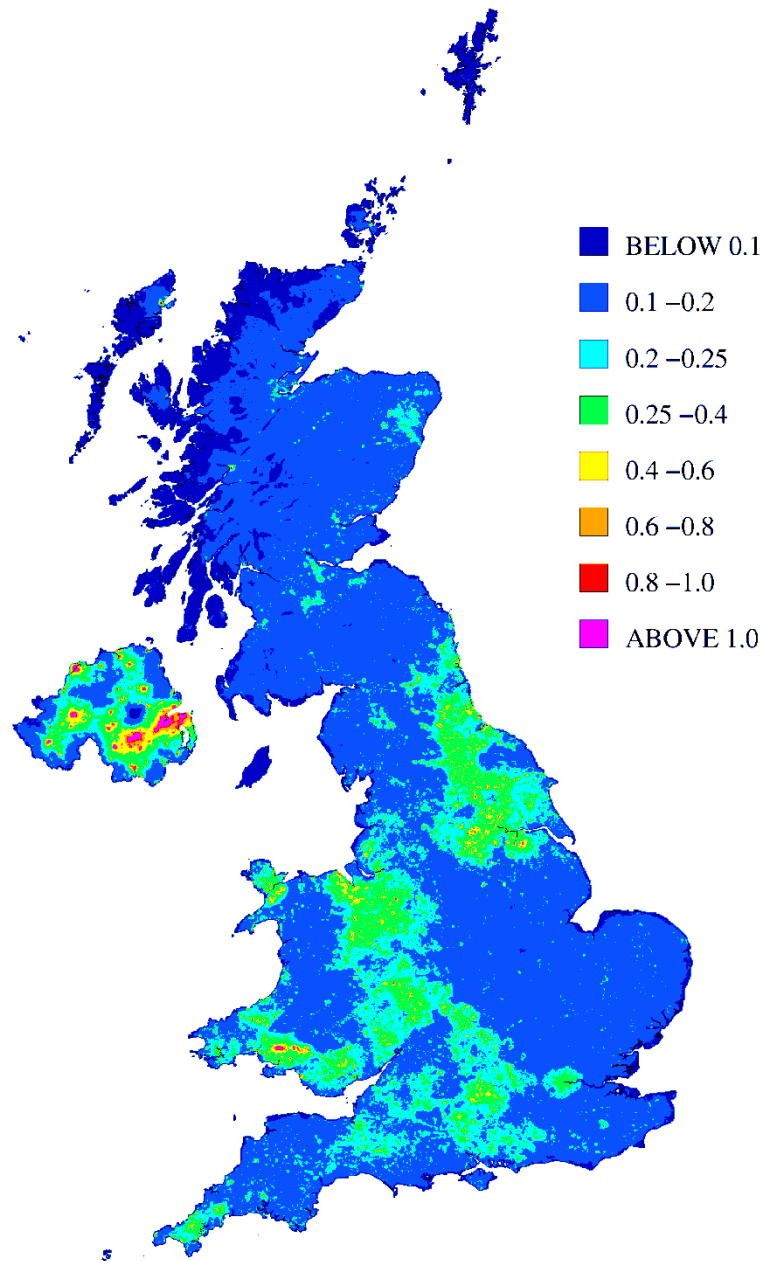
3.5.2 Source apportionment

A source apportionment graph has been plotted in Figure 3.6 to present the B(a)P 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.

3.5.3 Verification of mapped concentrations

An alternative presentation of the comparison between modelled and measured annual mean B(a)P concentrations in 2010 at different monitoring site locations are shown in Figure 3.7 to Figure 3.9. 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 1.6).

Figure 3.5: Annual mean map of B(a)P concentrations for comparison with the B(a)P target value of 1 ng/m^3 , 2010 (ng/m^3)



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Figure 3.6: Source apportionment for B(a)P

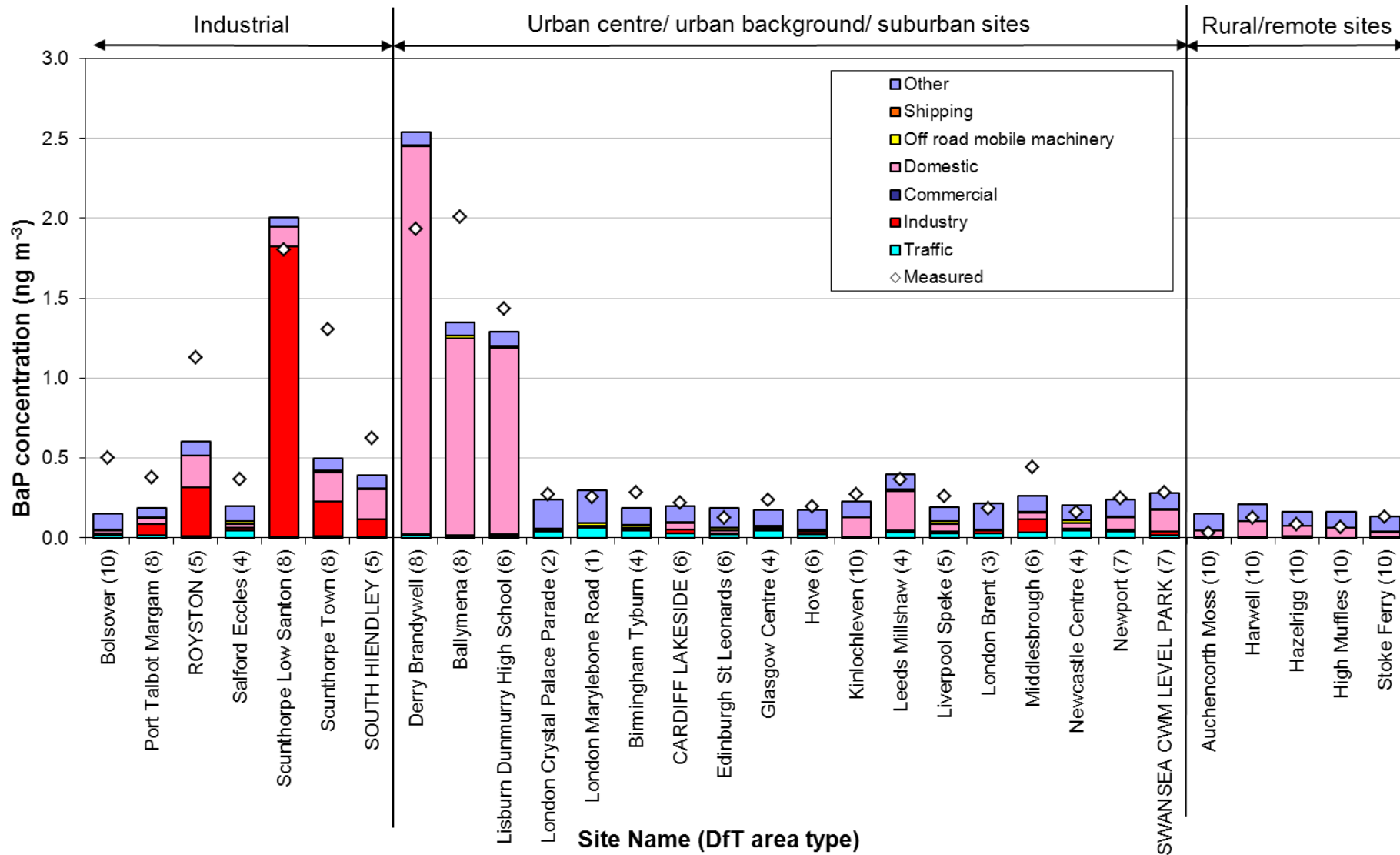


Figure 3.7: Verification of annual mean B(a)P at industrial sites

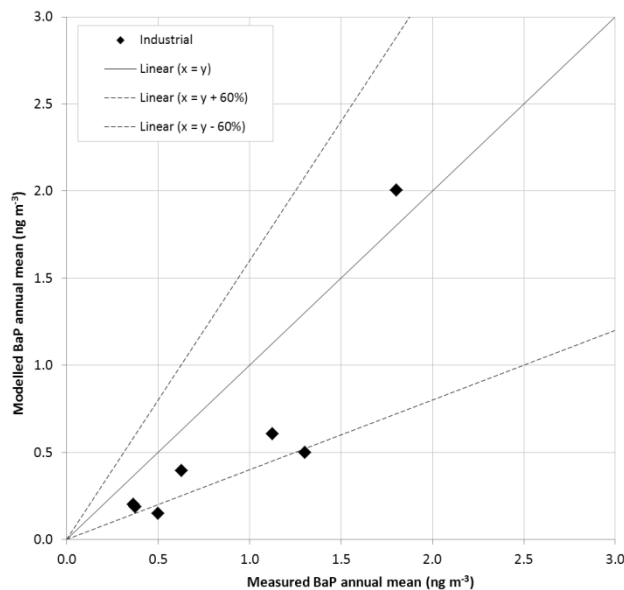


Figure 3.8: Verification of annual mean B(a)P at urban background sites

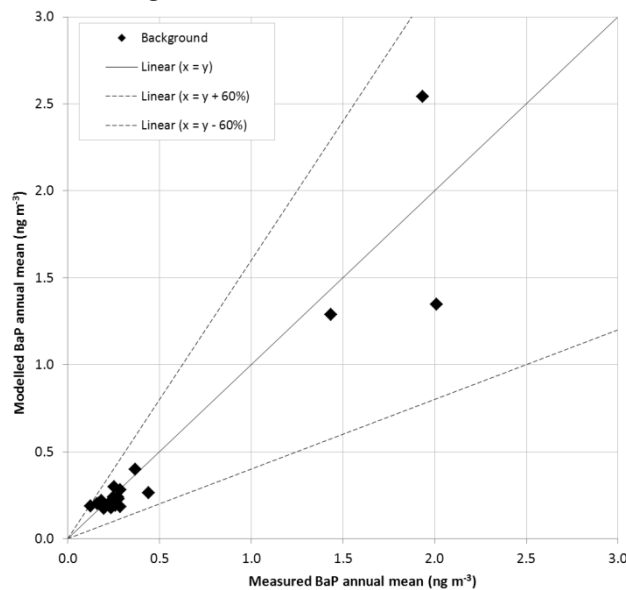
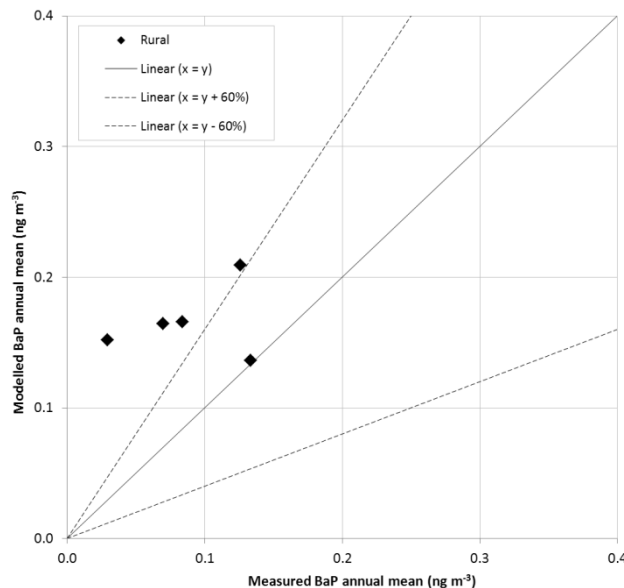


Figure 3.9: Verification of annual mean B(a)P at rural sites



Summary statistics for modelled and measured B(a)P concentrations are listed in Table 3.2, 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 good agreement for urban background and rural sites. The agreement between measured and modelled concentrations at industrial sites is less good. It is likely that variation of B(a)P concentrations in close proximity to these major sources is not as well represented in 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 3.2: Summary statistics for comparison between modelled and measured annual mean B(a)P concentrations at different monitoring sites, 2010

	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	0.87	0.58	0.77	29	7
Urban background sites	0.51	0.48	0.87	0	18
Rural sites	0.09	0.17	0.06	80	5

3.5.4 Comparison of modelling and measurement results with the target value

Tabular results for the supplementary assessment for B(a)P are presented in Table 3.3.

Exceedances of the 1 ng/m³ target value have been modelled for eight zones.

The exceedances in the North Wales zone, South Wales zone and West Midlands zone were associated with domestic combustion with the exception of 1 km² in South Wales zone which was exceeding the target value as a result of industrial emissions. The exceedances in Belfast Metropolitan Urban Area and the Northern Ireland zone were also associated with domestic solid fuel use and this sector was calibrated separately for Northern Ireland as described in the methodology above.

The exceedances in the Yorkshire & Humberside zone were associated with coking operations at Monkton and Scunthorpe and domestic solid fuel use.

The exceedances in the Teesside Urban Area and North East zone were associated with coking operations at Redcar and Southbank.

Measured concentrations also exceeded the target value in the Yorkshire & Humberside and Northern Ireland zones and measured exceedances have therefore been reported for these zones in the air quality assessment.

Table 3.3: Tabular results of and methods used for supplementary assessment for B(a)P

Zone	Zone code	Above TV for health (annual mean)			
		Area		Population exposed	
		Km ²	Method	Number	Method
Greater London Urban Area	UK0001	0	B	0	B
West Midlands Urban Area	UK0002	0	B	0	B
Greater Manchester Urban Area	UK0003	0	B	0	B
West Yorkshire Urban Area	UK0004	0	B	0	B
Tyneside	UK0005	0	B	0	B
Liverpool Urban Area	UK0006	0	B	0	B
Sheffield Urban Area	UK0007	0	B	0	B
Nottingham Urban Area	UK0008	0	B	0	B
Bristol Urban Area	UK0009	0	B	0	B
Brighton/Worthing/Littlehampton	UK0010	0	B	0	B
Leicester Urban Area	UK0011	0	B	0	B
Portsmouth Urban Area	UK0012	0	B	0	B
Teesside Urban Area	UK0013	2	B	263	B
The Potteries	UK0014	0	B	0	B
Bournemouth Urban Area	UK0015	0	B	0	B
Reading/Wokingham Urban Area	UK0016	0	B	0	B
Coventry/Bedworth	UK0017	0	B	0	B
Kingston upon Hull	UK0018	0	B	0	B
Southampton Urban Area	UK0019	0	B	0	B
Birkenhead Urban Area	UK0020	0	B	0	B
Southend Urban Area	UK0021	0	B	0	B
Blackpool Urban Area	UK0022	0	B	0	B
Preston Urban Area	UK0023	0	B	0	B
Glasgow Urban Area	UK0024	0	B	0	B
Edinburgh Urban Area	UK0025	0	B	0	B
Cardiff Urban Area	UK0026	0	B	0	B
Swansea Urban Area	UK0027	0	B	0	B
Belfast Metropolitan Urban Area	UK0028	128	B	411513	B
Eastern	UK0029	0	B	0	B
South West	UK0030	0	B	0	B
South East	UK0031	0	B	0	B
East Midlands	UK0032	0	B	0	B
North West & Merseyside	UK0033	0	B	0	B
Yorkshire & Humberside	UK0034	8	B	2052	B
West Midlands	UK0035	2	B	1618	B
North East	UK0036	4	B	2488	B
Central Scotland	UK0037	0	B	0	B
North East Scotland	UK0038	0	B	0	B
Highland	UK0039	0	B	0	B
Scottish Borders	UK0040	0	B	0	B
South Wales	UK0041	28	B	12755	B
North Wales	UK0042	2	B	1446	B
Northern Ireland	UK0043	275	B	343987	B
Total		449		776121	

Method 'B' is the modelling methodology described in this report.

4 Results of the air quality assessments

The results of the air quality assessments for As, Cd, Ni, and B(a)P are listed in Table 4.1. This table presents information from Form 9b of the questionnaire.

The tables have been completed as follows:

- Where all measurements were within the relevant target values in 2010, the table shows this as “OK”;
- Where compliance was determined by modelling only, this is shown as “OK (m)”;
- Where locations were identified as exceeding a target value this is identified as “>TV”;
- Where an exceedance was determined by modelling, this is indicated by (m).

Zones that complied with the relevant target values are shaded blue, while those in exceedance are shaded in yellow.

If both measurements and model estimates show that a threshold has been exceeded then the measurements are regarded as the primary basis for compliance status. Where locations have been identified as exceeding from modelling this indicates that modelled concentrations were higher than measured concentrations, or on rare occasions that measurements were not available or not required for that zone (measurements are not required where the Article 5 Assessment illustrates that concentrations are lower than the Lower Assessment Threshold) 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. Compliance can be determined by modelling where measurements are not available for a zone.

Table 4.1: List of zones and agglomerations where levels exceed or do not exceed target values for arsenic, cadmium, nickel and benzo(a)pyrene (2004/1007/EC, Annex I)

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	OK	OK	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	OK	OK	> 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 (m)	OK
Belfast Metropolitan Urban Area	UK0028	OK	OK	OK	> TV (m)
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	OK
North West & Merseyside	UK0033	OK	OK	OK	OK
Yorkshire & Humberside	UK0034	OK	OK	OK	> TV
West Midlands	UK0035	OK (m)	OK (m)	OK (m)	> TV (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 (m)	OK (m)	> TV (m)	> TV (m)
North Wales	UK0042	OK (m)	OK (m)	OK (m)	> TV (m)
Northern Ireland	UK0043	OK (m)	OK (m)	OK (m)	> TV

5 Acknowledgements

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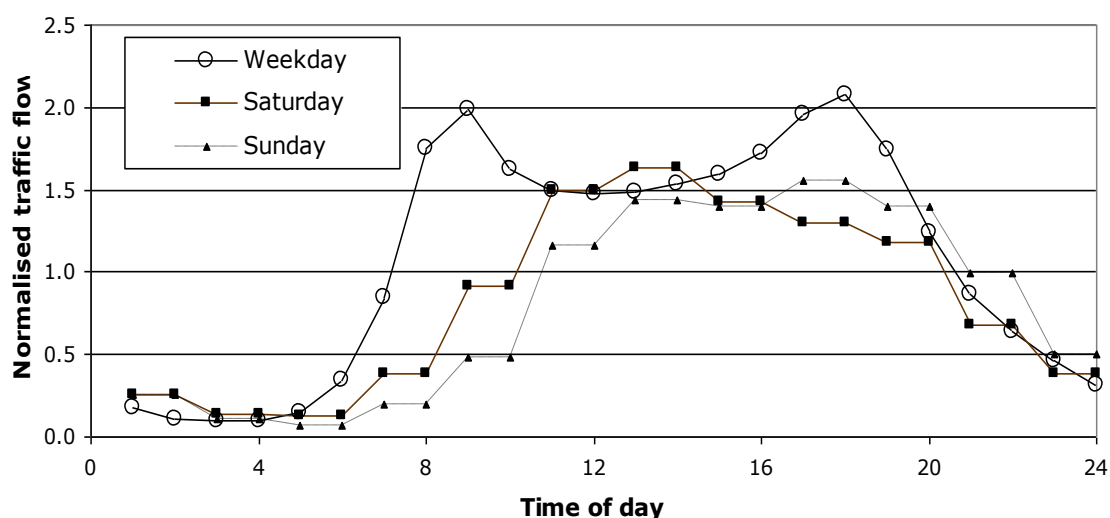
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Appendix 1 - Dispersion kernels for area source model

Dispersion kernels for 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 4.2. Separate kernels were calculated for traffic and other area sources (which were assumed to have a constant temporal profile of emissions). Kernels were generated for 2010 using sequential meteorological data from Waddington. The dispersion parameters used to calculate the kernels are listed in Table A.1. The emission profile used to represent traffic emissions for the traffic kernels is shown in Figure A.1. This was obtained from a distribution of all traffic in the United Kingdom by time of day (DETR, 2000).

Figure A.1. Temporal profile of traffic emissions



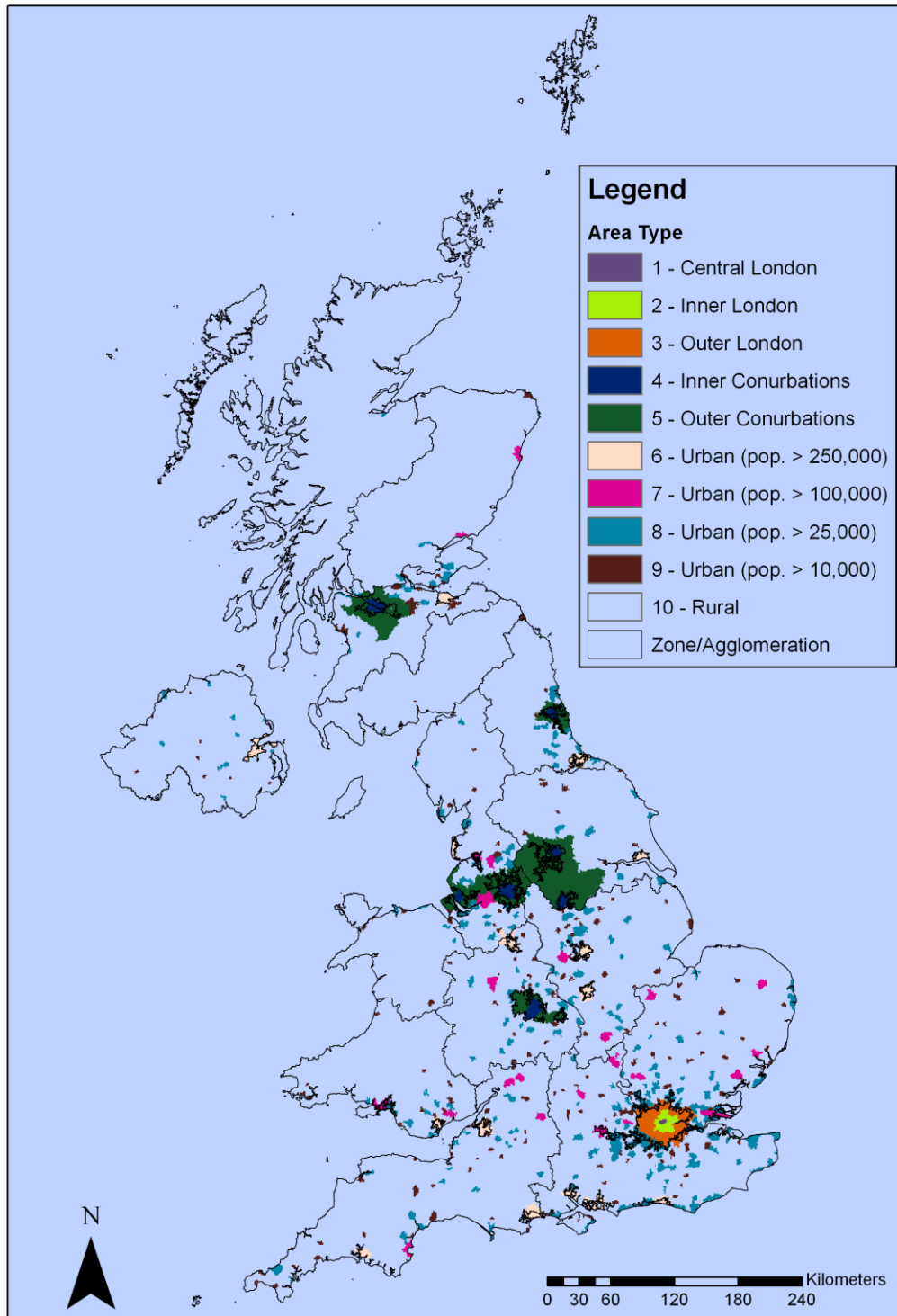
The dispersion kernels were revised for the 2007 modelling for all pollutants and the same method has been applied to derive the dispersion kernels for 2010. For NO_x, PM₁₀, benzene and CO the kernels are now on a 1 km x 1 km resolution matrix and are made using ADMS 4.2 (rather than the 3 km x 3 km resolution matrix used in previous years). 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. Previously this was accounted for in the PCM models by the application of different empirical calibration coefficients in inner conurbations and other locations. The kernels have been made specific to different types of location by varying minimum Monin Obukhov Length (LMO). The location of the different area types are shown in Figure A.2 and surface roughness due to different land use.

ADMS 4.2 recommends using a minimum Monin Obukhov Length (LMO) of 30 m for an urban area. However, sensitivity testing showed 20 m works better in ADMS 4.2.

Table A.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
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

Figure A.2. Map of UK area types



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