

Comparison of the Modelled National Air Quality Maps with 2017 Welsh AQ monitoring data

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1 Introduction

The purpose of this report is to compare the concentrations of the modelled 2017 UK Air Pollution Climate Mapping (PCM) carried out by Ricardo Energy & Environment for Defra and the Devolved Administrations (DAs), with the concentrations measured by the automatic monitoring sites in the Welsh Air Quality Database.

The locations of the monitoring sites considered in this study are shown in Figure 2-1. Comparisons of mapped concentrations with the automatic monitoring data from sites are presented in Figures 2-2 to 2-4 for nitrogen oxides (NO_X), nitrogen dioxide (NO₂), PM_{2.5}, PM₁₀ and sulphur dioxide (SO₂). Previous reports also showed modelled maps of the annual maximum 8-hour mean CO concentration at background locations and along major urban roads. However, the ambient concentrations of this pollutant throughout the UK have been well within the limit value for many years, therefore maps are no longer produced for CO. The modelled background and roadside maps are shown in Figures 2-5 to 2-14. All maps have been prepared from national modelled maps and cropped to present Wales only.

2 Methodology

The modelled maps of ambient concentrations were calculated from National Atmospheric Emissions Inventory (NAEI) data using a dispersion modelling approach. The model output for NO_x, NO₂, SO₂ PM₁₀ and PM_{2.5} was calibrated using monitored data from the national monitoring networks. These modelled maps were then verified against independent monitoring data held by Ricardo-Energy & Environment (local authority sites within the Ricardo-Energy & Environment 'Calibration Club'). The technical report on modelling for 2017 presenting maps of the UK and detailed explanations of the modelling methodology and verification is currently in preparation (Brookes et al., 2017) the most recent published report is the technical report on modelling for 2015 (Brookes et al., 2015).

The maps produced by Ricardo Energy & Environment for Defra and the Devolved Administrations include:

- NO_X annual mean concentration (μg m⁻³)
- NO₂ annual mean concentration (μg m⁻³)
- PM₁₀ (gravimetric) annual mean concentration (μg m⁻³)
- PM_{2.5} (gravimetric) annual mean concentration (μg m⁻³)
- SO₂ annual mean concentration (μg m⁻³)
- SO₂ 99.73rd percentile of hourly means (μg m⁻³)
- SO₂ 99.18th percentile of daily means (μg m⁻³)

The locations of each of the Welsh Air Quality Database monitoring sites were plotted on the modelled pollution maps and the corresponding modelled background concentration for the relevant 1x1 km grid square extracted. A 75% data capture threshold was applied to the monitoring data for this analysis. Any site with data capture below this threshold was omitted.

At roadside sites, where available, the corresponding modelled road link was used to ascertain a modelled roadside value rather than the modelled background concentration. The PM₁₀ and PM_{2.5} modelling was performed in gravimetric units for direct comparison against European legislation set out in the Air Quality Directive (AQD) (2008/50/EC). In order to provide a meaningful comparison against the model output, only measured data from reference method equivalent instruments or TEOM data corrected with the Volatile Correction Model (VCM) were used in this analysis.

The PM₁₀ monitoring undertaken with OSIRIS light scattering instruments at the Anglesey Brynteg, Anglesey Llynfaes, Anglesey Felin Cafnan and Anglesey Penhesgyn sites was excluded from the analysis. The OSIRIS monitors do not fulfil the EC reference method criteria and the data are therefore considered only as indicative.

The NO₂ and SO₂ monitoring undertaken with Differential Optical Absorption Spectroscopy (DOAS) technique at Swansea Hafod and Swansea St Thomas were not used for the analysis. This is because data from the DOAS instrument is not directly comparable to fixed point measurements and is difficult to fit to UK modelling procedures.

SO₂ is not modelled at roadside locations because roadside values are not significantly different from background values. As a result, modelled background concentrations were used for comparison with the monitored data at roadside sites instead. The only significant contribution to SO₂ concentrations at roadside comes from sulphur in petrol and diesel. Up to 1990 these emissions were increasing as a result of increasing numbers of road vehicles in the national fleet. Since 2000 emissions have declined with the introduction of the regulation for the sulphur content of petrol and diesel, and now road transport emissions of SO₂ account for less than 1% of the total SO₂ emissions (Murrells *et al.*, 2008).

The modelled information was directly compared with the corresponding monitored metric from each site and plotted in a scatter plot. Lines at 30% or 50% are shown on the scatter plots – these are the modelling data quality objectives (DQO) for each limit value (LV) for each pollutant. The LVs and DQOs are specified in Annex 1 of the Air Quality Directive (2008/50/EC). Lines at 50% were plotted for the annual mean PM_{10} concentration and the high percentile metrics for SO₂. Lines at 30% were plotted for the annual mean NO_x and NO_2 concentration, and the annual mean SO_2 concentration. The scatter plots are presented with tabulated statistics including the number of sites in the analysis for each metric, the average of the modelled and monitored data for all sites and the number of sites within the data quality objectives. The analysis was performed separately for background (non-roadside) and roadside sites.

The Air Quality Directive concerning ambient air quality and clean air in Europe entered into force in June 2008, and was brought into law in Wales by the Air Quality Standards (Wales) Regulations 2010 – transposing both the new Directive and the Fourth Daughter Directive.

A list of sites which form part of Defra Automatic Urban and Rural Network (AURN) and from the local networks in Wales used in the analysis is presented in Table 2-1. The AURN sites in Wales were included in the calibration of the UK scale models.

The data from all the monitoring sites listed in Table 2-1 have been fully ratified by Ricardo-Energy & Environment.

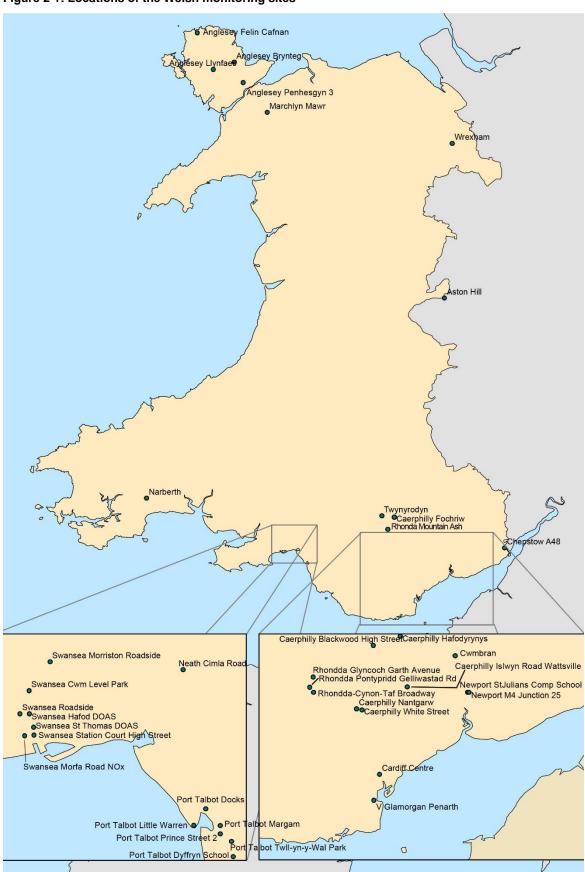
AURN sites	Non-AURN sites
Cardiff Centre	Anglesey Brynteg
Aston Hill	Anglesey Felin Cafnan
Chepstow A48	Anglesey Llynfaes
Cwmbran	Anglesey Penhesgyn 3
Newport	Caerphilly Blackwood High Street
Port Talbot Margam	Caerphilly Fochriw
Hafod-yr-ynys Roadside	Caerphilly Islwyn Road Wattsville
Swansea Roadside	Caerphilly Nantgarw
Wrexham	Caerphilly White Street
Narberth	Cwmbran PM ₁₀
	Marchlyn Mawr
	Neath Cimla Road

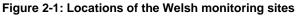
Table 2-1: Welsh air quality monitoring sites

Newport M4 Junction 25
Port Talbot Docks
Port Talbot Dyffryn School
Port Talbot Little Warren
Port Talbot Prince Street
Port Talbot Talbot Road
Port Talbot Theodore Road
Port Talbot Twll-yn-y-Wal Park
Rhondda Broadway
Rhondda Pontypridd Gelliwastad Rd
Rhondda Mountain Ash
Rhondda Glyncoch Garth Avenue
Swansea Cwm Level Park
Swansea Hafod DOAS
Swansea Morriston Roadside
Swansea St Thomas DOAS
Swansea Station Court High Street
Twynyrodyn
V Glamorgan Windsor Road Penarth

All of these Welsh Air Quality Database sites were considered for analysis in 2017. Some sites have been omitted due to low data capture statistics (low data capture is defined as anything below 75%), instruments that were incomparable with the model or local factors that make the monitoring data unrepresentative in 2017 and therefore not comparable with the corresponding modelled data. Monitoring sites that were omitted due to non-representative instruments and low data capture are listed below:

- Anglesey Brynteg (for PM₁₀ and PM_{2.5})
- Anglesey Felin Cafnan (for PM₁₀ and PM_{2.5})
- Anglesey Llynfaes (for PM₁₀ and PM_{2.5})
- Anglesey Penhesgyn 3 (for PM₁₀ and PM_{2.5})
- Marchlyn Mawr
- Swansea Hafod DOAS (NO₂)
- Swansea St Thomas DOAS (for SO₂)
- Newport
- Narberth (NO₂)
- Port Talbot Dyffryn School (PM₁₀)
- Port Talbot Theodore Road (PM₁₀)
- Rhondda Glyncoch Garth Avenue (PM₁₀)





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2.1 Comparison results

The scatter plots in Figures 2-2 to 2-4 show that the relationships between the national modelled maps and the Welsh monitoring data for 2017 were generally satisfactory. The results of this exercise from the 2017 model outputs were broadly consistent with the findings from earlier comparisons between measured and modelled concentrations in Wales.

2.1.1 Nitrogen Oxides and Nitrogen Dioxide

The comparison of modelled and measured annual mean NO_x and NO₂ concentrations at the monitoring sites locations is shown in Figure 2-2. Generally, the model did not exhibit systematic under or over prediction of NO_x and NO₂ concentrations. The relationship between NO_x and NO₂ tends to be non-linear, for this reason the percentage of the monitoring sites for which the modelled annual mean concentrations fall outside the data quality objectives is greater for NO_x than for NO₂ (Tables 2-2 and 2-3). In 2017, 20 sites were used to compare modelled and measured NO_x and NO₂ concentrations. The agreement between measured and modelled background concentrations is fair, although two sites (Caerphilly Hafodyrynys and Swansea Station Court High Street) are considerably higher than modelled concentrations. The model under predicts the roadside NO_x and NO₂ concentrations or traffic flow information on the road link. The Caerphilly Hafodyrynys and Swansea Station Court High Street sites are examples of where measured NO_x concentrations are far higher than the model predicts.

The main reason for the NO_x discrepancy at Caerphilly Hafodyrynys is because the site is on a main road and gateway to Caerphilly County Borough Council. The site is on a hill and on the opposite side of the road there is a large retaining wall which creates a canyon effect. There is a signalised junction at the bottom of the hill which can create a build-up of traffic. The main reason for the discrepancy at Swansea Station Court High Street is because there is a bus stop immediately outside the site. It is also close to congestion caused by signal-controlled lights and mini roundabouts. There is also Swansea Railway station opposite the site.

A very good agreement between modelled and monitored concentrations is found at the Caerphilly White Street and Cwmbran sites. The concentrations measured reflect very well the amount of traffic passing the monitoring stations. This shows that the combination of available spatial information (measured concentrations and traffic counts) allows the model to predict the concentrations accurately. Swansea Cwm Level Park, Aston Hill, Narberth, Cardiff and Wrexham sites also show a very good agreement between modelled and measured values.

The largest outlier in the NO₂ analysis is again found at Caerphilly Hafodyrynys. This is a roadside location with very high measured concentrations.

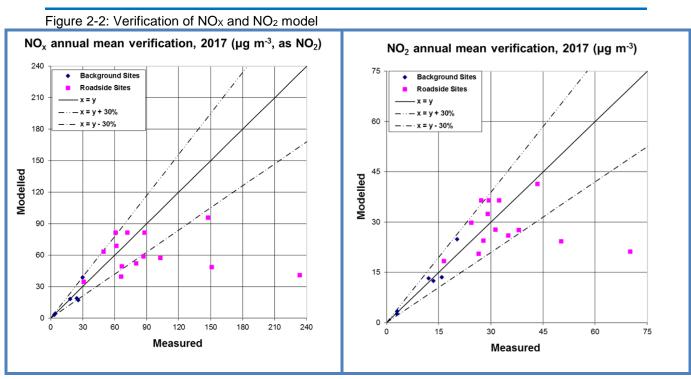


Table 2-2: Summary statistics for comparison between modelled and measured annual mean concentrations of NO_x at background and roadside sites, $\mu g m^{-3}$ (as NO₂)

NO _x annual mean	Average modelled	Average measured	Number of sites used	Number within range	Percentage within range
Background	16.8	17.6	6	4	67
Roadside	61.0	92.7	14	6	43

Table 2-3: Summary statistics for comparison between modelled and measured annual mean concentrations of NO₂ at background and roadside sites, $\mu g m^{-3}$

NO ₂ annual mean	Average modelled	Average measured	Number of sites used	Number within range	Percentage within range
Background	11.7	11.3	6	6	100
Roadside	28.8	34.4	14	11	79

2.1.2 PM₁₀ and PM_{2.5} Particulate Matter

 PM_{10} and $PM_{2.5}$ concentrations are measured using a variety of different methods in the Welsh Air Quality Database. The gravimetric equivalent PM_{10} model results were compared with reference method equivalent data or TEOM monitoring data corrected with VCM. TEOM data were recorded at the Cwmbran PM_{10} and Twynrodyn sites in 2017. The agreement between the model output for gravimetric PM_{10} , and $PM_{2.5}$ for all the monitoring sites at background and roadside locations was very good (Table 2-4 and Figure 2-3), with the exception of PM_{10} at Port Talbot Prince Street and Port Talbot Little Warren these sites are close to a major industrial pollution source. For $PM_{2.5}$ Twynrodyn falls outside the agreement between the model and the actual measured data. Twynrodyn is next to an open cast mine which could be why it has higher modelled data.



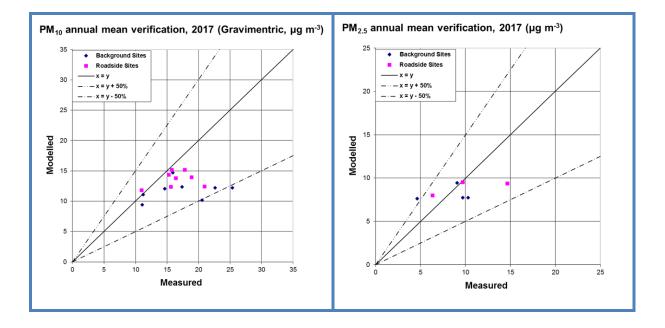


Table 2-4: Summary statistics for comparison between modelled and measured annual mean concentrations of gravimetric equivalent PM_{10} at background and roadside sites, $\mu g m^{-3}$

PM ₁₀ annual mean	Average modelled	Average measured	Number of sites used	Number within range	Percentage within range
Background	11.8	17.4	10	8	80
Roadside	13.6	16.5	8	8	100

Table 2-5: Summary statistics for comparison between modelled and measured annual mean concentrations of gravimetric equivalent $PM_{2.5}$ at background and roadside sites, $\mu g m^{-3}$

PM _{2.5} annual mean	Average modelled	Average measured	Number of sites used	Number within range	Percentage within range
Background	8.1	8.4	6	5	83
Roadside	9.0	10.2	3	3	100

2.1.3 Sulphur Dioxide

The comparison of modelled and measured SO_2 concentrations in 2017 at the monitoring site locations is shown in Figure 2-4. The agreement between measured and modelled SO_2 concentrations in 2017 was less favourable than for other pollutants. Only Port Talbot Margam shows a reasonable agreement between modelled and measured annual mean SO_2 concentrations. Narberth and Wrexham have fair agreement on hourly and daily measures. The model over-predicts the SO_2 measured concentrations at Cardiff Centre, in contrast, in 2016 the model was found to be under-predicting SO_2 concentrations at Cardiff Centre.

Concentrations of SO₂ are at very low levels and this means that differences between modelled and measured data are exaggerated, for example the measured concentration of SO₂ at Narberth is 1.3 μ g m⁻³ while the modelled data is 0.6 μ g m⁻³. This is less than half the measured data but is still actually within 1 μ g.

The current model is deemed to be appropriate for the metrics calculated around the range of the limit values. The high percentile metrics are very sensitive to meteorological conditions, thus very difficult to model. There have been improvements made to the model for smaller industrial sources in an effort to improve the model performance in the range of the assessment thresholds (i.e. lower concentrations than the LVs).

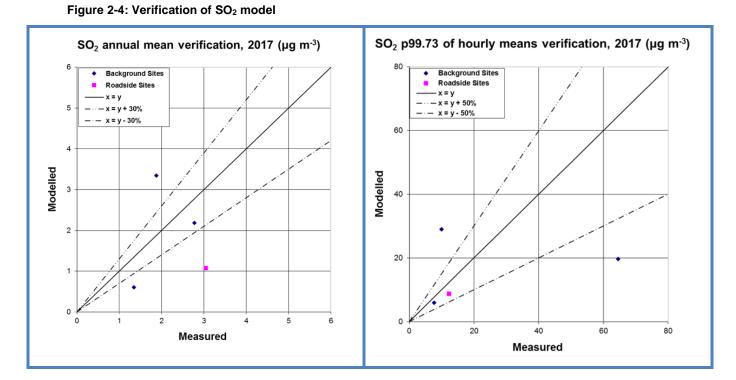
It should be noted that the model is known to under predict the concentrations at roadside sites, which were compared to background modelled concentrations. It is believed that there is no significant roadside increment in SO_2 nationally. However, it is possible that specific individual road links experience higher concentrations than predicted by the national SO_2 background model for this pollutant.

There is considerable scatter displayed in the verification charts of all SO_2 metrics shown in Figure 2-4, this was also the case in previous years. The high percentile of the concentration is generally associated with a higher level of uncertainty than the annual mean concentration due to the influence of large sources. The measured data, for the higher percentile SO_2 modelling, depends greatly on the particular combination of meteorological conditions and hour-by-hour emissions. However, hour-byhour emissions are not known and reported monthly emission totals and typical profiles have been used as a surrogate in the modelling process.

Summary statistics for modelled and measured SO₂ concentrations and 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 presented in Table 2-6 to Table 2-8. The mean measured and modelled concentrations for each averaging time has poor agreement.

The agreement between measured and modelled concentrations on a site-by-site basis has historically been poor for all SO₂ metrics both for sites in the national network and the verification sites. Reasons for the poor agreement include:

- There are few SO₂ measurement points and overall ambient concentrations are low compared to the uncertainties of both monitoring and modelling;
- 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;
- The modelling method does not explicitly model concentrations arising from non-UK sources.



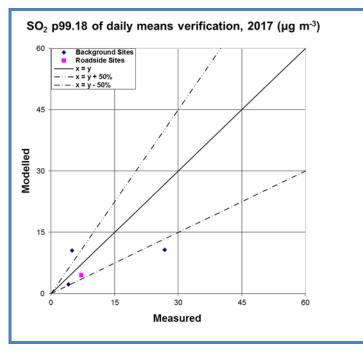


Table 2-6: Summary statistics for comparison between modelled and measured annual mean concentrations of SO₂ at background and roadside sites, μ g m⁻³

SO₂ annual mean	Average modelled	Average measured	Number of sites used	Number within range	Percentage within range
Background	2.0	2.0	3	1	33
Roadside	1.1	3.0	1	0	0

Table 2-7: Summary statistics for comparison between modelled and measured 99.73^{rd} percentile of 1-hour concentrations of SO₂ at background and roadside sites, $\mu g m^{-3}$

SO₂ p99.73 1-hour means	Average modelled	Average measured	Number of sites used	Number within range	Percentage within range
Background	18.2	27.4	3	1	33
Roadside	8.7	12.3	1	1	100

Table 2-8: Summary statistics for comparison between modelled and measured 99.18th percentile of 24-hour concentrations of SO₂ at background and roadside sites, $\mu g m^{-3}$

SO ₂ p99.18 daily means	Average modelled	Average measured	Number of sites used	Number within range	Percentage within range
Background	7.8	12.0	3	1	33
Roadside	4.6	7.2	1	1	100

2.2 2017 Maps

2.2.1 Background concentration maps

The modelling methods used for background locations closely follow those used in the 2016 mapping report. Background maps for NO_x and NO₂ are presented in Figures 2-5 and 2-6. Firstly, a map of NO_x concentrations from all sources was calculated. The map of estimated annual mean NO₂ concentrations was then calculated from modelled NO_x concentrations using a calibrated version of the updated oxidant-partitioning model (Jenkins, 2004; Murrells et al., 2008, Jenkin, 2012). This model uses representative equations to account for the chemical coupling of O₃, NO and NO₂ within the atmosphere.

A map of annual mean PM_{10} and $PM_{2.5}$ in 2017 at background locations is shown in Figure 2-7 and Figure 2-8. The 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 2017. Measurements from gravimetric instruments 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.

The maps of annual mean background PM_{10} and $PM_{2.5}$ concentrations have been calculated by summing contributions from different sources:

 Secondary inorganic aerosol (derived by interpolation and scaling of measurements of SO₄, NO₃ and NH₄ at rural sites)

- Secondary organic aerosol (semi-volatile organic compounds formed by the oxidation of nonmethane volatile organic compounds. Estimates derived from results from the NAME model)
- Large point sources of primary particles (modelled using ADMS and emissions estimates from the NAEI)
- Small point sources of primary particles (modelled using the small points model and emissions estimates from the NAEI)
- Regional primary particles (from results from the TRACK model and emissions estimates from the NAEI and EMEP)
- Area sources of primary particles related to domestic combustion (modelled using a dispersion kernel and emissions estimates from the NAEI)
- Area sources of primary particles related to combustion in industry (modelled using the small points model and emissions estimates from the NAEI)
- Area sources of primary particles related to road traffic (modelled using a dispersion kernel and emissions estimates from the NAEI)
- Other area sources of primary particles (modelled using a dispersion kernel and emissions estimates from the NAEI)
- EU Emissions Trading Scheme¹ (ETS) point sources modelled using the small points model and emissions estimates from the NAEI 2016
- 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 land 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)

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 then aggregated to a single 1km x 1km background PM_{10} grid. An additional roadside increment is added for roadside locations.

The map of annual mean of SO_2 at background locations is presented in Figure 2-9. Maps of 99.73 percentile of 1-hour mean and 99.18 percentile of 24-hour mean SO_2 concentration in 2017 are shown in Figures 2-10 and 11 and these were calculated for comparison with the 1-hour and 24-hour limit values for SO_2 . The methodology to produce the SO_2 maps follows closely the methodology used in previous mapping reports.

In common with the 2016 maps the background models for SO₂, NO_x, NO₂, PM₁₀ and PM_{2.5} now include Emissions Trading Scheme point emissions estimates for Air Quality pollutants based on reported carbon emissions. Other recent changes to the modelling approach include the introduction of a time varying dispersion kernel approach for area source emissions from domestic combustion and treating combustion from smaller industrial sources with the small point's model approach in line with the improvements made to the background model for SO₂ (included since the 2011 modelling).

¹ Emissions Trading Scheme point emissions estimates for Air Quality pollutants based on reported carbon emissions



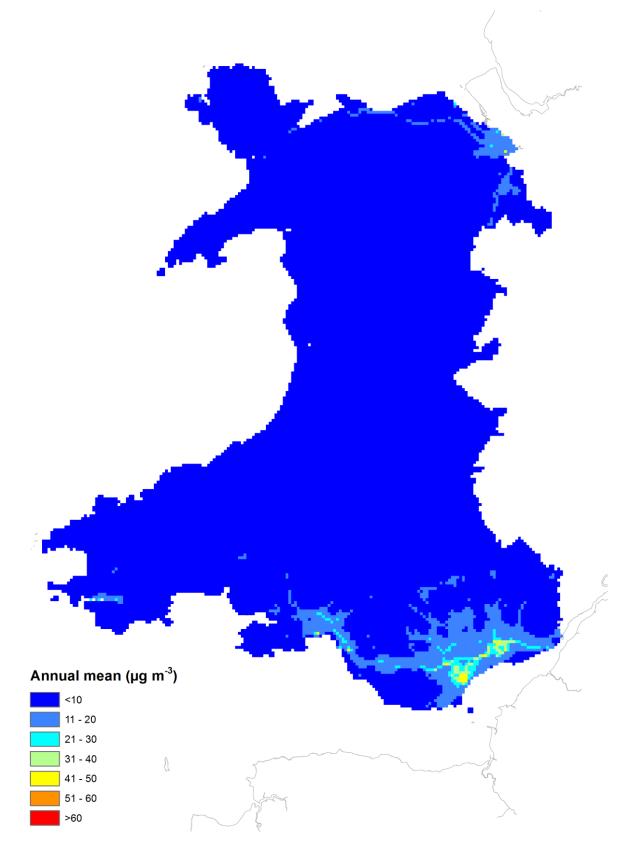


Figure 2-6: Estimated 2017 NO₂ annual mean, $\mu g m^{-3}$

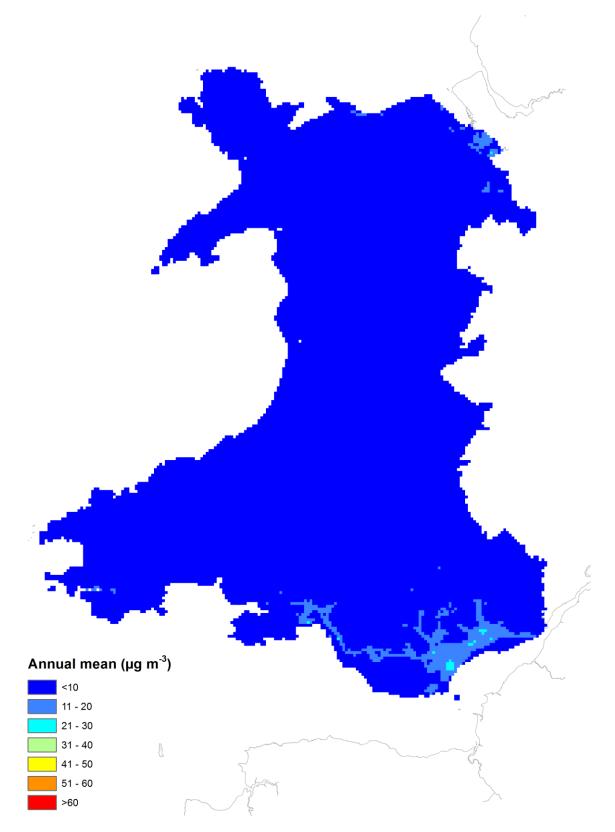


Figure 2-7: Estimated 2017 PM₁₀ annual mean, $\mu g m^{-3}$

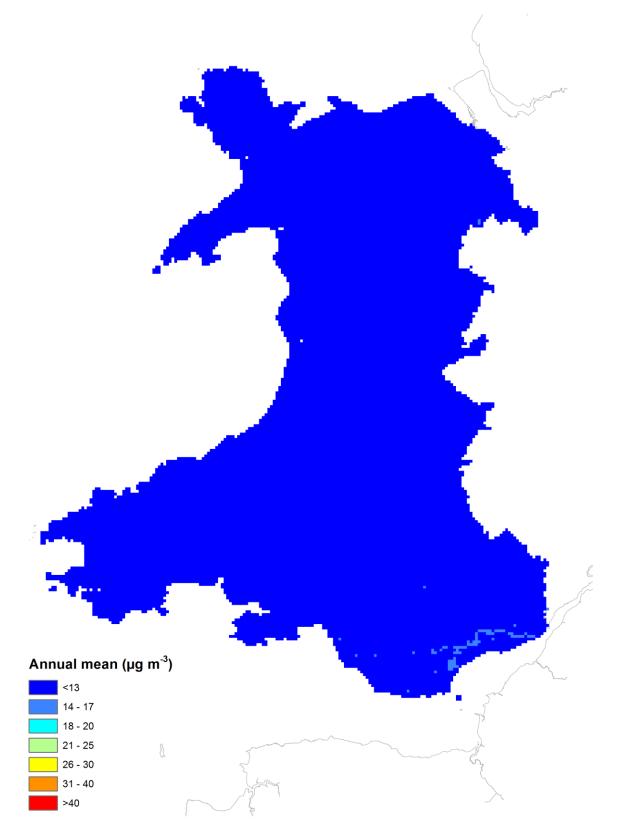


Figure 2-8: Estimated 2017 $PM_{2.5}$ annual mean, $\mu g \ m^{-3}$

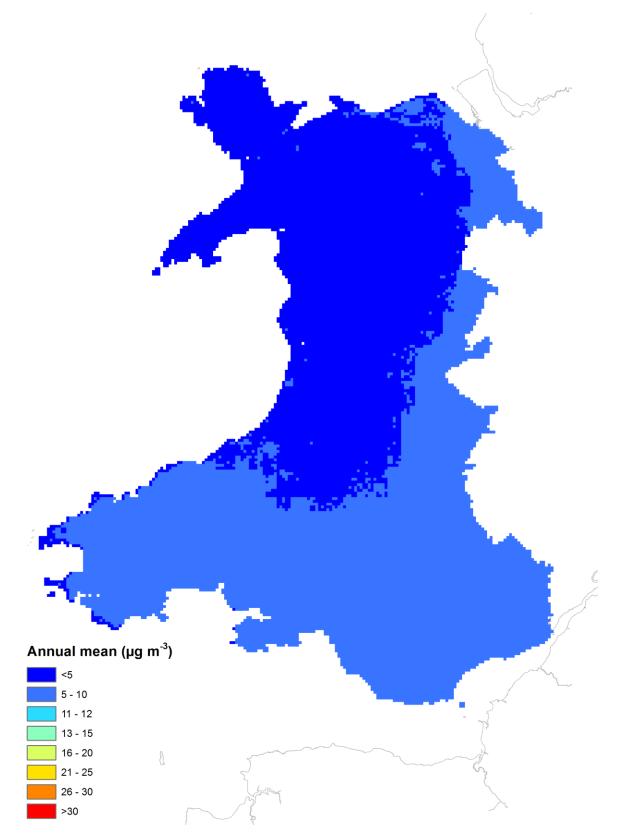


Figure 2-9: Estimated 2017 SO₂ annual mean, $\mu g m^{-3}$

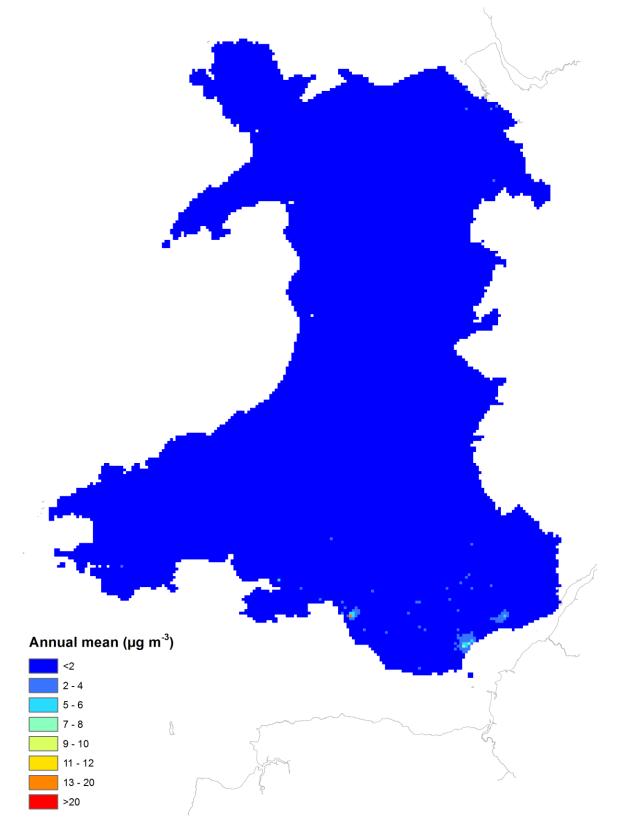


Figure 2-10: Estimated 2017 SO₂ 99.73rd percentile of hourly means, µg m⁻³

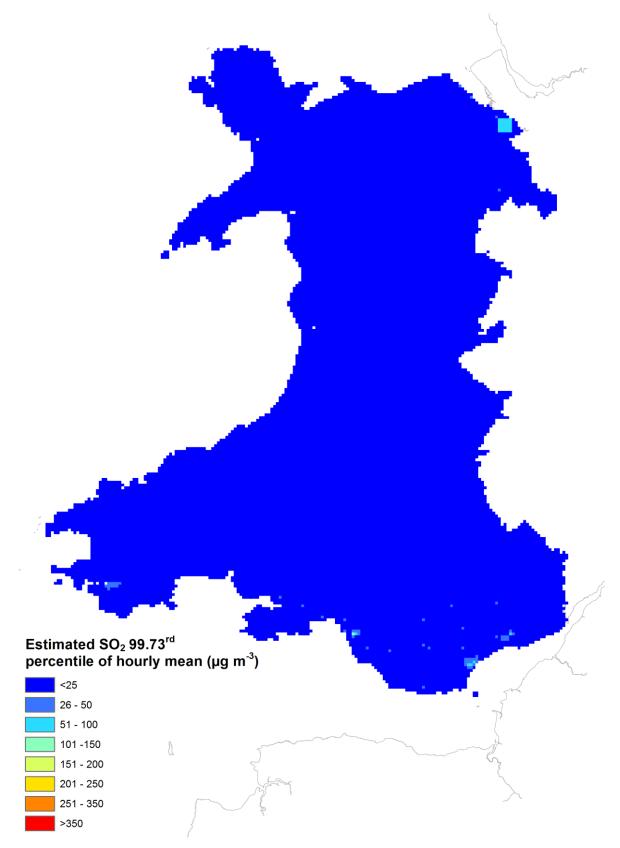
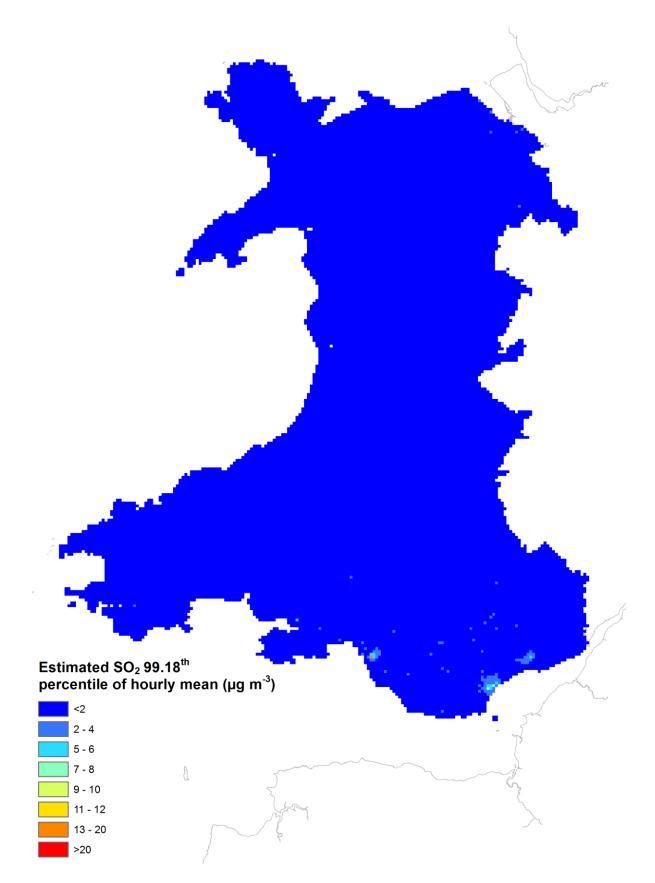


Figure 2-11: Estimated 2017 SO₂ 99.18th percentile of daily means, $\mu g m^{-3}$



2.2.2 Roadside concentration maps 2017

Modelling of roadside concentrations in 2017 was performed in the same way as in previous years using the 2016 NAEI emissions for all major road links.

These emissions were adjusted to provide estimates of emissions in 2017. The annual mean concentrations at roadside locations have been assumed to be made up of two parts, the background concentration (described above) and a roadside increment:

roadside concentration = background concentration + roadside increment.

Roadside maps are not prepared for SO_2 because variations in SO_2 concentrations between background and roadside locations are negligible. Although roadside concentrations of NO_x are calculated as an intermediate stage in modelling roadside NO_2 roadside concentrations, this is not presented because there is no corresponding legislative objective. Figure 2-12: Estimated 2017 NO2 roadside annual mean, µg m-3

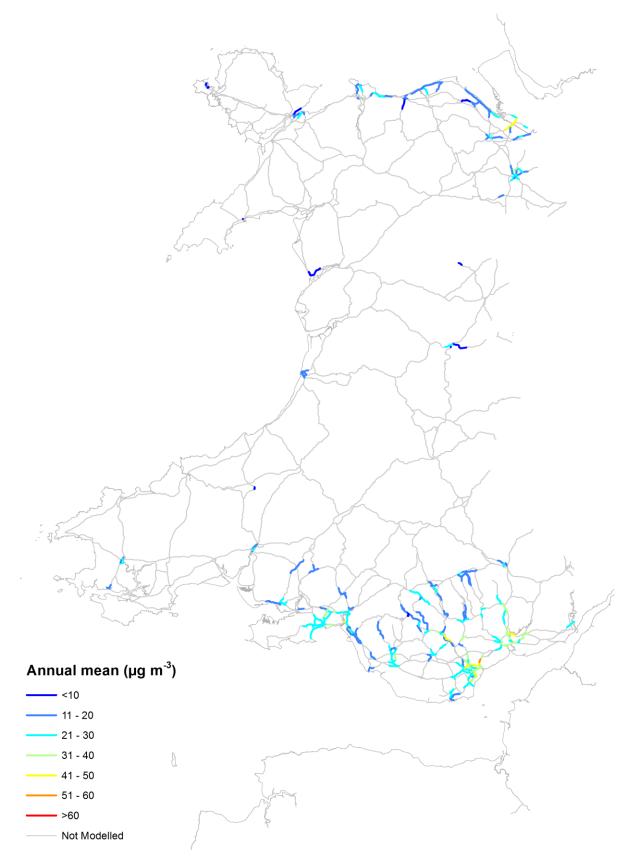
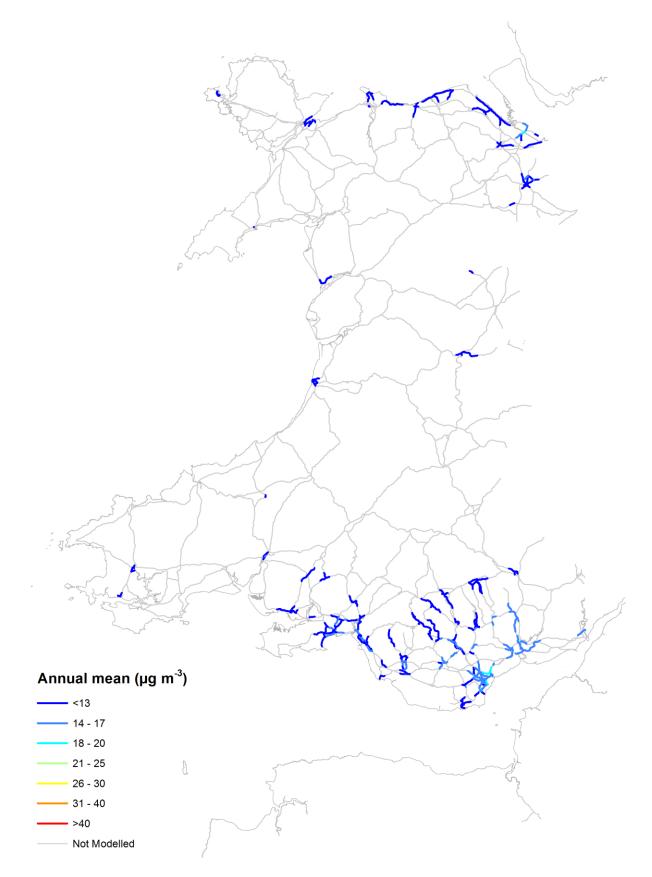


Figure 2-13: Estimated 2017 PM_{10} (gravimetric) roadside annual mean, $\mu g \ m^{-3}$



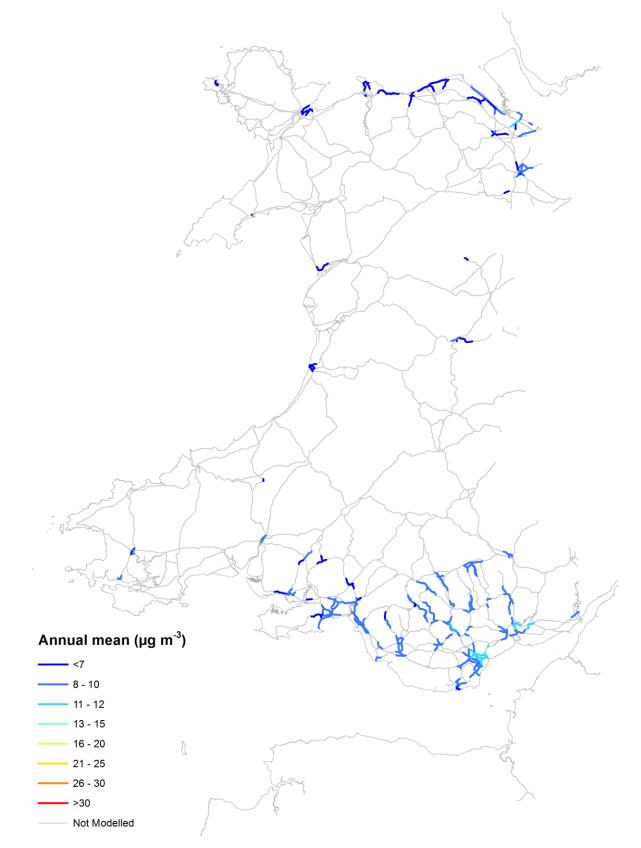


Figure 2-14: Estimated 2017 $PM_{2.5}$ (gravimetric) roadside annual mean, μg m-3

2.2.3 References

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