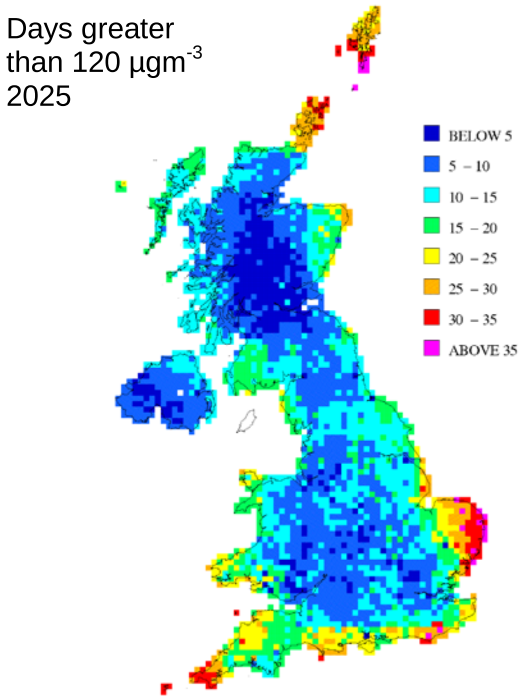
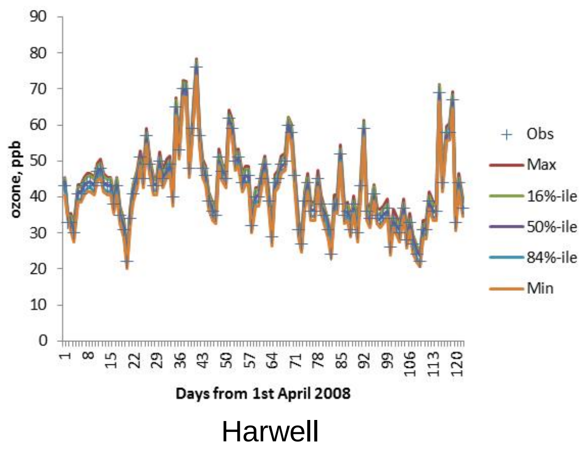
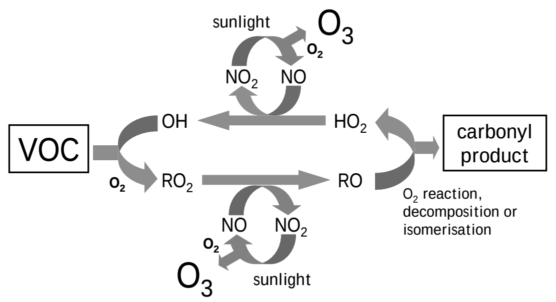
Modelling of Tropospheric Ozone

Annual Report 2013/14







Report for Defra

Ricardo-AEA/R/ED57616
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Executive summary

Ozone is an air pollutant that affects human health, vegetation and materials. The concentrations of ground-level ozone widely exceed environmental quality standards across the UK and Europe. Ozone is not emitted directly into the atmosphere, but is a secondary air pollutant formed in the lower atmosphere by sunlight-initiated reactions of ozone precursors - volatile organic compounds (VOCs) in the presence of nitrogen oxides (NO_x). It therefore requires sophisticated models combining meteorology, emissions and atmospheric chemistry processes to understand the factors affecting the production and subsequent control of ground-level concentrations of ozone.

This report describes work undertaken during 2013/14 in the project "*Modelling of Tropospheric Ozone*" funded by the Department for Environment, Food and Rural Affairs (Defra) and the Devolved Administrations (the Scottish Executive, the Welsh Assembly Government and the Department of the Environment for Northern Ireland).

This project aims to maintain two models that have been previously developed and demonstrated to quantify the rate of production and loss of ozone in the UK and to use them to support the analysis and development of Defra's policies on ozone air quality. The two models are the **Ozone Source Receptor Model (OSRM)** and the **Photochemical Trajectory Model (PTM).**

The OSRM and PTM were used to model and interpret the UK ground level ozone concentrations for 2012. The OSRM gave the overall picture for ozone throughout the year and across the UK. The PTM was used to diagnose and understand the nature of the high ozone concentration episodes observed in 2012 by modelling the responses of peak ozone concentrations at twelve sites. At many sites, the PTM model did not capture the seasonal maxima well. This may reflect deficiencies in the emissions inventories with the decline in European NO_x emissions being overstated, but overprediction of ozone deposition rates may also be partly responsible.

Box 1: Ozone in the UK in 2012

- **Overall, as the EU Air Quality Directive compliance metrics are concerned, 2012 was a year with relatively low ozone. However, there were a number of ozone episodes.**
- **Most (though not all) of the episodes in 2012 at the twelve sites modelled by PTM were dominated by emissions from the rest of Europe.**

UK ozone has been modelled for a range of different emission reduction scenarios of relevance to Defra's ozone air quality policy.

Box 2: Ozone concentrations for different emission scenarios

- **The OSRM was used to model UK ozone for:**
  - **An arbitrary 10% reduction in UK NOx and VOC emissions for 2012. This was to provide Defra with the information to update health, crop and materials damage cost functions in relation to ozone.**
  - **Three different UK emissions scenarios for 2025 and three 2030 scenarios.**
  - **Four 2025 scenarios and two 2030 scenarios developed by Defra from their estimates of what might be in the European Commission proposal for UK and European emission reductions as a result of revisions to the EU National Emissions Ceilings Directive.**

- **The simulations consistently show how ozone concentrations expressed as the national-scale metrics are predicted to be higher in future years when emissions are reduced and all other conditions are maintained the same.**

- **The PTM was used to model the impacts on ground-level ozone under 2008 episodic conditions for a central case emission reduction scenario for 2025 and 2030.**
  - **The impact on peak ozone was found to be substantial, bringing about a decrease in ozone at Harwell between 2008 and 2025 and 2030.**
  - **Although the episodic peak levels decreased by 2025 and 2030, the extremes of the distributions were not reduced enough to protect against the exceedance of the World Health Organisation air quality guideline**

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1 Introduction

Ozone is an air pollutant that affects human health, vegetation and materials. In light of this the concentrations of ambient ozone near ground level are of concern.

Ozone is not emitted directly into the atmosphere, but is a secondary air pollutant formed in the lower atmosphere by sunlight-initiated reactions of ozone precursors - volatile organic compounds (VOCs) in the presence of nitrogen oxides (NO_x). These precursors are emitted from both natural and man-made sources. Formation of atmospheric ozone occurs over a large spatial scale and as such ground level concentrations of ozone experienced in the UK are the result of emissions from sources within the UK, across Europe and further afield.

Concentrations are strongly influenced by meteorological conditions. Elevated concentrations over the UK occur in the spring and summer when slow-moving, or stagnant, high pressure (anticyclonic) weather systems bring in photochemically reacting air masses from mainland Europe. Concentrations of ozone are also influenced by ozone entering the UK in the free troposphere from the north Atlantic under prevailing meteorological conditions, providing a so-called hemispheric baseline ozone concentration upon which regional contributions are superimposed.

Local effects can play a part in both removing and forming ozone. Local emissions of highly reactive VOCs can lead to rapid photochemical production of ozone under favourable meteorological conditions. However, in urban areas these are usually offset by ozone removal through reaction with locally emitted NO_x from sources such as road traffic.

Recognising the transboundary nature of ozone formation, a series of European directives have been introduced to reduce emissions of ozone precursor gases. The Gothenburg Protocol to Abate Acidification, Eutrophication and Ground-level Ozone, under the Convention on Long-range Transboundary Air Pollution, set national emission ceilings for 2010 on total emissions of sulphur dioxide, nitrogen oxides, volatile organic compounds and ammonia. This was amended in 2012 to include national emission reduction commitments to be achieved in 2020 and beyond. There are similar ceilings set under the EU National Emissions Ceiling Directive (NECD). A proposal for the revised NECD has been published and sets out emission ceilings to be respected by 2020 and 2030. There is also a series of complementary EU Directives targeting specific sources that emit ozone precursor gases such as use of solvents, large combustion plant and road transport.

The EU Air Quality Directive sets target values and long-term objectives for ambient ozone concentrations for the protection of human health and vegetation. The two target values for ambient ozone both came into force from 1/1/2010:

- A maximum daily 8-hour mean concentration of 120 μgm^{-3}, not to be exceeded on 25 days per calendar year averaged over 3 years;
- AOT40 (calculated from 1-hr values) 18000 μgm^{-3}.h averaged (May to July) over five years.

National emissions inventories show that VOC and NO_x emissions have been falling in the UK and the rest of Europe over the last two decades. In spite of this there are still exceedances of the target values and the more challenging, long term objective values.

Understanding past trends in ozone concentrations and quantifying how measures aimed at reducing emissions of ozone precursor gases are likely to affect ground level ozone concentrations in the future is challenging. The complex nature of ozone production requires the use of sophisticated models that combine meteorological effects, emissions data and descriptions of chemical processes that occur in the atmosphere in order to quantify the rate of ozone production and loss in a moving air mass that receives precursor emissions over a wide spatial scale.

This project aims to maintain two models that have been previously developed and demonstrated to quantify the rate of production and loss of ozone in the UK and to use them to support the analysis and development of Defra's policies on ozone air quality. More specifically, the project uses these models to predict future concentrations of ozone and allow assessments of how concentrations respond to changes in precursor emissions. The results will be used to inform policy makers in the development of policies on precursor emission control and to evaluate their effects on UK ambient ozone concentrations (including compliance with the EU Air Quality Directive). Importantly the models will be used to assess the effects of alternative emission reduction scenarios on UK ambient ozone concentrations in 2020, 2030 and other years as part of the review of the EU Air Quality Directive and proposed revised NECD.

The two models used in this project are both Lagrangian-type models: the Ozone Source Receptor Model (OSRM) and the Photochemical Trajectory Model (PTM).

The following section provides a brief description of these models. The overall aims and objectives of the project, which started in March 2012 and runs until March 2014, are then described. These can be summarised as:

- **Objective 1:** The modelling of UK ozone in 2011 and 2012 using the OSRM and PTM.

- **Objective 2:** Policy application of the OSRM and PTM by modelling the formation and loss of ozone for alternative emission scenarios. This work is undertaken on a call-off basis;

- **Objective 3:** Maps of ozone concentration and surface flux parameters for different agricultural crops and semi-natural species;

- **Objective 4:** Optimising the use of emissions inventory information in the OSRM.

This report summarises the work undertaken for Objective 1 concerning the modelling and analysis of ozone concentrations in the UK in 2012. In addition, the specific model simulations requested by Defra and carried out under Objective 2 during 2013/14 are described.

The work for Objectives 3 was completed in March 2012 and was reported then. The work for Objective 4 was reported in the project annual report for 2012/13 (Cooke et al, 2013).

2 The Ozone Source Receptor and Photochemical Trajectory Models

The OSRM and PTM models are both Lagrangian-type models, developed and supported by Defra over the years through previous tropospheric ozone modelling contracts. Their performance has been demonstrated in peer-reviewed scientific journals and both models have been assessed in Defra's air quality Model Intercomparison Exercise (Williams et al, 2011, Carslaw, 2011, Carslaw et al, 2013).

Both models have been the backbone of Defra's ozone policy development and analysis for some years, having been extensively used for formulating and testing alternative policies on precursor emission controls. These include vehicle emission and fuel quality directives and directives on biofuels, solvents and industrial emissions. They have also been used to assess the effects of domestic policies and measures on ozone including those considered in the review of the Air Quality Strategy. The models have been used to model the UK's future ground level ozone climate up to 2030 assuming different meteorology conditions. More recently, the models have been used to assess the effects of various emission reduction scenarios considered for different countries in revisions to the Gothenburg Protocol and National Emissions Ceilings Directive.

The Monks' review of Defra's future ozone modelling requirements (Monks et al, 2007) recommended that Defra should consider moving its ozone modelling activity to an Eulerian basis. Although Eulerian models such as EMEP4UK and CMAQ are being used in the UK for regional scale ozone modelling, Defra is still assessing their practical application for national scale modelling and for formulating and assessing ozone air quality policy. In the meantime, there is still an urgent need for efficient and tested ozone models such as the OSRM and PTM to support a range of policies currently being developed, most notably to address different future emission scenarios such as those proposed for the revisions to the Gothenburg Protocol and National Emissions Ceilings Directive as well as to the reviews of the European Air Quality Directive.

2.1 The Ozone Source Receptor Model

Details of the OSRM have been given elsewhere in project reports and publications and only a brief description of the model is given here (e.g. Hayman et al, 2010 and Murrells et al, 2012).

The OSRM simulates the photochemical production of ozone in reactive air masses as they arrive at different receptor points in the UK. Essentially, each parcel of air picks up emissions from natural and man-made sources as it moves over land and sea surfaces over a large spatial scale and these undergo a series of chemical reactions initiated by sunlight leading to the production of ozone. Gridded 1 x 1 km emissions data for the UK are taken from the NAEI[1] (Tsagatakis et al, 2013) and 50 x 50 km emissions data for the rest of Europe are taken from EMEP[2]. Emission terms to describe natural biogenic emissions from European forests and agricultural crops are derived from the European PELCOM project.

The model uses archived 96-hour back trajectory data from the Met Office NAME model providing boundary layer depth and other parameters. The chemical mechanism used to define the rate of ozone formation and loss is a modified version of the mechanisms used in the STOCHEM model, but an option is available to use the condensed CRIv2-R5 chemical scheme,

[1] National Atmospheric Emissions Inventory, http://naei.defra.gov.uk/
[2] http://www.ceip.at/webdab-emission-database/emissions-as-used-in-emep-models/

linked to the Master Chemical Mechanism[3]. Dry deposition processes are represented using a conventional resistance approach.

The OSRM calculates ozone concentrations at mid-boundary layer height at hourly intervals on a 10 x 10 km grid covering the whole of the UK. These are corrected to account for loss of ozone due to reaction with local emissions of NO_x and deposition to land and sea surfaces in order to generate concentrations at ground-level.

The OSRM is also used in conjunction with a Surface Ozone Flux Model which can be used to model the uptake of ozone by different types of vegetation species under different meteorological conditions.

In conjunction with GIS-based tools, the OSRM is used to derive population- and area-weighted means of different ozone concentration metrics to provide the information necessary to Defra policy makers for cost-benefit analysis of emission reduction policies.

Previous work had shown that the empirical type modelling approach used in Defra's UK Pollution Climate Mapping (PCM) model traditionally gives results for ozone concentration metrics that, in model verification, are more representative of the measured concentrations than corresponding outputs provided by the OSRM. Hence, the PCM model, under the UK Ambient Air Quality Assessments (UKAAQA) modelling contract is used to provide the supplementary ozone modelling required for EU Air Quality Directive reporting on ozone to the European Commission each year on behalf of Defra. The OSRM, on the other hand, has a stronger role to play in scenario analysis and policy development as the OSRM can model future emission scenarios and the chemistry involved in forming and removing ozone over a large spatial scale from the emitted precursor gases, NO_x and VOCs. The OSRM is therefore maintained and evaluated each year using appropriate meteorology and emissions data and comparing calculated ozone concentrations with those from the PCM model and with monitoring data at specific AURN sites.

The OSRM has been used to model the UK ground-level ozone climate based on meteorological conditions and emissions from 1999 to 2012 and for forecasting ozone under future UK and European-wide emission scenarios for different meteorological conditions represented by those of previous years. The model has been optimised for computational efficiency and has been a vital policy tool for Defra and is routinely used in quantifying the response of the UK's ground-level ozone climate to measures aimed at reducing emissions of the precursor species.

Both the PCM and OSRM modelling techniques are verified against measured data to provide confidence in their performance. The two models have been compared in previous years, most recently for 2004, 2005, 2007, 2009, 2010 and 2011, which were noted as relatively "low ozone" years (Hayman et al, 2006a, Murrells et al, 2009, Murrells et al, 2012, Cooke et al, 2013), 2006 which was a relatively "high ozone" year (Murrells et al, 2008) and 2008 which was a broadly moderate year for ozone concentrations (Murrells et al, 2011).

2.2 The Photochemical Trajectory Model

The PTM has been used to describe photochemical ozone formation as well as secondary inorganic and organic aerosol formation in north-western Europe. Details are given in Derwent et al (1996, 1998, 2009), Abdalmogith et al. (2006) and Johnson et al. (2006). The model describes the chemical development within an air parcel that follows a trajectory for up to 10 days. For each mid-afternoon of each day a large number of equally probable and randomly selected 96-hour air parcel trajectories are generated using the Met Office Numerical Atmospheric dispersion Model Environment (NAME) model. The PTM uses NAEI and EMEP gridded emissions data and inventories for natural biogenic emissions. Initial and background species concentrations are taken from the EMEP site at the Valentia Observatory and the atmospheric baseline station

[3] http://mcm.leeds.ac.uk/MCM/

at Mace Head, Ireland. The model has the option of using different chemical mechanisms. Dry deposition processes are represented using a conventional resistance approach.

The PTM has been used for a variety of purposes to support Defra policy on ozone and secondary particulate matter (PM). These include the estimation of photochemical ozone creation potentials (POCPs) of individual VOCs (Derwent et al., 1998) and more recently to estimate secondary organic aerosol formation potentials (SOAPs, Derwent et al, 2010a). It has also been used to evaluate the effectiveness of current precursor emission controls in Europe on levels of ground-level ozone in the UK (Derwent et al, 2010b) and the effectiveness of future potential emission controls.

The PTM is similar to the OSRM but uses 3-dimensional trajectories to specified receptors and is able to use much more detailed chemical mechanisms than the OSRM, including the Master Chemical Mechanism (MCM) and its reduced derivatives. Thus the PTM complements the OSRM in being able to address the impact of chemistry on ozone formation and removal by using alternative chemical schemes to get an appreciation of the sensitivity of predicted ozone concentrations to choice of chemical scheme. By using the MCM, the PTM can also be more aligned to the detailed speciation VOC emissions inventory produced by the NAEI (Passant 2002) and can be used to address policies targeted at more specific groups of VOCs.

As a summary, the OSRM is used to model ground-level ozone concentrations (and ozone flux to vegetation) across the UK domain at 10 x 10 km resolution so is well set up to provide metrics on a national scale for the damage costs of ozone and the effectiveness of emission reduction measures to be evaluated. The outputs generated in this project are mainly as population- and area-weighted concentration metrics. The PTM is mainly used in this project to model ozone ***episodes*** at specific receptors rather than the whole of the UK like the OSRM but is used to provide a detailed picture of the sources responsible for the episodes.

3 Overview of Project Aims and Objectives

The overall aim of the project is to maintain a level of modelling support for Defra's ozone air quality policy development and assessment using the existing OSRM and PTM models.

The work is divided into four main project objectives. These are aimed at maintaining the OSRM and PTM models for predicting ground-level ozone concentrations in the UK and applying them to future emission scenarios relevant to Defra's policies on air quality and impacts on health and vegetation. The emission scenarios are worked on throughout the year on an *ad-hoc* basis.

Objective 1: Modelling of UK ozone in 2011 and 2012 using the OSRM and PTM

This Objective involves incorporating the latest meteorology and emissions inventory data to model the ground-level ozone climate in the UK for 2011 and 2012. This creates a new OSRM "Basecase" so the model is primed for predicting future ozone concentrations when emissions or meteorological conditions are changed (Objective 2). It also involves an initialisation of the concentrations relevant to the model year. The work in this reporting year has involved modelling UK ozone in 2012.

Objective 2: Policy application of the OSRM and PTM

This Objective involves the use of the OSRM and PTM to model ozone concentrations in the UK for emission scenarios specified by Defra. The modelling normally entails forecasting ozone concentrations in future years, typically 2020, 2025 or 2030, for relevant emission changes assuming meteorological conditions represented by those of a historical year. These might be years characterised by particularly high levels of ozone during summer episodes such as 2006 or years characterised by cool summers with little photochemical activity such as 2007. The work involves national scale modelling at 10 x 10 km resolution using the OSRM, producing outputs specified by Defra. The PTM can be used to assess the probability distributions of the various outcomes of the emission scenarios in terms of ozone, normally in terms of the impacts on predicted ozone episodes.

Objective 3: Maps of ozone concentration and surface flux parameters for different agricultural crops and semi-natural species: 2007 and 2020

This Objective provided the Centre for Ecology and Hydrology (CEH) with UK maps for 24-hr mean ozone concentration outputs from the OSRM and ozone flux parameters for vegetation from the Surface Ozone Flux Model (SOFM) covering years 2007 and 2020. This work was reported in March 2012 and is not further mentioned in this report.

Objective 4: Optimising the use of emissions inventory information in the OSRM

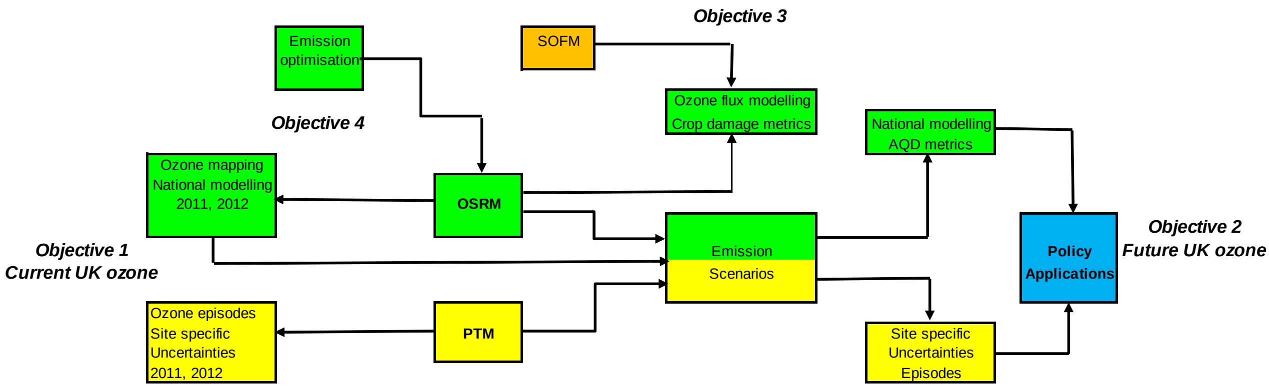
This Objective aims to improve the efficiency and transparency of the OSRM by optimising the use of emissions inventory information particularly in terms of

- The emission scenario pre-processor, and
- The treatment of shipping emissions

This work was reported in Cooke et al (2013) and is not further mentioned in this report.

Linkages between the four Objectives are shown in Figure 3.1.

Figure 3.1. Links between project objectives



Thus, the OSRM and PTM are used to model different aspects of the current ground level ozone climate using relevant emissions and meteorology data for the years 2011 and 2012 in Objective 1. Both models are used to predict future ozone concentrations for different emission scenarios. The OSRM predicts concentrations on a national scale, producing relevant health and vegetation-based metrics that can be compared with Air Quality Directive objectives and inform policies on regional differences in exposure. The PTM is used to predict future episodes and probabilistic uncertainty analysis of future trends based on modelling at specific locations. The improvements developed in Objective 4 improved the transparency and efficiency of OSRM runs for different emission scenarios in Objective 2. Objective 3 used the OSRM for a specific task on ozone flux modelling, but further work of this nature will benefit from the maintenance of the OSRM carried out in Objectives 1 and 4.

The work on the OSRM across all objectives has been undertaken by **Ricardo-AEA** who is the lead contractor with overall project management responsibilities for the project. Work involving the PTM model in Objectives 1 and 2 has been undertaken **by Professor Dick Derwent (rdscientific).**

4 Modelling UK Ground-Level Ozone Concentrations in 2012

4.1 UK Scale Modelling Using the OSRM

The OSRM was used to model hourly ground-level ozone concentrations at 10 x 10 km resolution for 2012 in the same way as done for previous years. Meteorology data from the Met Office NAME model at 6-hourly intervals covering 23 boundary layer parameters over a domain 30°W to 40°E and 20° to 80°N at 1 x 1° spatial resolution were used in conjunction with emissions inventory data for 2012. For UK emissions, the 1 x 1 km NAEI gridded data for 2011 were used,[4] projected to 2012 using the most up-to-date NAEI emission projections for each source sector based on DECC's UEP45 energy projections (Passant et al, 2013). For European emissions, the latest 50 x 50 km EMEP gridded data were used for 2010, also re-scaled to 2012 using PRIMES-2012 CLE (TSAP (2013)) projections of emissions total by country.

Ozone concentrations on each OSRM trajectory were initialised using daily concentration fields from the global tropospheric ozone model, STOCHEM, adjusted using monthly data for 2012 from measurements at Mace Head, Ireland, provided by Professor Derwent (rdscientific).

The OSRM was run to provide hourly ozone concentrations at mid-boundary layer height. The post-processor was then run to generate maps of ground-level ozone, taking account of surface deposition and losses due to reaction with locally emitted NO_x. The post-processor generated concentrations for the two Long-Term Objective ozone metrics used in the EU Air Quality Directive reporting:

- Days greater than 120 μgm^{-3} as a maximum daily running mean (DGT 120, the Long Term Objective for Human Health)
- AOT40 (Long Term Objective for Vegetation)

Concentrations for these metrics were also calculated at specific AURN monitoring sites for comparison with measurements.

4.1.1 Comparison of maps of OSRM and PCM outputs for ozone metrics in 2012

Figures 4.1(a) and 4.2(a) show maps of AOT40 and DGT 120 calculated by the OSRM. Corresponding maps from the PCM modelling technique used in the UK Ambient Air Quality Assessments (UKAAQA) programme are also shown in Figures 4.1(b) and 4.2(b). These are developed at finer resolution on a 1 x 1 km grid.

Although there are differences between the two models, there are broad similarities. The OSRM ozone metrics tend to be higher than those from the PCM. The OSRM shows higher concentrations to the east of the UK and along the south coast, features also shown by the PCM. However, the higher ozone metrics from the OSRM extend much further north around the coast of Scotland. In general, the level of performance of the OSRM seems to be in line with previous years.

[4] http://naei.defra.gov.uk/data/map-uk-das

Tests were carried out to show that the main difference between the OSRM results for 2012 and 2011 (presented by Cooke et al, 2013) was due to the different meteorological parameters for the two years rather than changes to the emissions.

An evaluation of OSRM and PCM model performance has also been undertaken, comparing model results for 2012 with measured concentrations and against each other.

Figure 4.1. AOT40 maps of ozone for 2012 from the OSRM and PCM models

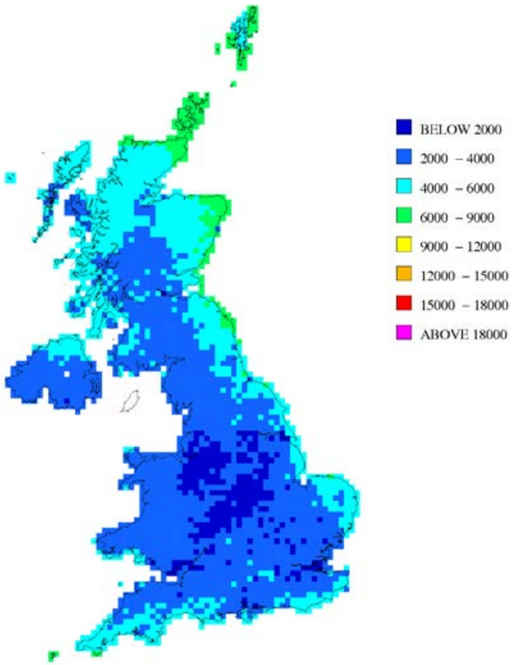
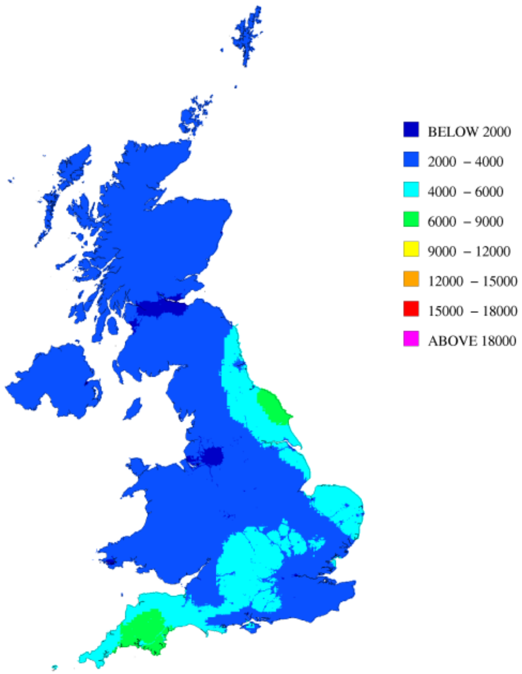
(a) AOT40 (2012) (μgm^{-3}.hours) (OSRM map)	(b) AOT40 (2012) (μgm^{-3}.hours) (PCM map)
	

Figure 4.2. Number of days exceeding 120 µgm^{-3} maps for 2012 from the OSRM and PCM models

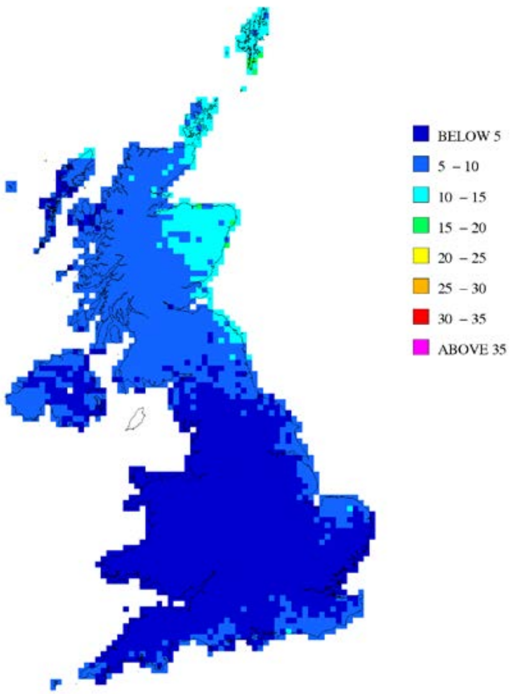
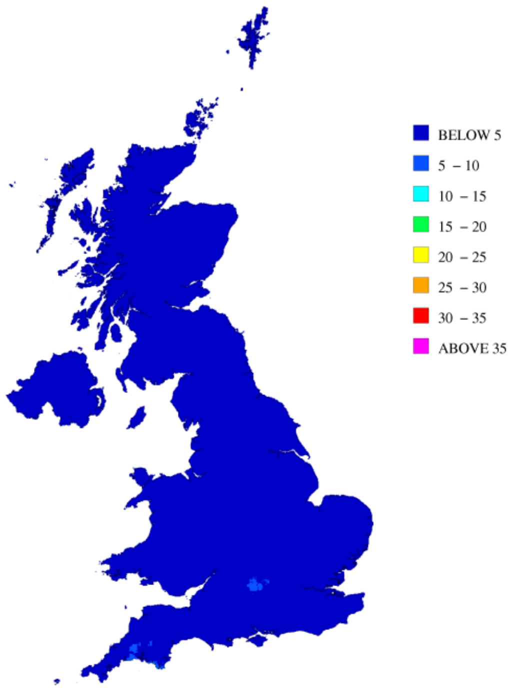
(a) Number of days exceeding 120 µgm^{-3} (2012) (OSRM map)	(b) Number of days exceeding 120 µgm^{-3} (2012) (PCM map)
	

Figure 4.3. AOT40 verification plots for 2012 for the OSRM and PCM models

(a) OSRM - AOT40 verification plot for 2012 (µgm^{-3}.hours)	**(b) PCM - AOT40 verification plot for 2012 (µgm^{-3}.hours)**

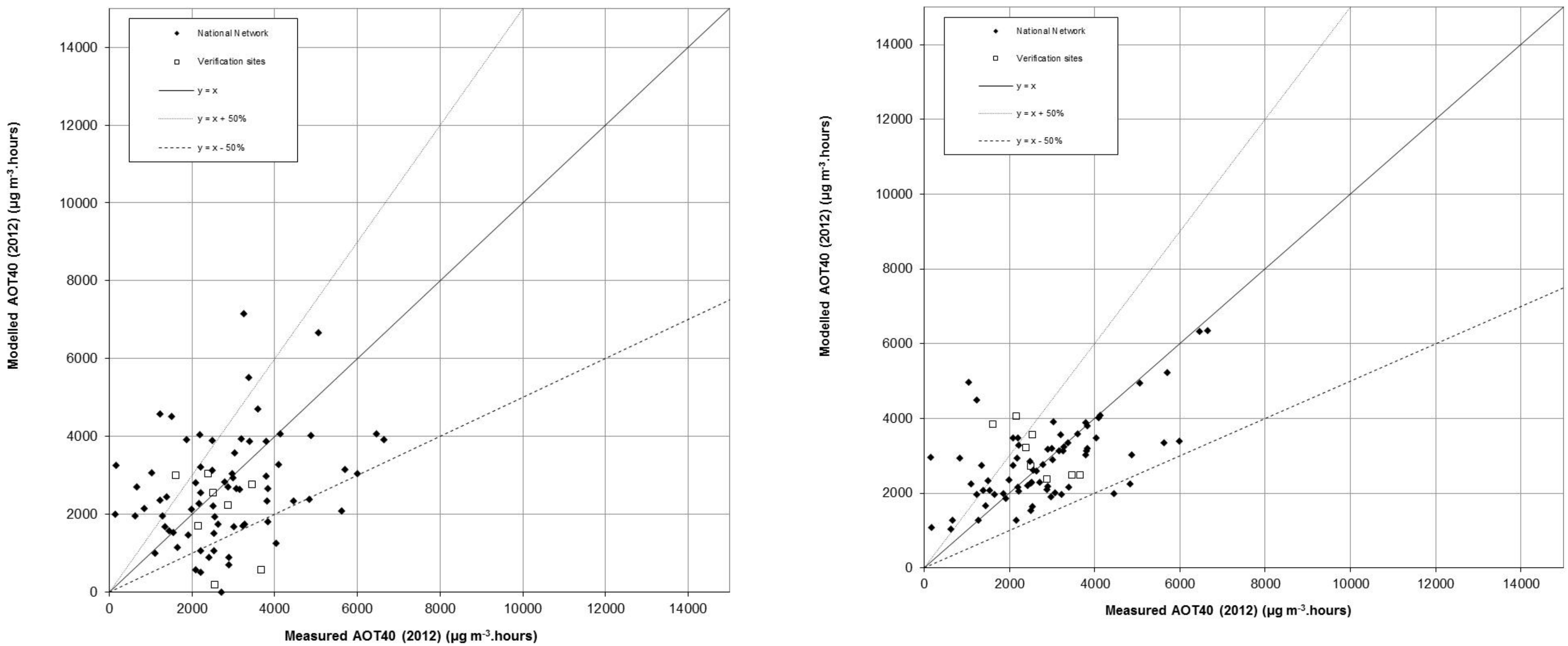
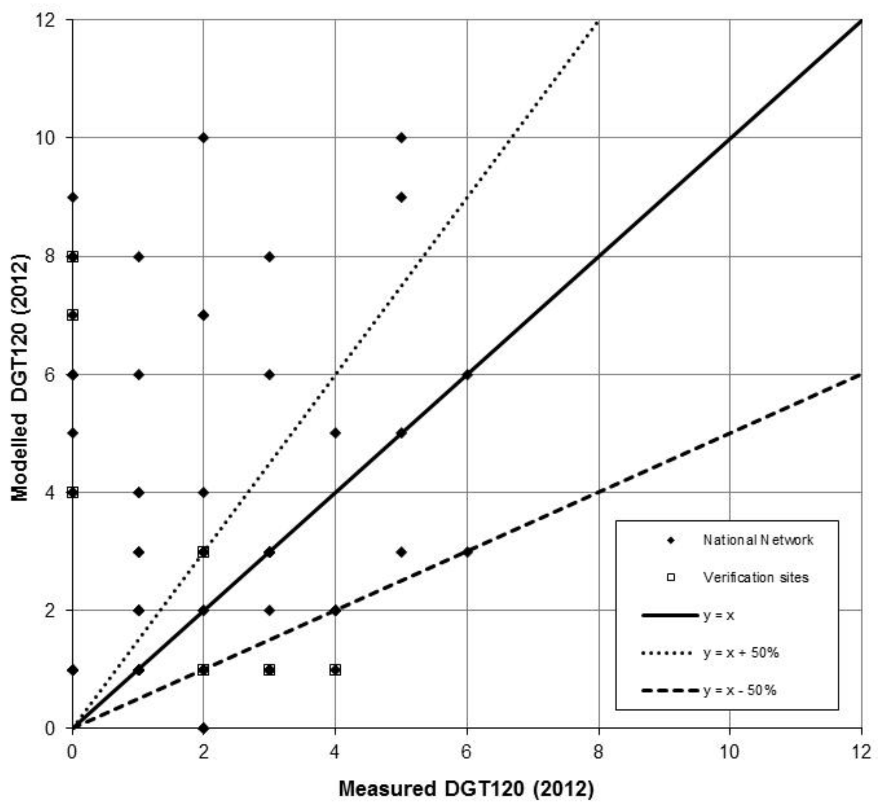
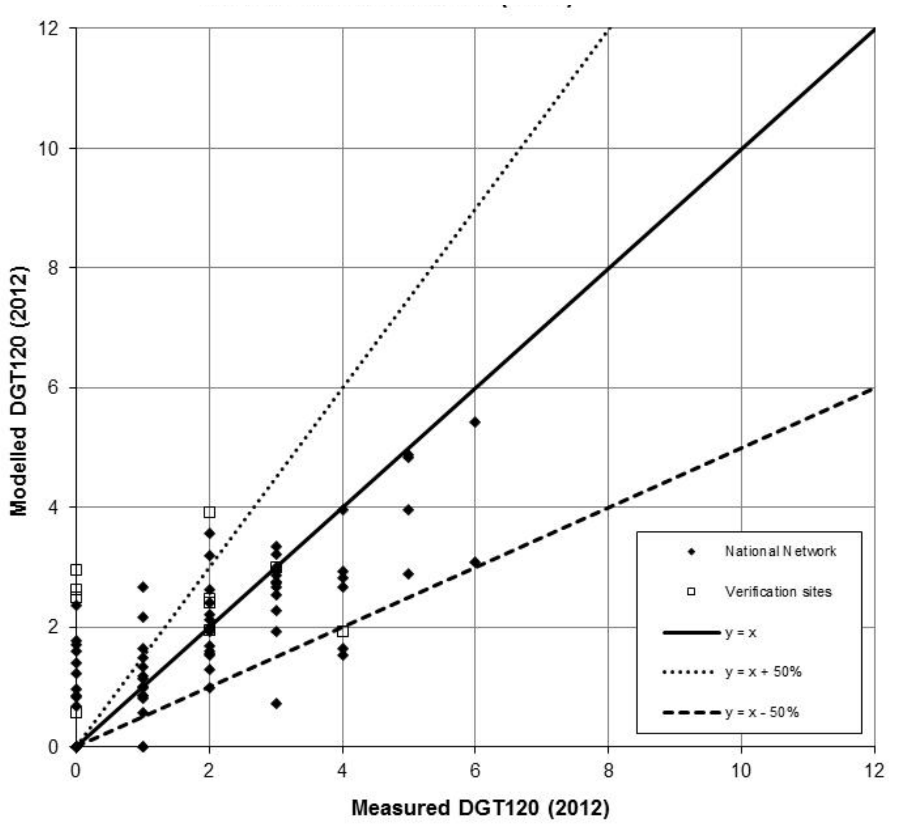


Figure 4.4. Number of days exceeding 120 µgm^{-3} verification plots for 2012 for the OSRM and PCM models

(a) OSRM - number of days exceeding 120 µgm^{-3} verification plot for 2012	(b) PCM - number of days exceeding 120 µgm^{-3} verification plot for 2012
	

Verification plots for the AOT40 and number of days exceeding 120 µgm^{-3} metrics are shown in Figures 4.3 and 4.4, respectively. Figures 4.3a and 4.4a show data for the OSRM and Figures 4.3b and 4.4b show data for the PCM. The 1:1 line and data quality objective (+/- 50%) lines are also shown. Two groups of sites are presented in the verification charts: national network (AURN) monitoring sites and verification sites. The AURN sites were used as a direct input to the PCM model and therefore provide a useful check during the verification process, but are not able to provide a completely independent representation of model performance. For this reason there is a separate group of sites labelled 'verification sites' that are completely independent from the PCM model. These typically come from local authorities, research institutions and ad-hoc monitoring campaigns for which Ricardo-AEA holds and ratifies the data. These monitoring data are ratified to the same standard as the AURN. Both groups of sites provide an independent verification of the OSRM because this is a process based model which does not use monitoring data as an input or a calibration method. A data capture threshold of 75% has been applied to the monitoring data prior to analysis.

Table 4.1 summarises the average of the measured AOT40 concentrations, the average of the modelled AOT40 estimates, the R^2 of the fit line (Figure 4.3), the number of monitoring sites used and the percentage of these monitoring sites that fall outside the Data Quality Objective (DQO) for both the OSRM and PCM results. Table 4.2 shows the equivalent data for the number of days exceeding 120 µgm^{-3} metric.

Table 4.1. AOT40 metric verification summary for the OSRM and PCM model results for 2012

	Mean of measurements (µgm^{-3}.hours)	Mean of model estimates (µgm^{-3}.hours)	R^2	% outside DQO	No. sites used in assessment
National network (PCM)	2814	2845	0.37	23%	70
Verification sites (PCM)	2647	3097	0.65	25%	8
National network (OSRM)	2814	2650	0.09	40%	70
Verification sites (OSRM)	2647	2413	0.12	38%	8

Table 4.2. Number of days exceeding 120 µgm^{-3} metric verification summary for the OSRM and PCM model results for 2012

	Mean of measurements (days)	Mean of model estimates (days)	R^2	% outside DQO	No. sites used in assessment
National network (PCM)	2.0	1.9	0.61	30%	70
Verification sites (PCM)	1.5	2.4	0.02	60%	10
National network (OSRM)	2.0	3.5	0.00	60%	70
Verification sites (OSRM)	1.5	3.3	0.65	60%	10

The mean measured values in the tables above for AOT40 and number of days exceeding 120 µgm^{-3} indicate that 2012 was a relatively low ozone year. It can be seen in Table 4.2 above that on average the OSRM over-predicts the number of days exceeding 120 µgm^{-3} for 2012.This over-prediction can also be seen in the verification plot (Figure 4.4). In Table 4.1 above, on average, the OSRM under-predicts the AOT40 metric for 2012. However, this under-prediction is not obvious in the verification plot (Figure 4.3).

Past analysis (Hayman et al, 2006b, Murrells et al, 2009, Murrells et al, 2012, Cooke et al., 2013) has shown that the OSRM slightly under-predicts measured concentrations in some cases and slightly over-predicts measured concentrations in others. In general, it has under-predicted ozone metrics in high ozone years (e.g. 2003 and 2006) and slightly over-predicted ozone metrics in low ozone years (2004, 2005, 2007, 2009 and 2010). In 2008, which was considered a moderate ozone year, the OSRM generally under-predicted AOT40 concentrations. For 2011, which was also a relatively low ozone year, the OSRM underpredicted these metrics.

Tables 4.3 and 4.4 below present the average measured and average OSRM modelled results for the years 2004-2011. These show the model performance in each year for both metrics, including during high (e.g. 2006) and low (e.g. 2004, 2005, 2007, 2009, 2010, 2011) ozone years. The OSRM results for later years are not directly comparable with earlier years because of model improvements to emissions and boundary conditions and changes in the meteorology data format. Nevertheless, the OSRM results seem to be consistent with the measurements for 2012 indicating that it was a relatively low ozone year in terms of the mean of these metrics.

Table 4.3. OSRM results for AOT40 (μgm^{-3}.hours) for the years 2004 - 2012

		National network		Verification sites	
Year Modelled	**NAEI Year**	**Mean of measured**	**Mean of modelled**	**Mean of measured**	**Mean of modelled**
2004	2003	2888	2056	3681	2256
2005	2004	3650	4165	3810	3088
2006	2005	10497	5043	5061	6574
2007	2006	2281	4503	3061	5211
2008	2007	6025	4444	4913	4559
2009	2008	3182	4274	2738	3818
2010	2009	2244	4404	2518	4150
2011	2010	2333	2171	2627	2158
2012	2011	2814	2650	2647	2413

Table 4.4. OSRM results for number of days exceeding 120 μgm^{-3} for the years 2004 - 2012

		National network		Verification sites	
Year Modelled	**NAEI Year**	**Mean of measured**	**Mean of modelled**	**Mean of measured**	**Mean of modelled**
2004	2003	13	12	7	6
2005	2004	3	6	4	5
2006	2005	13	8	8	8
2007	2006	2	4	2	6
2008	2007	5	6	5	7
2009	2008	1	4	1	4
2010	2009	1	8	2	9
2011	2010	3	2	3	2
2012	2011	2	4	2	3

4.2 Analysis of Episodes of Photochemical Ozone in the United Kingdom during 2012 Using the PTM

4.2.1 Overview of ozone episodes in 2012

The PTM was used to investigate ozone episodes that occurred in 2012.

There were several photochemically active periods during 2012. Maximum hourly ozone levels reached 90 ppb at Yarner Wood on 26th May and 87 ppb at Harwell on 26th July. Yarner Wood experienced 36 days with hourly mean levels in excess of 50 ppb, followed by High Muffles with 25 days. There were three main ozone episodes which extended from 24th March to 5th April, 17th May to 30th May and 22nd July to 27th July. Altogether 64 days exhibited maximum hourly ozone levels in excess of 50 ppb at any of the 12 rural monitoring sites studied. The ozone episodes started on 24th March in the west and north of Great Britain and ended with a widely distributed single day episode on 9th September that encompassed Auchencorth Moss, Eskdalemuir, Harwell, High Muffles, Lullington Heath, Narberth, Rochester and Sibton. The dates of each 50 ppb exceedance day and the maximum hourly mean ozone levels are tabulated by site in Tables 4.5 – 4.16.

Photochemical Trajectory Model (PTM) runs were performed for each 15:00 hrs. on each day of 2012 for each of the 12 sites studied. The PTM results for the days in which the maximum hourly ozone levels were observed to exceed 50 ppb are tabulated in Tables 4.5 – 4.16 together with the fractional bias achieved by the model. In addition, two sensitivity cases were performed in which man-made VOC emissions were reduced by 30% across-the-board in the UK and in the Rest of Europe (RoE). The responses (Base case – Scenario case) of the model to the 30% reductions in VOC emissions were estimated. If the ozone response to the 30% reduction in the UK case was greater than the response to the 30% reduction in the RoE case on a given day, then that day was assigned as UK-dominant and vice versa. If the model performance was considered satisfactory, that is to say the fractional bias achieved was within ± 0.1, then the UK- versus RoE-dominance was also tabulated in Tables 4.5 – 4.16.

The ozone episodes were then examined from the standpoint of the observations and the PTM results on an episode-by-episode basis in the paragraphs that follow.

4.2.1.1 24th March to 5th April ozone episode

This was the first ozone episode of the 2012 season and occurred whilst the weather was exceptionally sunny and warm with notably elevated temperatures in Wales and Scotland. During 24th and 25th March, elevated ozone levels above 50 ppb were observed at Yarner Wood, Narberth, Eskdalemuir, Auchencorth Moss and Strath Vaich. Strath Vaich monitored 61 ppb on 25th March, the highest hourly value at this site observed during the entire ozone season. The ozone episode spread to Aston Hill on 27th March and to High Muffles and Rochester on 28th March. Levels were generally lower towards the end of March but the episode returned during the first few days of April with elevated levels at Strath Vaich on 1st April, Yarner Wood and Harwell on 2nd April and Rochester on 5th April.

The episode was generally well predicted by the PTM. Auchencorth Moss, High Muffles and Narberth had elevated ozone levels on two days and these were predicted within ± 10% accuracy by the PTM. Strath Vaich, Eskdalemuir and Rochester had accurate PTM predictions on half of the days with observed elevated ozone levels. Three out of eight episode days at Yarner Wood were predicted by the PTM. The episode maximum at Strath Vaich was well predicted by the PTM within the accuracy of ± 10%. The observed elevation at Harwell was not predicted by the PTM.

The sensitivity analyses performed with the PTM pointed to the UK being the more important source of the photochemical ozone predicted at Strath Vaich during the early part of the episode rather than the Rest of Europe. The source of the elevated ozone levels at Yarner Wood appeared to have been largely baseline in origin.

4.2.1.2 17th May to 30th May ozone episode

This was the second ozone episode of the 2012 season and began with mostly sunny weather in Scotland from the 20th to 22nd and from the 22nd onwards over central and eastern England. The weather became somewhat cooler and cloudier towards the end of May. This ozone episode began at Yarner Wood on 17th May and spread to Glazebury and Narberth on 21st May and to the rest of the UK on 22nd May. The 28th May was the last day with elevated ozone levels at a number of sites, with elevated ozone levels only being observed at Glazebury and Rochester on the 29th May and Harwell on 30th May. Auchencorth Moss saw its highest ozone level of the season on 25th May, with 56 ppb, Narberth on 26th May with 71 ppb, Yarner Wood on 26th May with 90 ppb, Aston Hill on 27th May with 72 ppb. Eskdalemuir, Glazebury and High Muffles all saw their highest ozone levels of the season on 28th May with levels between 72 and 76 ppb.

The PTM model performance was best at the Aston Hill site where the ozone maxima on 6 out of the 8 episode days were predicted within ± 10%. Apart from High Muffles where 4 out of 9 ozone maxima were predicted accurately, the PTM performance at the other sites was poor. Although 7 sites showed their season maxima during this episode, none were predicted accurately by the PTM model.

Sensitivity analyses carried out with the PTM at Aston Hill pointed to the Rest of Europe as the more likely source of the photochemical ozone observed during this episode, rather than the UK.

4.2.1.3 22nd July to 27th July ozone episode

It was dry and sunny over much of the UK on 21st July but rain returned to Scotland and Northern England on the 22nd July. Meanwhile southern and central parts of England became sunny and very warm between 23rd and 26th July. The warm weather was confined to southern England by 27th July and then showers and rain set in for the remainder of the month. The ozone episode began on 22nd July at Harwell then spread to Lullington Heath, Sibton and Rochester on 23rd July. Its most westerly extent was reached on 24th July when elevated ozone levels were observed at Yarner Wood and its most northerly extent on 25th when elevated ozone levels were observed at Aston Hill. July 25th saw Sibton reach its ozone maximum of the season with 84 ppb, Rochester with 75 ppb and Lullington Heath with 80 ppb. July 26th saw the season maximum being reached at Harwell with 87 ppb. The episode ended on 27th July with elevated ozone levels observed at Harwell, Lullington Heath and Rochester.

This ozone episode was reasonably well predicted by the PTM. The season maxima at Harwell, Rochester and Sibton were predicted accurately to within ± 10% but that at Lullington Heath was missed altogether. Three of the 5 days with elevated ozone levels were predicted for Rochester and 2 out of 4 for Sibton. Elsewhere model performance was poor.

On those sites and days when model performance was satisfactory, better than ± 10%, sensitivity analyses indicated that the more likely source of the photochemical ozone was from the Rest of Europe rather than the UK.

Table 4.5. Days at the Aston Hill site with maximum hourly ozone levels in excess of 50 ppb, the observed maximum ozone levels, the PTM model predictions, their fractional bias and comments of whether the ozone levels were dominated by VOC sources in the UK or in the Rest of Europe.

Date	Observed peak, ppb	PTM peak, ppb	Fractional bias	Comments
27th March	51	45.82	-0.10	UK
28th March	53	41.51	-0.22	
17th April	52	45.04	-0.13	
24th April	51	43.84	-0.14	
30th April	52	51.49	-0.01	UK
12th May	51	42.56	-0.17	
21st May	54	49.24	-0.09	UK
22nd May	57	56.98	0	RoE
23rd May	54	50.84	-0.06	UK
24th May	54	52.83	-0.02	RoE
25th May	63	62.32	-0.01	RoE
26th May	58	53.65	-0.08	RoE
27th May	72	58.77	-0.18	
28th May	51	48.73	-0.04	UK
20th June	55	48.06	-0.13	
26th July	69	58.55	-0.15	
11th August	59	53.27	-0.01	UK

Table 4.6. Days at the Auchencorth Moss site with maximum hourly ozone levels in excess of 50 ppb, the observed maximum ozone levels, the PTM model predictions, their fractional bias and comments of whether the ozone levels were dominated by VOC sources in the UK or in the Rest of Europe.

Date	Observed peak, ppb	PTM peak, ppb	Fractional bias	Comments
25th March	52	49.91	-0.04	RoE
26th March	55	51.55	-0.06	UK
5th May	51	44.15	-0.13	
7th May	53	45.28	-0.15	
24th May	55	50.03	-0.09	UK
25th May	56	39.91	-0.29	
26th May	54	42.31	-0.22	
28th May	55	35.52	-0.35	
15th August	55	51.02	-0.07	RoE
9th September	53	53.99	0.02	RoE

Table 4.7. Days at the Eskdalemuir site with maximum hourly ozone levels in excess of 50 ppb, the observed maximum ozone levels, the PTM model predictions, their fractional bias and comments of whether the ozone levels were dominated by VOC sources in the UK or in the Rest of Europe.

Date	Observed peak, ppb	PTM peak, ppb	Fractional bias	Comments
25th March	54	51.21	-0.05	UK
27th March	53	44.23	-0.17	
28th March	52	49.08	-0.06	RoE
29th March	53	43.57	-0.18	
22nd May	62	55.51	-0.11	
23rd May	54	50.16	-0.07	RoE
24th May	53	40.28	-0.24	
25th May	62	44.87	-0.28	
26th May	54	42.30	-0.22	
27th May	54	50.67	-0.06	UK
28th May	72	52.92	-0.27	
9th September	51	46.86	-0.08	RoE

Table 4.8. Days at the Glazebury site with maximum hourly ozone levels in excess of 50 ppb, the observed maximum ozone levels, the PTM model predictions, their fractional bias and comments of whether the ozone levels were dominated by VOC sources in the UK or in the Rest of Europe.

Date	Observed peak, ppb	PTM peak, ppb	Fractional bias	Comments
24th April	51	46.70	-0.08	UK
21st May	52	46.44	-0.10	UK
22nd May	52	52.44	0	RoE
25th May	52	42.79	-0.18	
26th May	53	40.21	-0.24	
27th May	65	55.38	-0.15	
28th May	76	61.11	-0.20	

Table 4.9. Days at the Harwell site with maximum hourly ozone levels in excess of 50 ppb, the observed maximum ozone levels, the PTM model predictions, their fractional bias and comments of whether the ozone levels were dominated by VOC sources in the UK or in the Rest of Europe.

Date	Observed peak, ppb	PTM peak, ppb	Fractional bias	Comments
2nd April	53	45.51	-0.14	
24th April	51	48.05	-0.06	RoE
30th April	54	47.73	-0.12	
12th May	51	43.20	-0.15	
13th May	52	43.16	-0.17	
22nd May	65	48.14	-0.26	
23rd May	60	55.22	-0.08	
24th May	59	49.79	-0.16	
25th May	67	55.53	-0.17	
26th May	68	50.06	-0.26	
27th May	82	59.63	-0.27	
20th June	53	45.52	-0.14	
22nd July	52	50.88	-0.02	UK
23rd July	51	36.20	-0.29	
24th July	70	40.82	-0.42	
25th July	86	52.30	-0.39	
26th July	87	77.49	-0.10	RoE
27th July	55	35.11	-0.36	
9th August	54	40.63	-0.25	
10th August	61	45.4	-0.26	
11th August	62	50.28	-0.19	
9th September	63	44.52	-0.29	

Table 4.10. Days at the High Muffles site with maximum hourly ozone levels in excess of 50 ppb, the observed maximum ozone levels, the PTM model predictions, their fractional bias and comments of whether the ozone levels were dominated by VOC sources in the UK or in the Rest of Europe.

Date	Observed peak, ppb	PTM peak, ppb	Fractional bias	Comments
28th March	54	54.16	0	UK
29th March	51	51.11	0	UK
22nd April	52	45.39	-0.13	
24th April	53	50.97	-0.04	UK
26th April	52	47.31	-0.09	UK
30th April	53	50.98	-0.04	UK
4th May	51	39.20	-0.23	
5th May	51	41.30	-0.19	
6th May	54	41.34	-0.23	
7th May	51	40.26	-0.21	
18th May	51	47.32	-0.07	RoE
22nd May	58	62.23	0.07	RoE
23rd May	62	45.26	-0.27	
24th May	65	62.65	-0.04	RoE
25th May	64	48.83	-0.24	
26th May	63	46.19	-0.27	
27th May	60	54.02	-0.10	RoE
28th May	72	53.70	-0.25	
29th May	54	46.09	-0.15	
20th June	56	40.06	-0.29	
21st June	59	48.89	-0.17	
5th July	58	57.50	-0.01	RoE
12th August	54	46.32	-0.14	
15th August	66	75.60	0.15	
9th September	59	45.47	-0.23	

Table 4.11. Days at the Lullington Heath site with maximum hourly ozone levels in excess of 50 ppb, the observed maximum ozone levels, the PTM model predictions, their fractional bias and comments of whether the ozone levels were dominated by VOC sources in the UK or in the Rest of Europe.

Date	Observed peak, ppb	PTM peak, ppb	Fractional bias	Comments
22nd May	60	53.38	-0.11	
24th May	68	52.62	-0.23	
25th May	66	51.99	-0.21	
26th May	70	52.12	-0.26	
27th May	66	51.90	-0.21	
20th June	52	50.80	-0.02	RoE
23rd July	56	41.59	-0.26	
24th July	69	53.96	-0.22	
25th July	80	64.58	-0.19	
26th July	69	65.90	-0.05	RoE
27th July	70	68.41	-0.02	UK
10th August	53	51.38	-0.03	UK
17th August	56	38.62	-0.31	
8th September	58	44.50	-0.23	
9th September	54	48.90	-0.09	RoE

Table 4.12. Days at the Narberth site with maximum hourly ozone levels in excess of 50 ppb, the observed maximum ozone levels, the PTM model predictions, their fractional bias and comments of whether the ozone levels were dominated by VOC sources in the UK or in the Rest of Europe.

Date	Observed peak, ppb	PTM peak, ppb	Fractional bias	Comments
24th March	55	54.99	0	RoE
28th March	53	51.06	-0.04	RoE
24th May	55	54.62	-0.01	UK
25th May	67	57.34	-0.14	
26th May	71	57.02	-0.20	
27th May	70	60.02	-0.14	
10th August	58	56.55	-0.03	UK
11th August	67	56.55	-0.16	
12th August	54	32.61	-0.40	
9th September	55	45.48	-0.17	

Table 4.13. Days at the Rochester site with maximum hourly ozone levels in excess of 50 ppb, the observed maximum ozone levels, the PTM model predictions, their fractional bias and comments of whether the ozone levels were dominated by VOC sources in the UK or in the Rest of Europe.

Date	Observed peak, ppb	PTM peak, ppb	Fractional bias	Comments
28th March	52	48.37	-0.07	UK
5th April	53	45.53	-0.14	
20th April	53	47.49	-0.10	UK
26th April	57	44.25	-0.22	
27th April	54	47.77	-0.12	
13th May	55	48.30	-0.12	
22nd May	53	47.85	-0.10	RoE
24th May	59	56.13	-0.05	RoE
25th May	65	53.02	-0.18	
26th May	63	39.82	-0.37	
27th May	67	57.34	-0.14	
28th May	53	57.29	0.08	RoE
29th May	57	48.85	-0.14	
20th June	65	53.50	-0.18	
23rd July	59	64.52	0.09	RoE
24th July	72	63.59	-0.12	
25th July	75	76.93	0.03	RoE
26th July	62	47.35	-0.24	
27th July	58	56.65	-0.02	UK
1st August	51	38.98	-0.24	
10th August	59	50.21	-0.15	
9th September	68	48.43	-0.29	

Table 4.14. Days at the Sibton site with maximum hourly ozone levels in excess of 50 ppb, the observed maximum ozone levels, the PTM model predictions, their fractional bias and comments of whether the ozone levels were dominated by VOC sources in the UK or in the Rest of Europe.

Date	Observed peak, ppb	PTM peak, ppb	Fractional bias	Comments
26th April	53	51.48	-0.03	UK
30th April	53	52.04	-0.02	UK
1st May	53	44.13	-0.17	
7th May	59	41.24	-0.30	
24th May	65	64.63	-0.01	RoE
25th May	59	52.56	-0.11	
26th May	57	50.07	-0.12	
27th May	67	49.47	-0.26	
28th May	52	53.92	0.04	UK
30th May	52	45.96	-0.12	
20th June	61	48.10	-0.21	
23rd July	61	53.99	-0.12	
24th July	74	56.82	-0.23	
25th July	84	75.28	-0.10	RoE
26th July	55	55.80	0.01	RoE
10th August	53	54.16	0.02	UK
11th August	51	37.11	-0.27	
12th August	57	47.23	-0.17	
15th August	53	52.15	-0.02	RoE
18th August	70	76.03	0.09	UK
19th August	76	59.45	-0.22	
9th September	60	51.84	-0.14	

Table 4.15. Days at the Strath Vaich site with maximum hourly ozone levels in excess of 50 ppb, the observed maximum ozone levels, the PTM model predictions, their fractional bias and comments of whether the ozone levels were dominated by VOC sources in the UK or in the Rest of Europe.

Date	Observed peak, ppb	PTM peak, ppb	Fractional bias	Comments
25th March	61	59.92	-0.02	UK
26th March	56	49.92	-0.10	UK
27th March	61	52.46	-0.14	
28th March	59	63.06	0.07	RoE
29th March	55	41.78	-0.24	
1st April	55	44.09	-0.20	
22nd April	52	52.75	0.01	UK
24th April	52	43.81	-0.16	
25th April	52	48.38	-0.07	RoE
1st May	51	42.52	-0.17	
2nd May	54	40.75	-0.25	
22nd May	54	50.94	-0.06	RoE
23rd May	57	47.43	-0.17	
25th May	56	48.37	-0.14	
26th May	55	40.74	-0.26	
27th May	53	38.96	-0.27	
22nd June	53	50.97	-0.04	RoE
15th August	52	50.86	-0.02	RoE

Table 4.16. Days at the Yarner Wood site with maximum hourly ozone levels in excess of 50 ppb, the observed maximum ozone levels, the PTM model predictions, their fractional bias and comments of whether the ozone levels were dominated by VOC sources in the UK or in the Rest of Europe.

Date	Observed peak, ppb	PTM peak, ppb	Fractional bias	Comments
24th March	51	49.33	-0.03	Baseline
25th March	56	47.43	-0.15	
27th March	58	47.57	-0.18	
28th March	64	47.23	-0.26	
29th March	58	48.73	-0.16	
30th March	52	41.87	-0.20	
2nd April	51	47.44	-0.07	Baseline
3rd April	51	47.74	-0.06	Baseline
12th April	51	47.57	-0.07	Baseline
16th April	53	50.12	-0.05	Baseline
17th April	52	44.82	-0.14	
20th April	51	47.62	-0.07	Baseline
24th April	52	43.83	-0.16	
25th April	56	45.87	-0.18	
27th April	52	47.58	-0.09	Baseline
30th April	54	47.96	-0.11	
1st May	53	42.63	-0.20	
2nd May	54	42.89	-0.21	
12th May	54	45.31	-0.16	
13th May	55	48.13	-0.13	
14th May	51	41.75	-0.18	
17th May	52	44.50	-0.14	
19th May	55	39.80	-0.28	
20th May	52	50.89	-0.02	RoE
21st May	56	51.08	-0.09	UK
22nd May	51	42.07	-0.18	
23rd May	75	54.85	-0.27	
25th May	82	58.78	-0.28	
26th May	90	50.48	-0.44	
27th May	61	42.83	-0.30	

20th June	51	48.83	-0.04	RoE
24th July	53	50.45	-0.05	RoE
25th July	68	45.33	-0.33	
26th July	84	66.96	-0.20	
10th August	62	53.99	-0.13	
11th August	56	42.87	-0.24	

4.2.2 PTM model performance during 2012

The performance of the PTM over the 2012 ozone season at the 12 sites is summarised in Table 4.17. Overall, model performance was far from satisfactory. Model performance in terms of predicting within ± 10%, the seasonal ozone maxima at each site was only satisfactory at Harwell, Rochester, Sibton and Strath Vaich. Elsewhere the seasonal maxima were grossly underestimated. Model performance in terms of predicting the number of days with over 50 ppb ozone was satisfactory only at Aston Hill and Auchencorth Moss. Elsewhere model performance was poor against this metric and a significant number of episode days were completely missed. Of the three main ozone episodes, only the first from 24th March to 5th April and the third from 22nd July to 27th July, were reasonably well predicted by the PTM. Model performance was comprehensively poor for the second episode.

Table 4.17. PTM model performance against observations over the 2012 ozone season at all twelve rural ozone monitoring stations.

Station	Number of ozone episode days with > 50 ppb	Number of episode days predicted by PTM	Seasonal maxima
Aston Hill	17	10	not predicted
Auchencorth Moss	10	5	not predicted
Eskdalemuir	12	5	not predicted
Glazebury	7	3	not predicted
Harwell	22	3	predicted
High Muffles	25	11	not predicted
Lullington Heath	15	5	not predicted
Narberth	10	4	not predicted
Rochester	22	8	predicted
Sibton	22	9	predicted
Strath Vaich	18	8	predicted
Yarner Wood	36	11	not predicted

The reasons behind the poor PTM performance over the 2012 ozone season are not completely clear. It is possible that the emissions inventories have overstated the decline in NO_x emissions as indexed by the EMEP national NO_x emission totals. This would lead to an underestimation of the long range transport of ozone because of NO_x depletion. It is also possible that the PTM treatment of ozone dry deposition is no longer appropriate due to changes in climatic conditions across Europe and the more likely drying out of soils earlier in the year. This possibility is further explored in Section 4.2.4.

4.2.3 Uncertainty analysis for episodic peak ozone at Aston Hill during 2012

The highest 8-hour mean ozone level observed by the Defra AURN network during 2012 was 72 ppb at Aston Hill on 27th May. Using ‘best estimate’ PTM model input data and the CB-05 chemical mechanism, the peak mid-afternoon predicted ozone level was 58.8 ppb, indicating a level of model performance that was less than satisfactory (fractional bias -0.19). Monte Carlo uncertainty analysis was employed to investigate the origins of the poor model performance on 27th May.

The PTM model was set up for mid-afternoon conditions for 27th May using input parameters selected by Monte Carlo sampling. Table 4.18 presents the uncertainty ranges that were sampled by the Monte Carlo analysis for each of the 342 PTM model input parameters required by the PTM model version which utilises the CB-05 chemical mechanism. A total of 10,000 PTM model runs were then completed, of which 532 runs were considered acceptable, based on an acceptance criterion of the fractional bias lying in the range -0.05 to +0.05 about the observed 8-hour maximum ozone mixing ratio of 72 ppb. Table 4.19 shows the distribution of acceptable PTM runs for each of the 30 equi-probable back-track air mass trajectories generated by the NAME atmospheric dispersion model and randomly sampled by the Monte Carlo analysis. It appears that five trajectories out of the 30 (numbered 27, 9, 5, 10 and 18) had between them 254 acceptable results, that is about 48% of the total. These trajectory cases were then studied in some further detail.

The Monte Carlo uncertainty analysis was repeated by completing a further 10,000 PTM runs. The input parameters were selected as above, except that the random sampling of the 30 equi-probable trajectories was replaced by selecting trajectory number 27, the case that gave the greatest number of acceptable results. With the trajectory case fixed, 1980 out of the 10,000 runs were found to generate acceptable results with fractional biases in the range from -0.05 to +0.05. Trajectory number 27 was initialised over St Petersburg then travelled in a south-westerly direction over the Baltic States, Poland and Germany, before turning westerly over Belgium then north-westerly to reach Aston Hill after 4 days of travel.

Multiple regression was then applied across the entire model output from all 10,000 PTM model runs. The independent parameters for the multiple regression analysis were the 342 scaling parameters selected by the Monte Carlo sampling for each of the 10,000 model runs and the dependent variables were the 10,000 predicted mid-afternoon ozone mixing ratios for 27th May. In this way, the parameters that contributed most to bridging the gap between the ‘best estimate’ model predicted mixing ratio and the observed peak mixing ratio could be identified. Table 4.20 presents the multiple regression correlation coefficients (R) for a selected number of the 342 scaling parameters for trajectory number 27 on 27th May. Only the input parameters with the largest positive or negative regression correlation coefficients are shown.

Multiple regression analyses were then repeated for the output from four further sets of 10,000 PTM model runs using trajectory numbers 9, 5, 10 and 18 in exactly the same manner as that described for trajectory number 27 above. The results from all five multiple regression analyses are collected together in Table 4.20.

The most important chemical kinetic parameters that influence the model predicted peak ozone mixing ratio are the chemical reaction coefficients that form the photostationary state involving NO, NO_2 and O_3, the reactions that control PAN and its homologues involving C_2O_3 and C_XO_3 and the fast photochemical reactions that control the OH and HO_2 radicals involving NO, NO_2, CO, CH_4 and O_3. The multiple regression coefficients for these chemical kinetic input parameters are largely independent of the chosen trajectory in both sign and magnitude.

The most important non-chemical kinetic input parameters involved trajectory position bias, emissions of VOCs, NO_x and isoprene, ozone deposition velocity, boundary layer depth and air temperature. Again, these multiple regression coefficients were largely independent of chosen trajectory in both sign and magnitude.

Table 4.18. Representation of the uncertainties in the PTM model input parameters in a Monte Carlo study of parametric uncertainties.

Input parameter	Representation	Range
CO emissions	multiplicative scaling	x 0.5 – 2.0
CH_4 emissions	multiplicative scaling	x 0.5 – 2.0
C_5H_8 emissions	multiplicative scaling	x 0.25 – 4.0
NH_3 emissions	multiplicative scaling	x 0.5 – 2.0
NO_x emissions	multiplicative scaling	x 0.5 – 2.0
SO_2 emissions	multiplicative scaling	x 0.5 – 2.0
VOC emissions	multiplicative scaling	x 0.5 – 2.0
VOC speciation	multiplicative scaling	x 0.5 – 2.0
Air parcel longitude	additive	± 0 – 0.45 ^{o}
Air parcel latitude	additive	± 0 – 0.28 ^{o}
Boundary conditions	multiplicative scaling	
Boundary layer depth	multiplicative scaling	x 0.5 – 2.0
Choice of mechanism	random	
Choice of trajectory	random	
Dry deposition velocity	multiplicative scaling	x 0 – 1.0
Photolysis rate coefficient	multiplicative scaling	x 0.7 – 1.3
Rate coefficient	multiplicative scaling	x 0.7 – 1.3
Relative humidity	multiplicative scaling	x 0.5 – 2.0
Temperature	additive	± 0 – 3 ^{o}C

Notes:

- All assignments in this table are subjective.
- A scaling factor of unity represents ‘best estimate’ model input.
- Uncertainties in longitudes and latitudes have ‘Gaussian’ shapes, remainder have ‘top hat’.

Table 4.19. The number of acceptable PTM runs found by random sampling from 30 equi-probable NAME model back-track air mass trajectories on 27th May in the Monte Carlo uncertainty analysis.

Trajectory number	Number acceptable	Trajectory number	Number acceptable	Trajectory number	Number acceptable
1	20	11	41	21	5
2	0	12	9	22	0
3	0	13	0	23	2
4	14	14	8	24	0
5	48	15	1	25	26
6	15	16	18	26	0
7	0	17	36	27	61
8	1	18	42	28	14
9	57	19	25	29	10
10	46	20	22	30	11

4.2.4 Sensitivity of ozone episodes at Mace Head, Ireland, calculated by the PTM to dry deposition velocity

To investigate possible reasons for the inability of the PTM to predict some of the ozone episodes over the 2012 season, simulations were carried out for Mace Head, Ireland, for different assumptions about ozone deposition velocity.

This station is the most remote of all the EMEP ozone monitoring stations and provides a stringent test of model performance over the long range transport scale. Observations revealed that 1-hourly mean ozone levels exceeded 50 ppb on 15 days during 2012 and exceeded 60 ppb on 3 days: 25th May with 61.2 ppb, 29th March with 63.0 ppb and 26th May with 65.5 ppb.

PTM model performance of the 15 >50 ppb episode days is presented in Figure 4.5. This plot covers the 15 days in rank order of their observed maximum hourly ozone levels. Also shown are the PTM results for the base case model with the deposition velocity for ozone set at 0.5 cm s^{-1} (vg=0.5 cm s^{-1}, see Figure 4.5) and for four sensitivity cases with decreasing step-wise values for the deposition velocity. On the highest ozone episode day, 26th May, the base case model dramatically underestimated the observed ozone maximum hourly level. This underestimation decreased steadily through the sensitivity cases. The model bracketed the observed ozone maximum with the lowest vg values. On the second highest ozone episode day, 29th March, the base case model underestimated the observed ozone maximum of 63 ppb and overestimated it in all four sensitivity cases. The behaviour on the 3rd highest ozone episode day, 25th May, is exactly the same as for the highest ozone episode day.

Decreasing the ozone deposition velocity improved model performance on 7 further days out of the 15 >50ppb ozone episode days. However, there were 5 days when decreasing the ozone deposition velocity failed to change the PTM model performance and gross underestimation was found for all the PTM sensitivity cases. These episodes were therefore identified as ‘background’ episodes, that is to say, the elevated ozone levels were advected directly to Mace Head across the North Atlantic Ocean and had had no significant European continental influence.

These sensitivity cases suggest that the ozone deposition velocity in the base case PTM model run is set too high for the ozone episode conditions at Mace Head during 2012. It may be that significant drying out of the vegetated surfaces had occurred such that the PTM model was overestimating the strength of the ozone dry deposition sink along the several hundred kilometres fetch from the ozone precursor sources regions out to Mace Head, Ireland.

Figure 4.5: Maximum 1-hourly observed ozone levels on 15 >50 ppb ozone episode days at Mace Head, Ireland, in 2012 together with the base case PTM model results and those for four sensitivity cases involving different ozone dry deposition rates (vg).

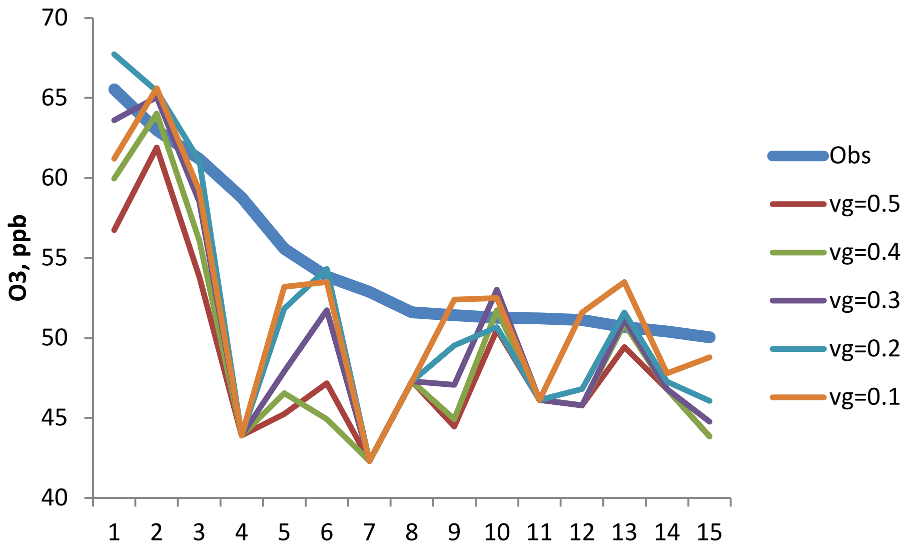


Table 4.20. Multiple regression coefficients (R) for each PTM model input parameter in five separate Monte Carlo uncertainty analyses.

Parameter	Trajectory number 27	Trajectory number 9	Trajectory number 5	Trajectory number 10	Trajectory number 18
Chemical kinetic input					
$NO+O_3$	-0.325	-0.347	-.0337	-0.316	-0.395
NO_2+O_3	-0.082	-0.072	-0.107	-0.081	-0.168
O^1D+H_2O					-0.035
$OH+O_3$			-0.034	-0.036	
OH+CO			+0.094	+0.090	
HO_2+O_3	-0.053		-0.055	-0.049	
$OH+NO_2$	-0.278	-0.198	-0.277	-0.262	-0.241
HO_2+NO	+0.157	+0.083	+0.210	+0.179	+0.200
O_3+hv		-0.030			-0.051
NO_2+hv	+0.388	+0.411	+0.389	+0.369	+0.477
$OH+CH_4$	+0.122	+0.058	+0.162	+0.139	+0.127
FORM+hv	+0.057	+0.053	+0.037	+0.043	+0.035
ALD_2+hv		+0.035			
C_2O_3+NO	+0.086	+0.183	+0.068	+0.072	+0.109
$C_2O_3+NO_2$	-0.087	-0.171	-0.060	-0.065	-0.105
$PAN=C_2O_3+NO_2$	+0.058	+0.102		+0.036	+0.078
ALD_X+hv		+0.031			
C_XO_3+NO	+0.051	+0.082	+0.045	+0.041	+0.089
$C_XO_3+NO_2$	-0.053	-0.075		-0.032	-0.057
$PANx=C_XO_3+NO_2$	+0.047	+0.071	+0.034	+0.045	+0.085
PAR+OH	+0.047	+0.087			
N_2O_5=NA+NA		-0.037			-0.033
Non-chemical kinetic input					
Air parcel longitude	-0.066		+0.072	+0.186	+0.081
Air parcel latitude		-0.309	+0.082	+0.149	+0.168
VOC emissions	+0.127	+0.058		+0.071	+0.040
NO_x emissions		+0.265	+0.153	+0.145	+0.300
C_5H_8 emissions	+0.258		+0.108	+0.074	+0.040
O_3 deposition velocity	-0.578	-0.361	-0.612	-0.557	-0.314
Boundary layer depth	-0.107	-0.183		+0.128	+0.093
Air temperature	+0.176	+0.225	+0.109	+0.106	+0.180

5 Policy Applications of the OSRM and PTM

Objective 2 involves the use of the OSRM and PTM to model ozone concentrations in the UK for different emission scenarios or meteorological conditions specified by Defra. During 2013/14 the OSRM has been used to model twelve future year emission scenarios, all involving national scale annual runs producing maps of ozone concentrations and population- and area-weighted means of health- and ecosystem-based metrics. The PTM has been used to model episodic peak ozone at the Harwell site in 2025 and 2030 for a central case scenario.

5.1 Modelling of scenarios based on the UEP45 emissions projections for the UK

5.1.1 OSRM modelling

The OSRM was used to run three different UK NAEI emissions scenarios for the year 2025. These were a central UK case, a high UK case and an optimistic UK case. These are emission scenarios derived from DECC's UEP45 energy projections. The same three scenarios were run for the year 2030. All of the scenarios were run twice, once with 2006 meteorology and once with 2007 meteorology, giving a total of 12 simulations.

These runs were carried out using the emissions data described below:

- 2011 NAEI UEP45 projections using 2010 NAEI base maps for the UK
- PRIMES-2012 CLE projections from the TSAP (2013) report with EMEP2010 base maps for the rest of Europe.

The runs carried out are shown in Table 5.1 below. Details of the 2011 NAEI UEP45 projections for the different scenarios are given in Passant et al (2013). In general, the high case refers to higher emissions than the central case, while the optimistic case refers to a lower emission scenario than the central case.

Table 5.1. Details of scenarios run and meteorology used

Met Year	UK Inventory	Non-UK UNECE inventory	Projected Inventory Year
2006	NAEI11 UEP45 projections central case (with NAEI10 maps)	PRIMES-2012 CLE[1] projections (with EMEP2010 maps).[2]	2025
2006	NAEI11 UEP45 projections high case (with NAEI10 maps)	PRIMES-2012 CLE[1] projections (with EMEP2010 maps).[2]	2025
2006	NAEI11 UEP45 projections optimistic case (with NAE10 maps)	PRIMES-2012 CLE[1] projections (with EMEP2010 maps).[2]	2025
2006	NAEI11 UEP45 projections central case (with NAEI10 maps)	PRIMES-2012 CLE[1] projections (with EMEP2010 maps).[2]	2030
2006	NAEI11 UEP45 projections high case (with NAEI10 maps)	PRIMES-2012 CLE[1] projections (with EMEP2010 maps).[2]	2030
2006	NAEI11 UEP45 projections optimistic case (with NAEI10 maps)	PRIMES-2012 CLE[1] projections (with EMEP2010 maps).[2]	2030

2007	NAEI11 UEP45 projections central case (with NAEI10 maps)	PRIMES-2012 CLE[1] projections (with EMEP2010 maps).[2]	2025
2007	NAEI11 UEP45 projections high case (with NAEI10 maps)	PRIMES-2012 CLE[1] projections (with EMEP2010 maps).[2]	2025
2007	NAEI11 UEP45 projections optimistic case (with NAEI10 maps)	PRIMES-2012 CLE[1] projections (with EMEP2010 maps).[2]	2025
2007	NAEI11 UEP45 projections central case (with NAEI10 maps)	PRIMES-2012 CLE[1] projections (with EMEP2010 maps).[2]	2030
2007	NAEI11 UEP45 projections high case (with NAEI10 maps)	PRIMES-2012 CLE[1] projections (with EMEP2010 maps).[2]	2030
2007	NAEI11 UEP45 projections optimistic case (with NAEI10 maps)	PRIMES-2012 CLE[1] projections (with EMEP2010 maps).[2]	2030

1 – From the TSAP (2013) report
2 – EMEP2010 projections were used for countries and pollutants that were not available in this dataset.

The tables below show the scenario results for different ozone metrics. Table 5.2 shows the area-weighted annual mean ozone for all scenarios, Table 5.3 shows the area-weighted AOT40 (Crops) for all scenarios, Table 5.4 shows population-weighted annual mean ozone for all scenarios, Table 5.5 shows the population-weighted number of days when the daily maximum running 8 hourly ozone concentration exceeds 120μgm^{-3} for all scenarios, Table 5.6 shows the population-weighted SOMO0 metric, Table 5.7 shows the population-weighted SOMO10 and Table 5.8 shows the population-weighted SOMO35.

Table 5.2. OSRM Scenario Results for Area-Weighted Annual Mean Ozone (μgm^{-3})

Scenario	Scotland	Wales	Northern Ireland	Inner London	Outer London	Rest of England	All UK
2025 UEP45 central case UK (Met 2006)	68.3	70.5	68.2	62.6	61.7	65.5	67.0
2025 UEP45 high case UK (Met 2006)	68.2	70.2	68.1	61.4	60.6	65.0	66.7
2025 UEP45 optimistic case UK (Met 2006)	68.5	70.9	68.5	65.2	63.9	66.5	67.6
2030 UEP45 central case UK (Met 2006)	69.2	71.5	69.0	64.0	63.0	66.7	68.0
2030 UEP45 high case UK (Met 2006)	69.1	71.1	68.8	62.4	61.6	66.0	67.6
2030 UEP45 optimistic case UK (Met 2006)	69.5	72.0	69.4	67.2	65.8	67.8	68.8
2025 UEP45 central case UK (Met 2007)	71.4	71.4	70.9	62.3	61.7	66.1	68.5
2025 UEP45 high case UK (Met 2007)	71.3	71.1	70.8	61.0	60.4	65.5	68.2
2025 UEP45 optimistic case UK (Met 2007)	71.6	72.0	71.2	65.2	64.1	67.0	69.2
2030 UEP45 central case UK (Met 2007)	72.3	72.5	71.8	63.8	63.0	67.2	69.6
2030 UEP45 high case UK (Met 2007)	72.2	72.1	71.6	62.1	61.5	66.6	69.2

2030 UEP45 optimistic case UK (Met 2007)	72.5	73.2	72.1	67.3	66.0	68.4	70.4

Table 5.3. OSRM Scenario Results for Area-Weighted AOT40 - Crops (µgm^{-3}.hours)

Scenario	Scotland	Wales	Northern Ireland	Inner London	Outer London	Rest of England	All UK
2025 UEP45 central case UK (Met 2006)	7760	8330	7187	11278	10727	10935	9439
2025 UEP45 high case UK (Met 2006)	7838	8322	7196	10537	10108	10790	9386
2025 UEP45 optimistic case UK (Met 2006)	7600	8314	7188	12948	12046	11179	9520
2030 UEP45 central case UK (Met 2006)	8731	9333	8037	12824	12203	12242	10583
2030 UEP45 high case UK (Met 2006)	8839	9330	8053	11806	11364	12054	10517
2030 UEP45 optimistic case UK (Met 2006)	8406	9212	7956	15049	13906	12406	10556
2025 UEP45 central case UK (Met 2007)	8700	8102	6837	8817	8559	8982	8687
2025 UEP45 high case UK (Met 2007)	8856	7981	6925	8224	8123	8910	8693
2025 UEP45 optimistic case UK (Met 2007)	8442	8307	6626	10125	9464	9070	8658
2030 UEP45 central case UK (Met 2007)	9666	9261	7786	10243	9882	10188	9795
2030 UEP45 high case UK (Met 2007)	9860	9099	7915	9433	9289	10094	9801
2030 UEP45 optimistic case UK (Met 2007)	9231	9386	7347	11891	10979	10155	9626

Table 5.4. OSRM Scenario Results for Population-Weighted Annual Mean Ozone (µgm^{-3})

Scenario	Scotland	Wales	Northern Ireland	Inner London	Outer London	Rest of England	All UK
2025 UEP45 central case UK (Met 2006)	63.2	68.7	66.9	62.4	62.1	62.8	63.2
2025 UEP45 high case UK (Met 2006)	62.7	68.3	66.6	61.1	61.0	62.0	62.4
2025 UEP45 optimistic case UK (Met 2006)	64.2	69.6	67.4	65.0	64.4	64.3	64.7
2030 UEP45 central case UK (Met 2006)	64.2	69.8	67.7	63.7	63.4	64.0	64.4
2030 UEP45 high case UK (Met 2006)	63.6	69.3	67.3	62.1	62.0	63.0	63.4

2030 UEP45 optimistic case UK (Met 2006)	65.4	70.8	68.4	67.0	66.3	65.9	66.2
2025 UEP45 central case UK (Met 2007)	65.8	69.3	69.2	62.1	62.1	63.2	63.8
2025 UEP45 high case UK (Met 2007)	65.3	68.8	68.8	60.7	60.9	62.4	62.9
2025 UEP45 optimistic case UK (Met 2007)	66.8	70.3	69.7	65.0	64.6	64.8	65.3
2030 UEP45 central case UK (Met 2007)	66.8	70.5	70.1	63.5	63.5	64.4	65.0
2030 UEP45 high case UK (Met 2007)	66.1	69.8	69.7	61.8	61.9	63.4	63.9
2030 UEP45 optimistic case UK (Met 2007)	68.0	71.7	70.7	67.2	66.6	66.3	66.9

Table 5.5. OSRM Scenario Results for Population-Weighted Number of Days when the Daily Maximum Running 8 Hourly Ozone Concentration exceeds 120µgm^{-3}

Scenario	Scotland	Wales	Northern Ireland	Inner London	Outer London	Rest of England	All UK
2025 UEP45 central case UK (Met 2006)	6.6	10.3	7.8	7.7	8.1	11.6	10.5
2025 UEP45 high case UK (Met 2006)	6.6	10.1	7.7	7.5	7.8	11.2	10.2
2025 UEP45 optimistic case UK (Met 2006)	6.7	11.0	8.1	9.9	10.4	12.3	11.3
2030 UEP45 central case UK (Met 2006)	8.4	12.6	9.3	9.6	9.8	13.2	12.2
2030 UEP45 high case UK (Met 2006)	8.2	12.3	9.5	7.9	9.1	12.6	11.7
2030 UEP45 optimistic case UK (Met 2006)	8.3	13.0	8.9	12.4	12.4	14.1	13.2
2025 UEP45 central case UK (Met 2007)	7.8	5.3	3.4	9.2	10.2	7.3	7.5
2025 UEP45 high case UK (Met 2007)	8.0	4.8	3.1	7.8	9.0	7.1	7.1
2025 UEP45 optimistic case UK (Met 2007)	7.9	5.9	3.7	12.3	12.0	7.9	8.2
2030 UEP45 central case UK (Met 2007)	9.6	7.6	4.3	10.9	12.1	9.4	9.4
2030 UEP45 high case UK (Met 2007)	9.6	7.0	4.2	9.7	11.3	8.9	9.0
2030 UEP45 optimistic case UK (Met 2007)	9.2	8.2	4.4	15.9	14.2	10.0	10.2

Table 5.6. OSRM Scenario Results for Population-Weighted SOMO0 (μgm^{-3}.days)

Scenario	Scotland	Wales	Northern Ireland	Inner London	Outer London	Rest of England	All UK
2025 UEP45 central case UK (Met 2006)	27391	29382	28238	27559	27435	27640	27701
2025 UEP45 high case UK (Met 2006)	27247	29244	28159	27148	27066	27402	27463
2025 UEP45 optimistic case UK (Met 2006)	27660	29624	28386	28420	28172	28081	28151
2030 UEP45 central case UK (Met 2006)	27773	29807	28574	28064	27927	28090	28147
2030 UEP45 high case UK (Met 2006)	27600	29639	28480	27549	27469	27800	27855
2030 UEP45 optimistic case UK (Met 2006)	28089	30093	28739	29146	28848	28628	28697
2025 UEP45 central case UK (Met 2007)	27997	29342	28863	27309	27251	27435	27598
2025 UEP45 high case UK (Met 2007)	27872	29191	28782	26870	26863	27196	27357
2025 UEP45 optimistic case UK (Met 2007)	28238	29617	29007	28232	28022	27880	28055
2030 UEP45 central case UK (Met 2007)	28379	29811	29231	27868	27791	27912	28072
2030 UEP45 high case UK (Met 2007)	28226	29626	29136	27320	27312	27619	27776
2030 UEP45 optimistic case UK (Met 2007)	28666	30139	29381	29017	28747	28454	28629

Table 5.7. OSRM Scenario Results for Population-Weighted SOMO10 (μgm^{-3}.days)

Scenario	Scotland	Wales	Northern Ireland	Inner London	Outer London	Rest of England	All UK
2025 UEP45 central case UK (Met 2006)	20164	22210	20995	20447	20321	20497	20551
2025 UEP45 high case UK (Met 2006)	20029	22083	20918	20055	19971	20275	20328
2025 UEP45 optimistic case UK (Met 2006)	20417	22432	21137	21271	21021	20909	20973
2030 UEP45 central case UK (Met 2006)	20540	22624	21325	20933	20797	20934	20983
2030 UEP45 high case UK (Met 2006)	20377	22469	21235	20441	20361	20663	20710
2030 UEP45 optimistic case UK (Met 2006)	20835	22882	21483	21973	21673	21435	21498

2025 UEP45 central case UK (Met 2007)	20740	22091	21596	20125	20074	20228	20386
2025 UEP45 high case UK (Met 2007)	20618	21943	21516	19699	19697	19997	20153
2025 UEP45 optimistic case UK (Met 2007)	20976	22359	21739	21030	20825	20658	20829
2030 UEP45 central case UK (Met 2007)	21118	22552	21962	20673	20605	20696	20852
2030 UEP45 high case UK (Met 2007)	20968	22372	21867	20141	20137	20413	20565
2030 UEP45 optimistic case UK (Met 2007)	21399	22871	22110	21799	21533	21219	21391

Table 5.8. OSRM Scenario Results for Population-Weighted SOMO35 (μgm^{-3}.days)

Scenario	Scotland	Wales	Northern Ireland	Inner London	Outer London	Rest of England	All UK
2025 UEP45 central case UK (Met 2006)	4154	5688	4485	4836	4754	4728	4726
2025 UEP45 high case UK (Met 2006)	4098	5619	4450	4587	4538	4613	4606
2025 UEP45 optimistic case UK (Met 2006)	4261	5812	4551	5386	5210	4950	4961
2030 UEP45 central case UK (Met 2006)	4433	6036	4753	5209	5118	5058	5055
2030 UEP45 high case UK (Met 2006)	4363	5948	4712	4885	4839	4913	4904
2030 UEP45 optimistic case UK (Met 2006)	4550	6177	4821	5916	5698	5329	5344
2025 UEP45 central case UK (Met 2007)	4256	5300	4624	4432	4390	4236	4322
2025 UEP45 high case UK (Met 2007)	4203	5219	4585	4203	4196	4130	4211
2025 UEP45 optimistic case UK (Met 2007)	4363	5449	4687	4943	4796	4443	4542
2030 UEP45 central case UK (Met 2007)	4537	5662	4911	4829	4768	4572	4659
2030 UEP45 high case UK (Met 2007)	4470	5560	4867	4530	4519	4436	4517
2030 UEP45 optimistic case UK (Met 2007)	4662	5841	4967	5470	5277	4825	4929

The following figures show UK maps of the days greater than 120μgm^{-3} ozone metric for the central scenario. Figure 5.1 is for 2025 with 2006 meteorology, Figure 5.2 is for 2030 with 2006 meteorology and Figure 5.3 is for 2025 with 2007 meteorology. Maps are available for all combinations of scenarios, ozone metrics and meteorology years, but for a given meteorology year, the maps appear very similar for all scenarios.

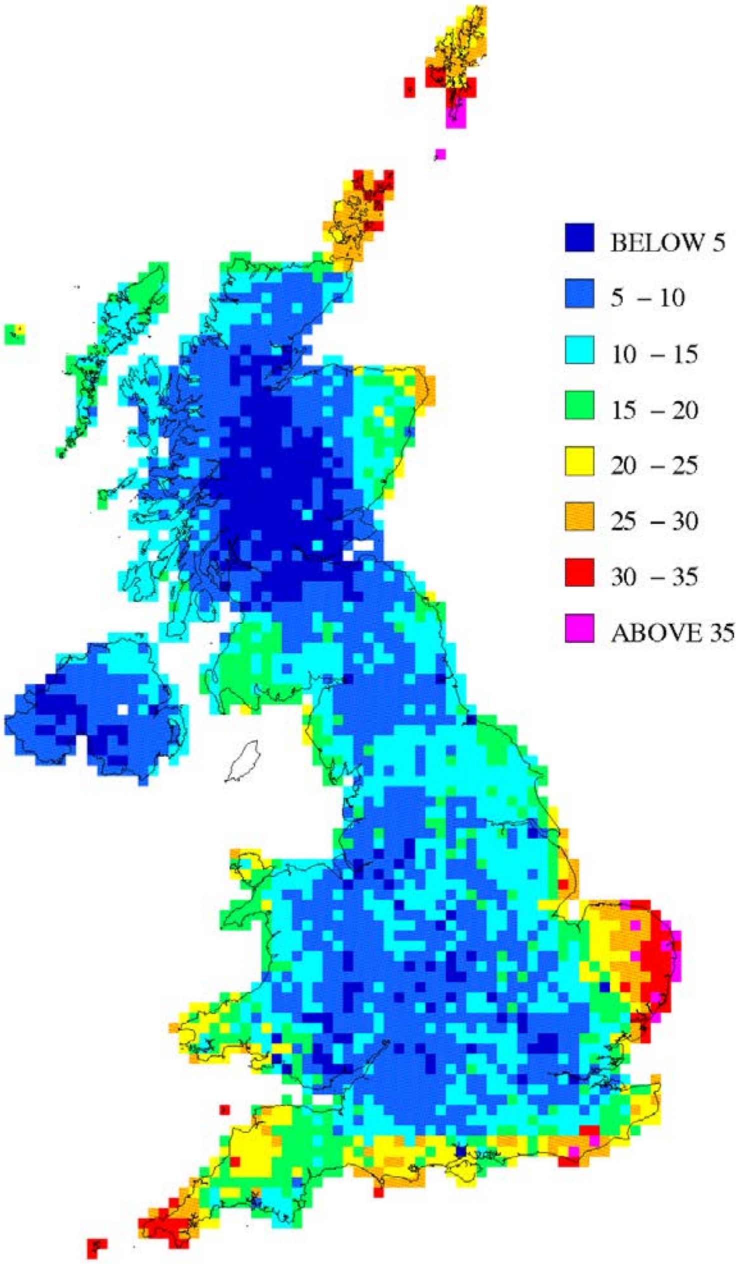


Figure 5.1. Map of Days Greater than 120µgm^{-3} for 2025 Central Case Scenario with 2006 Meteorology

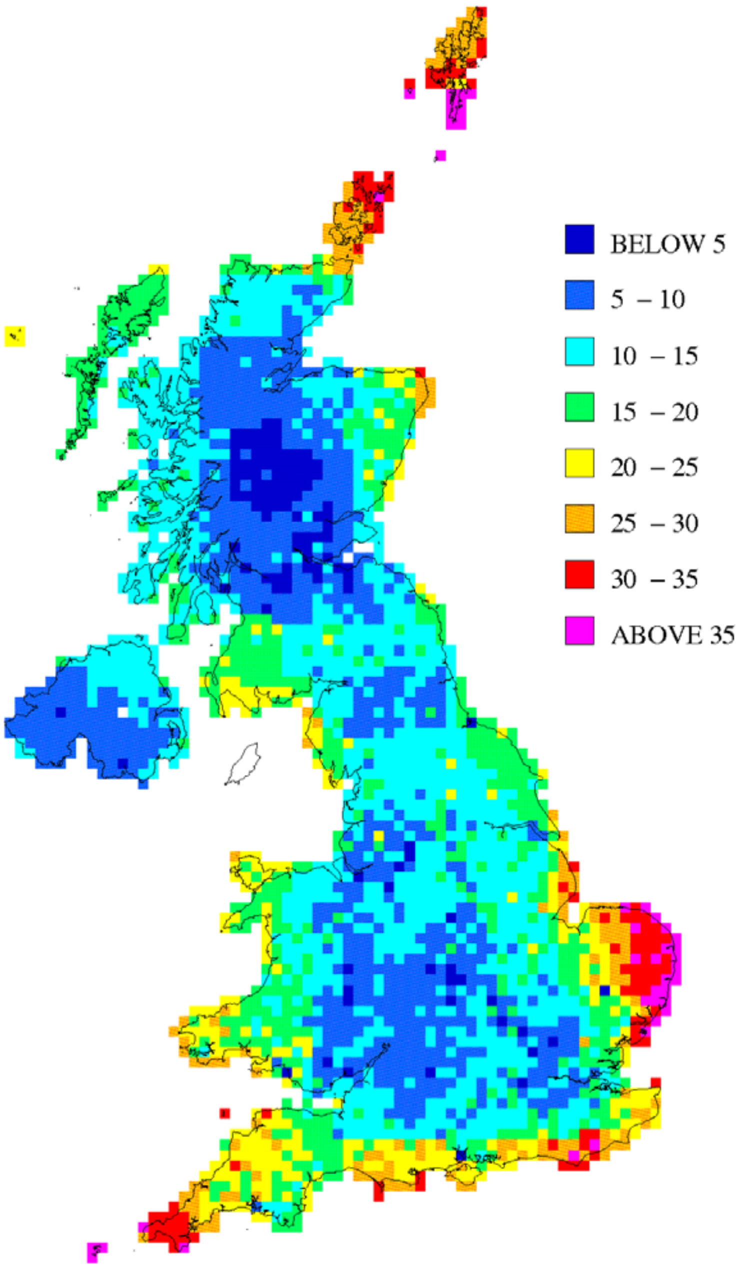


Figure 5.2. Map of Days Greater than 120µgm^{-3} for 2030 Central Case Scenario with 2006 Meteorology

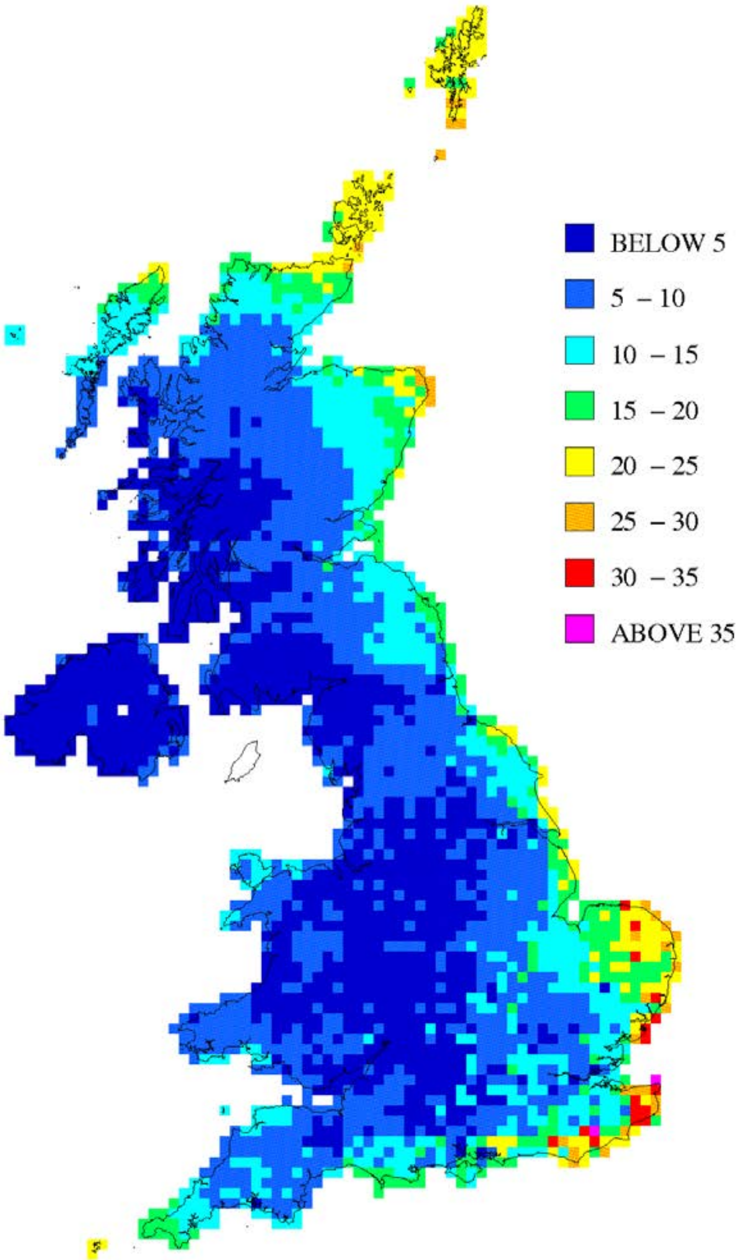


Figure 5.3. Map of Days Greater than 120µgm^{-3} for 2025 Central Case Scenario with 2007 Meteorology

The results for the year 2025 (using both 2007 meteorology and 2006 meteorology) indicate that the optimistic low emission scenario generally leads to higher ozone than the central scenario and the high scenario generally leads to lower ozone than the central scenario. This is found for all metrics and regions analysed, except the AOT40 and days greater than 120µgm^{-3} metrics for a few regions.

The results for the 2030 central case indicate higher ozone than the 2025 central case.

The differences between the results for the 2030 scenarios are generally consistent with the differences seen for the 2025 scenarios; the optimistic scenario generally leads to higher ozone than the central scenario and the high scenario generally leads to lower ozone than the central scenario.

These conclusions were consistent with the results we have seen for previous OSRM scenarios. Specifically, that reducing emissions tends to lead to an increase in the ozone metrics, especially the population-weighted means. We believe this is due in part to a reduction in the NOx titration effect.

5.1.2 PTM modelling

The PTM was used to model the impacts on ground-level ozone of the UEP45 Central case emission projections for 2025 and 2030 together with the PRIMES-2012 European emission projections for the rest of Europe. The study focussed on changes in ***episodic peak*** ozone at the rural Harwell site in Oxfordshire in southern England.

The PTM was set up using the CB-05 chemical mechanism for a 122-day base case covering the period from the 1st April to 31st July 2008 for the rural Harwell site in Oxfordshire in southern England. Ozone observations from the AURN Network demonstrated the occurrence of photochemical episodes at this site producing level in excess of 50 ppb on 24th – 26th April, 5th – 12th May, 21st – 24th May, 8th – 9th June, 1st July and 24th – 28th July 2008. During the entire year, the daily maximum 1-hour and 8-hour running mean ozone levels were related through the equation:

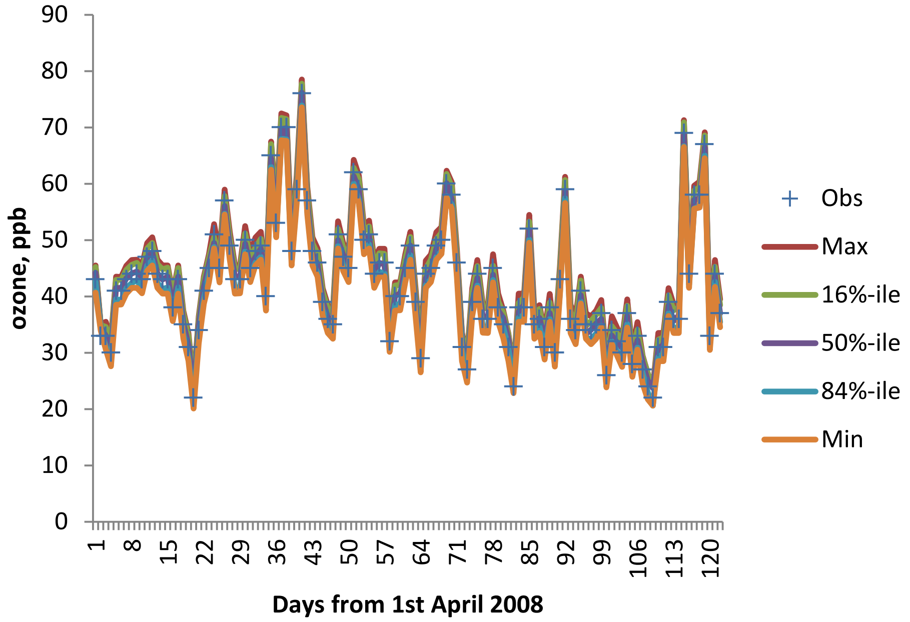
Maximum 8-hour running mean = maximum 1-hour mean x 0.9496 - 1.5785 (R^2 = 0.83).

On this basis, it was possible to move accurately between the 1-hour and 8-hour averaging times. So, for example, the World Health Organisation air quality guideline of 50 ppb for a maximum 8-hour running mean ozone level was found to be equivalent to a maximum 1-hour mean level of 54.3 ppb.

An uncertainty framework has been developed for the PTM based on Monte Carlo sampling of predefined model input uncertainty ranges for all model input parameters. A large number, 12200, of PTM runs were performed for the base case, mid-afternoon conditions for the 122-day period from 1st April to 31st July 2008 for Harwell, Oxfordshire. The PTM results for the 2008 base case are compared with AURN network observations in Figure 5.4, showing how the PTM is able to account accurately for the observed day-by-day variability in the observed maximum hourly ozone levels. PTM performance was considered entirely satisfactory using the model evaluation benchmarks discussed by Derwent et al., (2010c).

The 50-percentile PTM simulations for 2008 indicated the presence of a number of photochemical episodes in agreement with observations, culminating in a predicted maximum 1-hour mean level of 76.2 ppb on the 11th May. There were altogether 16 days on which the PTM predicted exceedances of the World Health Organisation 50 ppb maximum 8-hour running mean air quality guideline.

Figure 5.4. Comparison of the daily maximum ozone levels observed at Harwell, Oxfordshire during 1st April to 31st July 2008 and calculated with the PTM, showing the maximum, 84%-ile, 50%-ile, 16%-ile and minimum predictions from the Monte Carlo uncertainty analysis.



5.1.2.1 PTM simulations for 2025 and 2030

Those parameter sets that performed well against the AURN observations in the 2008 base case runs were deemed ‘acceptable’ and were used again for the 2025 and 2030 projections cases. The results from the base case run were paired up with those from the projections cases and the impacts of the emission projections were found by taking differences in the mid-afternoon maximum ozone levels for each day from the 2008 base case. The 2025 and 2030 emission projections cases took NO_x, SO_2, VOC, CO and NH_3 emissions for each year and each EU member state from the PRIMES-2012 European emission projections. The corresponding emissions for the United Kingdom were taken from the UEP45 Central Case emission projections.

The 50-percentile maximum 1-hour mean ozone level was predicted to decrease from 76.2 ppb to 63.2 ppb and 61.3 ppb by 2025 and 2030, respectively. These reductions amount to 17% and 20%, respectively. Although substantial, they were not enough to bring the maximum 1-hour mean level down to the levels approaching those of the World Health Organisation air quality guideline that is close to 54.3 ppb, equivalent to a 50 ppb maximum 8-hour running mean. The distributions of the acceptable ozone levels predicted for the 11th May for 2008, 2025 and 2030 are plotted as box-and-whisker plots in Figure 5.5. This figure shows that although the episodic peak levels decreased between 2008 and 2025 and 2030, the extremes of the distributions were not reduced enough to protect against the exceedance of the World Health Organisation air quality guideline.

Although there were 16 days in which the 50-percentile PTM predictions indicated that the World Health Organisation 8-hour running mean air quality guideline was exceeded in 2008, this number decreased substantially, by over one half, to 7 days in 2025 and 2030.

SOMO35 decreased from 1036 ppb days in 2008 to 799 ppb days in 2025 and 768 ppb days in 2030. These reductions amounted to 23% and 26%, respectively.

In general terms, the PTM predictions for 2025 and 2030 were substantially lower than those for 2008 against a range of ozone policy metrics. However, there was correspondingly little difference between the predictions for the 2025 and 2030 emission projection cases.

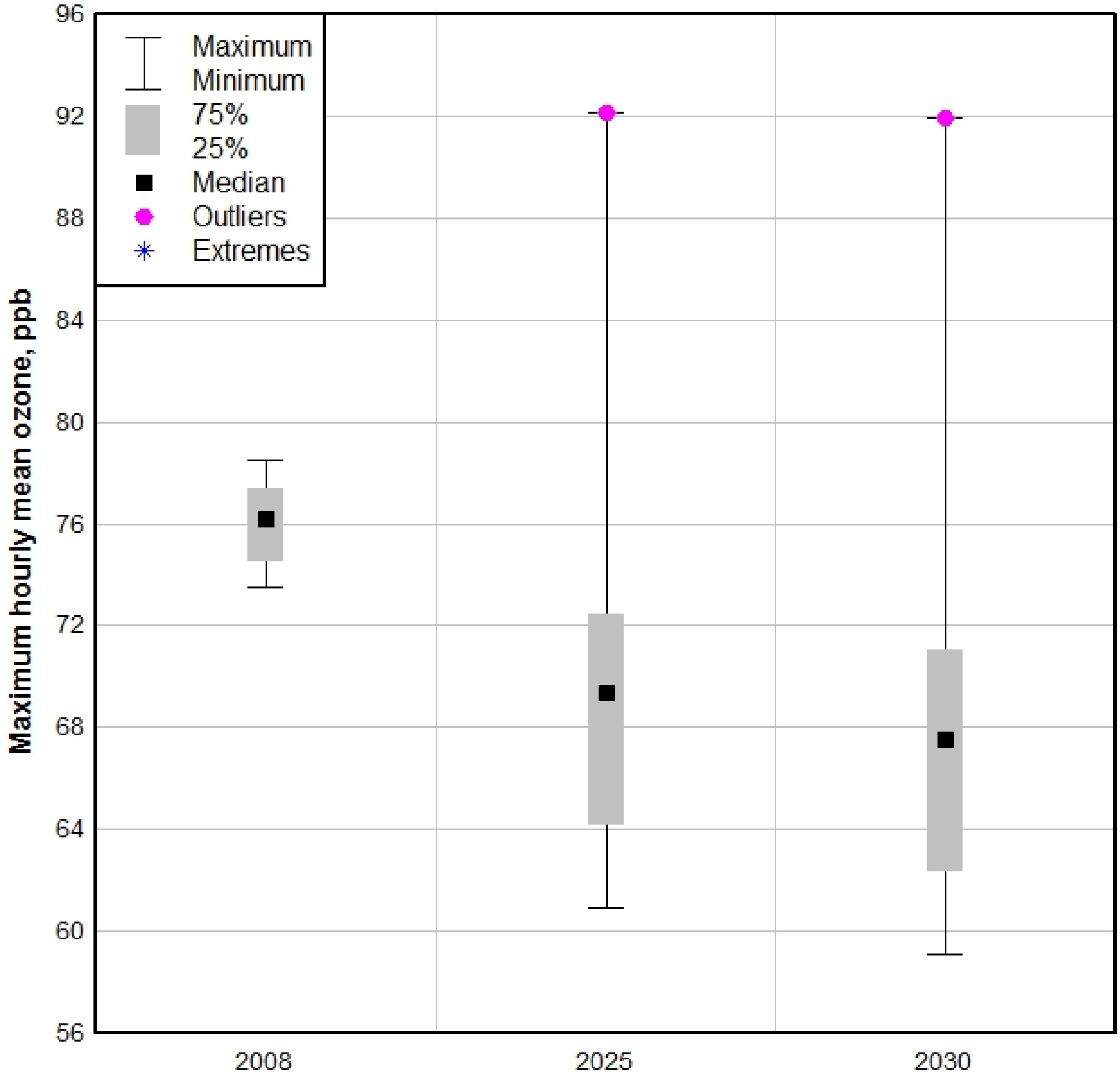


Figure 5.5. Box-and-whisker plots for the maximum hourly mean ozone levels on the 11th May 2008 with 2008, 2025 and 2030 emissions. The 50%-iles are shown as black squares, the interquartile ranges as grey shaded rectangles and the maxima and minima as short lines.

5.2 OSRM modelling of scenarios based on the UEP45 emissions projections and estimates of what might be in the European Commission proposal for a revised/replacement NECD

For this analysis, four scenarios for the year 2025 were run using the OSRM. These were a 75% of MTFR (maximum technically feasible reduction) scenario, a 50% of MTFR scenario, a 25% of MTFR scenario and a 75% of MTFR scenario with a reduction in European methane emissions reflected in the OSRM (through reductions in methane boundary conditions, as independently calculated by the Met Office). Two of these four scenarios (75% MTFR and 75% MTFR with a reduction in European methane emissions) were also run for the year 2030. All of the scenarios were run twice, once with 2006 meteorology and once with 2007 meteorology, leading to a total of twelve model runs.

The scenarios presented here were developed by Defra from their estimates of what might be in the European Commission proposal for a revised/replacement NECD (before the proposed revised NECD was published). These estimated emissions reductions were applied to NO_x, VOC and SO_2 emissions in all scenarios and additionally to CH_4 as changes in boundary condition concentrations in the specific scenarios including this.

The basecase used for these scenarios is the central case scenario described in Section 5.1 above. This used the emissions data described below:

- 2011 NAEI UEP45 projections using 2010 NAEI base maps for the UK
- PRIMES-2012 CLE projections from the TSAP (2013) report with EMEP2010 base maps for the rest of Europe.

Details of the scenario runs for which results are presented in this section are shown in Table 5.9 below. In general, the 25% MTFR scenario refers to lower emissions than the base case, the 50% MTFR scenario refers to lower emissions than the 25% MTFR scenario and the 75% MTFR scenario refers to lower emissions than the 50% MTFR scenario.

Table 5.9. Details of scenarios run and meteorology used

Met Year	UK Inventory	Non-UK UNECE inventory	Boundary conditions change	Projected Inventory Year
2006	NAEI11 UEP45 projections optimistic case (with NAE10 maps) with 25% MTFR emissions reduction for NOx, VOC and SO_2.	PRIMES-2012 CLE[1] projections (with EMEP2010 maps)[2] with 25% MTFR emissions reduction for NOx, VOC and SO_2.	None	2025
2006	NAEI11 UEP45 projections optimistic case (with NAE10 maps) with 50% MTFR emissions reduction for NOx, VOC and SO_2.	PRIMES-2012 CLE[1] projections (with EMEP2010 maps)[2] with 50% MTFR emissions reduction for NOx, VOC and SO_2.	None	2025
2006	NAEI11 UEP45 projections central case (with NAE10 maps) with 75% MTFR emissions reduction for NOx, VOC and SO_2.	PRIMES-2012 CLE[1] projections (with EMEP2010 maps)[2] with 75% MTFR emissions reduction for NOx, VOC and SO_2.	None	2025
2006	NAEI11 UEP45 projections high case (with NAE10 maps) with 75% MTFR emissions reduction for NOx, VOC and SO_2.	PRIMES-2012 CLE[1] projections (with EMEP2010 maps)[2] with 75% MTFR emissions reduction for NOx, VOC and SO_2.	Equivalent change in boundary conditions CH_4 concentration for 75% MTFR emissions reduction for CH_4	2025
2006	NAEI11 UEP45 projections high case (with NAE10 maps) with 75% MTFR emissions reduction for NOx, VOC and SO_2.	PRIMES-2012 CLE[1] projections (with EMEP2010 maps)[2] with 75% MTFR emissions reduction for NOx, VOC and SO_2.	None	2030
2006	NAEI11 UEP45 projections high case (with NAE10 maps) with 75% MTFR emissions reduction for NOx, VOC and SO_2.	PRIMES-2012 CLE[1] projections (with EMEP2010 maps)[2] with 75% MTFR emissions reduction for NOx, VOC and SO_2.	Equivalent change in boundary conditions CH_4 concentration for 75% MTFR emissions reduction for CH_4	2030
2007	NAEI11 UEP45 projections optimistic case (with NAE10 maps) with 25% MTFR emissions reduction for NOx, VOC and SO_2.	PRIMES-2012 CLE[1] projections (with EMEP2010 maps)[2] with 25% MTFR emissions reduction for NOx, VOC and SO_2.	None	2025
2007	NAEI11 UEP45 projections central case (with NAE10 maps) with 50% MTFR emissions reduction for NOx, VOC and SO_2.	PRIMES-2012 CLE[1] projections (with EMEP2010 maps)[2] with 50% MTFR emissions reduction for NOx, VOC and SO_2.	None	2025

2007	NAEI11 UEP45 projections central case (with NAE10 maps) with 75% MTFR emissions reduction for NOx, VOC and SO_2.	PRIMES-2012 CLE[1] projections (with EMEP2010 maps)[2] with 75% MTFR emissions reduction for NOx, VOC and SO_2.	None	2025
2007	NAEI11 UEP45 projections high case (with NAE10 maps) with 75% MTFR emissions reduction for NOx, VOC and SO_2.	PRIMES-2012 CLE[1] projections (with EMEP2010 maps)[2] with 75% MTFR emissions reduction for NOx, VOC and SO_2.	Equivalent change in boundary conditions CH_4 concentration for 75% MTFR emissions reduction for CH_4	2025
2007	NAEI11 UEP45 projections high case (with NAE10 maps) with 75% MTFR emissions reduction for NOx, VOC and SO_2.	PRIMES-2012 CLE[1] projections (with EMEP2010 maps)[2] with 75% MTFR emissions reduction for NOx, VOC and SO_2.	None	2030
2007	NAEI11 UEP45 projections high case (with NAE10 maps) with 75% MTFR emissions reduction for NOx, VOC and SO_2.	PRIMES-2012 CLE[1] projections (with EMEP2010 maps)[2] with 75% MTFR emissions reduction for NOx, VOC and SO_2.	Equivalent change in boundary conditions CH_4 concentration for 75% MTFR emissions reduction for CH_4	2030

1 – From the TSAP (2013) report
2 – EMEP2010 projections were used for countries and pollutants that were not available in this dataset.

The tables below show the scenario results for different ozone metrics. In addition the base case results (the UEP45 central case) are also included (in grey text). Table 5.10 shows the area-weighted annual mean ozone for all scenarios, Table 5.11 shows the area-weighted AOT40 (Crops) for all scenarios, Table 5.12 shows population-weighted annual mean ozone for all scenarios, Table 5.13 shows the population-weighted number of days when the daily maximum running 8 hourly ozone concentration exceeds 120µgm^{-3} for all scenarios, Table 5.14 shows the population-weighted SOMO0, Table 5.15 shows the population-weighted SOMO10 and Table 5.16 shows the population-weighted SOMO35.

Table 5.10. OSRM Scenario Results for Area-Weighted Annual Mean Ozone (µgm^{-3})

Scenario	Scotland	Wales	Northern Ireland	Inner London	Outer London	Rest of England	All UK
2025 UEP45 central case UK (Met 2006)	68.3	70.5	68.2	62.6	61.7	65.5	67.0
2025 UEP45 25% MTFR UK & EU (Met 2006)	**68.3**	**70.5**	**68.3**	**63.3**	**62.3**	**65.8**	**67.2**
2025 UEP45 50% MTFR UK & EU (Met 2006)	**68.3**	**70.6**	**68.3**	**64.0**	**62.9**	**66.0**	**67.3**
2025 UEP45 75% MTFR UK & EU (Met 2006)	**68.3**	**70.6**	**68.3**	**64.6**	**63.5**	**66.2**	**67.4**
2025 UEP45 75% MTFR UK & EU with CH4 reduction (Met 2006)	**68.2**	**70.6**	**68.3**	**64.6**	**63.5**	**66.2**	**67.4**
2030 UEP45 central case UK (Met 2006)	69.2	71.5	69.0	64.0	63.0	66.7	68.0
2030 UEP45 75% MTFR UK & EU (Met 2006)	**69.1**	**71.6**	**69.1**	**66.3**	**65.2**	**67.4**	**68.4**
2030 UEP45 75% MTFR UK & EU with CH4 reduction (Met 2006)	**69.1**	**71.6**	**69.1**	**66.3**	**65.2**	**67.4**	**68.4**
2025 UEP45 central case UK (Met 2007)	71.4	71.4	70.9	62.3	61.7	66.1	68.5
2025 UEP45 25% MTFR UK & EU (Met 2007)	**71.4**	**71.5**	**71.0**	**63.1**	**62.3**	**66.3**	**68.7**

2025 UEP45 50% MTFR UK & EU (Met 2007)	**71.3**	**71.6**	**71.0**	**63.8**	**63.0**	**66.6**	**68.8**
2025 UEP45 75% MTFR UK & EU (Met 2007)	**71.3**	**71.7**	**71.0**	**64.5**	**63.6**	**66.8**	**68.9**
2025 UEP45 75% MTFR UK & EU with CH4 reduction (Met 2007)	**71.3**	**71.7**	**70.9**	**64.5**	**63.6**	**66.8**	**68.9**
2030 UEP45 central case UK (Met 2007)	72.3	72.5	71.8	63.8	63.0	67.2	69.6
2030 UEP45 75% MTFR UK & EU (Met 2007)	**72.1**	**72.8**	**71.8**	**66.4**	**65.4**	**68.1**	**70.0**
2030 UEP45 75% MTFR UK & EU with CH4 reduction (Met 2007)	**72.1**	**72.8**	**71.8**	**66.4**	**65.4**	**68.0**	**70.0**

Table 5.11. OSRM Scenario Results for Area-Weighted AOT40 - Crops (μgm^{-3}.hours)

Scenario	Scotland	Wales	Northern Ireland	Inner London	Outer London	Rest of England	All UK
2025 UEP45 central case UK (Met 2006)	7760	8330	7187	11278	10727	10935	9439
2025 UEP45 25% MTFR UK & EU (Met 2006)	**7505**	**8098**	**6991**	**11512**	**10910**	**10785**	**9247**
2025 UEP45 50% MTFR UK & EU (Met 2006)	**7231**	**7843**	**6779**	**11717**	**11059**	**10596**	**9025**
2025 UEP45 75% MTFR UK & EU (Met 2006)	**6934**	**7564**	**6551**	**11880**	**11157**	**10362**	**8768**
2025 UEP45 75% MTFR UK & EU with CH4 reduction (Met 2006)	**6913**	**7536**	**6531**	**11833**	**11112**	**10323**	**8737**
2030 UEP45 central case UK (Met 2006)	8731	9333	8037	12824	12203	12242	10583
2030 UEP45 75% MTFR UK & EU (Met 2006)	**7485**	**8210**	**7112**	**13379**	**12503**	**11188**	**9475**
2030 UEP45 75% MTFR UK & EU with CH4 reduction (Met 2006)	**7460**	**8177**	**7089**	**13322**	**12450**	**11142**	**9439**
2025 UEP45 central case UK (Met 2007)	8700	8102	6837	8817	8559	8982	8687
2025 UEP45 25% MTFR UK & EU (Met 2007)	**8416**	**7976**	**6567**	**8905**	**8570**	**8821**	**8483**
2025 UEP45 50% MTFR UK & EU (Met 2007)	**8118**	**7828**	**6275**	**8962**	**8552**	**8631**	**8256**
2025 UEP45 75% MTFR UK & EU (Met 2007)	**7807**	**7652**	**5960**	**8982**	**8500**	**8409**	**8004**
2025 UEP45 75% MTFR UK & EU with CH4 reduction (Met 2007)	**7788**	**7630**	**5943**	**8948**	**8469**	**8382**	**7981**
2030 UEP45 central case UK (Met 2007)	9666	9261	7786	10243	9882	10188	9795
2030 UEP45 75% MTFR UK & EU (Met 2007)	**8345**	**8536**	**6458**	**10298**	**9654**	**9254**	**8732**
2030 UEP45 75% MTFR UK & EU with CH4 reduction (Met 2007)	**8324**	**8509**	**6439**	**10256**	**9615**	**9222**	**8705**

Table 5.12. OSRM Scenario Results for Population-Weighted Annual Mean Ozone (μgm^{-3})

Scenario	Scotland	Wales	Northern Ireland	Inner London	Outer London	Rest of England	All UK
2025 UEP45 central case UK (Met 2006)	63.2	68.7	66.9	62.4	62.1	62.8	63.2
2025 UEP45 25% MTFR UK & EU (Met 2006)	63.5	68.9	67.0	63.1	62.7	63.3	63.6
2025 UEP45 50% MTFR UK & EU (Met 2006)	63.7	69.1	67.2	63.7	63.4	63.7	64.0
2025 UEP45 75% MTFR UK & EU (Met 2006)	64.0	69.3	67.3	64.4	63.9	64.1	64.4
2025 UEP45 75% MTFR UK & EU with CH4 reduction (Met 2006)	63.9	69.3	67.3	64.3	63.9	64.1	64.4
2030 UEP45 central case UK (Met 2006)	64.2	69.8	67.7	63.7	63.4	64.0	64.4
2030 UEP45 75% MTFR UK & EU (Met 2006)	65.1	70.5	68.2	66.1	65.6	65.5	65.8
2030 UEP45 75% MTFR UK & EU with CH4 reduction (Met 2006)	65.1	70.5	68.2	66.1	65.6	65.5	65.8
2025 UEP45 central case UK (Met 2007)	65.8	69.3	69.2	62.1	62.1	63.2	63.8
2025 UEP45 25% MTFR UK & EU (Met 2007)	66.0	69.6	69.3	62.8	62.8	63.7	64.2
2025 UEP45 50% MTFR UK & EU (Met 2007)	66.3	69.8	69.4	63.6	63.4	64.1	64.7
2025 UEP45 75% MTFR UK & EU (Met 2007)	66.5	70.1	69.6	64.3	64.1	64.5	65.1
2025 UEP45 75% MTFR UK & EU with CH4 reduction (Met 2007)	66.5	70.0	69.5	64.3	64.0	64.5	65.1
2030 UEP45 central case UK (Met 2007)	66.8	70.5	70.1	63.5	63.5	64.4	65.0
2030 UEP45 75% MTFR UK & EU (Met 2007)	67.6	71.4	70.5	66.2	65.9	66.0	66.6
2030 UEP45 75% MTFR UK & EU with CH4 reduction (Met 2007)	67.6	71.3	70.5	66.2	65.9	66.0	66.5

Table 5.13. OSRM Scenario Results for Population-Weighted Number of Days when the Daily Maximum Running 8 Hourly Ozone Concentration exceeds $120\mu gm^{-3}$

Scenario	Scotland	Wales	Northern Ireland	Inner London	Outer London	Rest of England	All UK
2025 UEP45 central case UK (Met 2006)	6.6	10.3	7.8	7.7	8.1	11.6	10.5
2025 UEP45 25% MTFR UK & EU (Met 2006)	6.1	9.7	7.8	8.1	8.1	11.4	10.3
2025 UEP45 50% MTFR UK & EU (Met 2006)	5.7	9.3	7.5	8.3	8.0	11.2	10.2
2025 UEP45 75% MTFR UK & EU (Met 2006)	5.4	8.6	7.1	8.4	8.1	11.0	9.9

2025 UEP45 75% MTFR UK & EU with CH4 reduction (Met 2006)	5.4	8.5	7.1	8.4	8.0	10.9	9.8
2030 UEP45 central case UK (Met 2006)	8.4	12.6	9.3	9.6	9.8	13.2	12.2
2030 UEP45 75% MTFR UK & EU (Met 2006)	6.2	10.2	7.8	9.8	10.4	12.2	11.2
2030 UEP45 75% MTFR UK & EU with CH4 reduction (Met 2006)	6.2	10.2	7.8	9.8	10.3	12.1	11.1
2025 UEP45 central case UK (Met 2007)	7.8	5.3	3.4	9.2	10.2	7.3	7.5
2025 UEP45 25% MTFR UK & EU (Met 2007)	7.5	5.1	3.4	9.4	10.1	7.2	7.3
2025 UEP45 50% MTFR UK & EU (Met 2007)	7.1	5.0	3.3	9.6	9.9	7.1	7.2
2025 UEP45 75% MTFR UK & EU (Met 2007)	6.6	4.9	3.2	9.3	9.8	6.9	7.0
2025 UEP45 75% MTFR UK & EU with CH4 reduction (Met 2007)	6.6	4.9	3.2	9.3	9.6	6.8	6.9
2030 UEP45 central case UK (Met 2007)	9.6	7.6	4.3	10.9	12.1	9.4	9.4
2030 UEP45 75% MTFR UK & EU (Met 2007)	7.5	6.6	3.7	12.9	11.9	8.3	8.5
2030 UEP45 75% MTFR UK & EU with CH4 reduction (Met 2007)	7.5	6.5	3.7	12.6	11.9	8.3	8.4

Table 5.14. OSRM Scenario Results for Population-Weighted SOMO0 (μgm^{-3}.days)

Scenario	Scotland	Wales	Northern Ireland	Inner London	Outer London	Rest of England	All UK
2025 UEP45 central case UK (Met 2006)	27391	29382	28238	27559	27435	27640	27701
2025 UEP45 25% MTFR UK & EU (Met 2006)	27426	29400	28247	27737	27596	27733	27792
2025 UEP45 50% MTFR UK & EU (Met 2006)	27456	29413	28251	27912	27752	27819	27877
2025 UEP45 75% MTFR UK & EU (Met 2006)	27478	29418	28249	28079	27901	27898	27955
2025 UEP45 75% MTFR UK & EU with CH4 reduction (Met 2006)	27471	29409	28243	28068	27889	27889	27945
2030 UEP45 central case UK (Met 2006)	27773	29807	28574	28064	27927	28090	28147
2030 UEP45 75% MTFR UK & EU (Met 2006)	27852	29822	28573	28681	28479	28374	28427
2030 UEP45 75% MTFR UK & EU with CH4 reduction (Met 2006)	27844	29812	28566	28667	28466	28363	28416
2025 UEP45 central case UK (Met 2007)	27997	29342	28863	27309	27251	27435	27598

2025 UEP45 25% MTFR UK & EU (Met 2007)	28026	29377	28868	27508	27425	27535	27696
2025 UEP45 50% MTFR UK & EU (Met 2007)	28050	29405	28864	27702	27593	27628	27787
2025 UEP45 75% MTFR UK & EU (Met 2007)	28069	29424	28853	27888	27753	27714	27872
2025 UEP45 75% MTFR UK & EU with CH4 reduction (Met 2007)	28062	29415	28847	27877	27742	27704	27862
2030 UEP45 central case UK (Met 2007)	28379	29811	29231	27868	27791	27912	28072
2030 UEP45 75% MTFR UK & EU (Met 2007)	28449	29885	29190	28559	28383	28228	28383
2030 UEP45 75% MTFR UK & EU with CH4 reduction (Met 2007)	28441	29875	29182	28546	28370	28217	28372

Table 5.15. OSRM Scenario Results for Population-Weighted SOMO10 (μgm^{-3}.days)

Scenario	Scotland	Wales	Northern Ireland	Inner London	Outer London	Rest of England	All UK
2025 UEP45 central case UK (Met 2006)	20164	22210	20995	20447	20321	20497	20551
2025 UEP45 25% MTFR UK & EU (Met 2006)	20192	22218	20999	20609	20466	20577	20629
2025 UEP45 50% MTFR UK & EU (Met 2006)	20214	22219	20998	20767	20605	20649	20701
2025 UEP45 75% MTFR UK & EU (Met 2006)	20228	22212	20992	20920	20739	20715	20765
2025 UEP45 75% MTFR UK & EU with CH4 reduction (Met 2006)	20221	22204	20986	20909	20728	20705	20755
2030 UEP45 central case UK (Met 2006)	20540	22624	21325	20933	20797	20934	20983
2030 UEP45 75% MTFR UK & EU (Met 2006)	20591	22599	21309	21500	21293	21168	21217
2030 UEP45 75% MTFR UK & EU with CH4 reduction (Met 2006)	20583	22589	21302	21488	21280	21157	21206
2025 UEP45 central case UK (Met 2007)	20740	22091	21596	20125	20074	20228	20386
2025 UEP45 25% MTFR UK & EU (Met 2007)	20766	22121	21600	20317	20240	20320	20478
2025 UEP45 50% MTFR UK & EU (Met 2007)	20788	22145	21596	20504	20399	20406	20562
2025 UEP45 75% MTFR UK & EU (Met 2007)	20803	22160	21584	20683	20550	20485	20640
2025 UEP45 75% MTFR UK & EU with CH4 reduction (Met 2007)	20797	22151	21577	20671	20539	20476	20631
2030 UEP45 central case UK (Met 2007)	21118	22552	21962	20673	20605	20696	20852
2030 UEP45 75% MTFR	21178	22613	21917	21335	21162	20987	21139

UK & EU (Met 2007)							
2030 UEP45 75% MTFR UK & EU with CH4 reduction (Met 2007)	21171	22603	21909	21323	21150	20977	21129

Table 5.16. OSRM Scenario Results for Population-Weighted SOMO35 (μgm^{-3}.days)

Scenario	Scotland	Wales	Northern Ireland	Inner London	Outer London	Rest of England	All UK
2025 UEP45 central case UK (Met 2006)	4154	5688	4485	4836	4754	4728	4726
2025 UEP45 25% MTFR UK & EU (Met 2006)	4138	5664	4467	4920	4822	4745	4743
2025 UEP45 50% MTFR UK & EU (Met 2006)	4118	5635	4443	4999	4884	4756	4756
2025 UEP45 75% MTFR UK & EU (Met 2006)	4091	5600	4415	5071	4937	4760	4761
2025 UEP45 75% MTFR UK & EU with CH4 reduction (Met 2006)	4086	5592	4410	5061	4928	4752	4753
2030 UEP45 central case UK (Met 2006)	4433	6036	4753	5209	5118	5058	5055
2030 UEP45 75% MTFR UK & EU (Met 2006)	4324	5898	4647	5474	5320	5064	5067
2030 UEP45 75% MTFR UK & EU with CH4 reduction (Met 2006)	4318	5889	4641	5463	5309	5055	5058
2025 UEP45 central case UK (Met 2007)	4256	5300	4624	4432	4390	4236	4322
2025 UEP45 25% MTFR UK & EU (Met 2007)	4243	5292	4603	4511	4448	4254	4341
2025 UEP45 50% MTFR UK & EU (Met 2007)	4228	5278	4575	4585	4499	4267	4354
2025 UEP45 75% MTFR UK & EU (Met 2007)	4209	5258	4542	4650	4545	4274	4362
2025 UEP45 75% MTFR UK & EU with CH4 reduction (Met 2007)	4204	5251	4537	4641	4536	4266	4355
2030 UEP45 central case UK (Met 2007)	4537	5662	4911	4829	4768	4572	4659
2030 UEP45 75% MTFR UK & EU (Met 2007)	4461	5591	4781	5073	4934	4595	4685
2030 UEP45 75% MTFR UK & EU with CH4 reduction (Met 2007)	4455	5583	4775	5062	4924	4586	4677

Maps are available for all combinations of scenarios, metrics and meteorology years. However, for a given meteorology year, the maps appear very similar for all scenarios and the base case, so they are not presented here.

For the 2025 75% MTFR, 50% MTFR and 25% MTFR scenarios some of the metrics show an increase in the population- or area-weighted means in all regions compared to the basecase, while other metrics show an increase in some regions and a decrease in others. This is the case for the runs using the 2006 meteorology and the runs using the 2007 meteorology. For almost all metrics there is an increase in the London regions for all scenarios. Generally the results for the 25% MTFR scenario are between those for the basecase and those for the 50% MTFR scenario, and the results for the 50% MTFR scenario are between those for the 25% MTFR scenario and those for the 75% MTFR scenario .

The differences between the results for the 2030 scenarios are generally consistent with the differences seen for the 2025 scenarios. The results for the 2030 75% MTFR scenario generally indicate higher ozone than the 2025 75% MTFR scenario (though this is not the case for all metrics and regions).

These conclusions are consistent with the results we have seen for previous OSRM scenarios. Specifically, that reducing emissions tends to lead to an increase in the ozone metrics, especially the population-weighted means. We believe this is due in part to a reduction in the NO_x titration effect.

The changes in the results for the 75% MTFR scenario with the methane change compared to the 75% MTFR scenario without the change in methane are consistent across the different metrics and regions (for both 2025 and 2030). The methane change leads to a very small decrease in all metrics and all regions. However, it should be noted that for these scenarios only the initial methane concentration was changed and we have therefore assumed that changing methane does not have an effect on any of the other initialised concentrations.

5.3 OSRM Modelling for Updating Ozone Damage Costs Relationships with Emissions

The PCM model has previously been used to establish relationships between various pollution concentration metrics and incremental changes in UK emissions in order for Defra to update health-, crop- and materials damage cost functions. Previous relationships for ozone had used the OSRM to provide outputs on the changes in various ozone concentration metrics for decreases in precursor NO_x and VOC emissions in the UK.

Defra required these relationships between ozone metrics and emission changes to be updated. The approach was to model ozone from a 2012 basecase (meteorology and emissions) for an arbitrary 10% reduction in UK NO_x and VOC emissions separately.

The year and emissions data used were chosen to be as consistent as possible with the assessments for other pollutants made using the Pollution Climate Mapping (PCM) model in the UKAAQA programme and was the most recent year for which modelled results were available. The PCM damage costs runs for 2012 used the 2011 NAEI emissions scaled forward to 2012 and 2012 meteorology. An equivalent OSRM base case run (2012 modelled using the 2011 NAEI) was already available, so a new base case for 2012 run was not needed.

Two simulations were therefore carried out for Defra to provide the necessary information:

- 2012 using 2012 meteorology and NAEI emissions and 2012 PRIMES-2012 CLE emissions (TSAP (2013)) with 10% reduction in UK NO_x emissions
- 2012 as above with 10% reduction in UK VOC emissions

Various ozone metrics were calculated from the OSRM output. These metrics were specified by Defra in the previous damage cost runs (for 2010) to calculate human health impacts, materials damage and crops/vegetation damage.

For calculating the human health impacts the population-weighted mean (PWM) of FOUR metrics were calculated:

- Sum of the daily maximum of the running 8-hour mean ozone, calculated with a cut off at 0 μgm^{-3} (SOMO0).
- Sum of the daily maximum of the running 8-hour mean ozone, calculated with a cut off at 20 μgm^{-3} (SOMO10).
- Sum of the daily maximum of the running 8-hour mean ozone, calculated with a cut off at 70 μgm^{-3} (SOMO35).
- Sum of the daily maximum of the running 8-hour mean ozone, calculated with a cut off at 100 μgm^{-3} (SOMO50).

For calculating materials damage the population-weighted annual mean concentration was calculated.

For calculating crops/vegetation damage the area-weighted mean of the AOT40 metric was calculated.

5.3.1 Results for Damage Cost Runs

The results for the 2012 basecase (in grey) and the two new emission reduction scenarios are shown for each ozone metric in Tables 5.17 to 5.22. Results are shown for each country in the UK and for London as well as the UK as a whole.

Table 5.17: Population-weighted SOMO0 (μgm^{-3}.days)

	Scotland	Wales	Northern Ireland	Inner London	Outer London	Rest of England	All UK
Base 2012 (2011 NAEI)	24532	24896	26072	22397	22321	23014	23243
10% reduction in VOC emissions 2012	24423	24772	25976	22266	22188	22876	23109
10% reduction in NOx emissions 2012	25055	25547	26360	23945	23819	24094	24284

Table 5.18: Population-weighted SOMO10 (μgm^{-3}.days)

	Scotland	Wales	Northern Ireland	Inner London	Outer London	Rest of England	All UK
Base 2012 (2011 NAEI)	17420	17818	18882	15437	15359	16006	16223
10% reduction in VOC emissions 2012	17313	17697	18789	15309	15228	15870	16092
10% reduction in NOx emissions 2012	17900	18408	19147	16916	16782	17012	17195

Table 5.19: Population-weighted SOMO35 (μgm^{-3}.days)

	Scotland	Wales	Northern Ireland	Inner London	Outer London	Rest of England	All UK
Base 2012 (2011 NAEI)	2925	2894	3243	2013	1980	2171	2280
10% reduction in VOC emissions 2012	2882	2837	3196	1957	1920	2112	2222
10% reduction in NOx emissions 2012	3050	3075	3335	2565	2495	2500	2602

Table 5.20: Population-weighted SOMO50 (μgm^{-3}.days)

	Scotland	Wales	Northern Ireland	Inner London	Outer London	Rest of England	All UK
Base 2012 (2011 NAEI)	434	216	343	170	147	187	210
10% reduction in VOC emissions 2012	428	211	337	159	137	179	202
10% reduction in NOx emissions 2012	440	224	350	250	223	225	248

Table 5.21: Population-weighted annual mean ozone (μgm^{-3})

	Scotland	Wales	Northern Ireland	Inner London	Outer London	Rest of England	All UK
Base 2012 (2011 NAEI)	54.5	54.8	59.3	46.2	46.2	48.8	49.6
10% reduction in VOC emissions 2012	54.2	54.5	59.1	45.9	45.8	48.4	49.2
10% reduction in NOx emissions 2012	56.5	57.3	60.6	50.7	50.5	52.2	52.9

Table 5.22: Area-weighted AOT40 (μgm^{-3}.hours)

	Scotland	Wales	Northern Ireland	Inner London	Outer London	Rest of England	All UK
Base 2012 (2011 NAEI)	4459	2868	3302	2587	2450	3053	3516
10% reduction in VOC emissions 2012	4351	2748	3205	2376	2244	2903	3385
10% reduction in NOx emissions 2012	4391	2946	3274	3816	3506	3495	3735

The results for all the metrics show a consistent trend whereby the 10% reduction in VOC emissions leads to a small decrease in all the metrics calculated. The decrease is apparent in all the different regions. On the other hand the 10% reduction in NO_x emission leads to an increase in all the metrics calculated, other than AOT40 in Scotland and Northern Ireland. Where there is an increase due to the reduction in NOx emission, the increase is generally larger than the decrease apparent from the same percentage reduction in VOC emissions.

These results will be used in the update of the damage cost calculations.

6 Model Intercomparison Activities

Both the OSRM and PTM have taken part in the Defra Model Intercomparison Exercise (MIE). Partners attended a final meeting of the regional group in April 2013 and the MIE has now come to an end. The report on Phase 2 of the MIE demonstrates the performance of both models compared with other models and with observations.

The final report from the regional scale model evaluation Phase 2 (Carslaw et al, 2013) can be found at http://uk-air.defra.gov.uk/research/air-quality-modelling?view=intercomparison .

7 Summary and Conclusions

The OSRM and PTM were used to model and interpret the UK ground level ozone concentrations for 2012 and a range of different emission reduction scenarios to support Defra's ozone air quality policies.

As far as the EU Air Quality Directive compliance metrics are concerned, the average of the measurements indicate that 2012 was a year with relatively low ozone concentrations and this was supported by model runs using the OSRM. On average the OSRM tended to over-predict the number of days exceeding 120 μgm^{-3} for 2012 and under-predict the AOT40 metric (but was overall fairly consistent with the measurements).

In 2012 there were a number of ozone episodes and maximum hourly ozone levels reached 90 ppb. The PTM was used to diagnose and understand the nature of the 2012 episodes by modelling the responses of peak ozone concentrations at twelve sites to hypothetical changes in NO_x and VOC emissions in the UK and rest of Europe. From the results, it was concluded that most (though not all) of the episodes in 2012 at these sites were dominated by emissions from the rest of Europe.

Overall, the performance of the PTM over the 2012 ozone season at the twelve sites modelled was far from satisfactory, with episodes at some sites being missed. Model performance in terms of predicting within ± 10%, the seasonal ozone maxima at each site was only satisfactory at Harwell, Rochester, Sibton and Strath Vaich.

Further analysis of ozone episodes at Mace Head, Ireland, addressed the sensitivity of modelled peak ozone predictions to ozone deposition velocity. Reducing the ozone deposition velocity increased peak ozone to levels closer to measured values on some days, although not all, indicating this could be one reason why the PTM underpredicts peak ozone.

The OSRM and PTM were used to model UK ozone for a range of different emission reduction scenarios of relevance to Defra's ozone air quality policy. The OSRM was used to model UK ozone for three different UK NAEI emissions scenarios for 2025 and three 2030 scenarios. The OSRM was also used to model UK ozone for four 2025 scenarios and two 2030 scenarios developed by Defra from their estimates of what might be in the European Commission proposal for a revised/replacement NECD. The simulations consistently show how ozone concentrations are predicted to be higher in future years when emissions are reduced and all other conditions are maintained the same. The increase has been attributed to less efficient titration of ozone by NO_x in urban and suburban areas when NO_x emissions are reduced, in an area of NW Europe still saturated in NO_x. Moreover, there is an increasing trend in the emitted VOC/NO_x ratio in these future scenarios in an area of NW Europe which is VOC-limited.

Some scenarios were modelled in which European CH_4 emissions were reduced as well as NMVOCs. The reduction in CH_4 emissions was reflected by a change in the methane initialised boundary concentrations in the specific model runs and led to a very small reduction in ozone concentrations. The overall effect of changing the initialised methane boundary concentrations was found to be very small compared with the changes caused by other VOC emissions.

The PTM was used to model the impacts on ground-level ozone (under 2008 episodic conditions) of the UK NAEI UEP45 central case emission projections for 2025 and 2030 together with the PRIMES-2012 European emission projections for the rest of Europe. The study focussed on changes in episodic peak ozone at the rural Harwell site in Oxfordshire in southern England. Although the episodic peak levels decreased between 2008 and 2025 and 2030, the extremes of the distributions were not reduced enough to protect against the exceedance of the World Health Organisation air quality guideline. There were 16 days in which the 50-percentile PTM predictions indicated that the World Health Organisation 8-hour running mean air quality guideline was exceeded in 2008, this number decreased substantially, by over one half, to 7 days in 2025 and 2030.

The OSRM was also used to model various ozone metrics for an arbitrary 10% reduction in UK NO_x and VOC emissions separately for 2012. The results will be used by Defra to update health-, crop- and materials damage cost functions in relation to ozone to combine with those updated for other air pollutants. Under the conditions modelled, all metrics and all regions (other than AOT40 for some regions) show a small decrease for the 10% VOC reduction scenario and a larger increase for the 10% NO_x reduction scenario.

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