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EMission Scenario Toolkit for CMAQ-UK

Phase 2 of the Defra CMAQ Development for UK National Modelling Project

Report for Department for Environment, Food & Rural Affairs

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Executive summary

Emissions inventory data are key inputs to chemical transport air pollution models such as CMAQ. In Phase 2 of the Defra project "*CMAQ Development for UK National Modelling*", UK and European emissions inventory data have been collated for an optimised CMAQ-UK version of the model. The data must be processed to make them model-ready, e.g. by converting maps of annual emission rates to hourly emissions and to divide pollutants into their chemical components. To make the operational version of CMAQ-UK efficient for use in Defra policy applications, it is important that the inventory data can be modified in an efficient, flexible and transparent manner to be able to model different emission scenarios and model years.

This report describes an Emission Scenario Toolkit, EMST, developed for CMAQ-UK, but potentially applicable to other air pollution models used for Defra policy, such as EMEP4UK. An Anthropogenic Emissions Tool (AET) combines UK anthropogenic emissions inventory data from the NAEI and European inventory data from other sources. The EMST provides an environment to combine data from AET with biogenic emissions data calculated from the MEGAN model and processes them to provide model-ready data for CMAQ-UK.

The report describes the key sources of inventory input data, the various conversion factors used to create hourly and chemically-resolved emissions and provides a demonstration of emission outputs from the processor. These are outputs used for simulating air quality in the UK by CMAQ-UK for the years 2006, 2009-2011 and 2019-2021.

A User Guide for the AET developed in this project is available in a separate document.

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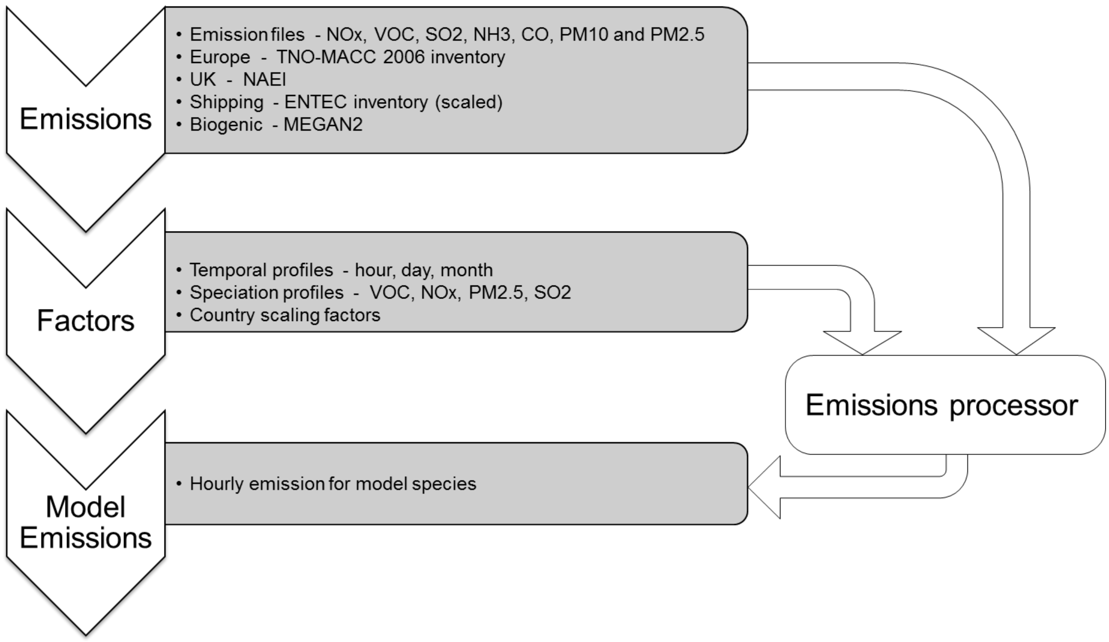
1 Introduction

The emissions scenario toolkit **(EMST**) is a model environment developed to combine emissions inventory data for anthropogenic and biogenic sources to create model-ready emissions for chemical transport air pollution models such as CMAQ. The European and UK anthropogenic inventories are converted using a new anthropogenic emissions tool (**AET**) and biogenic emissions are generated using the Model of Emissions of Gases and Aerosols from Nature (MEGAN). EMST is a flexible and transparent system capable of creating emissions scenario for modelling. It can be expanded to incorporate new sources of emissions or factors as they are required or become available.

Creating emissions for CMAQ modelling involves identifying suitable emissions inventories and applying factors to convert the annual emission rates to hourly emissions for the chemical species required for the chemical transport model as shown in Figure 1. The air quality model requires all anthropogenic and natural emissions.

Figure 1: Flow diagram inventory data to model data for CMAQ-UK



This report includes an overview of the inventories and methods used to produce model emissions for CMAQ-UK model. Examples of datasheets are in the Appendix.

Note that a User Guide for the AET is available in a separate document.

2 Sources of Emissions Inventory Data for CMAQ-UK

Emissions inventory data are collated primarily in formats for compliance with international inventory reporting commitments to the UNECE and EU.

These inventory data sets, maps and projections are expressed as annual rates of emissions and are used to create the hourly emissions required by CMAQ. Creating emissions for CMAQ modelling involves identifying suitable emissions inventories and applying factors to convert the annual emission rates to hourly emission rates for the chemical species required for the chemical transformation schemes in the CMAQ model.

The National Atmospheric Emissions Inventory (NAEI) programme has recently undertaken a number of tasks to prepare emissions data suitable for all of Defra's air quality modelling activities. These studies focused on developing a range of supplementary data for the air pollution modelling community including profiles defining the temporal (hourly, daily and monthly) variation in emissions for different source sectors and pollutant species, recommendations for methods to calculate biogenic emissions, specific data to characterise point source emissions and recommended sources of inventory data to convert emission maps for the UK and rest of Europe for current years back to 2005 and forward to 2020 on a consistent basis.

More specifically, these include:

- Recommendations on European Emission Inventories for air pollution modelling in the UK
- Updated gridded emissions data for 2005 (used for 2006 modelling) based on the 2010 NAEI inventory methodology and source-specific scaling factors for other years
- Temporal emission profiles for source sectors at the SNAP 1 level[1].
- More detailed information on the temporal variation in emissions from road transport
- Monthly profiles for ammonia emissions from agriculture

In Phase 1, the emissions were created using 2006 emission maps generated in 2008, but the European and UK maps have since been updated using methodologies consistent with more recent versions of the inventory. The emissions have been recreated using these latest NAEI updates and recommendations.

In evaluating the most suitable emissions to use, the following criteria were taken into account:

- suitability for Defra policy scenarios, i.e. the potential for changing emissions of specific pollutants from specific source sectors and for specific groups of countries
- suitability for temporal disaggregation at an appropriate sector level, i.e. how can the data be used in conjunction with temporal data also developed by the NAEI for air pollution modelling purposes
- accessibility of the maps and suitability for using on the CMAQ-UK grids
- provenance of the maps

This section makes frequent reference to year-, sector- and pollutant-specific scaling factors used to create an emissions map for a specific year from an existing map developed for another year. Further details of these scaling factors and other factors used to further disaggregate emissions by hour and by chemical species are given in Section 3.

[1] Selected Nomenclature for sources of Air Pollution (SNAP) is a system for categorising sources of emissions in inventories reported to the UNECE

Anthropogenic emissions

Table 1 summarises the sources of anthropogenic emissions used to prepare CMAQ-UK data. The base inventory maps are developed periodically e.g. the NAEI has recently redeveloped the 2005 NAEI maps using the same methodology as for the 2010 inventory and for the years between 2005 and 2010 scaling factors are applied to generate maps for the required year based on trends in the national totals for each sector.

Table 1 Summary of inventory data used for the European (EU 50x50km) and UK (UK 10x10km) anthropogenic emissions

	European 50km grid	UK 10km grid
Europe – area	TNO-MACC (2006) (including UK)	TNO-MACC (2006) (excluding UK and shipping)
Europe - point	TNO-MACC (2006) (including UK)	TNO-MACC (2006) (excluding UK)
UK - area		NAEI (2005 scaled to 2006) (2011 scale to 2009, 2010, 2019, 2020, 2021)
UK - point		NAEI (from the 2011 database)
Shipping	TNO-MACC (2006)	Entec shipping inventory (for 2007) scaled by the NAEI to other years consistent with shipping emission regulations

The NAEI and TNO-MACC pollutant maps are available for activity sectors. Historically these maps have only been available for sectors as SNAP level 1 detail for the main pollutants, however a few sub-sector maps are now available. The emissions preparation can be adapted to reflect the available maps. Table 2 shows the sectors available for the NAEI and TNO-MACC emissions.

2.1.1 European Emissions - TNO-MACC (2006)

The two main sources of European emissions data are:

- EMEP - European Monitoring and Evaluation Programme. Emissions data are freely available on the internet at SNAP 1 sector level on the EMEP 50km grid.
- TNO-MACC - Emissions prepared by the Netherlands Organisation for Applied Scientific Research (TNO) as part of the MACC II (Monitoring Atmospheric Composition and Climate) project. The finer resolution SNAP sector data are not available via the MACC data catalogue however and were provided by TNO directly. Permission has been given to use these emissions. These data are available at SNAP sector level at ~7km resolution.

EMEP and TNO emissions are based on the same basic source. The EMEP emissions are based on the emissions reported under the UNECE CLRTAP and are the basis for the TNO emissions. The difference is how the non-reported emissions are estimated.

Table 2 Sectors available for TNO-MACC and NAEI emissions

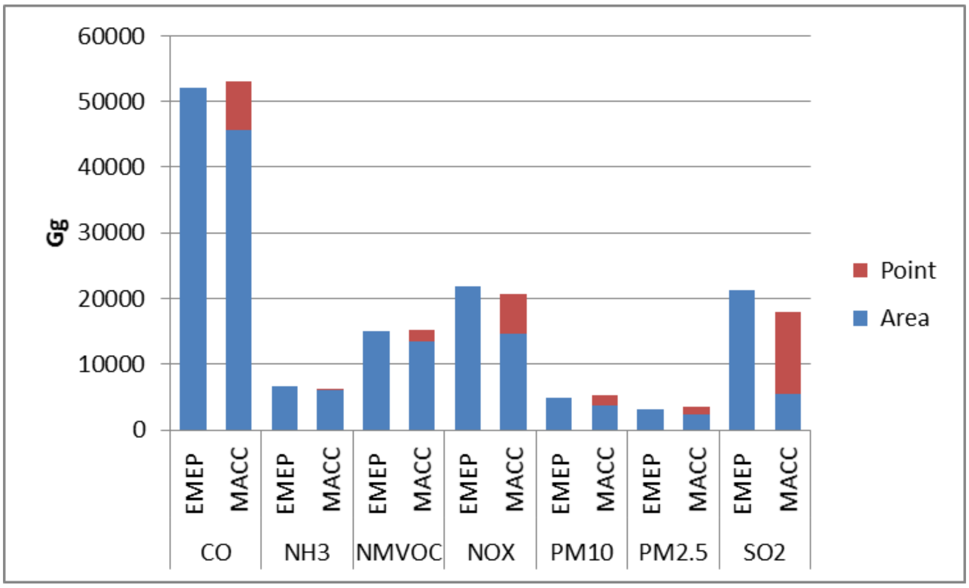
		TNO-MACC sub-sector detail	NAEI sub-sector detail
SNAP 1	Combustion in energy and transformation industries		
SNAP 2	Non-industrial combustion plants		Domestic*
SNAP 3	Combustion in manufacturing industry		
SNAP 4	Production processes		
SNAP 5	Extraction and distribution of fossil fuels and geothermal energy		
SNAP 6	Solvent use and other product use		
SNAP 7	Road transport	exhaust, gasoline exhaust, diesel exhaust, LPG/ natural gas gasoline evaporation Tyre /brake/road wear	Major roads ALL traffic Major roads CARS Major roads BUS Major roads HGV Major roads LGV Major roads M/C Minor roads ALL Tyre and Brake (PM only) Road Abrasion (PM only)
SNAP 8	Other mobile sources and machinery	Shipping Non-shipping	Shipping Non-shipping (Rail and Air)*
SNAP 9	Waste treatment and disposal		
SNAP 10	Agriculture		
SNAP 11	Other sources and sinks		

Where sub-snap sector data are available they are only used if different factors are applied otherwise they are aggregated into one sector.

* Additional sectors are generated for Defra projects and can be made available if required.

The European area total emissions for TNO-MACC and EMEP are very similar as shown in **Figure 1**, the main difference being the TNO-MACC emissions are split into area and point sources. The TNO-MACC emissions are well characterised and have been used for several international studies. The TNO-MACC emission data set is widely used in Europe, including the MACC II regional air quality forecast and the international model intercomparison initiative, AQMEII, coordinated by the EC JRC and the US EPA.

Figure 1 European area total emission for EMEP and TNO-MACC emission inventories (2006)



The MACC II[2] emissions inventory for Europe for area and point sources (based on 2006) is widely used in Europe, including the MACC II regional air quality forecast and the international model intercomparison initiative, AQMEII, coordinated by the JRC in the EU and the US EPA. Based on the completeness of the data coverage, the spatial representation and the ability to manipulate the data to represent hourly emissions and policy scenarios the TNO-MACC maps are recommended[3]. However this will be reviewed as new maps become available from EMEP, MACC and TNO.

Maps have been developed for use with the CMAQ-UK modelling activities and are available on request to the NAEI helpline[4]. TNO-MACC emissions data for 2006 were projected onto a 50x50km grid compatible with the NAEI's UK 1x1km grid.

TNO-MACC emissions data are also available for 2009, but could not be processed on the timescale of this project. However, the 2006 TNO-MACC data have been scaled to 2009 using country- and sector-specific trends data provided by TNO. This has been cross-checked against 2009 data available from EMEP and found to be consistent at the country level.

To develop consistent European gridded emissions data for 2010 and 2011, the TNO-MACC data have been scaled to these years using country-specific data reported to EMEP. Country-specific scaling factors are used to derive maps for future years (2019-2021 in the CMAQ-UK project) based on the TSAP_Mar13_CLE ("Current Legislation") scenario available through the GAINS Europe modelling system[5]. More details of these year-specific scaling factors are given in Section 3.

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[2] Pouliot, G., Pierce, T, Denier van der Gon, H., Schaap, M., Nopmongcol, U., 2012. Comparing Emissions Inventories and Model-Ready Emissions Datasets between Europe and North America for the AQMEII Project. Atmospheric Environment (AQMEII issue) 53, 4–14
[3] NAEI report "Recommendations on European Emission Inventories for Air Pollution Modelling in the UK" available from http://naei.defra.gov.uk/about-the-website
[4] http://naei.defra.gov.uk/about-the-website
[5] http://gains.iiasa.ac.at/index.php/gains-europe

2.1.2 UK Emissions - NAEI

For the UK, inventory data from the NAEI[6] is used. An updated 1x1km gridded dataset for UK emissions in 2005 was developed using factors and methodologies consistent with the latest NAEI emission maps developed for 2010. These maps are accompanied by a set of sector- and pollutant-specific scaling factors to enable a consistent set of gridded emissions for 2006 to be processed from the 2005 map.

The most recent NAEI maps for 2011 are used as the base for maps for 2009-2011 and 2019-2021 using sector- and pollutant-specific scaling factors representative of emissions in these years recommended by the NAEI. More details of these year-specific scaling factors are given in Section 3.

2.1.3 Point Source emissions

The NAEI has point source emissions data stored along with stack information in a data base. This is updated each year to take account of new and more accurate information e.g. new updated stack information. These are then applied to historic data to provide a consistent time series. The points data used for all years in this study are from the 2011 database.

The UK point source database has over 5000 records. A number of approaches have been considered for applying this to CMAQ-UK. In Phase 2 of this project, a simple method has been used based on the vertical profiles of distribution of emissions as outlined in Bieser[7] (2011). There are 73 profiles provided in the paper. Taking this and the vertical structure of CMAQ-UK into account, three vertical profiles are used for autumn/winter, spring and summer to release the emissions into layers 5, 6 and 7.

For Phase 2 all point sources were treated using standard profiles. Stack details are available for over 200 of the most polluting point sources of emissions for CO, NO_x, SO_2 or PM_{10}. If required these can be released directly into CMAQ using in-line processing (CMAQ v5).

The same vertical factors are used for the European point source emissions as no stack details are available with the TNO-MACC data.

2.1.4 Shipping emissions

A gridded shipping emissions inventory was developed by Amec (formerly Entec) under contract to Defra[8] in sea territories around the UK based on vessel movements in 2007. During the modelled period, the revised MARPOL Annex VI Regulations[9] came into force affecting SO_2 and PM emissions in different sea areas around the UK. UK grid maps have been created for 2006, 2009-2011 and 2019-2021 using a new method to take into account up-to-date and projected estimates of the impacts of MARPOL and European Sulphur Content of Marine Fuels Directive on PM and SO_2 emissions from ships operating within Sulphur Emission Control Areas[10]

2.2 Natural emissions

Experts in the field of biogenic emissions at the University of Lancaster were commissioned by the NAEI to review and recommend methodologies and data sources for estimating biogenic emissions in air pollution models. Professor Nick Hewitt's group have completed their assessment and their report has been peer-reviewed. The key recommendation is to use the MEGAN 2 methodology.

Model of Emissions of Gases and Aerosols from Nature (MEGAN) version 2.0.4 was used for the preparation of the biogenic emissions. Twenty biogenic emission species including isoprene and

[6] http://naei.defra.gov.uk/data/mapping
[7] J. Bieser, A. Aulinger, V. Matthias, M. Quante, H.A.C. Denier van der Gon, Vertical emission profiles for Europe based on plume rise calculations , Environmental Pollution 159 (2011)
[8]Entec (2010). UK Ship Emissions Inventory. Final Report to Defra, November 2010. http://uk-air.defra.gov.uk/reports/cat15/1012131459_21897_Final_Report_291110.pdf
[9] MARPOL (2010): Revised MARPOL Annex VI, Prevention of Air pollution from shipping. http://www.imo.org/OurWork/Environment/PollutionPrevention/AirPollution/Pages/Air-Pollution.aspx
[10] Tsagataskis, I., Brace, S., Passant, N., Cooke, S. (2013): UK Emission Mapping Methodology 2011 http://uk-air.defra.gov.uk/reports/cat07/1403100909_UK_Emission_Mapping_Methodology_2011-Issue_1.pdf

various terpenes were simulated with the MEGAN based on the meteorology[11]. The simulated biogenic emissions at the model's lowest layer were merged with the anthropogenic emissions data generated.

The sea salt contribution to particulate matter is calculated within CMAQ based on the meteorology.

[11] http://acd.ucar.edu/~guenther/MEGAN/MEGAN.htm

3 Emissions Processor

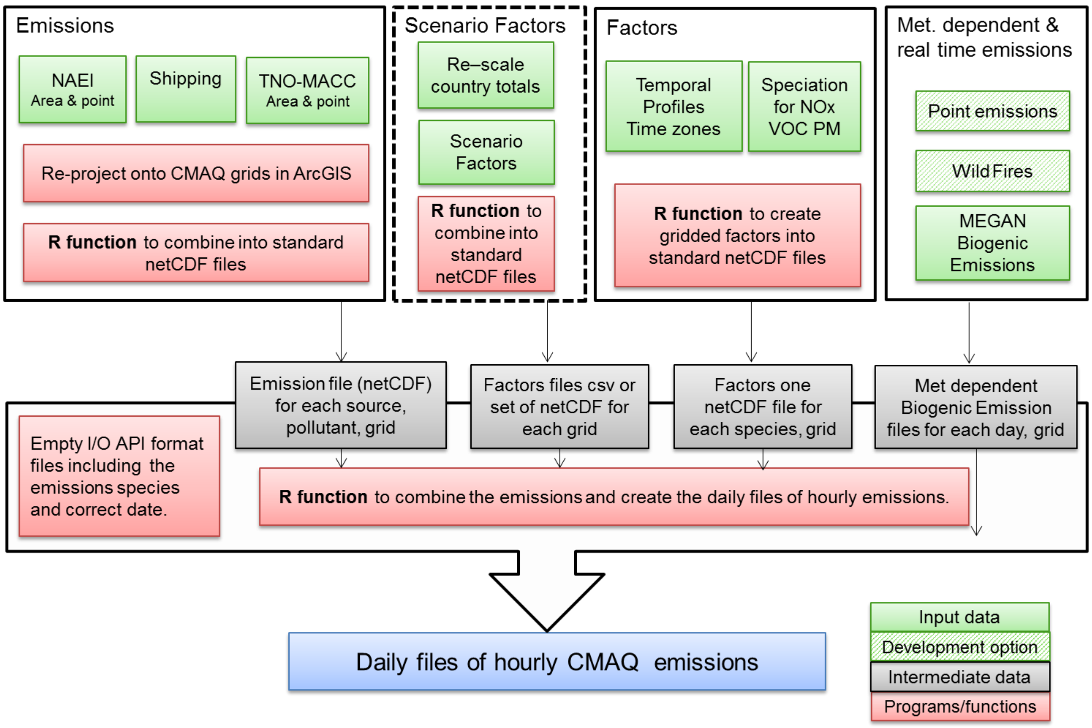
SMOKE, the model that accompanies CMAQ, is a complex model designed to build emissions inventory from components compatible with data available in the USA, then, using that inventory, it creates emission data ready for CMAQ. SMOKE has been adapted for applications in the UK. Having investigated SMOKE it was decided to create a more flexible and transparent tool that is suitable for a range of models including CMAQ that is not based on SMOKE and suitable for Defra scenario applications.

A system for processing the inventory data into CMAQ-ready data was developed. A new suite of programs was developed based on the R programming language to create the CMAQ emissions data. This will be described in a supplementary user guide document, but includes a series of models including:

- MEGAN biogenic model
- Anthropogenic Emissions Toolkit (AET). The process steps are written as a series of R functions; these are generic and can be applied to any modelling grid on which the base emissions have been created.
- The final stage combines the anthropogenic and biogenic emissions and writes the data into the CMAQ file format.

This is a flexible system, separating the preparation of the base emissions inventory data (annual emission rates) from the application of the scaling, temporal, speciation and scenario factors so that the choice of emission inventory or changes to the factors can be made independently without the need to reprocess all the data. The factors can be developed independently based on pollutant, emission sector, year and country to create CMAQ-ready emissions data for complex scenarios that may be required by Defra. It is only the final stage of the process that is CMAQ specific and this can be adapted for other models. Figure 2 shows a schematic of the emissions process.

Figure 2 Emissions process schematic.



3.1 Emission Conversion Factors

Factors are used to convert the basic annual inventory emission rates into gridded hourly emissions and to their chemical constituent parts required by CMAQ. As described above scaling factors are also used to generate emission maps for the years where maps are not available. Temporal and speciation factors have been developed based on UK activity patterns to convert the annual rate of emissions data into the hourly data required by CMAQ. Vertical profiles are used to introduce the point source emissions into the correct layer of the model.

3.1.1 Temporal emission profiles

The NAEI made recommendations for temporal profiles for each source sector following a review of UK activity data and profiles developed by TNO[12]. The UK temporal profiles are applied across the European area, taking into account time zones, and convert annual emission rates produced by inventories into hourly rates taking into account activity and other factors that vary by time-of-day, day-of-week and month.

Recommendations have been made for the following main SNAP sectors:

- **Power generation emissions –** new factors are based on 2010 and 2011 emissions data from primarily coal fired power stations in England and Wales.
- **Domestic and commercial and institutional combustion –** this SNAP sector is a complex mixture of emissions sources including domestic homes and institutions such as schools, hospitals, prisons, council offices which will have different temporal activity profiles. For 2006, SNAP 2 emission maps were not separated into sub SNAP sectors. To address this, weekly and hourly profiles were developed that took account of the relative contribution of residential and non-residential sources on a monthly basis. New monthly profiles based on daily temperature were developed from a degree-days concept.
- **Road transport –** the road transport profiles in Phase 1 were based on the London profiles developed by King's College and consisted of daily profiles for weekdays and weekends. New profiles for average UK traffic have been developed for passenger cars and commercial vehicles on different road types in Phase 2[13] based on DfT traffic statistics[14].
- **Ammonia emissions from agriculture –** Monthly estimates of ammonia emissions were estimated[15] using monthly activity data for different sources of emissions in agriculture. This includes estimates for cattle, pigs, poultry and sheep taking into account the different husbandry methods, emission from manure stores and application of nitrogen fertiliser. It is more difficult to allocate emission by hour of the day; many of the emission are continuous over 24hrs whilst others have a diurnal profile based on temperature or husbandry methods. In Phase 1 of the CMAQ-UK project, a constant (flat) profile was used, in Phase 2 a diurnal profile has been introduced.

3.1.2 Speciation factors

Chemical speciation factors are used to disaggregate total mass emissions of VOCs and PM reported by inventories into their chemical components. There has been no change in the VOC and PM speciation between Phase 1 and Phase 2.

- **VOC speciation**. – the speciation of VOCs into chemical forms relevant to different chemistry schemes used in CMAQ is calculated using the spreadsheet developed by Ricardo-AEA and is based on the NAEI's existing NMVOC speciation profile[16]. This provides a means of breaking down total VOC emissions from several hundred individual sources into over 600 individual VOC species.
- **PM Speciation** – the chemical speciation of $PM_{2.5}$ emissions is based on the AQMEII recommendations. The new species required for CMAQv5 have been introduced with zero values.

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[12] Temporal Emission Profiles – report of the NAEI (January 2014)
[13] Temporal variation in emissions from road transport - report of the NAEI (January 2014).
[14] https://www.gov.uk/government/statistical-data-sets/tra03-motor-vehicle-flow Table TRA0307
[15] Temporal Profiles for Ammonia Emissions from Agriculture - report of the NAEI (March 2013)
[16] Passant, N (2002). Speciation of UK emissions of non-methane volatile organic compounds. Report of the NAEI AEAT/ENV/R/0545 (February 2002). http://uk-air.defra.gov.uk/assets/documents/reports/empire/AEAT_ENV_0545_final_v2.pdf

- **NOx Speciation** – Based on the NAEI factors referring to the fraction of NO_x emitted directly as NO_2 (f-NO_2)[17] [18] from individual traffic sources, the overall profile for total road traffic emissions is year specific as the composition of the vehicle fleet changes. For 2006, the average f- NO_2 for all traffic is 12.7 % increasing to 19.9%, 20.4% and 21.5% for 2008, 2010 and 2011 respectively and 22.1%, 21.5% and 21.0% for 2019, 2020 and 2021.

The speciation profiles are used to represent the emissions in the chemical forms used in the chemical scheme in CMAQ. **Table 3** provides a cross reference between the inventory and the model emission species. The figures in this section use a model emission species as a surrogate for the inventory species to demonstrate a cross section of factors applied.

Table 3 Cross reference inventory and model emission species

Inventory Emissions	Model Emissions	Model Description
NMVOC	FORM	Formaldehyde (Methanal)
	PAR	Paraffin carbon bond (C-C) (Alkane)
CO	CO	Carbon monoxide
NOX	NO	Nitric oxide
	NO_2	Nitrogen dioxide
NH_3	NH_3	Ammonia
$PM_{2.5}$	PNO3 - Nitrate PM	Nitrate Particulate Matter (PM_NO_3)
SO_2	SO_2	Sulphur dioxide

3.1.3 Scaling factors for different years and scenarios

As described in Section 2, pollutant- and sector-specific scaling factors are used to convert the base emissions inventory maps into maps for other years. The emission processor is adaptable to allow these factors to be varied in order to run different emission scenarios for countries, sectors or pollutants.

For years 2009-2011, the 2006 TNO-MACC European inventory data have been scaled to 2009 using country- and sector-specific trends data provided by TNO. These have been further scaled to 2010 and 2011 using country-specific data reported to EMEP[19]. For all UK emissions the scaling factors are derived from trends in emissions for each sector reported by the NAEI over these years.

For 2019-2021, the European emissions are scaled using the TSAP_Mar13_CLE ("Current Legislation") scenario available through the GAINS Europe modelling system and UK emissions by the latest projections developed by the NAEI.

Table 4 summarises the scaling factors used to convert the 2009 TNO-MACC European emission maps to the 2020 emissions for a selection of countries in Europe. These are based on the ratios of national emission totals between these years.

[17] Murrells et al., (2010) An Emissions Inventory for Primary NO_2 and Projections for Road Transport: 2008 NAEI: NAEI reference 48954007 http://naei.defra.gov.uk/datachunk.php?f_datachunk_id=324. See also http://naei.defra.gov.uk/data/ef-transport for annually updated information on f-NO_2 factors for road transport
[18] Murrells, T., MacCarthy, J., Passant, N. An Emissions Inventory for Primary NO_2 and Projections for Road Transport: 2008 NAEI. Report 21 March 2010, NAEI Ref 48954007. Not published
[19] EMEP/CEIP (2014): Present state of emissions as used in EMEP models; http://www.ceip.at/ms/ceip_home1/ceip_home/webdab_emepdatabase/reported_emissiondata/

Table 4 Country scaling factors used to scale 2009 European maps to 2020

	CO	NH3	NOx	PM10	PM2.5	SO2	VOC
Austria	0.76	1.07	0.53	0.90	0.81	0.82	0.83
Belgium	1.43	0.91	0.70	0.87	0.77	0.77	0.84
Denmark	0.44	0.82	0.61	0.70	0.60	0.68	0.66
Finland	0.71	0.94	0.64	0.82	0.77	0.76	0.72
France	0.75	0.99	0.55	0.89	0.78	0.47	0.74
Germany	0.80	0.99	0.60	0.85	0.77	0.74	0.83
Greece	0.80	0.89	0.65	0.69	0.70	0.35	0.65
Ireland	1.12	0.97	0.82	1.00	0.95	0.75	0.90
Italy	0.67	1.01	0.60	0.82	0.77	0.65	0.69
Netherlands	0.76	0.87	0.62	0.89	0.78	0.89	0.85
Norway	1.12	1.04	0.83	0.95	0.92	0.98	0.65
Portugal	0.69	1.02	0.62	0.87	0.83	0.78	0.81
Spain	0.92	1.05	0.61	0.96	0.92	0.44	0.81
Sweden	0.69	0.92	0.56	0.93	0.87	0.87	0.80
Switzerland	0.63	1.00	0.63	0.84	0.74	0.76	0.81

3.1.4 Point Source vertical profiles

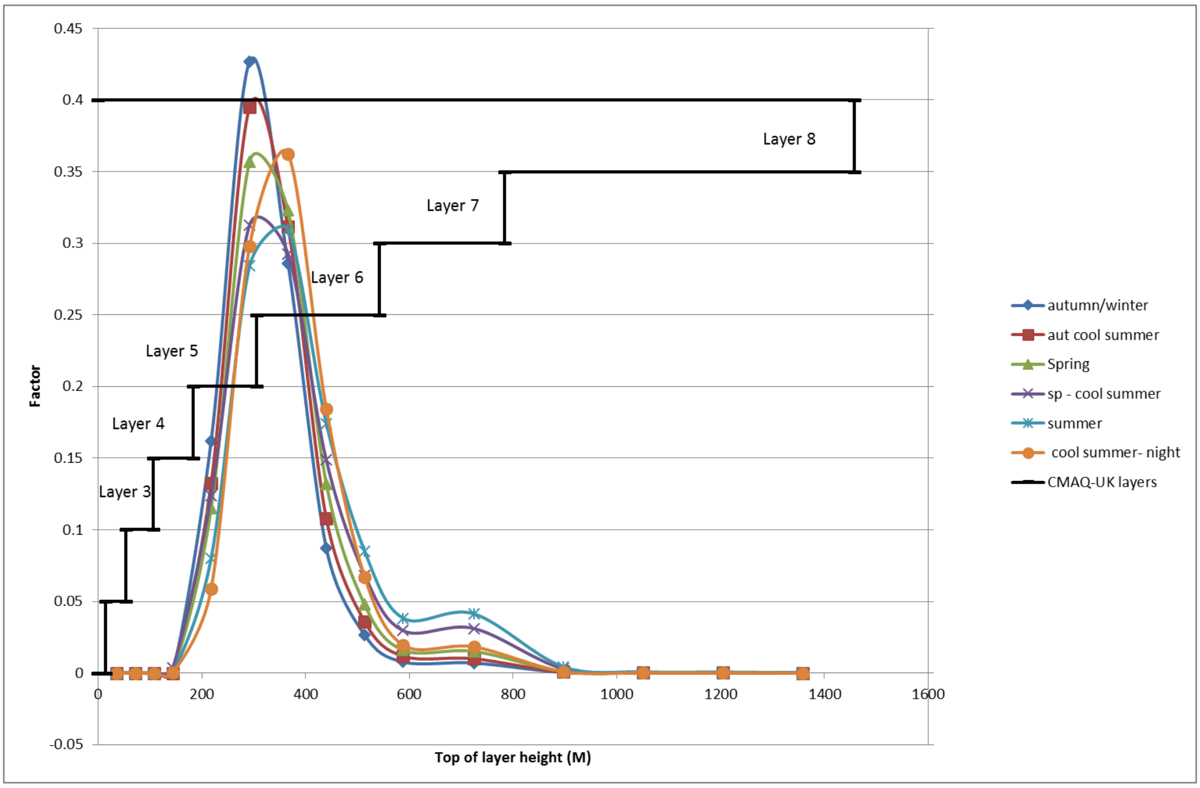
Figure 3 shows the UK vertical profiles from Bieser (2011) with the point on the blue line indicating the top of CMAQ-UK layers.

Calculating the plume rise for all UK points with stack details using the WRF met data (Phase 2), excluding very low wind speeds and taking into account the model vertical resolution, the range of effective release heights does not have a great effect. Taking this and the vertical structure of CMAQ-UK into account, we elected to standardise on three vertical profiles for autumn/winter, spring and summer - releasing the emissions into layers 5, 6 and 7. In Phase 1 point source emissions were released into layer 5.

There is a file of approximately 200 point sources above the 95th percentile of emissions for CO, NO_x, SO_2 or PM_{10} which includes all the stack details. These can be released directly into CMAQ using in-line processing (CMAQv5+) if required. For phase 2 all profiles were treated the same.

The same vertical factors are used for the European emissions as no stack details are available with the TNO-MACC data.

Figure 3 Point sources profiles for the UK from Bieser (2011). The black line indicates the height at the top of the CMAQ layers.



4 Demonstration of Emissions Data from EMST

For each set of emissions created by EMST for CMAQ modelling an information sheet is completed and a series of standard maps and plots are generated to demonstrate the emissions used. Appendix 1 includes the data sheets and check maps run for 2006, 2009-2011 and 2019-2021.

4.1 Mapped emissions for 2009-11 and 2020

The following maps show emissions in the lowest CMAQ-vertical level (i.e. ground level emissions). Emissions from point sources which are released into higher levels are not included in these plots.

Figure 4 shows NO_2 emissions over the UK (in mole/second) for the first Thursday in January and first Thursday in July for each of the years 2009, 2010, 2011 and 2020. **Figure 5** shows the corresponding data for SO_2 emissions. These figures are meant to demonstrate the trend in daily emissions over the years, reflecting changes in the inventory due to changes in activity rates and emission factors as a result of changes in activities, regulation and technologies.

Figure 6 shows the mapped difference in emissions between the first Monday in July of 2010 and 2020 (using the first Monday of the month eliminates variation due to day of the week). The maps on the left show differences in emissions in absolute terms, the maps on the right in fractional terms. For all species except ammonia there is a decrease in emissions over the years. The absolute reduction in emissions is centred on the urban areas for NO, VOC and CO, but in fractional terms are similar across the UK. PM and SO_2 emissions show larger differences over the areas of sea and clear demarcation of the marine sulphur emission control areas. The scaling factors applied for Ireland and France in the UK grid are based on the GAINS factors. These are at a country level and hence show no spatial variation.

4.2 Maps showing temporal variation

Figure 7 shows an example of NO_2 emissions over the UK at 3-hourly intervals over one day on 1st January 2009. **Figure 8** shows the corresponding data for SO_2. These figures are meant to demonstrate the diurnal variation in emissions for a given day.

Further demonstration of the diurnal variation is shown in the openair plots in **Figure 9**. These plots show the hourly, monthly and day of week variation in emissions and demonstrate the effect of the temporal factors. These plots are used to check the factors are being applied correctly. They show emissions released into the model at three locations, a rural and urban background monitoring site along with a location where shipping emissions are relatively high in the English Channel between Dover and Calais. Emissions of NO NO_2 and SO_2 for 2010 and 2020 have been put alongside each other for comparison. Shipping has a flat profile as it is considered to have the same level of activity at all times. The difference in total emission between rural and urban areas and the traffic temporal signature is clear. The difference in the NO and NO_2 profiles relative to shipping demonstrate that the ratio of NOx released as NO_2 is greater for road transport and has a greater influence in the urban areas. All emission are reduced by 2020; for NO and NO_2 the urban areas show the greatest reduction, and for SO_2 it is the shipping areas.

Figure 4 NO_2 emissions: comparison by year for the first Thursday in January (top row) and July (bottom row) for the years 2009, 2010, 2011 and 2020

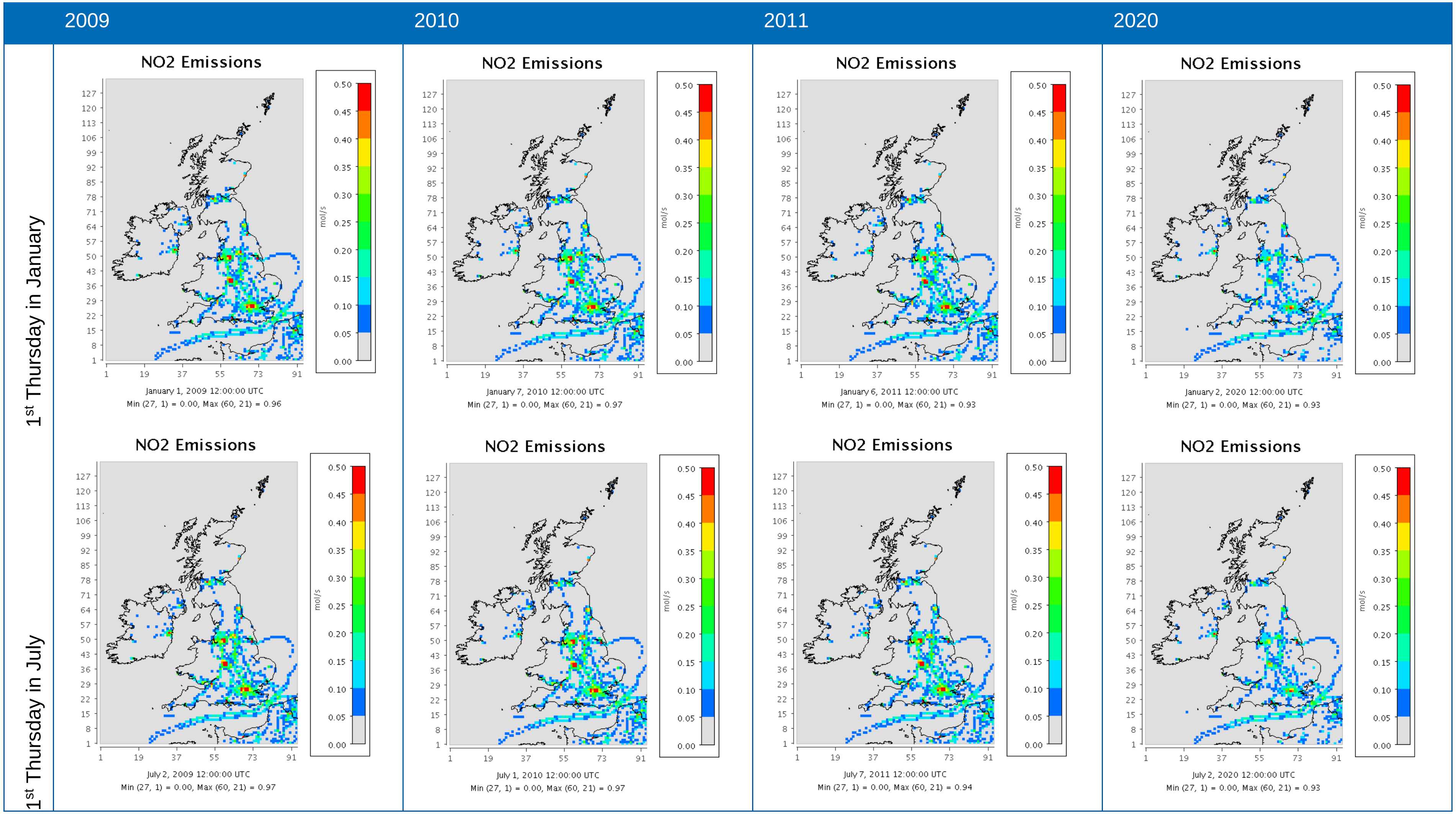


Figure 5 SO_2 emissions: comparison by year for the first Thursday in January (top row) and July (bottom row) for the years 2009, 2010, 2011 and 2020

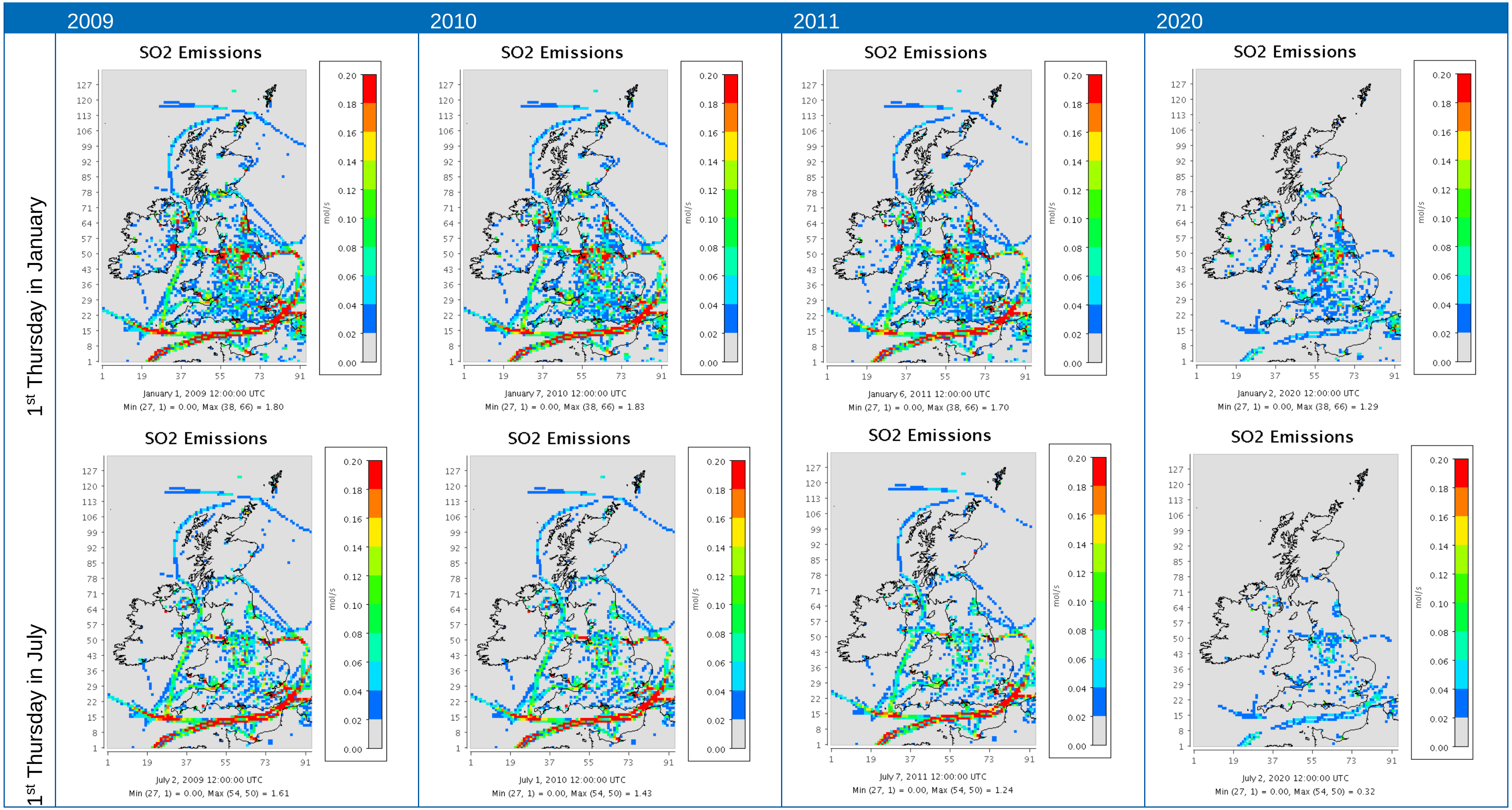


Figure 6 Maps of the difference in UK emissions for first Monday in July of 2010 and 2020 as a) moles s-1 except for PM nitrate (PM_NO3) which are g s-1 (left panel), and b) as factors (right panel)

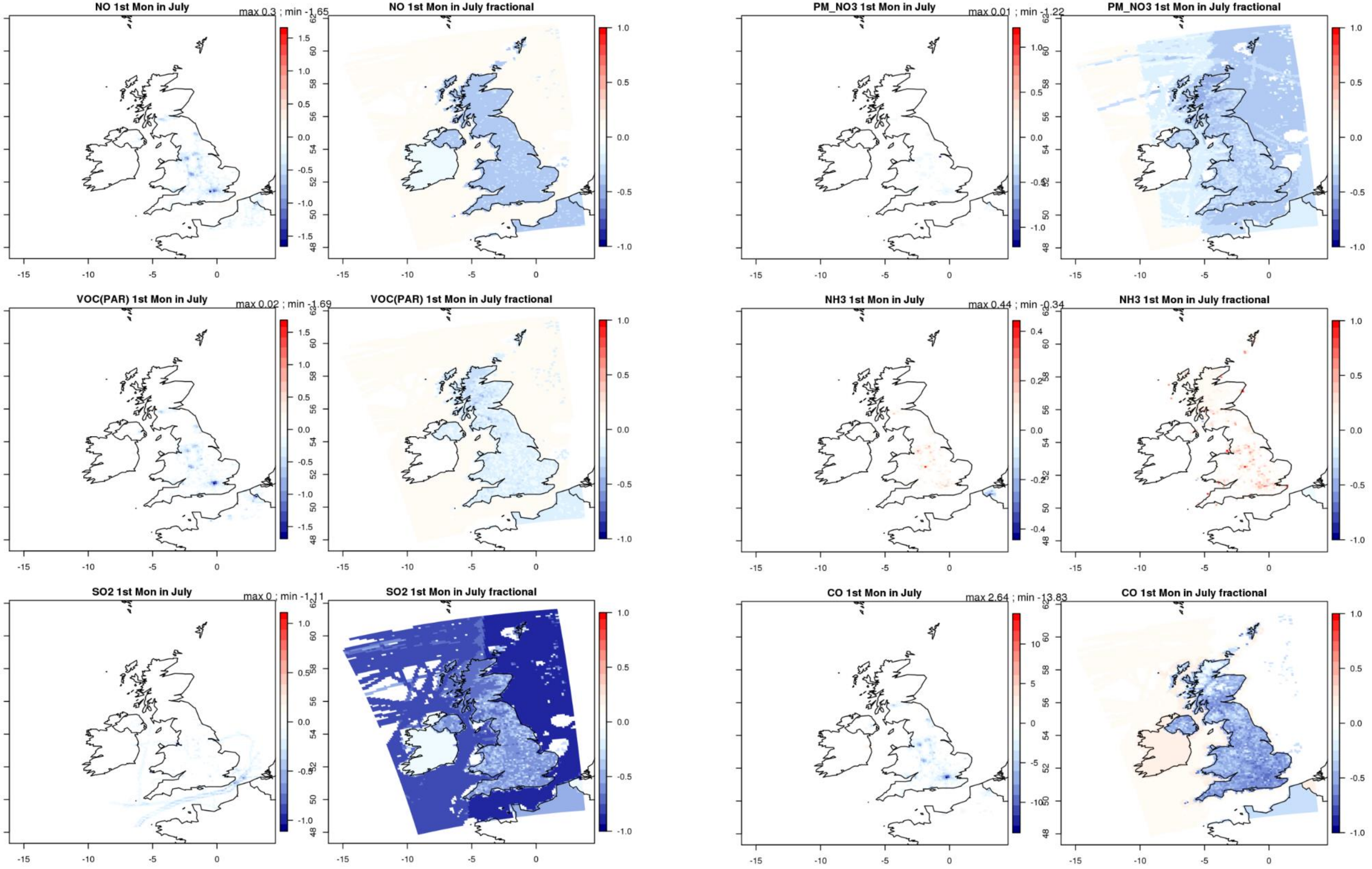


Figure 7 Time series of NO_2 emissions on 01/01/2009 at three-hourly intervals

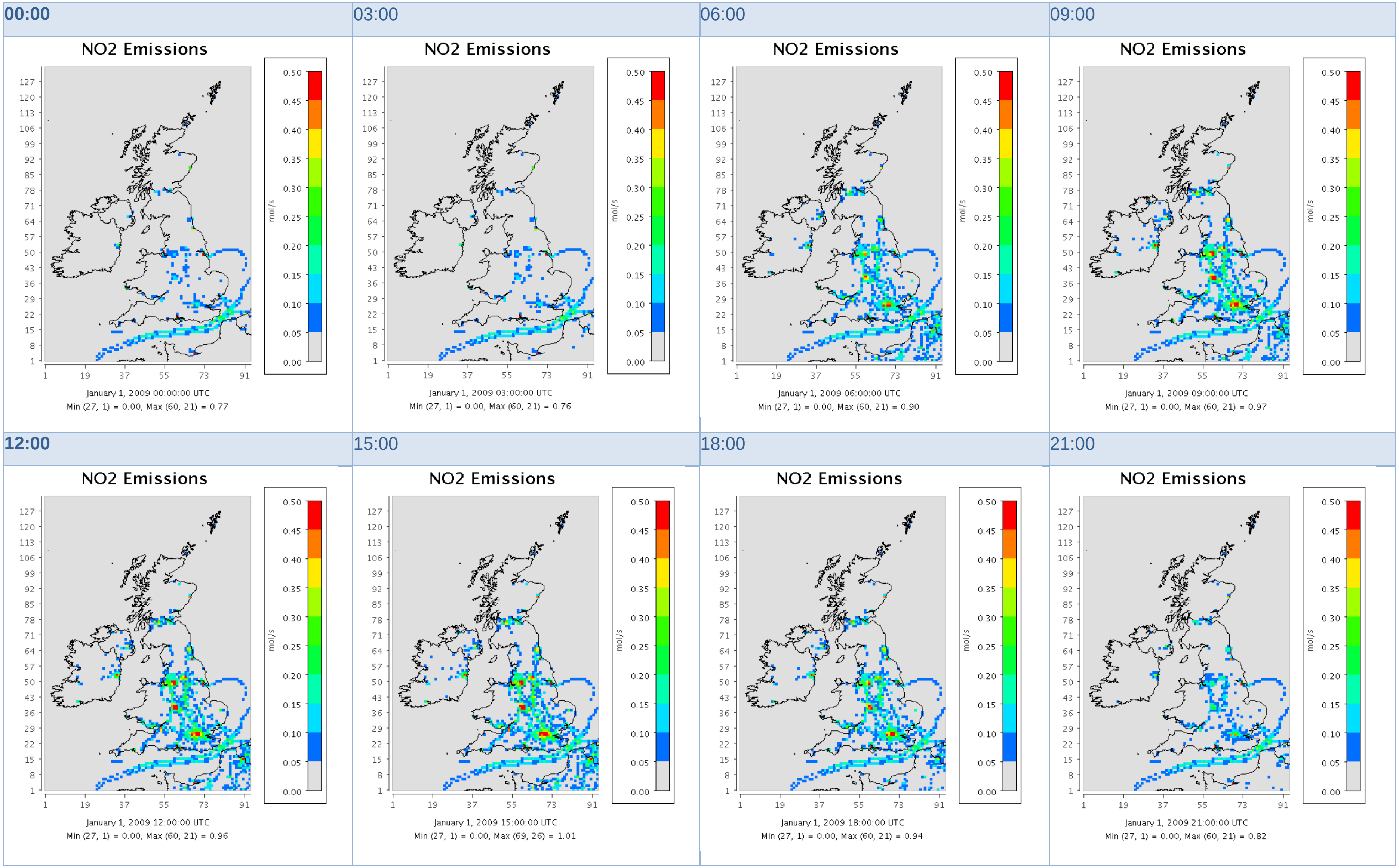


Figure 8 Time series of SO_2 emissions on 01/01/2009 at three-hourly intervals

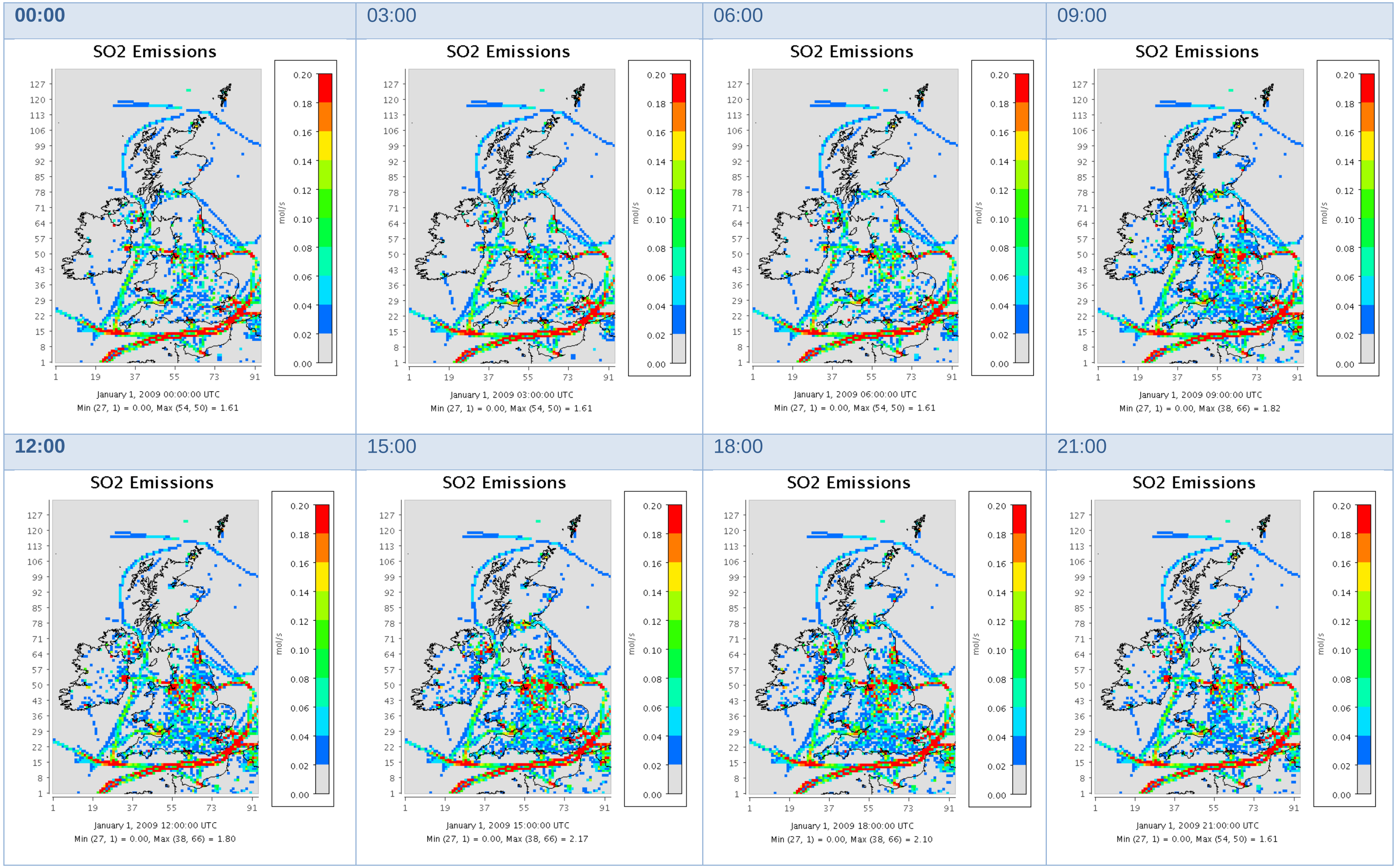
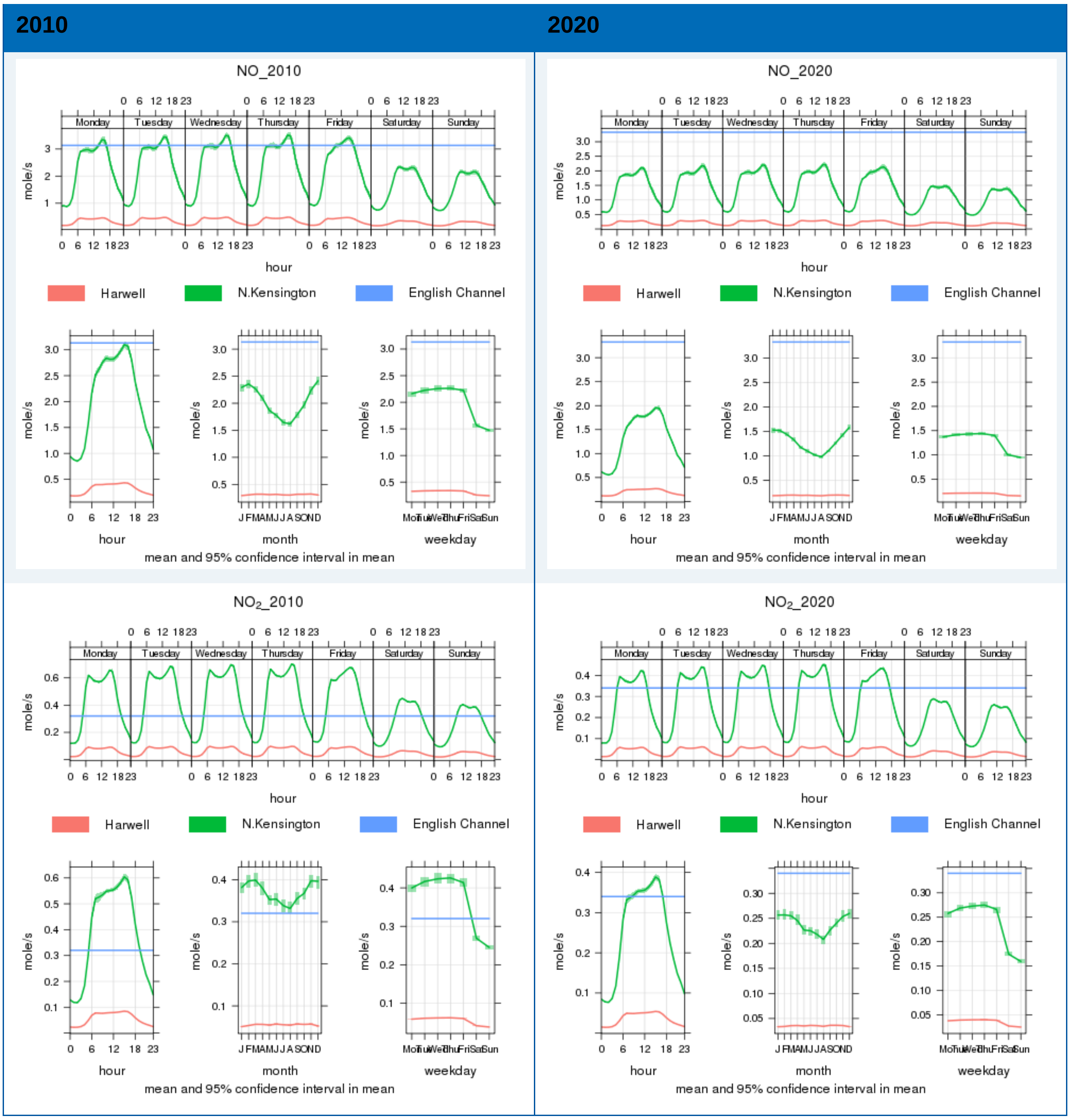
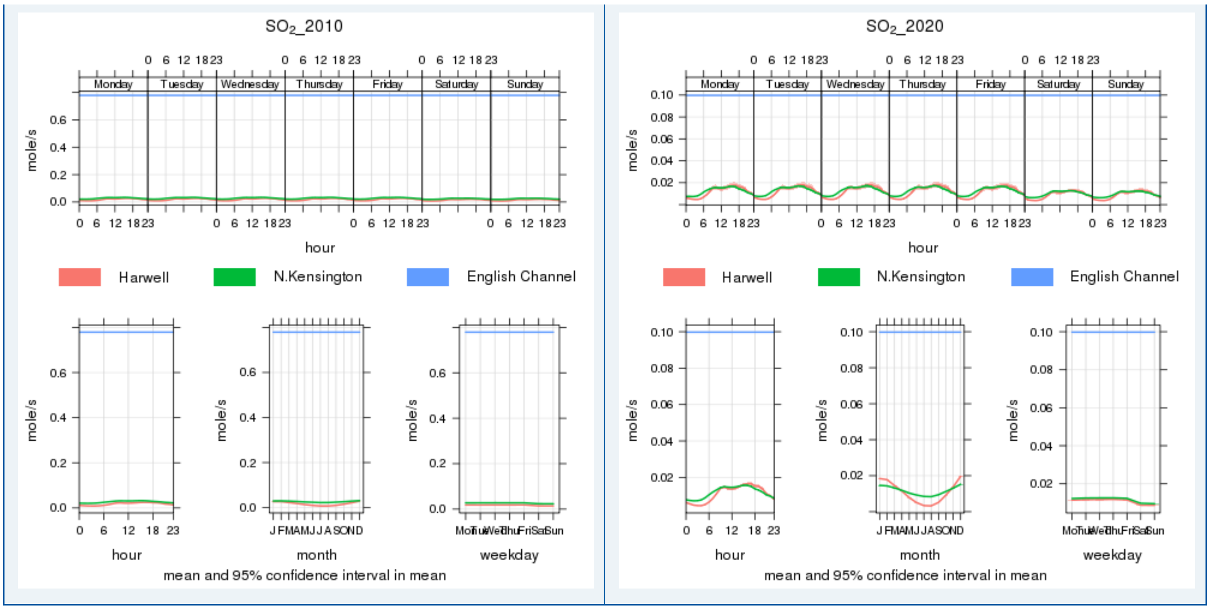


Figure 9 Time variation of emissions at a Rural (Harwell) Urban background (London N. Kensington) and sea (English Channel Dover-Calais)




SO2_2010
SO2_2020
Monday
Tuesday
Wednesday
Thursday
Friday
Saturday
Sunday
mole/s
hour
Harwell
N.Kensington
English Channel
month
weekday
mean and 95% confidence interval in mean

Appendices

Appendix 1: EMST datasheet and maps 2006, 2009-2011, 2019-2021

Appendix 1

EMST datasheet and maps: Emissions 2006

Version: e01 Year: 2006 Grid : EU50 and UK10

Summary

e01 is the base case scenario developed as part of the CMAQ-UK project. It represents a 'best modelling estimate' based on knowledge in December 2013. It incorporates the recommendation from the NAEI (2013) reports (detailed below).

Emissions Inventory

European EU50&UK10	**MACC-TNO 2006 maps (area and points)**
Shipping EU50	MACC-TNO 2006
UK UK10	Scaled to 2006 from 2005 emissions mapped by the NAEI using 2010 NAEI methodologies and scaling factors
Shipping UK10	Scaled from ENTEC 2007 to 2006 using NAEI factors (Military emission not included)
Points UK10	NAEI 2006 from 2012 points database
Biogenic EU50&UK10	Megan2.04 using the CB05SOA mechanism with UH correction

Country Scaling Factors EMST/emis_master/

NAEI spreadsheet: NAEI 11_2005-2011_SNAP_scalingfactors_2011_final.xlsx

AET file: UK10_files/input_data/scaling_factors/UK_factors_2005to2006.csv

Temporal Factors

NAEI report

AET file: UK10_files/input_data/profiles: DAY_factor.csv HR_factor.csv MTH_factor.csv

Speciation Factors

VOC speciation	**VOC speciation is calculated using the spreadsheet developed by Garry Hayman, based on the NAEI's NMVOC speciation profile.**
PM Speciation	PM2.5 speciation is based on the AQMEII recommendations.
NOx Speciation	Based on the NAEI factors, the road traffic profile is year specific, for 2006 NO2 is 12.8 % of NOx.

NAEI report

AET file: UK10_files/input_data/profiles: PM25_species_factors.csv VOC_species_fators.csv OTHER_species_factors.csv

Scenario modifications

No modifications

Figure 10 Evaluation emission maps for first Monday in January 2006: European 50km and UK 10km maps

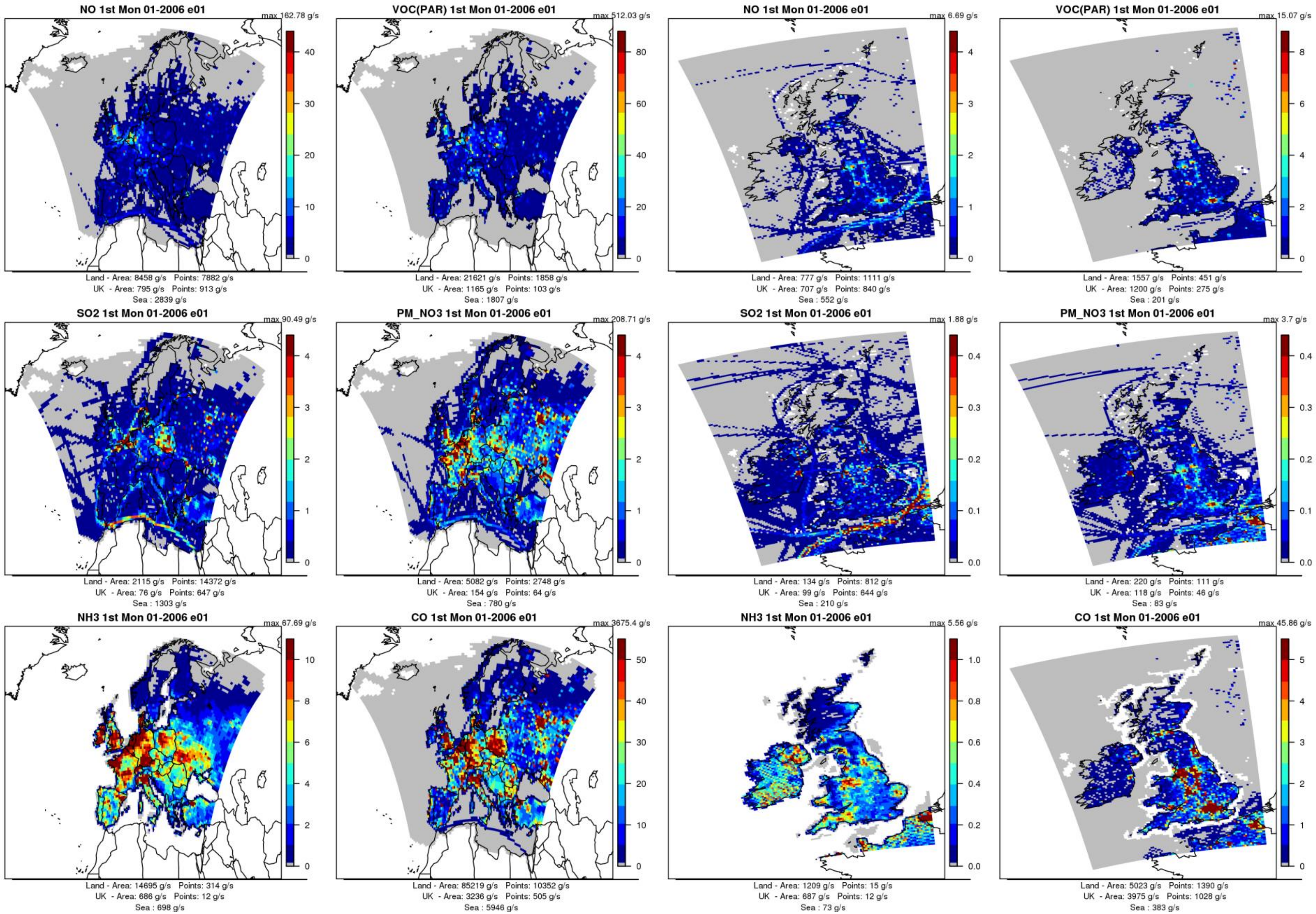
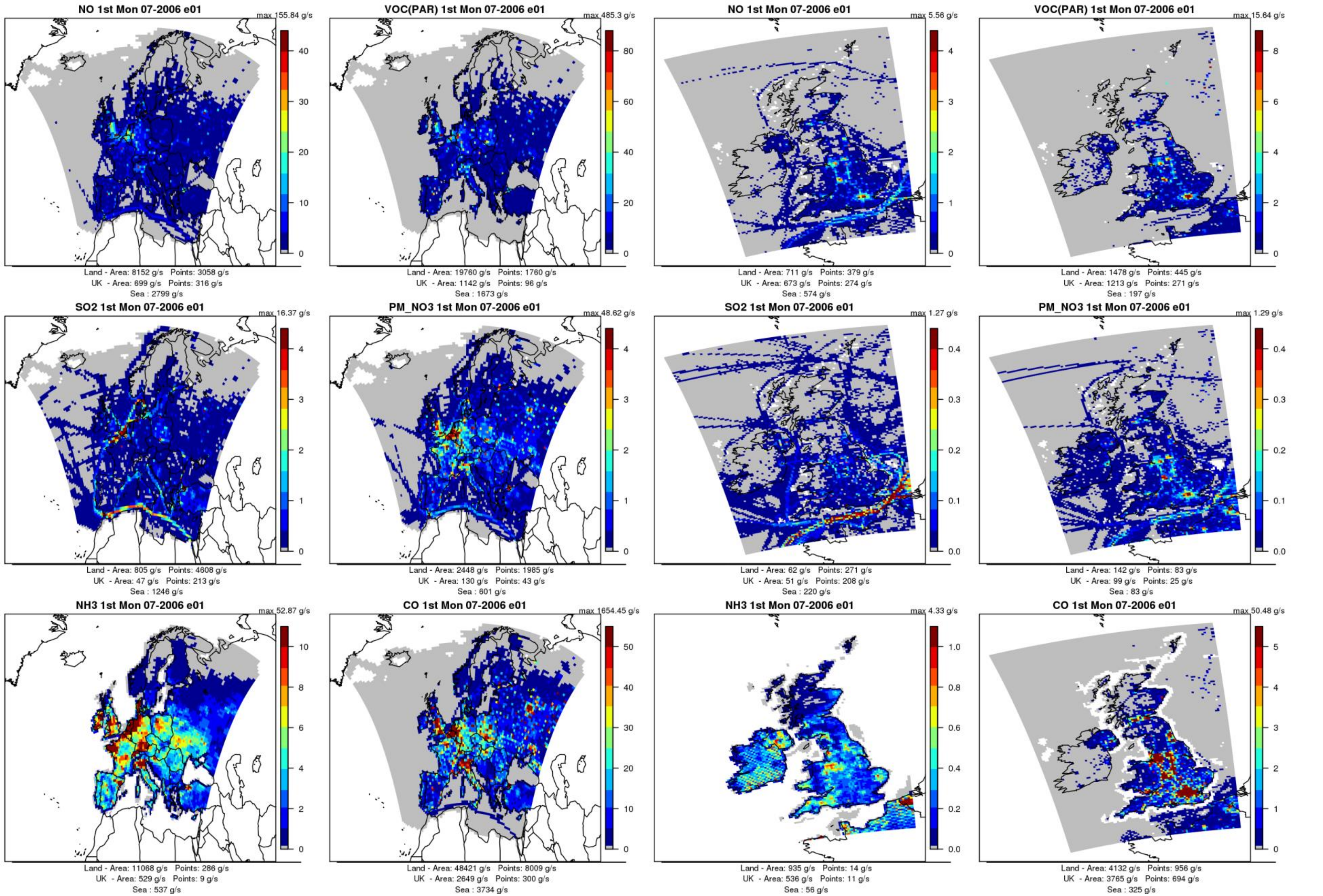


Figure 11 Evaluation emission maps for first Monday in July 2006: European 50km and UK 10km maps



EMST datasheet and maps: Emissions 2009, 2010, 2011

Version: e01 Year: 2009/2010/2011 Grid : EU50 and UK10

Summary

e01 is the base case scenario developed as part of the CMAQ-UK project. It represents a 'best modelling estimate' based on knowledge in December 2013. It incorporates the recommendation from the NAEI (2013) reports (detailed below).

Emissions Inventory

European EU50&UK10	**MACC-TNO 2006 maps (area and points) scaled to 2009 using the MACC-TNO country totals. Then scaled to 2010 and 2011 based on EMEP scaling factors.**
Shipping EU50	Scaled from MACC-TNO 2006 using EMEP trends for 2009,2010,2011 accounting for introduction of SECAs
UK UK10	Scaled from NAEI 2011 maps using the 2011 NAEI national total trends by sector and pollutant derived by the NAEI
Shipping UK10	Scaled from ENTEC 2007 using NAEI (2011) UK trends for 2009,2010, 2011 accounting for introduction of SECAs (Military emission not included)
Points UK10	NAEI 2009/2010/2011 from 2012 points database
Biogenic EU50&UK10	Megan2.04 using the CB05SOA mechanism with UH correction

Country Scaling Factors - EMST/emis_master/

NAEI spreadsheet: NAEI 11_SNAP ScalingFactors_2020_final.xlsx

AET file: /EU50_files/input_data/scaling_factors/2006to2009[10 11]EMEP.csv /EU50[UK10]_files/input_data/scaling_factors/UK_factors_2011to2009[10].csv

Temporal Factors

NAEI report

AET file: UK10_files/input_data/profiles: DAY_factor.csv HR_factor.csv MTH_factor.csv

Speciation Factors

VOC speciation	**VOC speciation is calculated using the spreadsheet developed by Garry Hayman, based on the NAEI's NMVOC speciation profile.**
PM Speciation	PM2.5 speciation is based on the AQMEII recommendations.
NOx Speciation	Based on the NAEI factors, the road traffic profile is year specific. 2009 NO2 is 19.9 % of NOx. 2010 NO2 is 20.4 % of NOx. 2011 NO2 is 21.5 % of NOx.

NAEI report

AET file: UK10_files/input_data/profiles: PM25_species_factors.csv VOC_species_fators.csv OTHER_species_factors.csv

Scenario modifications

No modifications

Figure 12 Evaluation emission maps for first Monday in January and July 2009: UK 10km

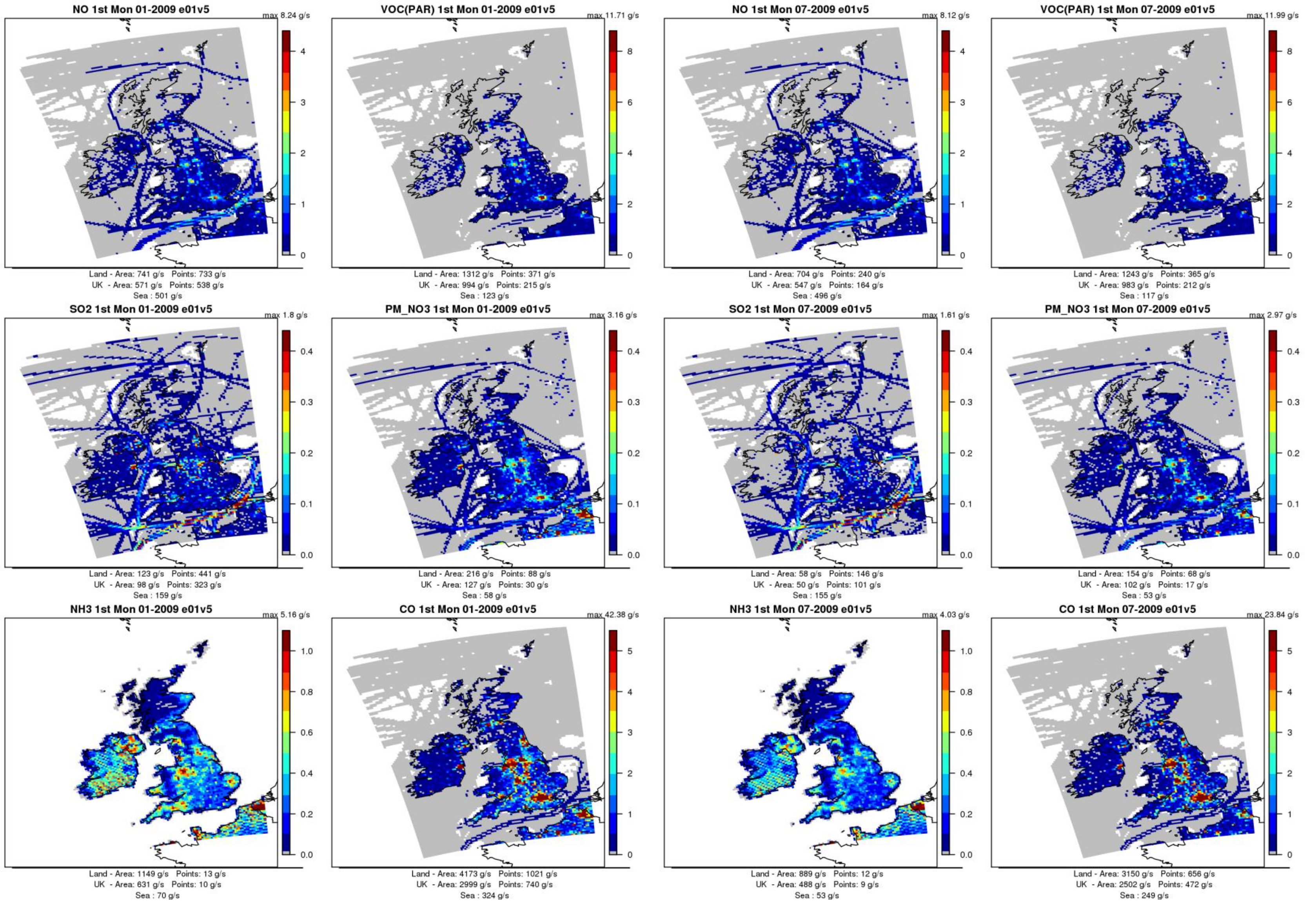


Figure 13 Evaluation emission maps for first Monday in January and July 2010: UK 10km

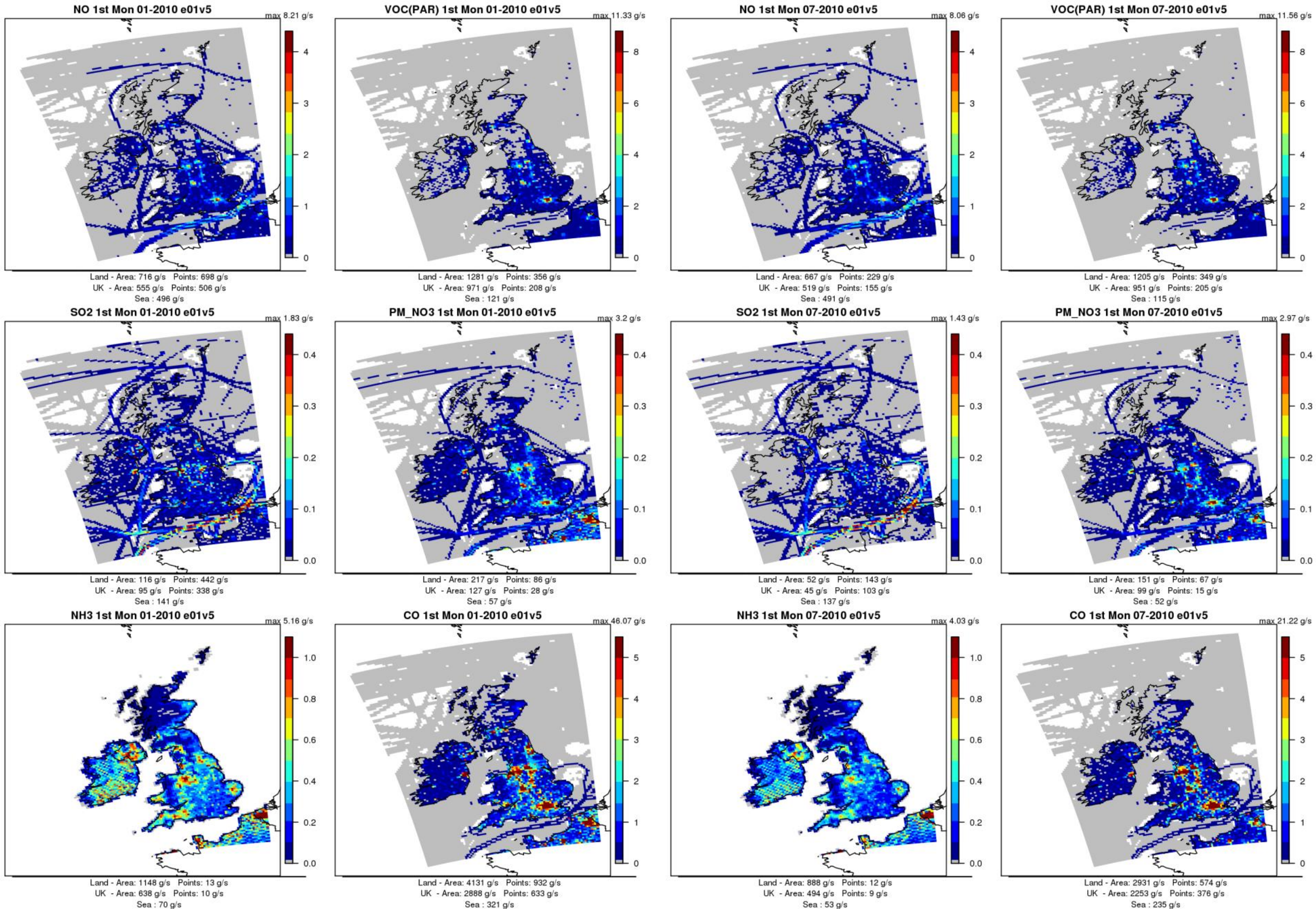
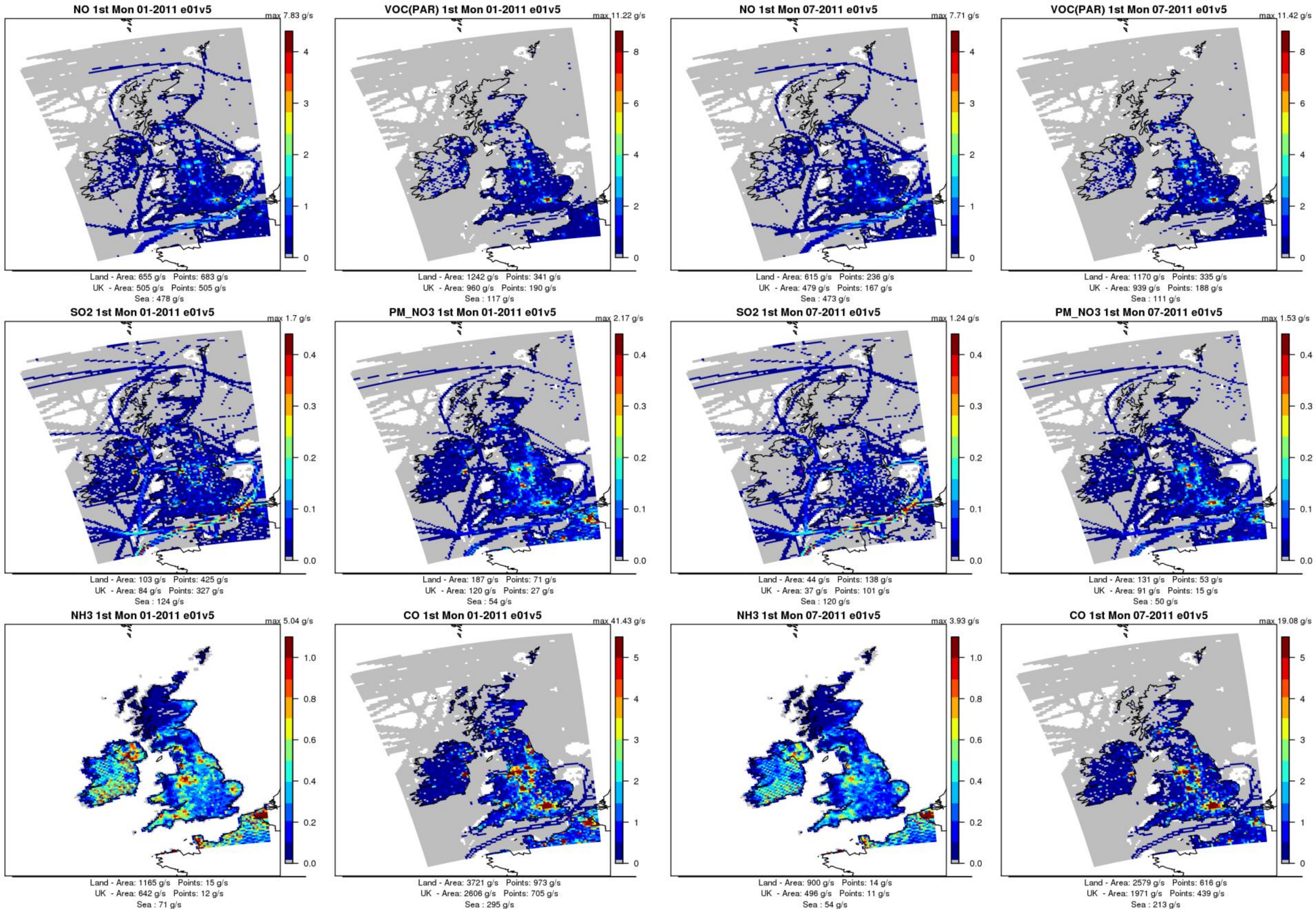


Figure 14 Evaluation emission maps for first Monday in January and July 2011: UK 10km



EMST datasheet and maps: Emissions 2019, 2020, 2021

Version: e01 Year: 2019/2020/2021 Grid : EU50 and UK10

Summary

e01 is the base case scenario developed as part of the CMAQ-UK project. It represents a 'best modelling estimate' based on knowledge in December 2013. It incorporates the recommendation from the NAEI (2013) reports (detailed below).

Emissions Inventory

European EU50&UK10	**Maps created for 2009 are scaled to 2019/2020/2021 using the PRIMES12_CLE projections from the TSAP2013 report #10.**
Shipping EU50	Scaled from 2009 emissions using the PRIMES12_CLE projections from the TSAP2013 report #10, including European SCMFD regulations for 2015
UK UK10	Scaled from NAEI 2011 maps using the 2011 NAEI national total trends by sector and pollutant derived by the NAEI from the UEP45 DECC energy projections and the NAEI Base 2013c road transport projections
Shipping UK10	ENTEC 2007 Scaled using NAEI projections, including European SCMFD regulations for 2015 (Military emission not included)
Points UK10	NAEI 2020 projections from 2012 database Scaled from MACC-TNO(2006)
Biogenic EU50&UK10	Megan2.04 using the CB05SOA mechanism

Country Scaling Factors - EMST/emis_master/

European projections PRIMES report - http://www.iiasa.ac.at/web/home/research/researchPrograms/MitigationofAirPollutionandGreenhousegases/TSAP-review.en.html report #10

NAEI spreadsheet: xxxxxxxxxxxxx

AET file: /EU50_files/input_data/scaling_factors/2006to2009[10 11]EMEP.csv /EU50[UK10]_files/input_data/scaling_factors/UK_factors_2011to2009[10].csv

Temporal Factors

NAEI report

AET file: UK10_files/input_data/profiles: DAY_factor.csv HR_factor.csv MTH_factor.csv

Speciation Factors

VOC speciation	**VOC speciation is calculated using the spreadsheet developed by Garry Hayman, based on the NAEI's NMVOC speciation profile.**
PM Speciation	PM2.5 speciation is based on the AQMEII recommendations.
NOx Speciation	Based on the NAEI factors, the road traffic profile is year specific, for 2019-2021 NO2 is 21.5 % of NOx.

NAEI report

AET file: UK10_files/input_data/profiles: PM25_species_factors.csv VOC_species_fators.csv OTHER_species_factors.csv

Scenario modifications

No modifications

Figure 15 Evaluation emission maps for first Monday in January and July 2019: UK 10km

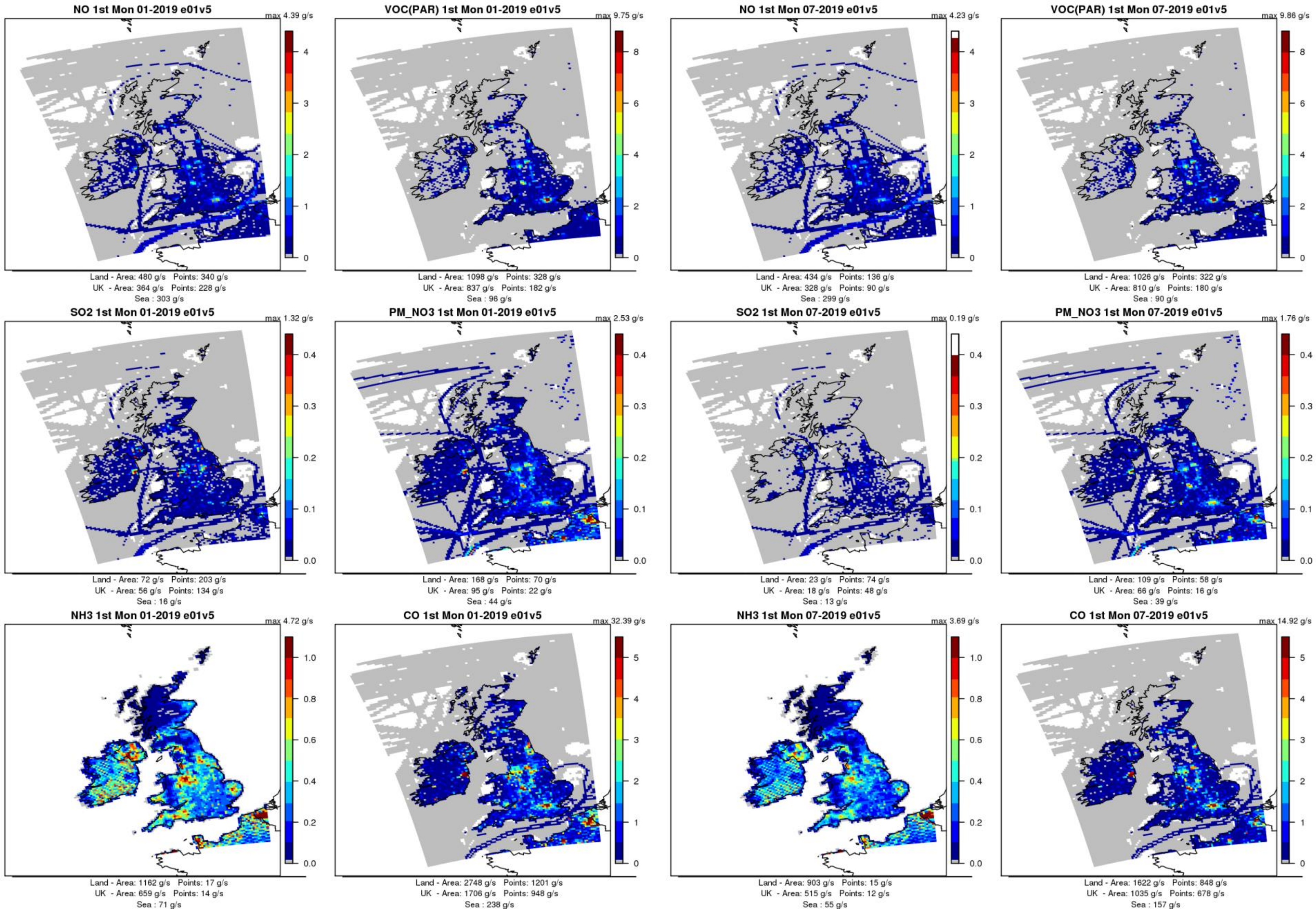


Figure 16 Evaluation emission maps for first Monday in January and July 2020: UK 10km

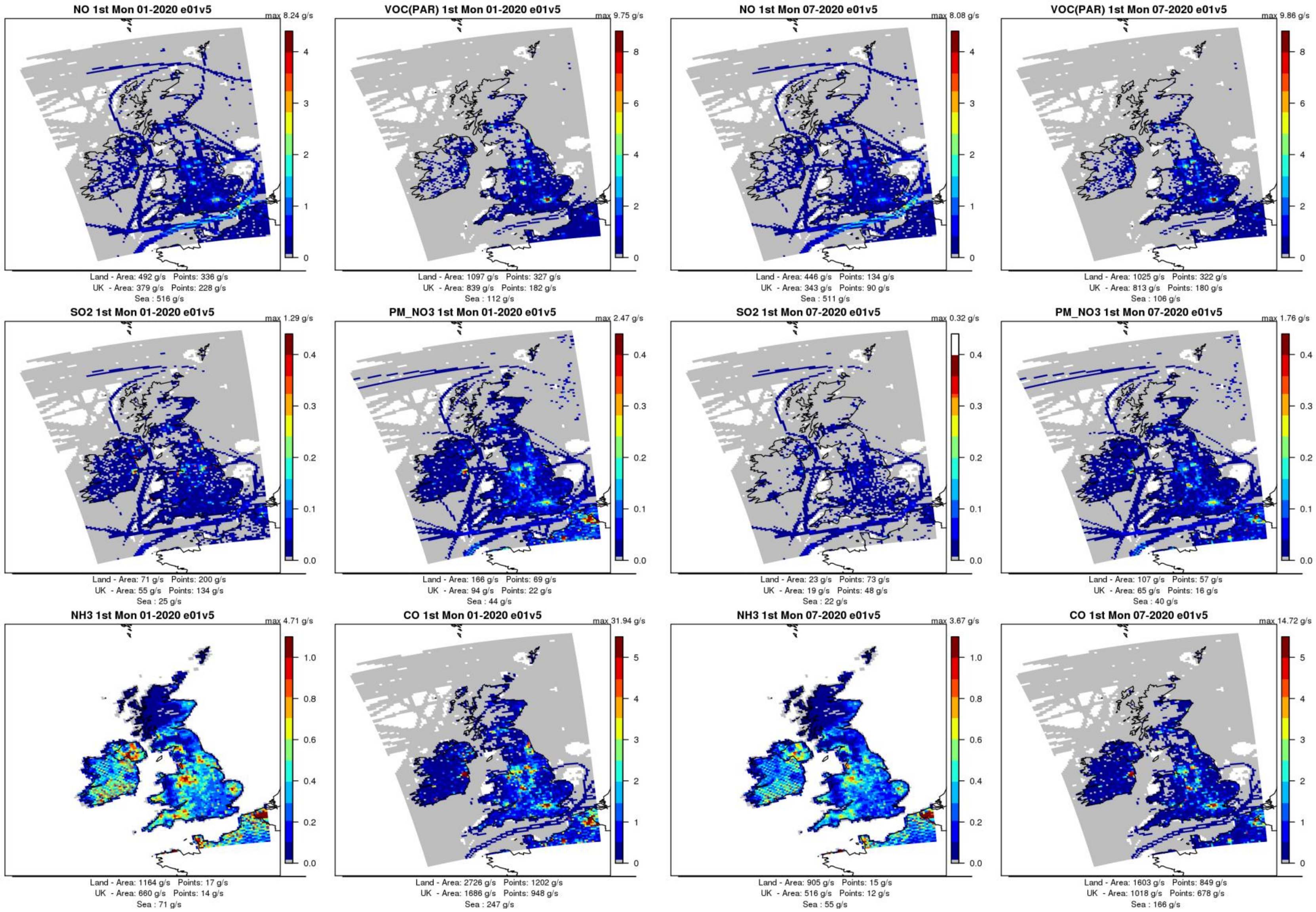
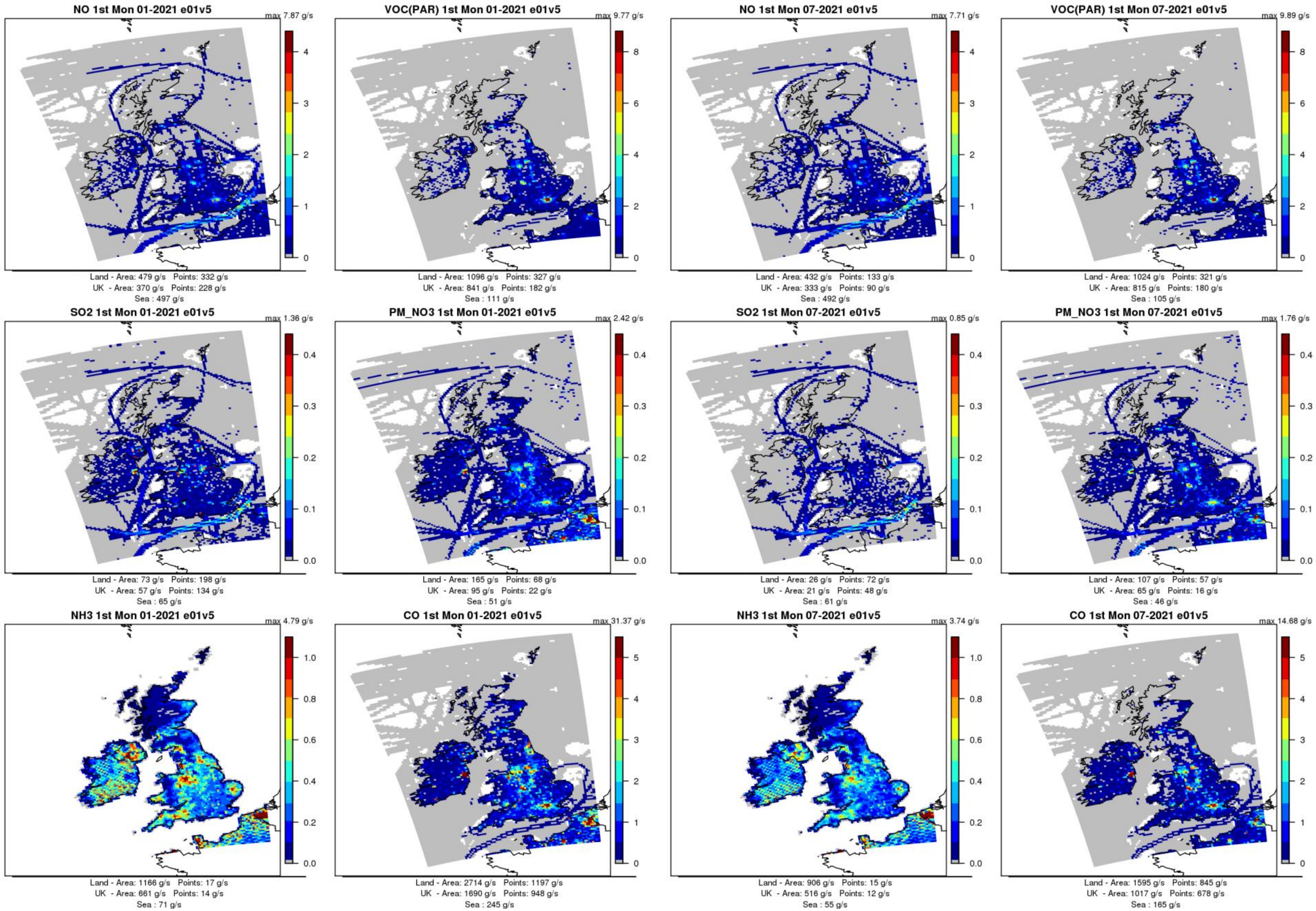


Figure 17 Evaluation emission maps for first Monday in January and July 2021: UK 10km



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