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ÉCLAIRE

Effects of Climate Change on Air Pollution Impacts and Response Strategies for European Ecosystems

Seventh Framework Programme

Theme: Environment

D8.4: Sub-Grid module for inclusion in the EMEP model

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PU	Public	☐
PP	Restricted to other programme participants (including the Commission Services)	☒
RE	Restricted to a group specified by the consortium (including the Commission Services)	☐
CO	Confidential, only for members of the consortium (including the Commission Services)	☐

1. Executive Summary

- Currently, chemical transport models applied at a European scale, such as the EMEP MSC-W model, lack the spatial resolution necessary to simulate the spatial variability of impacts of air pollution on European ecosystems
- This spatial variability is especially important for assessing the impacts of short-lived pollutants, such as ammonia (NH_3) or nitrogen dioxide (NO_2) or the impacts of nitrogen deposition, which strongly depend on land cover and precipitation patterns
- In order to simulate this spatial variability, two “sub-grid” models have been developed to estimate the spatial distributions (at a spatial resolution of 1×1 km^2) of atmospheric concentrations and nitrogen deposition rates within the grid squares of a chemical transport model (e.g. the 50 km × 50 km grid squares of the EMEP model)
- The sub-grid model for atmospheric concentrations of NO_2 and NH_3 combines high resolution emission data with a simple parameterisation of atmospheric dispersion to simulate the spatial distribution of concentrations within each grid square of the chemical transport model
- For NH_3, which is emitted mostly by agricultural sources, it is reasonable to assume that the emission occurs close to ground level. However, NO_x has both near-ground-level sources (e.g. road transport) and elevated sources (e.g. chimney stacks). The sub-grid model for NO_2 concentrations, therefore, includes an emission threshold that determines whether a source square is a ground-level source or an elevated source
- The sub-grid model for nitrogen deposition uses the high resolution NH_3 concentration data (from the first sub-model) to simulate the spatial distribution of dry deposition of reduced nitrogen. The spatial distributions of wet deposition of both reduced and oxidised nitrogen are based on the spatial distributions of high resolution precipitation maps. It has not been possible to develop a sub-grid model for the dry deposition of oxidised nitrogen
- Both sub-models have been applied to two contrasting areas (Central Scotland and the Netherlands) and model performance of both the EMEP model and the sub-grid model has been assessed using monitoring data of atmospheric concentrations and wet deposition for both study areas
- The sub-grid model for atmospheric concentrations represents a substantial improvement on the predictions of the EMEP model reducing both model error and increasing the spatial correlation with the measured concentrations
- The performance of the sub-grid model for wet deposition, however, is similar to that of the EMEP model and provides only a small improvement on the deposition predictions

2. Objectives:

The objective of this deliverable is the development of a parameterisation (module) that can simulate the sub-grid spatial distributions of mean annual concentrations and deposition rates of air pollutants (specifically ammonia, nitrogen dioxide and nitrogen deposition) within the grid cell of a chemical transport model (e.g. the EMEP MSC-W model) using high spatial resolution emission and land cover data.

3. Activities:

3.1. Development of a sub-grid model for mean annual air pollutant concentrations

A sub-grid model was developed that combines high-spatial-resolution emission data and a simple parameterisation of short-range dispersion to estimate the spatial distribution (at a resolution of 1 × 1 km^2) of the concentrations of ammonia (NH_3) and nitrogen dioxide (NO_2) within the 50 km × 50 km (approx.) grid squares of the EMEP (MSC-W) model (Simpson et al., 2003). Pollutant dispersion from emission sources was parameterised using a simple scenario of a single 1 × 1 km^2 source with a constant emission of 1 tonne km^{-2} yr^{-1} in the centre of a square domain (of dimensions 101 × 101 km^2).

For the dispersion of NH_3, the source was assumed to be at ground level (a suitable approximation for agricultural sources). For the dispersion of NO_2, two different source heights were used: ground level to represent traffic sources and 400 m to represent industrial stack sources. Since no information is available in the emission inventories on the source type or height, it was necessary to determine whether a 1 × 1 km^2 square is predominantly traffic sources or stack sources. This was done by setting a threshold for stack emissions of NO_x + SO_x of 150 tonnes km^{-2} yr^{-1}. The sum of NO_x and SO_x was used since it makes a larger distinction between traffic and industrial sources then using NO_x alone. The threshold value was chosen so that it was large enough to exclude known traffic sources (e.g. Rhine river traffic in the Netherlands) but include known power station sources (identified from the European Pollutant Release and Transfer Register). A range of values for both the stack source height (100, 200, 400 and 800 m) and stack emission threshold (100, 150, 250 and 250 tonnes km^{-2} yr^{-1}) were also used to analyse the sensitivity of the model to these parameters.

For the ground level sources, three dispersion models (ADMS 4, AERMOD v12345 and LADD) were used to simulate the annual mean near-ground-level concentrations of NH_3 and NO_2 on a 1 km grid (for the 101 × 101 km^2 domain) using data from the Lyneham meteorological station in the UK for 1995. This dataset was chosen because it has been used in various model evaluation studies (e.g. Spanton et al. (2004), Theobald et al. (2012)). In order to make the dataset less location-specific the wind direction data were randomised and the wind speed was scaled so that the annual mean value was equal to the annual domain mean value used in the EMEP model for the 2008 study year (5.1 m s^{-1}). The use of a single meteorological dataset for the development of a model applied at the European scale from a location in the UK for a year different to the study year may introduce a large amount of uncertainty in the predictions. In order to assess this uncertainty, two domain-specific meteorological datasets for the study year were also tested. These datasets were from Easter Bush, for Scotland (see Famulari et al., (2004) for site details) and Cabauw, for the Netherlands (obtained from the Cabauw Experimental Site for Atmospheric Research (Cesar) website).

For the elevated source scenario (NO_x stack emissions), only ADMS and AERMOD were used to simulate the annual mean concentrations because the LADD model is not suitable for simulating dispersion from elevated sources (Theobald et al., 2012). A height of 1.5 m was used for the near-ground-level concentrations, because this height is commonly used for concentration monitoring and impact assessments (Cape et al., 2009). No removal processes (chemical reactions, dry or wet deposition etc.) were simulated because these processes depend strongly on local conditions (concentrations of other chemical species, meteorological conditions, surface characteristics, etc.). For this reason, the concentration predictions for the ground level NH_3 and NO_x sources are identical. The result of these simulations was five concentration fields (three for ground level sources and two for elevated sources) centred on the source location from which the grid-square average concentration was calculated for each source type (Figure 1). The two resulting concentration fields (for a ground and elevated source) were then multiplied by the emission data using a “moving window” approach and the results summed over the entire test domain. Separate calculations were carried out for the NO_x ground and stack source squares, that were then added together.

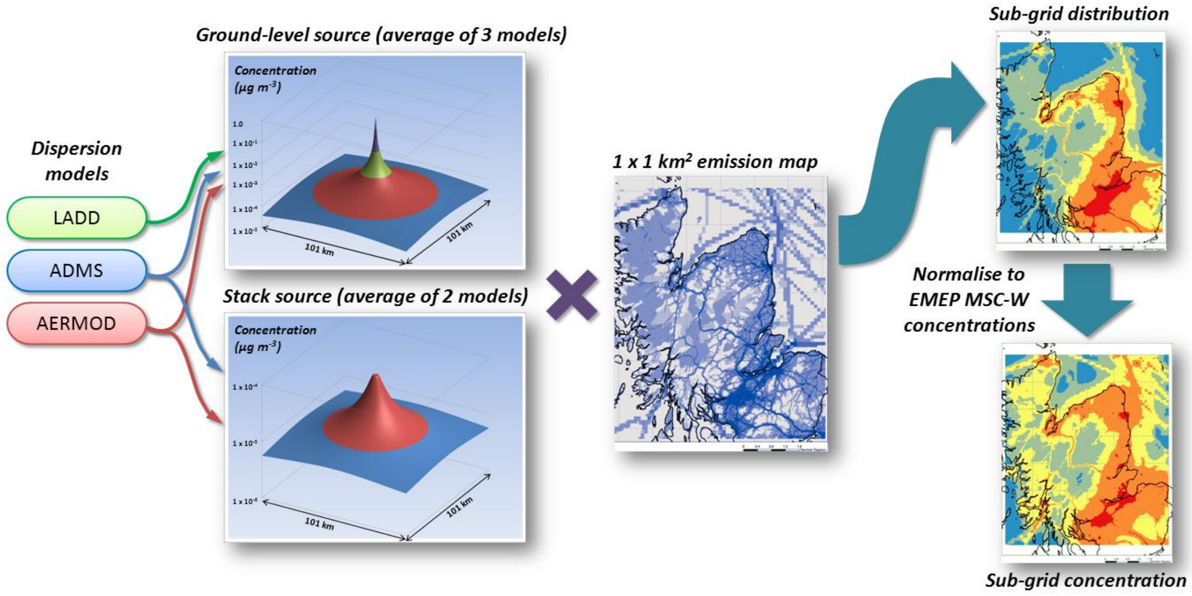

Figure 1: Schematic showing the process of producing the sub-grid concentration predictions from short-range dispersion model simulations and high spatial resolution emission data.

The resulting “sub-grid distributions” provide an estimate of the spatial variability of the concentrations at a 1 km resolution, which were then used to “redistribute” the 50 × 50 km^2 concentration predictions of the EMEP model. This was done by interpolating the concentration predictions of the EMEP model and the mean concentrations of the sub-grid distribution within each 50 × 50 km^2 grid square across the whole domain. The “sub-grid predictions” were then calculated by multiplying the sub-grid distributions by the interpolated EMEP predictions and then dividing by the interpolated sub-grid distribution (Figure 2).

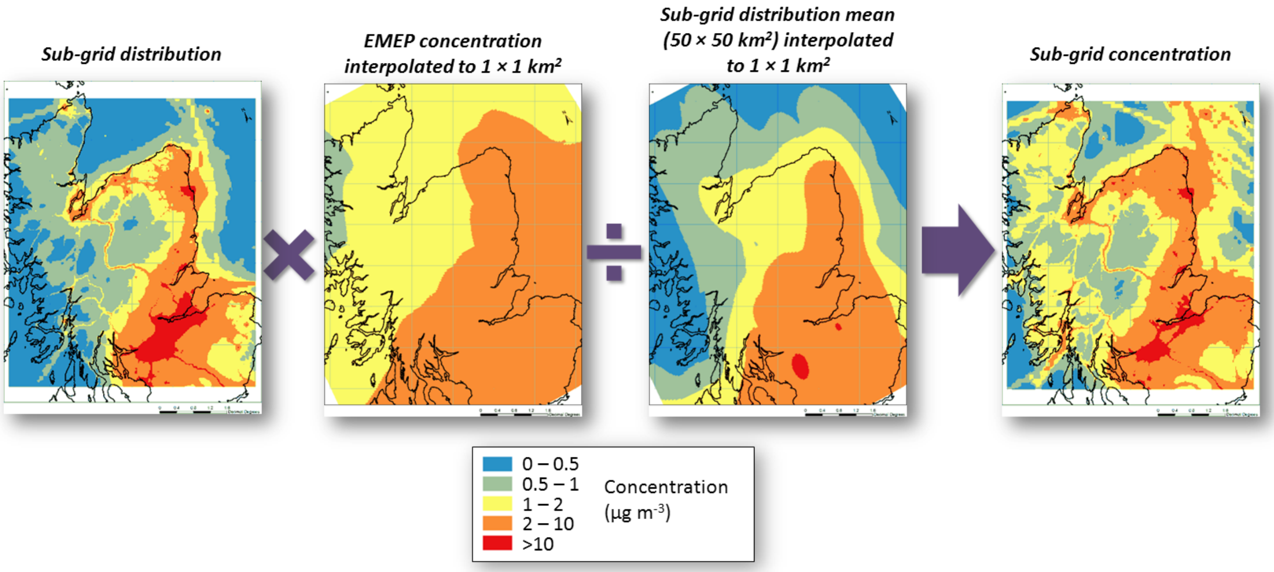

Figure 2: The process of converting the sub-grid distributions to sub-grid concentrations for an example dataset (NO_2 in Central Scotland).

The sub-grid model has been written in the “R” programming language (R Core Team, 2015) and the interpolation routines are carried out in ArcGIS 10.2 (Environmental Systems Research Institute, Redlands, CA, USA). Since the model has been designed as a “post-processor”, it can be run after atmospheric concentrations have been simulated with the EMEP model. The model therefore has not been incorporated into the EMEP model, thus allowing the flexibility of development outside of the development programme of the EMEP model and the possibility of applying the sub-grid model to historic runs of the EMEP model.

3.2. Development of a sub-grid model for mean annual wet and dry nitrogen deposition

Separate sub-grid parameterisations were developed for three of the four components of nitrogen deposition (wet oxidised, wet reduced and dry reduced). It was not possible to develop a simple parameterisation for dry deposition of oxidised nitrogen due to the contributions from multiple compounds, each affected by different transport and transformation processes. Dry deposition of reduced nitrogen is mainly the dry deposition of NH_3 and therefore the sub-grid distribution of NH_3 can be used for the sub-grid distribution of the dry deposition of reduced nitrogen. The spatial distribution of wet deposition of nitrogen is influenced both by the atmospheric concentrations of nitrogenous compounds and precipitation rates. The proxy used to estimate the sub-grid variability of wet deposition was the product of high spatial resolution annual precipitation data and the atmospheric concentrations of nitrate and ammonium (from the EMEP model), for deposition of oxidised and reduced nitrogen, respectively. Sub-grid total nitrogen deposition is calculated as the sum of the total wet deposition and the dry deposition of reduced nitrogen simulated by the sub-grid model plus the EMEP model estimate of dry deposition of oxidised nitrogen.

3.3. Application to two test domains for 2008

In order to test and evaluate the sub-grid parameterisations, they were applied to two test domains: the Netherlands and Central Scotland for the year 2008. For Central Scotland, high spatial resolution (1 × 1 km^2) NH_3, NO_x and SO_2 emission data, data were derived from the National Atmospheric Emission Inventory (NAEI, http://naei.defra.gov.uk). For the Netherlands, high spatial resolution (1 × 1 km^2) NH_3, NO_x and SO_2 emission data were obtained from RIVM. For the precipitation, high resolution (1 × 1 km^2) annual precipitation maps were simulated using the Weather Research and Forecast (WRF) model version 3.6.1 (www.wrf-model.org).

3.4. Evaluation of model performance

Evaluation of the performance of the sub-grid model for concentrations was carried out by comparing the predicted concentrations with 2008 mean annual concentration data from local and national monitoring networks in the two study domains. For the Scottish domain, NO_2 data from 49 monitoring stations were obtained from the Air Quality in Scotland website (http://www.scottishairquality.co.uk/) and NH_3 data from 14 sites of the National Ammonia Monitoring Network (NAMN) were obtained from the UK Pollutant Deposition website (http://pollutantdeposition.defra.gov.uk/networks). Of the 49 NO_2 monitoring stations, 38 are traffic stations (designated as either roadside or kerbside). The remaining 11 stations are designated as rural, suburban, urban background, urban industrial or airport. In addition, NH_3 monitoring data from a local network covering 36 km^2 (Vogt et al., 2013) was also used to assess sub-grid variability. Vogt et al. (2013) included some measurements made within 300 m of large poultry farms. Since these sites are not representative of the 1 × 1 km^2 grid square they are located in, they have been removed from the analysis. For the Dutch domain, national monitoring data for mean annual NH_3 and NO_2 concentrations for 112 and 43 sites, respectively, were provided by RIVM.

Evaluation of the performance of the sub-grid model for wet nitrogen deposition was carried out by comparing the predicted annual (2008) deposition rates of oxidised and reduced nitrogen with data from national monitoring networks in the two study domains. For the Scottish domain, precipitation and rain chemistry data (ammonium and nitrate concentrations) were obtained for 12 sites from the Defra website (http://uk-air.defra.gov.uk/data/) and for the Netherlands domain, data from 11 sites were provided by RIVM. Wet deposition rates were calculated by multiplying the precipitation for each measurement period by the ammonium and nitrate concentrations and summed over the whole year.

Model performance was assessed using the evaluation statistics of the R package "OpenAir" (Carslaw and Ropkins, 2012), that compare the modelled concentrations (M_i) with the observed values (O_i):

Fraction of model predictions within a factor of two of the observations (FAC2):

$$0.5 \le \frac{M_i}{O_i} \le 2.0$$

Normalised mean bias:

$$NMB = \frac{\sum_{i=1}^{n} M_i - O_i}{\sum_{i=1}^{n} O_i}$$

Normalised mean gross error:

$$NMGE = \frac{\sum_{i=1}^{n} |M_i - O_i|}{\sum_{i=1}^{n} O_i}$$

Pearson correlation coefficient:

$$r = \frac{1}{(n-1)} \sum_{i=1}^{n} \left(\frac{M_i - \overline{M}}{\sigma_M} \right) \left(\frac{O_i - \overline{O}}{\sigma_O} \right)$$

4. Results:

4.1. Sub-grid predictions for NO_2 and NH_3 concentrations

Figure 3 shows the sub-grid concentration predictions for NO_2 and NH_3 for the two domains. The EMEP model concentration fields are also shown for comparison.

Table 1 shows the evaluation statistics of the EMEP and sub-grid models for annual mean NO_2 concentrations for the Dutch and Scottish monitoring data. The EMEP model underestimates concentrations, on average, for all datasets (negative NMB). The error of the EMEP model is largest for the Scottish dataset with a NMGE of 82% and 70% for the datasets with and without traffic stations, respectively. The EMEP model performs considerably better for the Dutch dataset, with 92% of predictions within a factor of two of the observed values. The sub-grid model also performed best for the Dutch dataset, with a smaller bias and better correlation than the EMEP model, although the mean error is similar. The sub-grid model also out-performed the EMEP model for the Scottish dataset (both with and without traffic stations), as well of for the combined dataset (Netherlands + Scotland without traffic stations). Figure 4 shows the scatterplots of predictions of the EMEP and sub-grid model *vs.* the measured NO_2 concentrations.

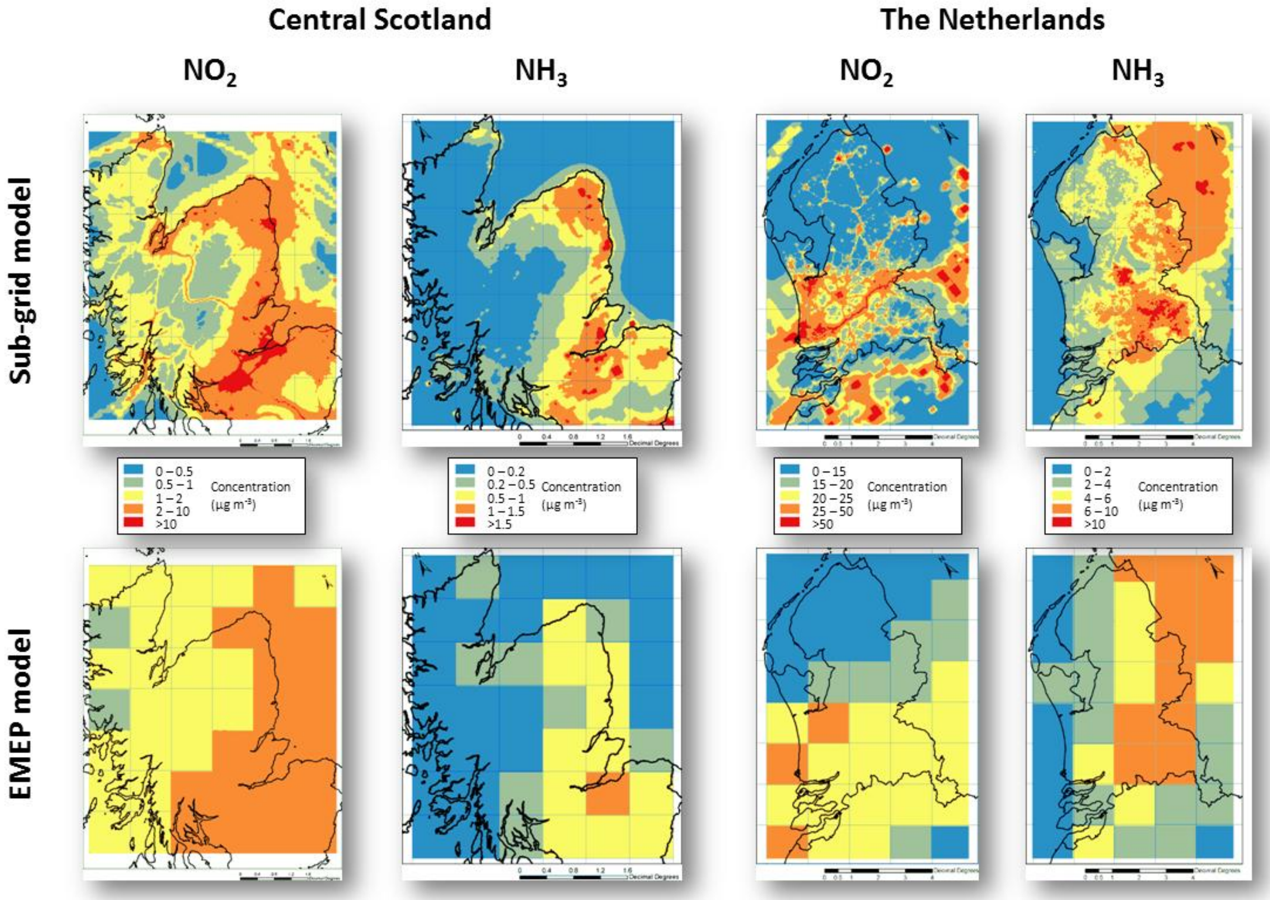

Figure 3: Sub-grid model predictions (top row) of mean annual concentrations of NO_2 and NH_3 for the two domains. EMEP model predictions at a resolution of 50 × 50 km^2 are shown for comparison (bottom row).

Table 1: Performance evaluation of the EMEP and sub-grid models for mean annual NO_2 concentrations. The best performing model for each statistic is highlighted in bold.

Dataset	n	EMEP				Sub-grid model			
		FAC2	NMB	NMGE	r	FAC2	NMB	NMGE	r
The Netherlands	43	0.91	-0.24	**0.31**	0.54	**0.98**	**0.10**	**0.31**	**0.80**
Scotland – All	49	0.06	-0.82	0.82	0.16	**0.77**	**-0.26**	**0.41**	**0.45**
Scotland – No traffic stations	11	0.27	-0.70	0.70	0.40	**0.82**	**0.32**	**0.40**	**0.79**
All (without Scotland traffic stations)	54	0.78	-0.31	0.37	0.52	**0.94**	**0.13**	**0.32**	**0.79**

Table 2 shows the evaluation statistics of the EMEP and sub-grid models for annual mean NH_3 concentrations for the Dutch and Scottish monitoring data. The EMEP model performed worse for the local monitoring network probably because all monitoring locations were within a single EMEP 50 km square. The sub-grid model also performs worst for this dataset, although its performance is better than that of the EMEP model, as it is for all the datasets. The values of all performance metrics are better for the sub-grid model except for the smaller bias of the EMEP model for the NAMN dataset. Figure 5 shows the scatterplots of predictions of the EMEP and sub-grid model *vs.* the measured NH_3 concentrations.

Table 2: Performance evaluation of the EMEP and sub-grid models for mean annual NH_3 concentrations. The best performing model for each statistic is highlighted in bold.

Dataset	n	EMEP				Sub-grid model			
		FAC2	NMB	NMGE	r	FAC2	NMB	NMGE	r
The Netherlands	112	0.85	0.23	0.39	0.69	**0.93**	**0.15**	**0.27**	**0.87**
Scotland - local network	21	0.52	-0.47	0.65	--	**0.62**	**-0.15**	**0.54**	**0.48**
Scotland - NAMN	14	0.71	**0.07**	0.46	0.73	**0.71**	0.26	**0.43**	**0.87**
All	147	0.79	0.17	0.42	0.74	**0.86**	**0.12**	**0.30**	**0.86**

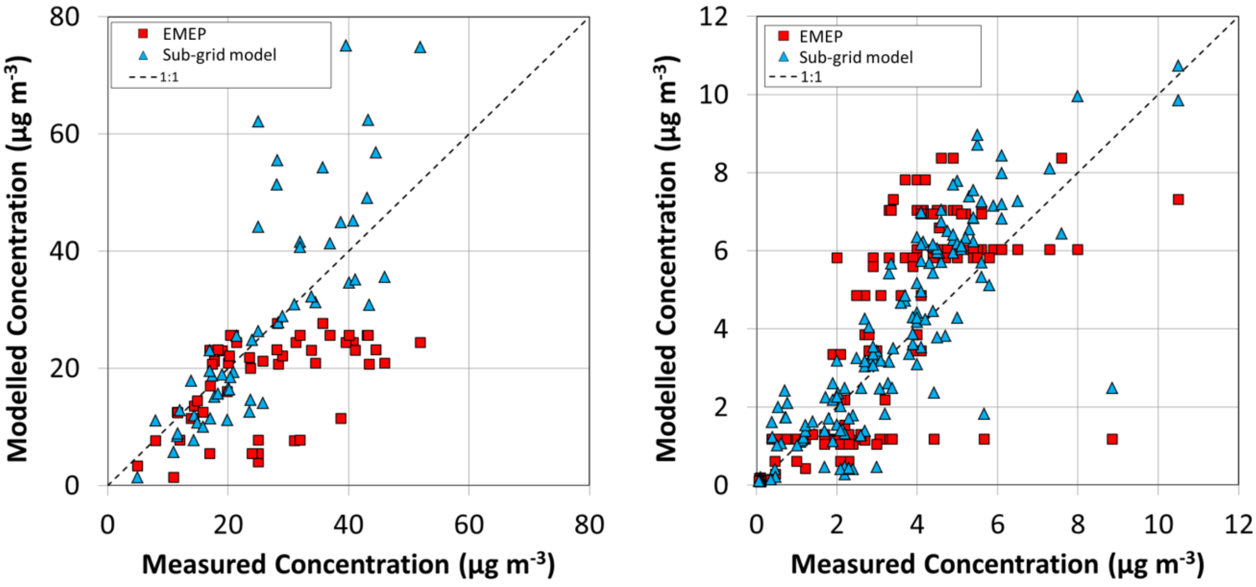

Figure 4: Modelled concentrations plotted against measured values for all sites for NO_2 (left) and NH_3 (right).

The use of domain-specific meteorological datasets only had a small effect on the concentration estimates of the sub-grid model, with a mean difference of 6% from the estimates using the generic meteorological dataset. Model performance was negligibly affected by the meteorological dataset used. The sub-grid model estimates are also not very sensitive to the NO_x stack parameters (emission height, emission threshold) for most of the monitoring sites. The range of concentrations at each site calculated using all combinations of stack parameters (four effective emission heights times four emission thresholds) is, on average, 9% of the value using the default parameters, with the maximum variation (39%) occurring at a monitoring site close to an industrial area in the Scottish domain.

4.1. Sub-grid predictions for wet deposition of oxidised and reduced nitrogen

Table 3 shows the evaluation statistics of the EMEP and sub-grid models for the wet deposition of oxidised and reduced nitrogen for the Dutch and Scottish monitoring data. Overall, both the EMEP and the sub-grid model underestimate wet deposition of oxidised and reduced nitrogen by an average of 50-50%. There is very little difference between the predictions of the models for the Netherlands as a result of low spatial variability of the precipitation. The performance of the two models is similar although the sub-grid model performs slightly better than the EMEP model for most of the evaluation statistics. Figure 5 shows the scatterplots of predictions of the EMEP and sub-grid model *vs.* the measured oxidised and reduced wet deposition for both domains.

Table 3: Performance evaluation of the EMEP and sub-grid models for annual wet deposition of oxidised and reduced nitrogen. The best performing model for each statistic is highlighted in bold.

Dataset		**n**	**EMEP**				**Sub-grid model**			
			FAC2	**NMB**	**NMGE**	**r**	**FAC2**	**NMB**	**NMGE**	**r**
Oxidised nitrogen	Scotland	11	**0.82**	-0.45	0.47	**0.76**	**0.82**	**-0.39**	**0.40**	0.72
	The Netherlands	11	**0.91**	-0.33	0.34	-0.11	**0.91**	**-0.32**	**0.33**	-0.03
Reduced nitrogen	Scotland	11	0.55	-0.47	0.52	0.76	**0.82**	**-0.42**	**0.44**	**0.82**
	The Netherlands	11	**1.00**	**-0.29**	**0.29**	0.70	**1.00**	**-0.29**	**0.29**	**0.72**

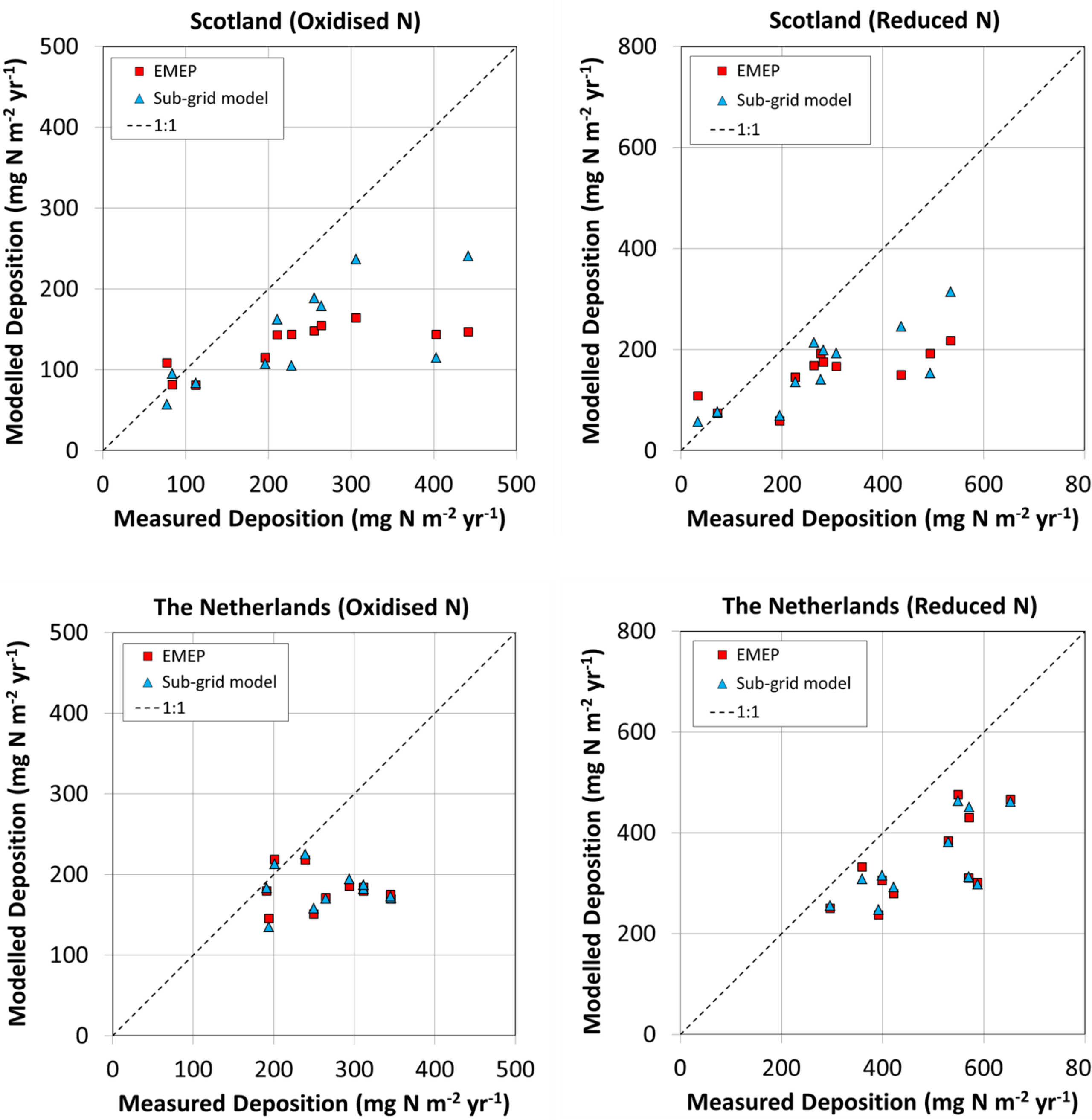

Figure 5: Modelled wet deposition of oxidised (left column) and reduced (right column) nitrogen for the Scotland (top row) and Netherlands (bottom row) domains.

5. Milestones achieved:

- MS38: Sub-grid module available for implementation in EMEP model

6. Deviations and reasons:

As explained in the WP8 periodic report for the second reporting period, this work was delayed by a few months as a result of personnel problems (long term sickness). In order to get this task back on schedule, UPM took the lead in this work. The delay in producing the sub-grid module for the EMEP model has not had any serious knock-on effect since the sub-grid parameterisation has been developed as a post-processor, which can be applied to the model output *a posteriori*.

7. Publications:

An article on the development and evaluation of the sub-grid model for atmospheric concentrations is currently in preparation.

8. Meetings:

The progress of this work has been discussed during WP8 sessions in the annual project meetings. In addition, frequent progress updates were sent by email to the WP participants to discuss the progress of the work and its work plan.

9. List of Documents/Annexes:

None

10. Acknowledgements:

We would like to thank Sim Tang at CEH Edinburgh for providing the NAMN data from the Defra project AQ0647 "UK Eutrophying and Acidifying Atmospheric Pollutants (UKEAP), Mhairi Coyle at CEH Edinburgh for providing the Easter Bush meteorological data, the Cabauw Experimental Site for Atmospheric Research (Cesar) database for the Cabauw meteorological data, Roy Wichink Kruit at RIVM for the Dutch NO_2 concentration and wet deposition data and Dorien Lolkema at RIVM for the Dutch NH_3 concentration data.

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