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**ÉCLAIRE**

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

**Seventh Framework Programme**

**Theme: Environment**

**D8.1 Synthesis report on the different local scale models dealing with  
atmosphere-biosphere exchange and their relevance for describing the  
climate change / air pollution interactions**

**D8.2 Report on local scale variability, based on modelling studies for  
selected regions**

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## 1. Executive Summary

The objective of Deliverable 8.1 is to provide a synthesis report on the different local scale models dealing with atmosphere-biosphere exchange and their relevance for describing the climate change / air pollution interaction. Furthermore, this report details results for Deliverable 8.2: describing the local scale variability, based on modelling studies for selected regions.

The results for Deliverable 8.1 are based on previous work describing various models on a local and regional scale. From this work it is clear that a full interaction between climate change and air pollution is not available for any of the models presented here. A higher degree of interaction is possible, but would require a complete redesign of the various models.

For Deliverable 8.2 the results are based on model calculations performed with the EMEP4UK model. They show a large variation in modelled concentrations and depositions with changing resolutions. This is of particular importance for use of these modelling results for e.g. calculation of critical loads exceedances (see WP17).

## Objectives:

One of the objectives of the ÉCLAIRE has been the study of the interaction between Air Quality and Climate Change. Various aspects of this interaction have been studied, such as the role it plays in the plant-atmosphere interaction, and the way it is represented in large scale models.

The report brings together a few aspects that play (perhaps in a more indirect way) a role in this interaction, and the way atmospheric transport and deposition models are able to deal with it. The first part of the next chapter gives an overview of local scale models for ammonia/nitrogen and their capability of describing the air quality/climate interaction (Deliverable 8.1) and the second part of the report describes the effect of modelling resolution on the concentration and deposition predictions used in the context of ÉCLAIRE (Deliverable 8.2).

## 2. Activities:

For Deliverable 8.1 the activities consisted mainly of a literature review, using existing work on model comparisons for local/regional scale models. The work for Deliverable 8.2 was based on EMEP4UK modelling on different spatial scales/resolutions. The results of these different activities are described below (Section 3), while a more detailed description of the different activities is given in the following paragraphs.

### 2.1 Model inventory

#### 2.1.1 General

This chapter gives an overview of different models that can be used, over different spatial scales, to make predictions of air pollutant concentrations and deposition rates (now or in the future). The purpose of this overview is to assess to what extent are these models capable of taking into account climate change. More and more is being discovered about the interaction between air quality and climate change, to which the ÉCLAIRE project has contributed.

Some interactions that exist between air quality and climate change are:

- Increasing volatilization of ammonia with increasing temperature
- Local cooling effect with increasing aerosol concentrations in the air
- Ozone formed from NO<sub>x</sub>/VOC emissions reduces plant productivity, and therefore reduces CO<sub>2</sub> uptake from the atmosphere
- Increasing biogenic VOC emissions with increasing temperature

However, to what extent is knowledge about these interactions incorporated in the models that are currently used for describing Air Quality and/or predicting the current or future situation with respect to concentrations and depositions? This inventory summarizes the different models that exist and gives an overview of the different ways in which these models take into account the interaction between air quality and climate.

#### 2.1.2 Local Scale atmospheric models

There are different models available, ranging from models describing processes on a plant level to global scale models. For the purpose of this overview, the main focus is on larger scale models: ranging from landscape scale to regional/global scale.

Most of the models described below are capable of dealing with different atmospheric components, although some are targeted at one particular species (mostly ammonia). Ammonia has been singled-out for special treatment as a result of its high spatial variability, especially close to emission sources. In order to correctly assess the ecological impacts of ammonia (either as the result of elevated concentrations or its contribution to nitrogen deposition), atmospheric processes need to be modelled at a higher resolution than required for the assessment of particulate nitrogen deposition, for example.

Most of the work presented here has been collated from previous activities published in:

- Atmospheric Ammonia – Detecting emission changes and environmental impacts (ISBN 978-1-4020-9120-9), 2009.
- Review and Integration of Biosphere-Atmosphere Modelling of Reactive Trace Gases and Volatile Aerosols (ISBN 978-94-017-7284-6), 2015.

Before providing details of the individual models, the next section first gives a brief overview of modelling concentrations and depositions of nitrogen/ammonia.

### **2.1.2.1 Overview of concentration and deposition modelling (taken from Atmospheric Ammonia)**

#### ***Brief overview of the most important atmospheric processes (with a focus on ammonia)***

Ammonia is emitted to the atmosphere mainly from agricultural sources. In essence the emission of ammonia is the evaporation from animal manure and is highly dependent on the specific agricultural activity and environmental circumstances. In the atmosphere ammonia is subject to dispersion and transport, removed by dry and wet deposition and transformed to aerosol-bound ammonium in reactions with acid gases and aerosols. Due to the relatively fast deposition and conversion process and the low emission height, the atmospheric lifetime of ammonia is typically a few hours. Aerosol-bound ammonium has generally a much longer lifetime in the atmosphere and may, therefore, be transported over long distances (>1,000km). The main removal path of the ammonium-containing aerosols is wet deposition.

#### ***Overview of modelling concepts and parameterisations***

Different approaches have been used in the modelling of the fate of ammonia in the atmosphere. The choice of the complexity of the parameterizations is often a function of among others (a) the state of knowledge of the process, (b) the availability of input parameters, (c) the purpose of the model, (d) the available computer power. The next section elaborates on the different processes. Several parts of the description were taken from Hertel et al. (2006), who give an overview of the status of ammonia modelling and further details can be found there.

#### ***Emissions***

In modelling emissions, the total amount as well as the temporal variation in the emission factors and the spatial resolution of the data, are very important. The emissions of ammonia mostly originate from animal housings and from the application of manures and slurries. The emission from animal housings depends mainly on the ventilation and the temperature inside the stables. The emissions of ammonia from manure and slurry applications are a function of the application method, the meteorological conditions and the soil type. Other sources of ammonia are grazing animals, storage facilities and fertilized crops. The total ammonia emission, therefore, varies to a large degree during the day and throughout the year.

Most chemical transport models (CTMs) deal with the seasonal and diurnal variations in a strongly simplified way. The main reason for this is the lack of input data.

#### ***Transport and Dispersion***

This process of dispersion of ammonia emitted into the atmosphere can be split into a local part (typically up to a distance of a few kilometres) and a longer range part (typically from tens to thousands of kilometres). The latter is often referred to as the mean transport of air pollution with the mean wind flow. For ammonia, which is generally emitted close to the ground, the local scale dispersion is particularly important with regards to ecological impacts. Describing the transport of ammonia at larger spatial scales is no different from that of other air pollutants. Besides the transport processes, all other physical and chemical processes included in the models may, in principle, be identical for the two main model types: Lagrangian and Eulerian.

### *Dry deposition*

The dry deposition is the most important removal process of ammonia from the atmosphere. The dry deposition process is a strong function of the transport rate from the ammonia in the air to the surface and the physical, chemical and biological characteristics of the surface.

In chemical transport models, the dry deposition of gases and particles is often calculated from a deposition velocity and the concentration of the substance at a reference height. The deposition velocity is often parameterized using a so-called resistance model in which the transport to the surface and the surface uptake is described using resistances. The dry deposition velocity for a gaseous compound is expressed as the reciprocal value of the total resistance to transport down to and removal onto the surface.

Generally speaking the resistance that describes the physical or meteorological part of this transport are well known, under the assumption that the aerodynamic roughness characteristics are known. Using the resistance methodology it is often assumed that the surface concentration of the air pollutant is zero. However, for ammonia this is not the case and formulations for the surface concentration are needed. This means that for ammonia the deposition process is in principle the net result of a bi-directional exchange process. The surface concentration of ammonia is often referred to as the compensation point, being the concentration where the exchange of ammonia changes from deposition to (re-) emission or vice versa.

Specific dry deposition sub-models for the surface resistance that include the description of a compensation point for ammonia have been derived and implemented in connection with the analysis of different plant surfaces. Overall the parameterization of the stomatal resistance is fairly established and can be found in the literature (e.g. Baldocchi et al., 1987; Wesely, 1989). The stomatal compensation point may be calculated from knowledge of the aqueous phase chemistry. It has been shown that the leaf surface may act as a capacitance for  $\text{NH}_3$  and  $\text{SO}_2$  uptake that increases with humidity. This transport is independent of solar radiation and contrary to stomatal uptake, will also take place during the night.

A special case is the dry deposition to marine waters. Experimental studies have shown that over the sea atmospheric fluxes of ammonia may be upward or downward, depending on the meteorological conditions and the relationship between the pH and contents of ammonium in the upper surface waters on the one hand, and the ammonia concentrations in ambient air just above the surface on the other.

### *Wet deposition*

Wet deposition takes place by uptake of pollutants in precipitation (rain, snow, hail) as well as in cloud droplets – termed below-cloud and in cloud scavenging, respectively. Uptake in cloud droplets may not necessarily lead to deposition, since clouds often evaporate without producing precipitation; on average every 10<sup>th</sup> cloud encountered by an air parcel precipitates.

Wet deposition is a very important removal process for ammonia since ammonia is highly soluble in water. For ammonia, both in-cloud and below-cloud scavenging are of importance. The uptake in rain and cloud droplets is limited by the diffusion into the droplet rather than the equilibrium concentration in the droplet.

The below-cloud scavenging of ammonia may be of importance in source regions. It has been shown from experimental results in America and South Korea that the wet deposition of ammonium is correlated to the local ammonia emission density. Also for the Netherlands a clear correlation between spatial distribution of the wet deposition and the ammonia emissions was found. When considering the contribution from a single farm, the wet deposition of ammonia will, however, be very limited. This is due to the short periods with precipitation compared with the dry periods, and at the same time a result of the short residence time of the pollutants near the farm.

### Chemical conversion

In the atmosphere ammonia is quickly transformed into particulate ammonium in the reaction with acid gases and aerosol particles. In a number of transport models the conversion of ammonia to ammonium is parameterized in a simplified way using pseudo first order reaction rates. For oxidized nitrogen, where the chemical reactions are more complex, the same holds: they are often only parameterized through simplified reaction rates.

#### 2.1.2.2 Model overview

In Table 1, an overview of the different models is given. These models are used in the context of dispersion and deposition studies for a wide variety of applications.

Table 1: Overview of landscape, regional scale and global dispersion and deposition models

Full model name	Acronym/short name	Reference
<b>Landscape</b>		
American Meteorological Society/Environmental Protection Agency Regulatory Model	AERMOD	Perry et al. (2004)
Atmospheric Dispersion Modelling System	ADMS	Carruthers et al. (1999)
DDR	DDR	Asman et al. (1989)
DEPO1	DEPO1	Asman (1998)
Flux Interpretation by Dispersion and Exchange over Short Range	FIDES-2D	Loubet et al. (2001)
Local Atmospheric Dispersion and Deposition	LADD	Hill (1998)
Model of Dispersion and Deposition of Ammonia over the Short-range	MODDAAS-2D	Loubet et al. (2006)
Operational Priority Substances (Pro 4.1)	OPS-Pro 4.1	Van Jaarsveld (2004)
Operational Priority Substances (Short Term)	OPS-st	Van Jaarsveld (2004), van Pul et al. (2008)
Operationelle Meteorologiske Luftkvalitetsmodeller Deposition	OML-DEP	Olesen et (2007); Sommer et al. (2009)
TREND/OPS	TREND/OPS	Asman and Van Jaarsveld (1992)
<b>Regional</b>		
A Unified Regional Air-quality Modelling System	AURAMS	Zhang et al. (2003)
CHIMERE	CHIMERE	Vautard et al. (2001)
Community Multiscale Air Quality	CMAQ	Byun and Schere (2006)
Danish Ammonia Modelling System	DAMOS	Geels et al. (2012)
European Monitoring and Evaluation Programme	EMEP	Simpson et al. (2012)
Regional application of the EMEP model	EMEP4UK	Vieno et al., (2010, 2014)
Fine Resolution Ammonia Exchange	FRAME	Singles et al. (1998)
Long Term Ozone Simulation European Operational Smog	LOTOS-EUROS	Wichink-Kruit et al. (2012)
Multi-Scale Atmospheric Transport and CHEmistry	MATCH	Klein et al. (2002)
<b>Global</b>		
Goddard Earth Observing System Chemical transport model	GEO-CHem	Bey et al. (2001), Wang et al. (1998)
Model of the Global Universal Tracer transport in the Atmosphere	MOGUNTIA	Dentener and Crutzen (1994)
Tracer Model version 5	TM5	Huijnen et al. (2010)
UK Met. Office Global Three-Dimensional Lagrangian Model	STOCHEM	Collins et al. (1997), Bouwman et al. (2002)

A further general description of these models is given below (taken from Review and Integration of Biosphere-Atmosphere Modelling)

### *Landscape Scale Models*

The specificity of the landscape scale, especially in agricultural areas, with respect to surface/atmosphere ammonia exchange modelling is characterised by the close proximity of large agricultural point sources and semi-natural ammonia sink areas such as forests, moorlands and wetlands. These hotspots of ammonia induce large horizontal ammonia concentration gradients downwind from sources, typically an exponential decay with distance, and a large spatial heterogeneity in ammonia concentration and exchange fluxes. This fine-scale variability occurs at spatial scales (typically 100m to 1 km) much smaller than, and therefore not 'seen' by regional CTMs (resolution typically 5x5 km<sup>2</sup> to 50x50 km<sup>2</sup>); from a regional modelling viewpoint the (unresolved) landscape scale generally falls under the header 'sub-grid issues'. Modelling studies have been applied to determine the fraction of emitted ammonia, which is recaptured locally downwind from the source. The results vary widely, showing recapture fractions within the first 2 km between 2% and up to 60%, but in most cases in the range between 10 and 40%.

The variability is in part due to variations in vegetation types, roughness and LAI over the patchwork of land uses, but also due to the nitrogen enrichment associated with large ammonia deposition rates close to sources (animal houses, manure storage facilities, fertilized fields).

The different processes involved and their coupled emission/dispersion/deposition modelling have recently been thoroughly reviewed by Loubet et al. (2009), and earlier by Hertel et al. (2006) and Asman (1998, 2002), and thus only a brief overview is presented here. Loubet et al. (2009) provided a technical comparison of 7 existing local atmospheric transport and deposition models for ammonia: DDR, TREND/OPS, LADD, DEPO1, FIDES-2D, MODDAAS-2D and OML-DEP. All models except MODDAAS-2D (multi-layer) use a 1-layer (big leaf) surface exchange architecture, and most models use a uni-directional dry deposition scheme by default. However, both MODDAAS-2D and FIDES-2D allowed bi-directional exchange with stomata, though they did not account for any potential soil emissions.

Theobald et al. (2012) presented the first intercomparison of 4 short-range atmospheric dispersion models (ADMS, AERMOD, LADD and OPS-st), which they applied to the case of ammonia emitted from agricultural sources. The intercomparison focused on atmospheric ammonia concentration prediction in two case study farms in Denmark and the USA. Wet deposition processes were not included in the simulations because dry deposition is likely the dominant deposition mechanism near sources. Similarly, chemical processing of ammonia in the atmosphere was also assumed to be negligible for short-range dispersion. Thus the only ammonia removal mechanism involved was surface dry deposition, with all models using the canopy resistance – deposition velocity ( $R_c/V_d$ ) schemes. The performance of all of the models for concentration prediction was judged to be 'acceptable' according to a set of objective criteria, although there were large differences between models, depending on which source scenarios (area of volume source, elevation above ground, exit velocity) were tested. The findings highlight that the rate of removal by dry deposition near such a source leads to a rather small effect on simulated near-source ammonia concentrations, which largely depended on sound treatment of source characteristics and dispersion rates.

A special case of landscape modelling is provided by the NitroScape model (Duret et al., 2011), which was developed in the NitroEurope Integrated Project and has been extended in ÉCLAIRE. NitroScape dynamically couples (on a daily time-step) a short-range dispersion and deposition model (OPS-st) to farm, ecosystem and hydrological models in order to simulate as many processes of nitrogen transfer and transformation as possible, at a landscape scale.

### *Regional Scale Models*

Despite unequivocal evidence and widespread consensus that ammonia exchange is bi-directional in most climates and ecosystem types, including unfertilized vegetation, most CTMs operating at national, regional and continental scales still use Rc/Vd deposition-only schemes for ammonia: e.g. an Rc/Vd approach is used in the EMEP MSC-W model and EMEP4UK; a Wesely approach is used in CHIMERE; DEPAC is used in OPS-Pro 4.1; the EMEP Rc/Vd approach is used in the coupled DEHM/OML-DEP system; combined DEPAC and EMEP parameterizations in MATCH; and land-cover-specific values of Rc are used in FRAME. Nevertheless, in some cases, parameterizations of bi-directional ammonia deposition schemes have been used: e.g. the LOTOS-EUROS model; the couples CMAQ-EPIC model; and AURAMS. Other CTMs have meanwhile focused on improving the treatment of sub-grid variability or the spatial and temporal distribution of ammonia emissions by field-applied mineral fertilizers.

### *Global Models*

Overall, the uncertainties in the global  $\text{NH}_3/\text{NH}_x$  cycle are very large, not least because the ammonia emission factors typically used for global emission upscaling, and the parameterizations for surface exchange modelling, are heavily biased towards NW European and N American measurements and conditions.

In global atmospheric CTMs, which are coupled to general circulation models (GCMs) or driven by analysed meteorological fields and use prescribed emissions of ammonia and other trace gases, often parameterise ammonia exchange following Wesely (e.g. TM5 model, STOCHEM, GEOS-Chem). However, in the MOGUNTIA model, Dentener and Crutzen (1994) – who were the first to reconcile the consistency on a global scale of upscaled ammonia emission inventories and atmospheric  $\text{NH}_3/\text{NH}_4$  concentration and deposition by modelling – did use a canopy compensation point to calculate ammonia emissions from continental natural ecosystems.

Dentener et al. (2006) reported a multi-model evaluation (23 global CTMs) of current and future (2030) deposition rates of reactive nitrogen as well as sulfate to land and ocean surfaces. Models predicted that ammonia dry deposition represents between 30 and 70% of total ammonia deposition. Present-day deposition using nearly all of the available information on wet deposition worldwide showed a good agreement with observation in Europe and North America. However, models systematically overestimated  $\text{NH}_x$  deposition in South Asia compared with available bulk wet deposition measurements.

### *In General*

The basic processes controlling surface/atmosphere ammonia exchange are relatively well understood, at least qualitatively. A wide range of factors are important, including: thermodynamics, meteorology, surface and air column heterogeneous chemistry, plant physiology and N uptake, ecosystem N cycling, compensation points, nitrogen inputs via fertilization and atmospheric deposition. Most of the fundamental process understanding was gained during the 1980s and 1990s, while many advances in modelling logically followed from the late 1990s onwards, spurred by the canopy compensation point concept of Sutton et al. (1995, 1998). There has been a gradual increase in the complexity of surface/atmosphere ammonia exchange models, from simple steady-state model to dynamic, multiple layer, multiple sink/source, multiple chemical species exchange models. This reflects both the improvements in process understanding and the increasing availability of flux datasets, which are needed to parameterize models.

### **2.1.3 Nitrogen & Climate interactions in atmospheric modelling**

In order to include the interactions of Nitrogen & Climate into a model, there are different options available, which depend on the extent of the modelling domain. This is not in terms of spatial scale, but what is (or is not) included in the model in terms of processes.

Most (all) models mentioned above have a nitrogen/climate interaction included in terms of the influence of a changing climate (temperature, precipitation, wind) on the transport and deposition of the different components. This is a fairly simple relation, which is taken into account through the possibility of including different meteorological datasets representative of different climatic conditions in the calculations.

Figure 1 shows this simple input/output relationship: information on land use, emissions and meteorology is used by the model, which will then provide predictions of concentrations and/or deposition.

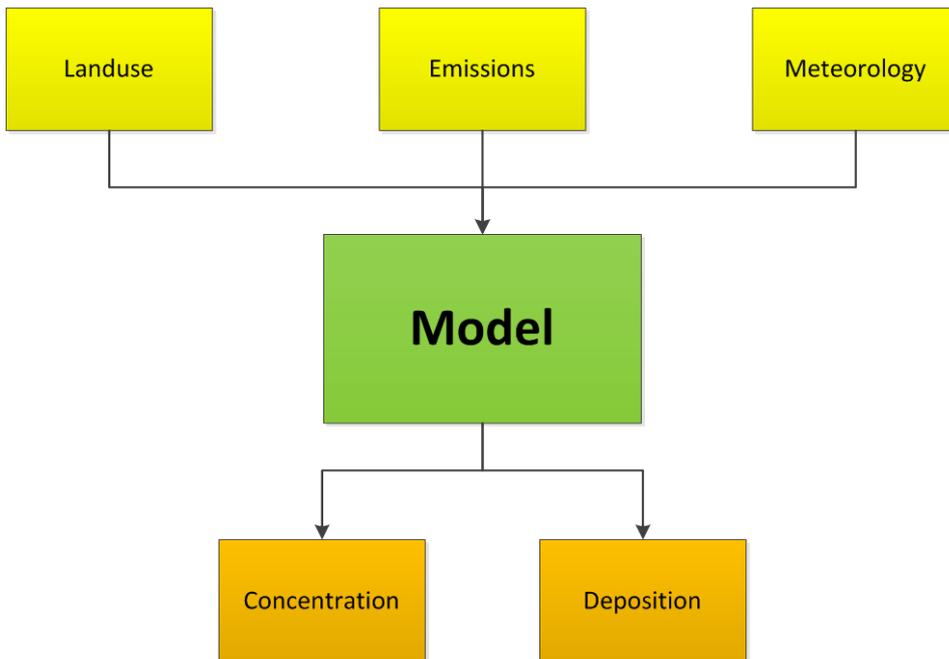


Figure 1: Overview a simple model input/output relationship.

As mentioned, many models will only incorporate the effect of a changing climate by means of varying meteorological input data from scenarios. In most cases there is a clear relation between a changing climate and changing emissions (or even land use; see below). However, these relationships are not automatically taken into account. For the different models, these inputs are taken from external data sources, which are very often not linked. This represents only a first step in trying to include the different interactions.

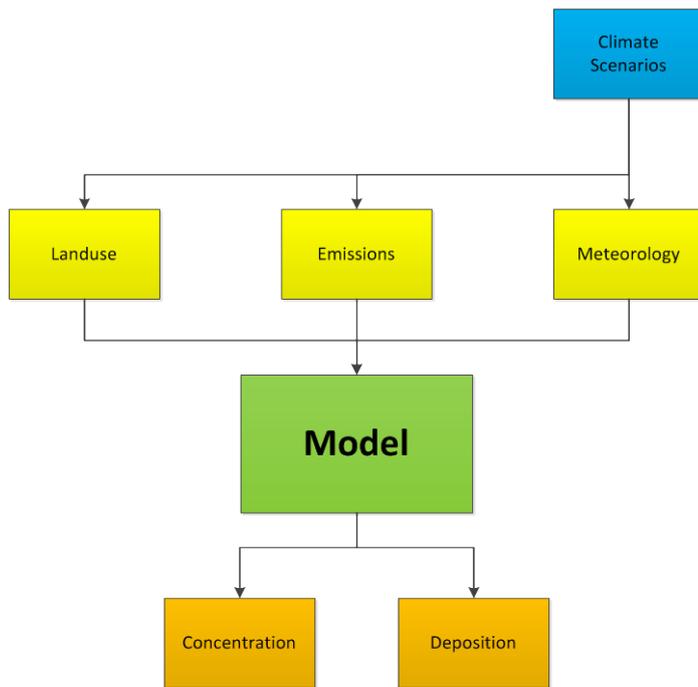


Figure 2: Next level of integration – including climate scenarios and their effects on landuse, emissions and meteorology.

Not only will climate scenarios have consequences for the different model inputs, there will also be emission and/or land use scenarios that will influence model inputs that also have interactions between them and with the climate scenarios.

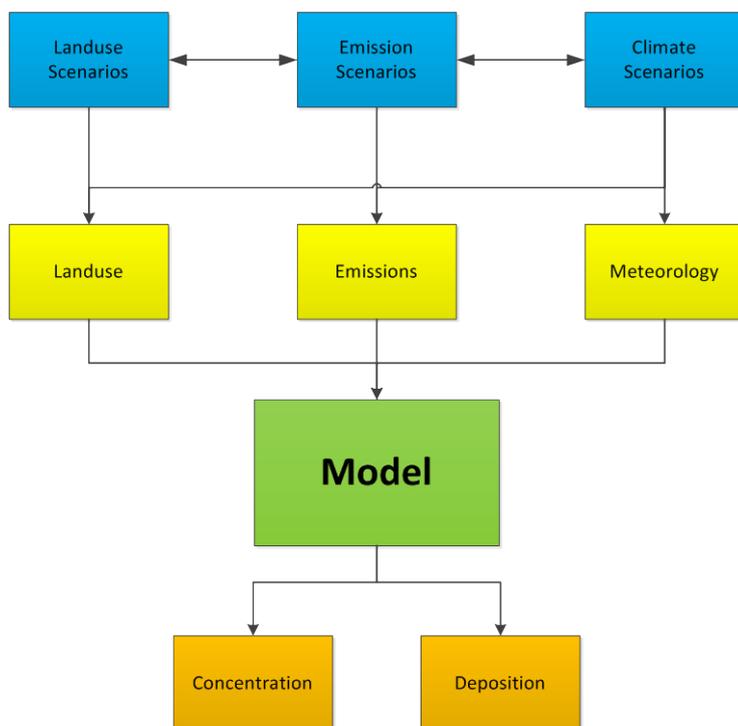


Figure 3: Next level of integration – including landuse, emission and climate scenarios and their effects on landuse, emissions and meteorology.

The level of complexity/interaction increases when also taking the changing depositions and concentrations and their potential influence on respectively emissions and/or meteorology into account.

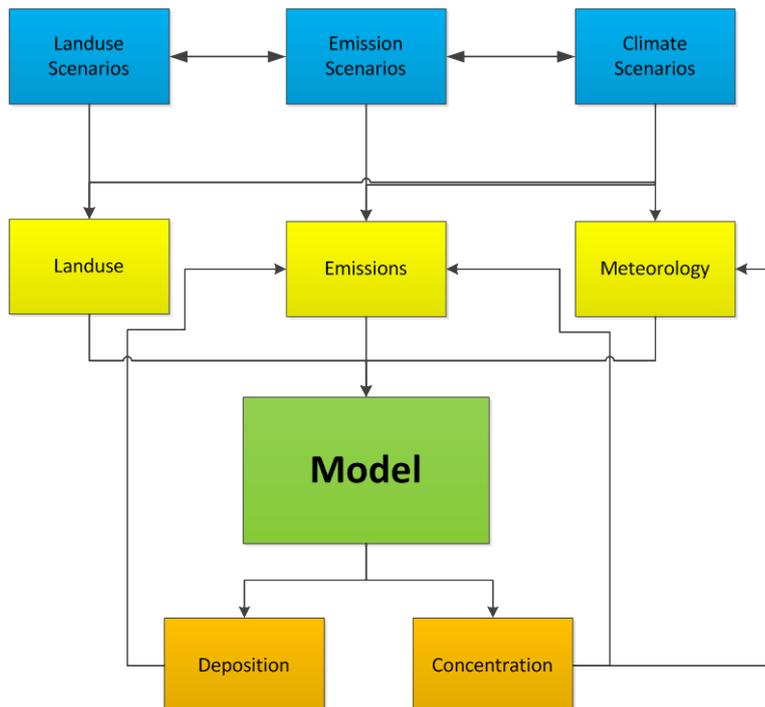


Figure 4: Full integration – effect of different scenarios on concentrations/depositions and vice versa.

There currently is no modelling system that has all these interactions included. There are, however, modelling systems available that perform these calculations in subsequent steps (see Figure 5: Sutton et al., 2013). They proposed a modelling architecture for treating the climate-dependence of ammonia fluxes in regional and global atmospheric transport and chemistry models. In this approach, static emission inventories are replaced by calculations depending on prevailing meteorology, while allowing for bi-directional exchange with area sources/sinks, giving the basis to assess climate change scenarios including the consequences of climate feedbacks through altered  $\text{NH}_3$  emissions. The effect of altered air chemistry may also be fed back into the climate model. In these cases however, full interaction is very difficult. Although models might seem to be coupled, full integration is only possible when all interactions are dealt with simultaneously (and not step by step).

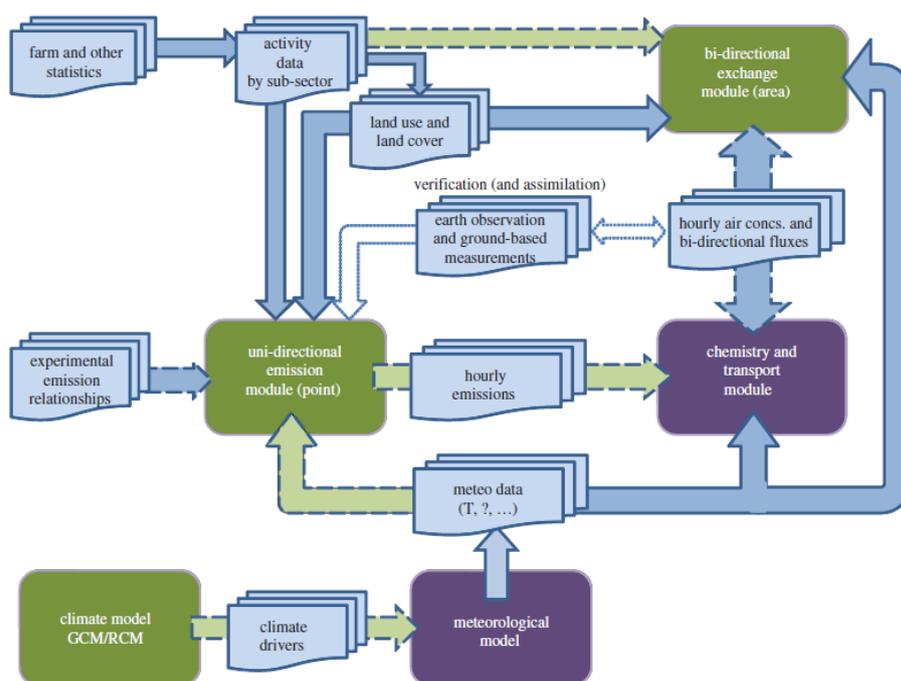


Figure 5: Proposed modelling architecture by Sutton et al. (2013).

## 2.2 Modelling resolution and consequences for concentrations / depositions

### 2.2.1. General

The EMEP4UK model used for the ÉCLAIRE project is a nested regional ACTM based on version v4.3 of the EMEP MSC-w model (Simpson et al., 2012). A detailed description of the EMEP4UK model framework and setup are given in (Vieno et al., 2010; Vieno et al., 2014) and only brief relevant details are shown here.

The EMEP4UK model is driven by the Weather Research Forecast (WRF) model version 3.6.1 ([www.wrf-model.org](http://www.wrf-model.org)). The model horizontal resolution scales down from 50 km x 50 km in ‘Greater European’ domain to 5 km x 5 km for the domain covering the British Isles, and the Netherland ‘Smaller European’ domain and two additional higher resolution regional domains (Scotland and the Netherlands) to a 1 km x 1 km. The boundary conditions are calculated from the largest domain to the inner domain (50 to 5 to 1) in a one-way nested setup. The EMEP4UK-ÉCLAIRE model domain is shown in Figure 6. The EmChem09 chemical scheme was chosen for the present study, as it has been extensively validated at the European scale (Simpson et al., 2012). The EmChem09 solver is based on Berge and Jakobsen (1998), but extended with photo-oxidant chemistry (Andersson-Skold and Simpson, 1999; Simpson, 1995). It has 72 species and 137 reactions. Full details of the chemical scheme are given by Simpson et al. (2012). Gas/aerosol partitioning uses the MARS equilibrium (Binkowski and Shankar, 1995).

The vertical domain of the model ranges from the surface up to 100 hPa (~ 16 km) in terrain following coordinates.

Anthropogenic emissions of NO<sub>x</sub>, NH<sub>3</sub>, SO<sub>2</sub>, primary PM<sub>2.5</sub>, primary PM<sub>coarse</sub> (the difference between PM<sub>10</sub> and PM<sub>2.5</sub>), CO, and non-methane volatile organic compounds (NMVOC) are included. PM<sub>10</sub> is the size fraction of particles with an aerodynamic diameter ≤ 10 μm. The TNO08 emissions are used for all domain and projected to the relevant resolution within the EMEP4UK model.

An example of EMEP4UK-ÉCLAIRE model nested domains for the surface concentrations of ozone and NO<sub>2</sub> is shown in Figure 7.

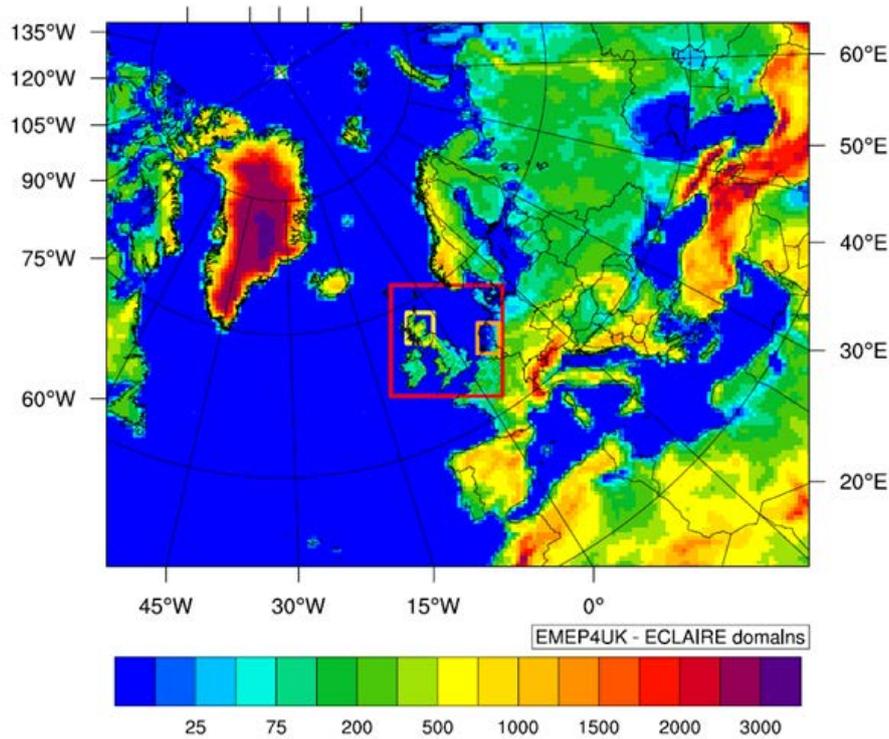


Figure 6 EMEP4UK model domain as used for the ÉCLAIRE project. The largest domain has a horizontal resolution of 50 km x 50 km, a nested 5 km x 5 km domain covering the British Isles, part of France, The Netherlands, Belgium (Red box), and two nested domains at 1km<sup>2</sup> horizontal resolution covering most of Scotland (Yellow box) and the Netherlands (Orange box) for detailed analyses.

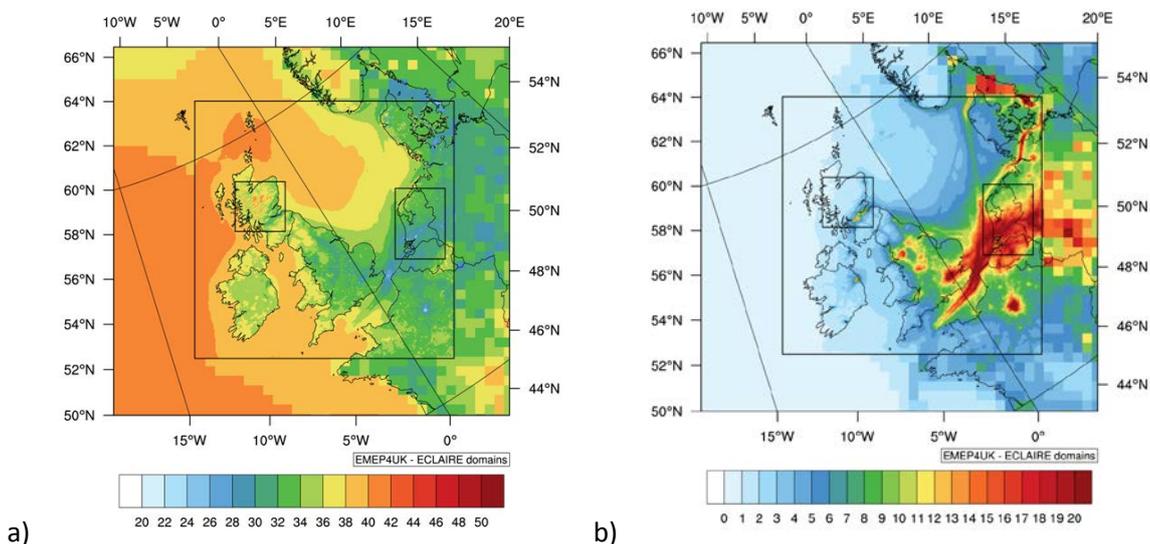


Figure 7. EMEP4UK 2008 annual average surface concentration of: (a) ozone in ppb and (b) NO<sub>2</sub> in µg m<sup>-3</sup>.

### 2.2.2 Differences in simulated surface concentrations and depositions at different scales

Figure 7 shows the annual average surface concentration of ozone calculated at the 3 horizontal resolutions used in the EMEP4UK-ÉCLAIRE model domain (50 km x 50 km, 5 km x 5 km and 1 km x 1 km). The EMEP4UK model and WRF model version are kept unchanged for each model resolution. All the interpolation and extrapolation needed for the model input file are calculated using online

conversion in the EMEP4UK model. Figure 8 the same area and resolutions as Figure 7 but for  $\text{NO}_2$  and  $\text{PM}_{2.5}$  surface concentrations.

The major driver of differences in the model results when applied at different resolutions are: the changes of chemical regime (ozone non linearity vs.  $\text{NO}_x$ ), emissions spatial distribution, and meteorological parameters such as rainfall.

When looking at the 50 km x 50 km, 5 km x 5 km, and 1 km x 1 km scale results for the Scottish domain ( $\text{NO}_2$  and  $\text{PM}_{2.5}$ ), the differences become clear. Especially the differences in the range of concentrations is a prominent aspect of the varying modelling resolutions. The implication of this is that even before any chemical conversion takes place in the model, large parts of the model domain overestimate (in rural areas, predominantly) or, in the case of urban areas, underestimate the  $\text{NO}_x$  surface concentrations directly changing the generation and/or titration of surface ozone. Moreover, the higher resolution better represented the mountain terrain in the Scottish highlands. The 1 km x 1 km Scottish domain also better resolved the higher ozone concentrations over elevated terrain with a difference of up to  $20 \mu\text{g m}^{-3}$  as shown in Figure 8.

Model resolution has a large influence on pollutants such as ozone where the non-linearity of the  $\text{NO}_x$  and VOC chemistry may lead to different results when the model is applied at different resolution. In a similar way, the spatio-temporal heterogeneity of  $\text{NH}_3$  emission patterns and the high rate of near-source deposition results in a strong influence of grid resolution on effects, e.g. the deposition of S and N on SSSIs or SACs as also shown in Hallsworth et al. (2010).

For particulate matter we found that the surface concentration was less resolution dependent compared to primary compound and depositions.  $\text{PM}_{2.5}$  surface concentration over the Dutch domain is shown in Figure 12.

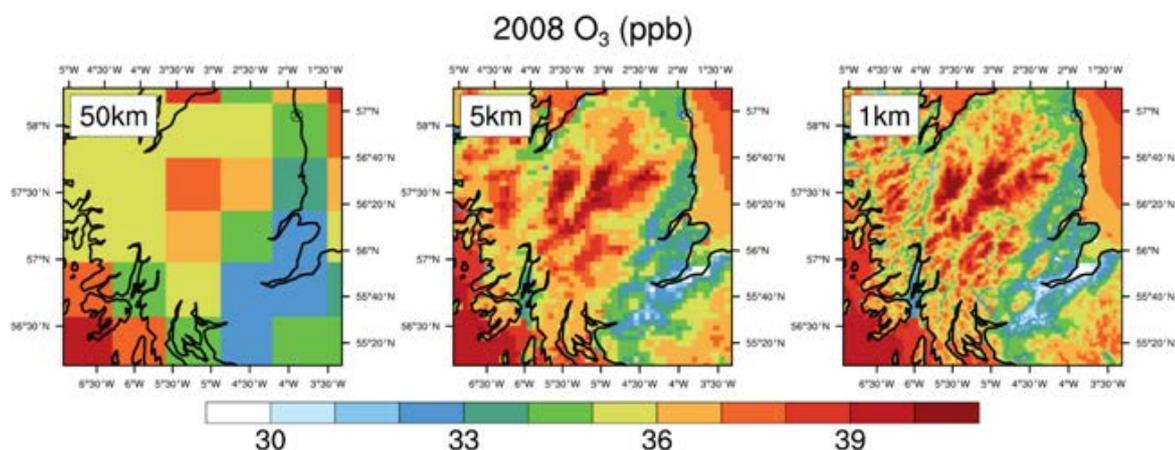


Figure 8. 2008 annual average surface concentration of ozone for a UK area of the EMEP4UK model for three horizontal resolutions: 50, 5 and 1 km x 1 km.

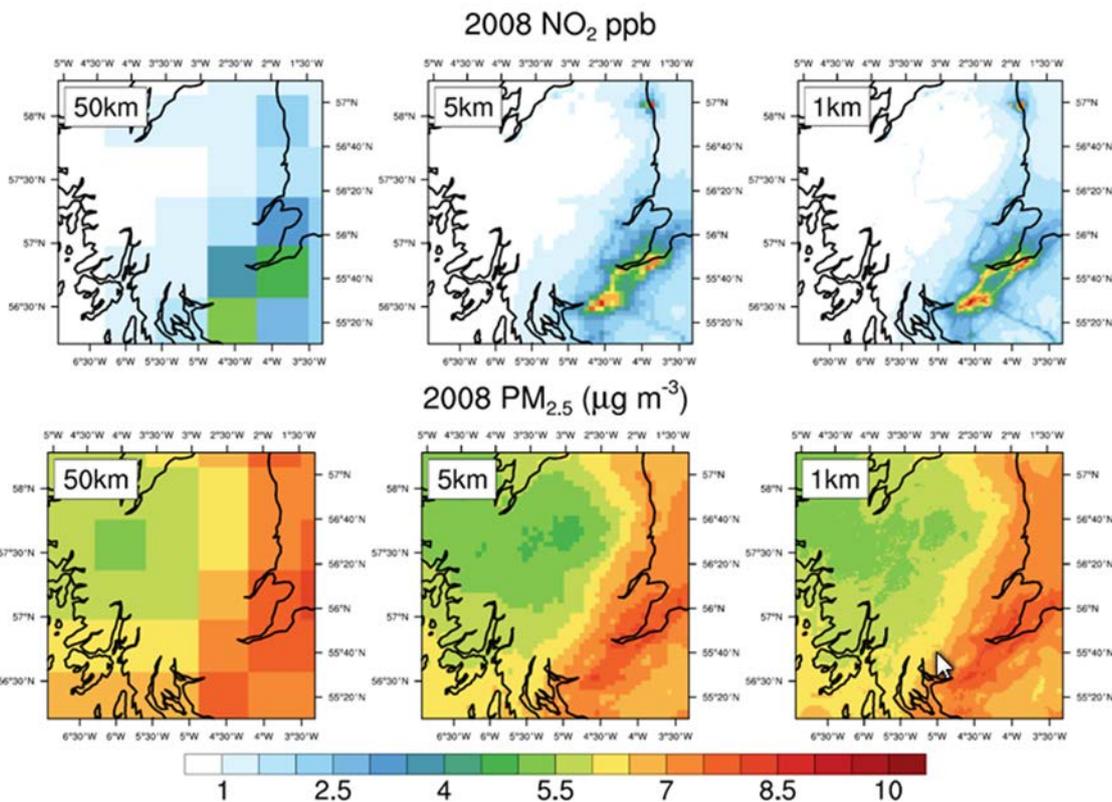


Figure 9. 2008 annual average surface concentration of  $\text{NO}_2$  and  $\text{PM}_{2.5}$  for a UK area of the EMEP4UK model for three horizontal resolutions: 50, 5 and 1 km x 1 km.

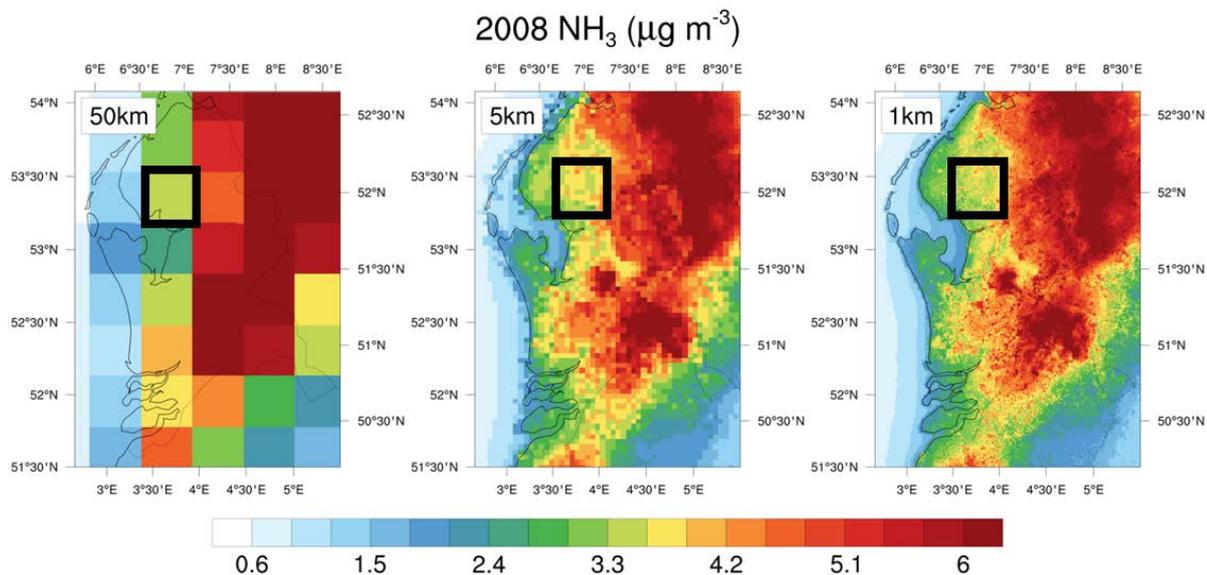


Figure 10. EMEP4UK modelled concentrations for the Dutch domain. The black box shows an arbitrary 50 km x 50 km where the concentration is  $\sim 3.5 \mu\text{g m}^{-3}$ . The range of concentrations in the same 50 km x 50 km grid square for: the 5 km x 5 km resolution is  $\sim 2.5 - 4.5 \mu\text{g m}^{-3}$ , and for the 1 km x 1 km resolution is  $\sim 2.5 - 5.5 \mu\text{g m}^{-3}$ .

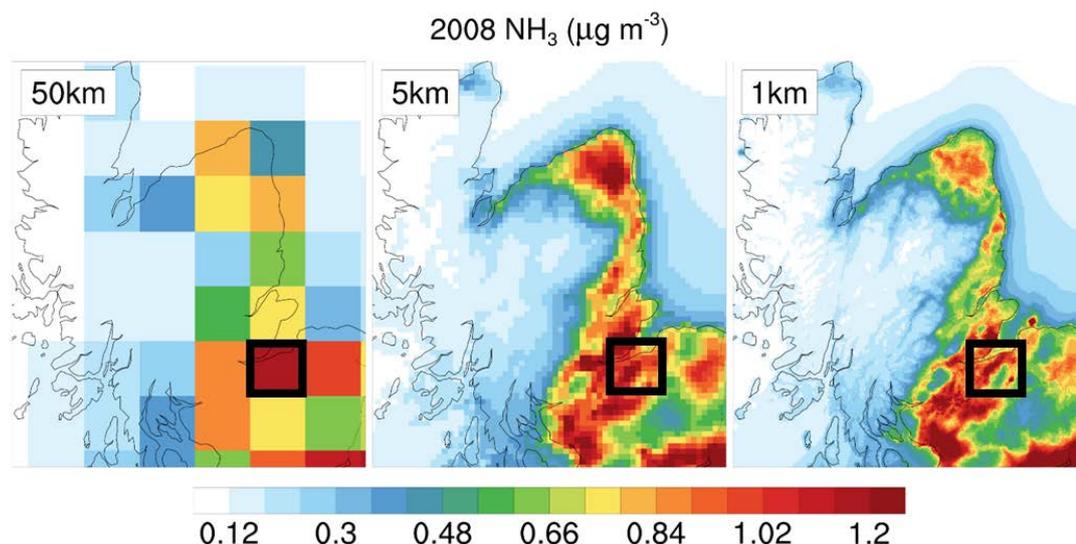


Figure 11. EMEP4UK modelled concentrations for the Scottish domain. The black box shows an arbitrary 50 km x 50 km where the concentration is >1.2 µg m<sup>-3</sup>. The range of concentrations in the same 50 km x 50 km grid square for: the 5 km x 5 km resolution is ~0.7 – >1.2 µg m<sup>-3</sup>, and for the 1 km x 1km resolution is ~0.4- >1.2 µg m<sup>-3</sup>.

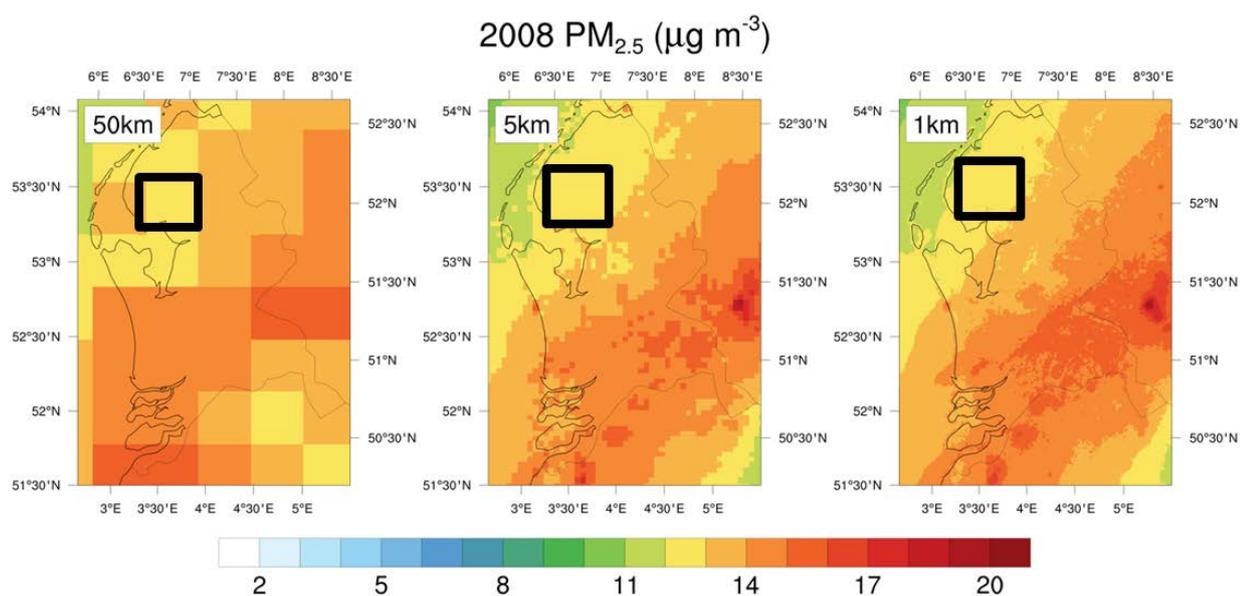


Figure 12. EMEP4UK modelled concentrations for the Dutch domain. The black box shows an arbitrary 50 km x 50 km where the concentration is 12 µg m<sup>-3</sup>. The range of concentrations in the same 50 km x 50 km grid square for: the 5 km x 5 km resolution is 12 – 14 µg m<sup>-3</sup>, and for the 1 km x 1km resolution is 12 - 14 µg m<sup>-3</sup>.

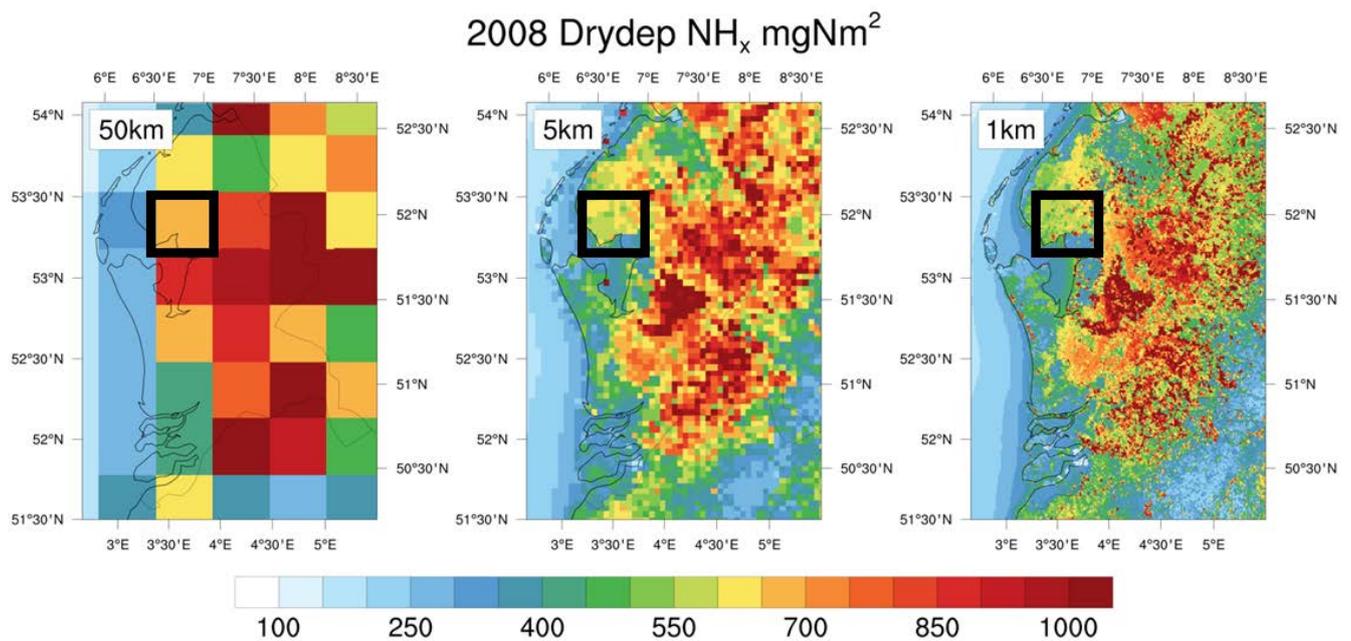


Figure 13. EMEP4UK modelled dry deposition for the Dutch domain. The black box shows an arbitrary 50 km x 50 km where the deposition is  $\sim 700 \text{ mgN m}^{-2}$ . The range of deposition in the same 50 km x 50 km grid square are: for the 5 km x 5 km resolution is  $\sim 250 - 750 \text{ mgN m}^{-2}$ , and for the 1 km x 1km resolution is  $\sim 250 - >850 \text{ mgN m}^{-2}$ .

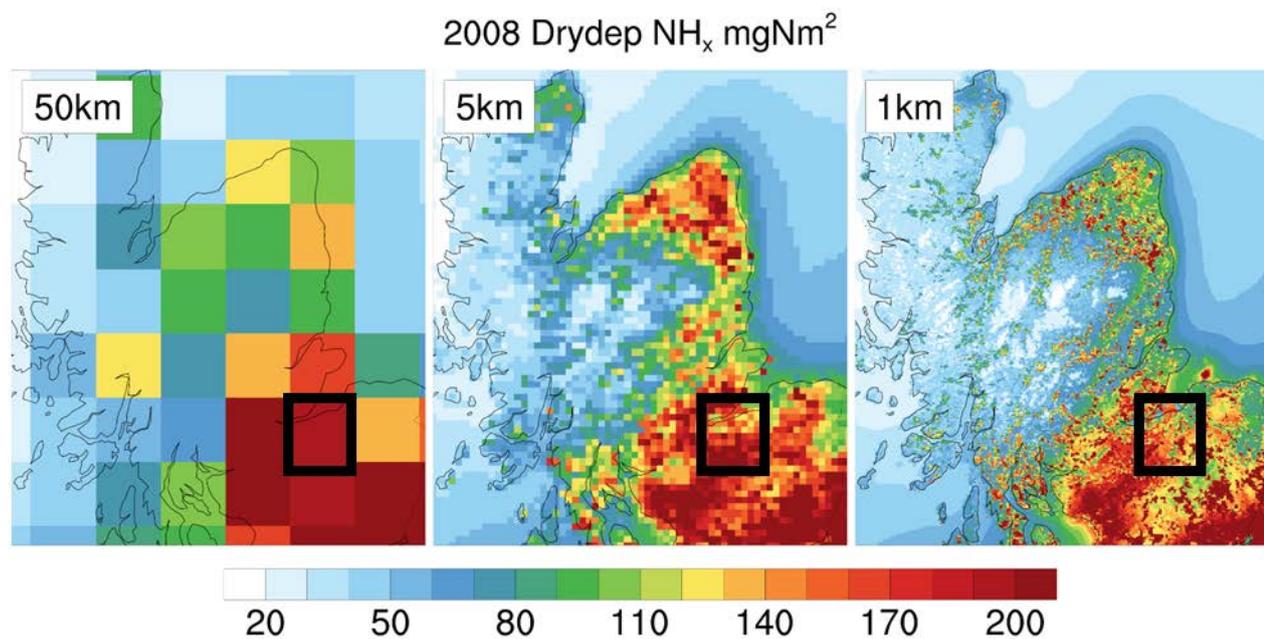


Figure 14. EMEP4UK modelled dry deposition for the Scottish domain. The black box shows an arbitrary 50 km x 50 km where the deposition is  $\sim 170 \text{ mgN m}^{-2}$ . The range of deposition in the same 50 km x 50 km grid square are: for the 5 km x 5 km resolution is  $\sim 110 - >200 \text{ mgN m}^{-2}$ , and for the 1 km x 1km resolution is  $\sim 50 - >200 \text{ mgN m}^{-2}$ .

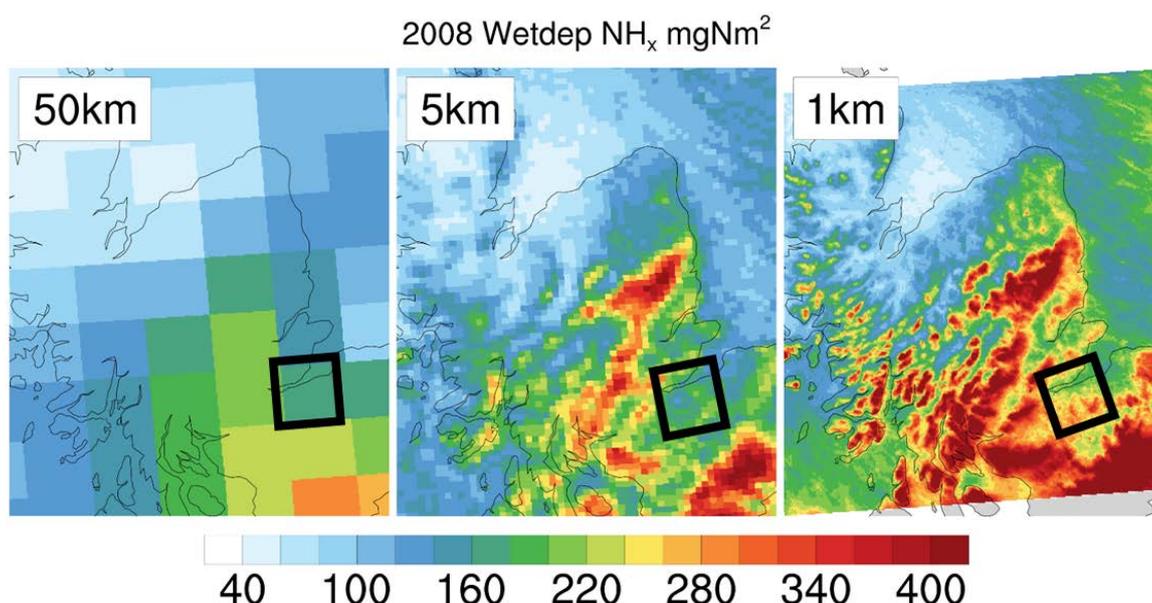


Figure 15. EMEP4UK modelled wet deposition for the Scottish domain. The black box shows an arbitrary 50 km x 50 km where the deposition is ~160 mgN m<sup>-2</sup>. The range of deposition in the same 50 km x 50 km grid square are: for the 5 km x 5 km resolution is ~110 – 250 mgN m<sup>-2</sup>, and for the 1 km x 1km resolution is ~100 - >350 mgN m<sup>-2</sup>.

**2.2.2.1 Effect of resolution on calculated concentrations**

When looking at the 50, 5 and 1 km<sup>2</sup> scale results for the Scottish domain (NO<sub>2</sub> and PM<sub>2.5</sub>), the differences become clear (see Figure 9). Especially the differences in the range of concentrations is a prominent aspect of the varying modellings resolutions.

When comparing the modelled and measured concentrations of e.g. O<sub>3</sub> for Aberdeen and Auchencorth (locations shown in Figure 16), large differences are introduced at different temporal and spatial resolutions.

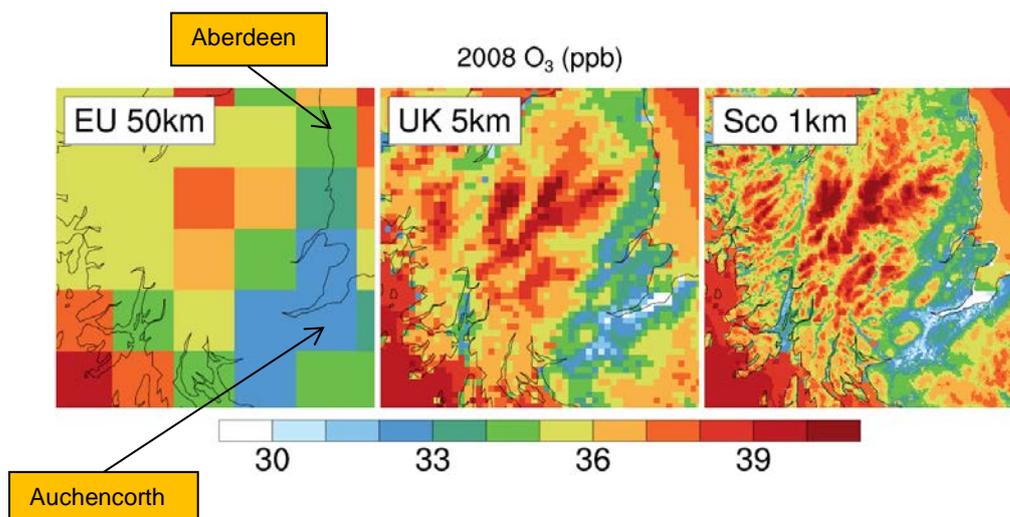


Figure 16. Locations of Aberdeen and Auchencorth on the ozone concentration maps for Scotland.

Figure 17 shows the detailed model results (2008 – O<sub>3</sub> and NO<sub>2</sub>) for the region of Aberdeen (square shown in Figure 16). Again, it is very clear how the range of concentrations changes for the different resolutions. The better resolved NO<sub>x</sub> spatial distribution allows the model to better represent the titration of O<sub>3</sub> in high NO<sub>x</sub> chemical regime (i.e. cities). In this specific example the surface ozone

concentration at a specific location (circle cross) changes from about 34 to 31 and 32 ppb, for the 50, 5 and 1 km horizontal model resolution, respectively.

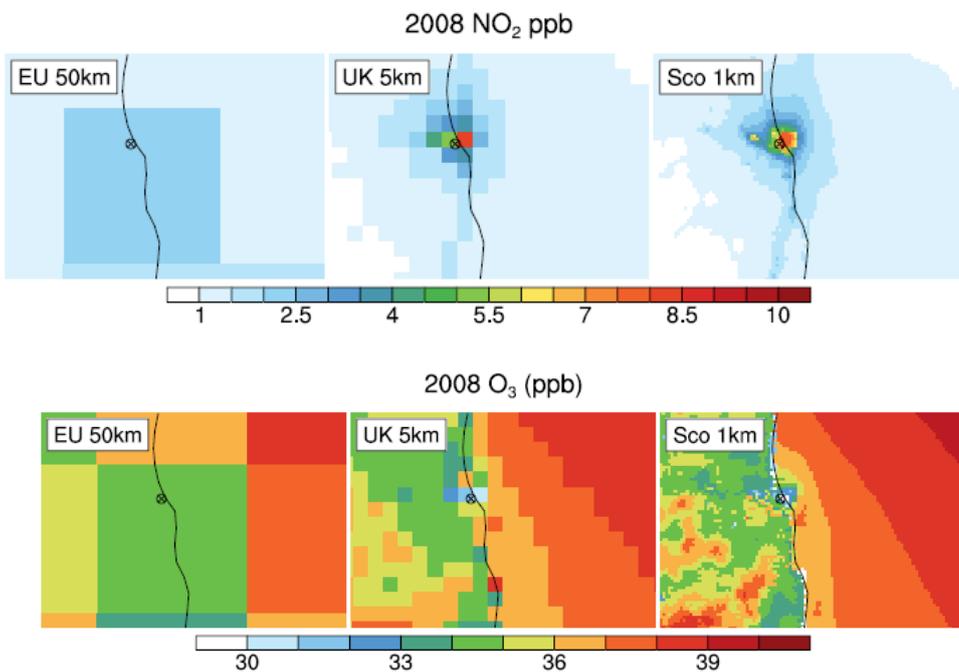


Figure 17. Detailed concentrations of NO<sub>2</sub> and O<sub>3</sub> for Aberdeen.

#### 2.2.2.2 Effect of resolution on calculated depositions

The differences in concentrations (shown in the previous paragraph) will eventually lead to differences in depositions. Looking at the earlier mentioned specific region in the Dutch modelling domain, the total dry deposition of reduced nitrogen will become less with increasing resolution.

For a resolution of 50 x 50 km<sup>2</sup>, the deposition is 800 mg N m<sup>-2</sup> (NL Budget = ~ 28 Gg N), for 5 x 5 km<sup>2</sup> this is 550-1000 mg N m<sup>-2</sup> (NL Budget ~ 25 Gg N), while for 1 x 1 km<sup>2</sup> this is 250 - >1000 mg N m<sup>-2</sup> (NL Budget ~ 24 Gg N). Dry deposition spatial distribution of reduced nitrogen is highly dependent of the spatial distribution of ammonia emissions and therefore the model resolution. Although different, the total NL budget, does not show a large differences between scales. Ammonia deposition velocity is relatively high and eventually most of available ammonia (not used to neutralise SO<sub>4</sub> and NO<sub>3</sub>) is eventually dry deposited within the NL domain. The changes in NL budget may be caused by the inclusion of fraction grid squares near the NL borders, in the budget calculation, due to the resolution approximations.

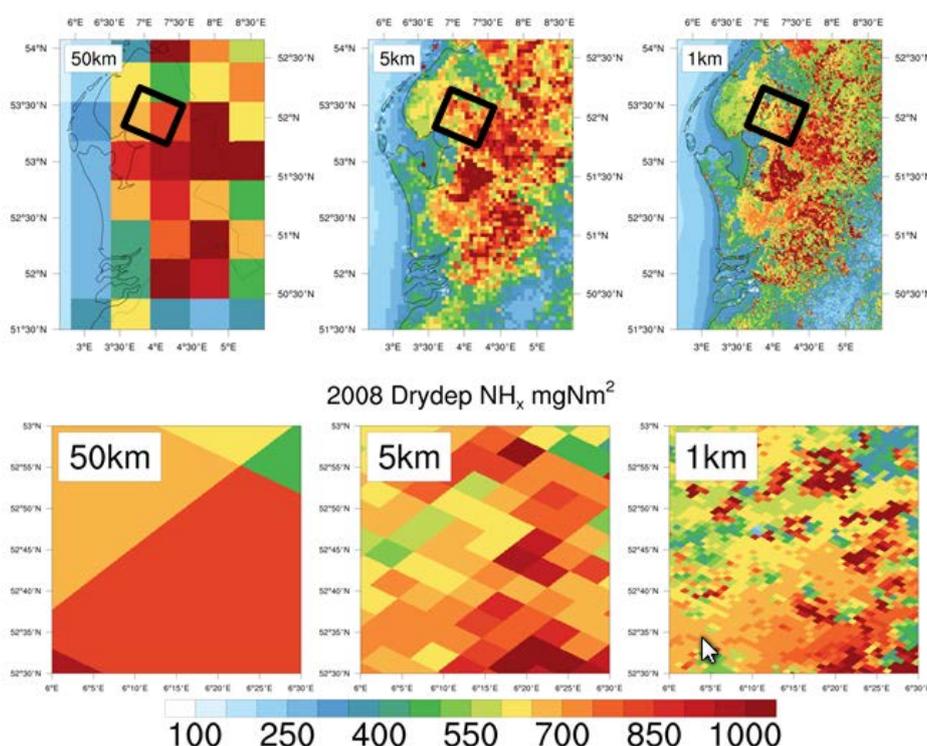


Figure 18: Changing deposition patterns for selected area in the Netherlands for different model resolutions

Overall, the differences in modelled depositions are larger than those for modelled concentrations. Not only the concentrations will have an effect on the depositions at different resolutions. Another factor influencing these differences in depositions are the local situations related to e.g. landuse / roughness length. They will also vary for the different resolutions and thus influence the calculated deposition. Eventually, this may have a larger effect on the differences than the modelled concentrations.

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### 3. Results:

With respect to the air quality / climate interaction it became clear from the model inventory that a full interaction is not available in the various models described here. Partly interactions exist when it comes to modelling the effect of a changing climate (with respect to meteorological conditions) on the modelled concentration/deposition.

As far as the modelled concentrations and depositions are concerned, it is clear that large differences will occur both in modelled concentrations and depositions with changing resolutions. While differences in modelled concentrations with changing resolutions will be of influence on the modelled depositions, the total difference for modelled depositions will also be the result of changing landuse/roughness lengths for the different resolutions. The latter likely to be of larger influence than the changing concentrations. Overall, the changes of concentrations/depositions with varying resolutions will have large effects on issues such as exceedance of critical levels/loads using these modelled maps.

### 4. Milestones achieved:

With these deliverables the following milestones have been achieved:

MS34: Report on local scale models inventory

MS37: Description of local scale interactions between air quality and climate change, based on e.g. NitroScape / EMEP4UK

**5. Deviations and reasons:**

The work presented here, was initially planned for an earlier stage of the project. Early delays were caused by illness and also the need to prioritise other parts of WP8 (further development of nitroscape for example, which encountered delays and required some refocussing of the work strategy). However, there was no knock on effects from late delivery of D8.1 as it turned out to be rather independent of other work.

**6. Publications:**

So far, no publications were developed based on the material presented here. However, a peer reviewed article is planned for the D8.2 material (will fall outside the project time-frame).

**7. Meetings:**

The plan for completing these deliverables has mainly been developed during the sessions held at the different annual project meetings.

**8. List of Documents/Annexes:**

None