Project Number 282910

ÉCLAIRE

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

Seventh Framework Programme

Theme: Environment

D13.3 Report on performance of site-based and regional-scale models

Due date of deliverable: **31/09/2013 (Month 24)** Actual submission date: **02/04/2015**

Start Date of Project: **01/10/2011** Duration: **48 months**

Organisation name of lead contractor for this deliverable :
NERC (Natural Environment Research Council – Centre for Ecology and Hydrology)

Project co-funded by the European Commission within the Seventh Framework Programme		
Dissemination Level		
PU	Public	X
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)	☐

Rowe EC, Hayes F, Sawicka K, Evans CD, Mills G, Emberson L, Briolat A & Büker P (2015) ECLAIRE Deliverable 13.3: Report on performance of site-based and regional-scale models.

1. Executive Summary

Modelling studies are an essential complement to empirical work, helping to develop understanding of processes and impacts and to identify and reduce uncertainty. The focus of this Working Package was to develop a predictive understanding of the combined effects of atmospheric ozone and nitrogen pollution on vegetation processes. Most of the work was on two dynamic models: DO_3SE, a model of gas exchange and photosynthesis at leaf-scale; and MADOC, a model of vegetation and soil processes at ecosystem scale.

The existing ozone (O_3) deposition model DO_3SE was improved by substituting the multiplicative with a photosynthesis (An) based stomatal conductance (gsto) algorithm (name of new model: An-gsto DO_3SE), which allows stomatal conductance to be estimated as a function of CO_2 concentration (as utilised by the photosynthesis) as well as other prevailing environmental conditions, e.g. N deposition (through varying levels of leaf N), relative humidity, irradiance, leaf temperature and soil moisture deficit. As such, a mechanism to incorporate an instantaneous O_3 damage function taking into account the combined effects of atmospheric O_3 and N pollution on An and hence biomass has been developed and incorporated into the DO_3SE model. The new modules developed within An-gsto DO_3SE representing the key physiological variables leaf temperature, gsto and photosynthesis were tested and evaluated through the application of An-gsto DO_3SE to the ECLAIRE Bangor dataset for birch (derived from field experiments carried out under WP 10), which offered the full set of required input and evaluation parameters. The model was found to be capable of simulating realistic ranges of these key physiological variables. The capability of An-gsto DO_3SE to predict NPP has also been demonstrated. Results suggest that higher leaf N may reduce the damaging effect of O_3, though further analysis is necessary.

The MADOC model was developed by combining submodels that simulated acid-base dynamics (VSD) and organic matter production and decomposition (N14C). Following a literature review (carried out within ECLAIRE WP9), two additional processes were included to represent effects of ozone concentration on plant productivity and leaf litter quality. The model was tested against data from long-term monitoring sites, and from an experiment (Alp Flix) in which both ozone and N exposure were manipulated. Although relevant empirical data on ozone-N interactions at ecosystem scale were scarce, model performance was considered to reflect the separate effects of ozone and N. Interactions were then explored in the model system. Ozone and N had opposite effects on plant productivity, with ozone causing an increasing proportional reduction in productivity at greater levels of N exposure. Increased plant productivity has both beneficial and negative effects (e.g. increased agricultural production, but loss of biodiversity). Ozone tended to make ecosystems more open or ‘leaky’ with respect to N. Increased N losses caused by greater ozone concentrations would have mainly harmful effects, such as more nitrate leaching and production of N_2O, a potent greenhouse gas.

2. Objectives:

The main aim of Working Package 13 was to develop existing dynamic vegetation models to better simulate the impacts of different air pollutants on plant growth and competition, and feedbacks on ecosystem carbon cycling. This was achieved via:

- Reviewing models that could be applied or adapted to simulate air pollution impacts, in particular combined impacts of ozone and N;

- Assessing data requirements for these models and determining which could realistically be applied;
- Adapting and improving the selected models;
- Collating data for setting up and testing the models;
- Assessing model performance against empirical data;
- Exploring effects of ozone and N pollution on key ecosystem processes and functions using the models.

3. Activities:

3.1 Data collation and model identification

An extensive set of models was initially proposed for use within WP13. The first task, carried out in Oct-Dec 2012, was to identify and summarise the scope, data requirements and outputs predicted by each model (Table 1). Data requirements were then compared against available data, including those collated during the NITROEUROPE project. It became clear that insufficient data were available to set up and test the majority of these models. The models remaining after this sift were:

i) DO_3SE

The DO_3SE (Deposition of Ozone for Stomatal Exchange) model simulates gas exchange and leaf-scale physiological processes, and has been applied to predict ozone impacts on a variety of plants including grassland species (Ashmore et al., 2007) evergreen trees (Alonso et al., 2008) and deciduous trees (Kinose et al., 2014). Further development and testing of DO_3SE are described below.

ii) VSD-N14C (i.e. MADOC)

The VSD model (Posch and Reinds, 2009) simulates acid-base exchange in soils and has been extensively applied to simulate impacts of acidifying pollutants at European scale. The N14C model (Tipping et al., 2012) simulates vegetation growth and the accumulation of soil organic matter. Within the ECLAIRE project, these two models have been fully integrated into a new model known as MADOC (Model of Acidity Dynamics and Organic Carbon) (Rowe et al., 2014). The model chain was not extended to include species-level responses predicted using MultiMOVE (Butler, 2010) as initially planned, due to a lack of data on species responses to ozone. The development and testing of MADOC are described below.

iii) VSD+

The VSD (Very Simple Dynamic) model (Posch and Reinds, 2009) has also been extended, using an alternative module for vegetation and organic matter dynamics, to form VSD+ (Bonten et al., 2010). This model has been combined with models of hydrology (MetHyd) and forest growth (GrowUp and FORSPACE) within the ECLAIRE project, and development of the VSD+ family of models is ongoing. However, it was considered that site-level data were insufficient to test these models. Development and testing of the VSD+ model family will be described instead in Working Package 14.

Work involving the LPJ-GUESS and DNDC-MOBILE models, as described in the original programme of work, has not taken place within WP13. Resources assigned to the respective participants (ULUND, KIT) have been utilised elsewhere in the project under C2 and C4. Additionally, it was agreed that different data (European-scale flux measurements) provided a more effective test of the large-scale

Dynamic Global Vegetation Models (DGVMs) than the site-based ecosystem experimental and monitoring data collated in C3; testing of these models has therefore been undertaken within C4 and will be reported on separately.

Table 1. Summary information for site-based and regional-scale models that were considered for inclusion in the study.

Model	Summary	Scale / spatial unit	Time units	Inputs summary	Outputs summary	Ecosystem impact indicators
DO3SE	The DO3SE model predicts the impact of O3 exposure, N and S deposition, diffuse radiation and climate on CO2 assimilation by different vegetation types.	point	hourly time-step	Atmopsheric component (hourly inputs of ozone and CO2 concentrations, reactive nitrogen treatments). Climate (hourly windspeed, radiation, precipitation, humidity)	Stomatal and total (inc-non stomatal) ozone deposition fluxes	Forest, grassland and crop growth/production impacts
VSD-N14C-MultiMOVE	Predicts soil and vegetation biogeochemistry (VSD+, VSD-N14C) and species occurrence (MultiMOVE)	point	yearly (VSD-N14C); not dynamic (MultiMOVE)	VSD-N14C inputs: Time-series of annual deposition of S, N, Ca, Mg, K, Na & Cl; observed C pool and C/N in a calibration year; organic and mineral horizon thicknesses; bulk density; average moisture content; precipitation surplus (drainage); cation exchange capacity; coefficients for ion selectivity (Al:Base cations, H:Base cations) & bicarbonate dissolution; weathering rates of Ca, Mg, K & Na; offtake rates of N, Ca, Mg & K. MultiMOVE inputs: %C, %N, moisture content and pH of 0-15 cm soil layer; canopy height; annual precipitation; min Jan and max July temperature.	Soil and biomass C & N pools (N14C); soil solution chemistry (VSD); Prevalence of individual species (803 higher plants and 327 bryophytes)	C & N storage; base saturation; soil solution nitrate and pH. Derived biodiversity indicators e.g. designated / typical / invasive species
LPJ-GUESS	Dynamic global vegetation model for simulation of interactions between climate, atmospheric burdens of trace gases and vegetation, biogeochemical cycles and trace gas exchange. The LPJ-GUESS model simulates the interactive effects of climate, CO2, O3 and N on plant C assimilation, C sequestration, growth, mortality and BVOC emissions	Spatial resolution deps. on climate and land cover input. Typically 10 minutes (Europe) or 0.5 degree (globe)	Shortest time-step daily; can be applied to past, present-day and 21st century simulations	Climate (monthly or daily radiation, precip, temperature (average), CO2 concentration, N deposition (under development), land use type if used in crop mode (or dynamic simulation of potential natural vegetation)	Forest and crop NPP or yield, soil and biomass C and N pools, trace gas emissions (BVOC, NOx, fire), forest potential natural species composition (Europe)	See outputs summary
LandscapeDNDC	LandscapeDNDC is the new name / version of DNDC-MOBILE. Biogeochemical process model simulaing major C and N cycling at ecosystem scale and associated ecosystem-atmosphere GHG exchange. Process parameterisation of the LandscapeDNDC model with regard to ecosystem GHG exchange, C sequestration, leaching losses and eutrophication will be further improved and uncertainty of key parameters will be assessed using, e.g., Bayesian calibration methods.	structured and unstructured grids. Spatial domain Europe	Daily outputs	Relevant information on meteorology and N deposition (daily), vegetation and soil properties needed.	Major C and fluxes, stock changes, GHG's/ NO fluxes, nitrate leaching	Changes in C/N ratios, nitrate leaching
GrowUp-MetHyd-VSD+-FORSPACE-VEG	dynamic process-based vegetation model (esp. forest, also semi -grasslands, shrubs). Describes mechanistically interactions between C, N, P, H2O, O3 and temp. in vegetation and soil	grid, polygons,	day	climate, soil, cover per species (or PFT for non-forest species), management	Processes: NPP, NEE, Evapotransp, biomass per species / PFT Current Annual Increment of trees. States: DBH, Basal area, volume of trees (per DBH class or height class). Standing and peak biomass.	impacts on growth. Measures of (fucntional) diversity.
ROMUL	Dynamic soil model with special attention to simulating successive change of different group of decomposers during litter decomposition. Model of soil organic matter (SOM) dynamics based on splitting SOM in correspondence with morphological soil horizons. Rates of decomposition, humification and flows between pools are obtained from laboratory data with accounting of soil fauna activities. Rates depend on nitrogen and ash contents in fresh litter and intermidiate pools, and from forest floor and soil temperature and moisture. Dynamics of nitrogen and basci cations is described by the same main equations but with correction functions for coefficients.	point, grid	month	Data on content of organic matter and nitrogen in soil horizons, climatic data, litterfall data	C and N stocks in main pools of soil organic matter	The amount of nitrogen availbale for plants

3.2 Model improvement and testing

i) DO_3SE

The DO_3SE (Deposition of Ozone for Stomatal Exchange) model (Büker et al., 2012; Emberson et al., 2000; Emberson et al., 2001a; Emberson et al., 2007; Emberson et al., 2001b) was improved by substituting the multiplicative version of the DO_3SE model with a photosynthetic based stomatal conductance algorithm based on (Farquhar et al., 1980) and (Ball et al., 1987), as described in the Deliverable 13.2 report in March 2013. The new photosynthetic algorithm allows stomatal conductance (g_{sto}) to be estimated as a function of CO_2 concentration as well as other prevailing environmental conditions, such as N deposition (through influence on leaf N content), relative humidity, irradiance (provided as diffuse and direct irradiance which can be influence by atmospheric aerosol load), leaf temperature (using energy balance equations to estimate leaf from air temperature) and soil moisture deficit (using methods developed for the original DO_3SE model).

The DO_3SE model has been developed so that it can be used to simulate site-specific experimental conditions. Importantly, this includes experiments that are performed in chambers (i.e. solardomes or open-top chambers) that are frequently used in filtration or fumigation studies to assess the effect of elevated pollution levels on plant growth and functioning. Within ECLAIRE a number of site-specific studies were conducted across Europe under such conditions. During the early stages of the project the DO_3SE modelling group were in collaboration with experimentalists to try to ensure, wherever possible, that data required for model application and evaluation would be collected within these experiments. Table 2 describes the data collected in these site-specific experiments from which suitability for use in DO_3SE modelling can be inferred.

To facilitate this Task 12.3 brought together the modellers or WP12 and WP13 with the experimentalists of WP10 and WP11 to design experimental protocols suitable for collecting physiological data that could be used to assess pollutant interactions at the physiological level. These protocols were applied in many of the C3 experimental studies over the 2012 and 2013 growing seasons and were uploaded to the ECLAIRE database during the first half of 2014.

Table 2 shows that only a few datasets (Bangor, Brandberg, Curno, Santa Olalla) have the full complement of input data necessary for DO_3SE modelling. Of these only Bangor includes evaluation data. Therefore, we focus the results presented in this report on the Bangor data and use this to describe the methods of application of the DO_3SE model that have been used at the other sites.

Table 2. Details of the experimental site-specific data and its suitability for use in DO3SE modelling.

Field site	Country	Vegetation type	Site design and exp. period	Met data (Temp, RH, VPD, u, P, PPFD, Pr, SW, $[O_3]$, $[CO_2]$)	Treatment	A_{net} data	g_{sto} data	T_{leaf} data	A/Ci & A/Q curves	Response data
Alpflix	Switzerland	Sub-alpine grassland	Field (2004 to 2010)	Temp, RH, u, $[O_3]$ (36% to 100%) Missing: PPFD	O3 and N treatments	×	×	×	×	Yield, above and below ground biomass (g m-2)
Bangor	UK	Birch	Solardome (2012 to 2013)	Temp, PPFD, VPD, $[O_3]$, $[CO_2]$, P. (87% to 100%)	O3 and N treatments.	✓	✓	✓	✓	Biomass (g m-2), Canopy height (m)
Bonn	Germany	Beech	Field 2012	Temp (100%) Missing: PPFD, VPD or RH, P, $[O_3]$	Water stress and N treatments	×	×	×	×	Canopy height (m), Biomass (total, foliage, stem) (g m-2)
Brandbjerg	Denmark	Grassland	Field 2006 to 2012	Temp, RH, u, $[O_3]$, PPFD, SWC, P, $[CO_2]$ (50% to 100%)	CO2, Temp, and O3 treatments	×	×	×	✓	Canopy height(m), LAI (m2/m2), above ground biomass g m-2
Curno	Italy	Oak & Hornbeam	Open to chamber 2012 to 2013	Temp, PPFD, P, Pr, $[O_3]$, VPD, LWP (60% to 100%)	N deposition and O3 treatments	×	×	×	✓	Biomass (leaf, stem, root (g m-2)
Santa Olalla	Spain	Mediterranean grassland (Dehesa)	Field 2011 to 2013	Temp, PPFD, $[O_3]$, VPD, PAW (~100%)	O3 treatments	×	×	×	×	Plant height (m)
Whim	UK	Bog	Field 2012 to 2013	Temp, PPFD, RH, u, P, (~100%) Missing: $[O_3]$	Ammonia and N treatments	×	×	×	×	Canopy height (m)

N.B. PPFD (Photosynthetic photon flux density), Temp (temperature), RH (Relative humidity), VPD (vapour pressure deficit), u (windspeed), SW (soil water), PAW (Plant available water), LWP (leaf water potential), Pr (air pressure), P (Precipitation), O3 (ozone), N deposition (nitrogen deposition). % denote data completeness for experimental period. Red text denotes missing data and highlights low data complements that complicates DO_3SE application and evaluation.

During the ECLAIRE project the DO_3SE model has been developed in a number of ways. Most importantly, a new photosynthetic based method has been implemented to derive stomatal conductance and hence stomatal O_3 flux. This has required the introduction of a new module to estimate leaf temperature (T_{leaf}) to allow an accurate estimate of the temperate dependant biochemical reactions that control photosynthesis within the leaf. This T_{leaf} module follows general principles of leaf energy balance and requires an analytical solution of the variables that control leaf gas exchange to optimise these variables for a particular set of conditions simultaneously. For T_{leaf} we follow the methods of Campbell & Norman (1998). Evaluation of T_{leaf}, net photosynthesis (A_n) and stomatal conductance (g_{sto}) is therefore a priority to ensure the DO_3SE model is fit for purpose and capable of simulating accumulated stomatal O_3 flux above a threshold 'y' or phytotoxic ozone dose (PODy) this being the metric that is used to characterise O_3 exposure for plant damage (Mills et al., 2011). The adoption of this coupled photosynthetic-stomatal conductance module (A_n-g_{sto}) also allows an assessment of the role of leaf N in determining PODy. This is important as is can eventually lead to an improved understanding of the combined stresses resulting from enhanced N deposition under elevated O_3 conditions. Leaf N content is strongly related to the maximum carboxylation efficiency (Vcmax) (the leaf capacity for photosynthesis) which is largely determined by the amount and activity of RUBISCO, the enzyme that catalyses CO_2 fixation). Vcmax can be estimated experimentally from A/Ci and A/Q curves which allow maximum photosynthesis under saturated conditions of internal CO_2 concentration (i.e. when CO_2 supply to photosynthesis is non-limiting) and irradiance (when irradiance saturates the supply of energy and electrons to the photosynthetic biochemistry. Ensuring the correct parameterisation of this Vcmax term is therefore also important.

Finally, a new method is under development to explore the role that O_3 (instantaneous stomatal O_3 flux (Fst)) may play in altering Vcmax. Identifying a relationship between Fst and Vcmax would provide an elegant means by which the effect of O_3 on C assimilation (and therefore plant growth) could be modelled according to core plant physiological processes which integrate to determine plant growth, biomass and yield. Further details of the new DO_3SE modules have been provided in other ECLAIRE deliverables (Deliverables 12.2 and 12.3)

In summary, the testing of the DO_3SE model has focussed on ensuring that the new modules developed within DO_3SE during the ECLAIRE project can simulate key physiological variables with a good degree of accuracy. These are T_{leaf}, A_n and g_{sto}. We have also used the experimental data to help calibrate the changes in Vcmax that occur with instantaneous O_3 flux so that the end of season Vcmax value reflects experimental observation for different O_3 and N deposition treatments.

i) VSD-N14C (i.e. MADOC)

The N14C and VSD models, and a simple model of dissolved organic matter formation and dissolution, were dynamically integrated to form the MADOC model (Rowe et al., 2014). Following an extensive review of the literature on ozone effects and ozone-nitrogen interactions (see ECLAIRE WP9 reports), strong and consistent evidence was found for two effects:

- A reduction in Net Primary Productivity (NPP);
- Early leaf senescence, resulting in reduced resorption of N and therefore a greater concentration of N in leaf litter.

These two effects were incorporated into the model using functions derived from empirical data in response to ozone, expressed as growing-season daylight-mean ozone concentration. Separate NPP reduction functions were fitted to biomass reduction data from: wet grassland and bog; other grassland; and woodland (Figure 1). It was assumed that overall woodland vegetation responded in the same way as trees. Fewer data were available on the effects of ozone on leaf N concentration in senescing leaves, and a single response function was fitted (Figure 2).

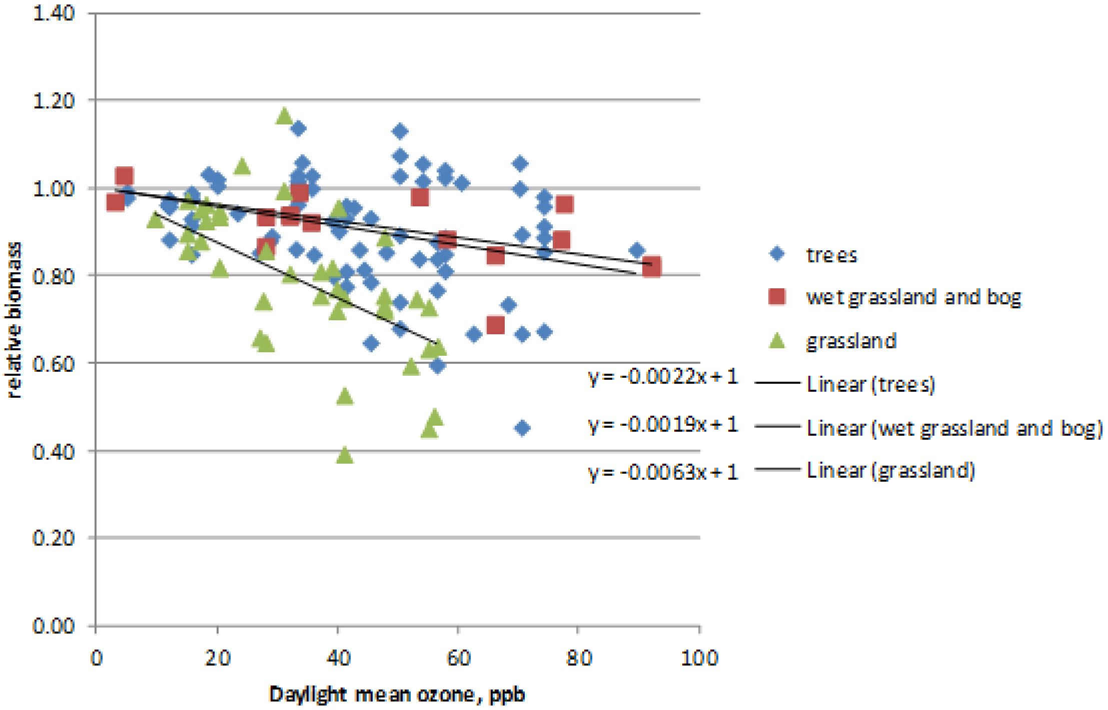

Figure 1. Effects of ozone pollution on biomass relative to unpolluted control, in wet grassland and bog, other grassland, and trees. Fitted lines were used within MADOC as response functions for reducing net primary productivity.

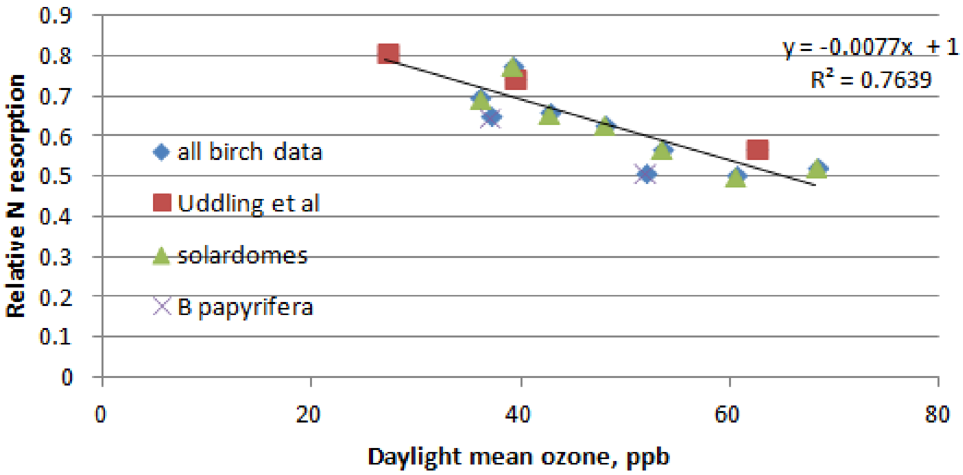

Figure 2. Effects of ozone pollution on the resorption of nitrogen from leaves before senescence. The fitted line was used within MADOC as a response function for reducing N resorption.

The revised MADOC model was tested against data from a set of experimental and long-term monitoring sites (Table 3; Figure 3). A full description of parameterisation and testing is given in Rowe et al. (in prep.) and Sawicka et al. (in prep.).

Table 3. Summary of sites used for testing the MADOC model. Long. = Longitude, degrees; Lat. = Latitude, degrees; Alt. = altitude, m above sea level; Precip. = mean annual precipitation, mm yr^{-1}; Temp. = mean annual temperature, ^{o}C; Factors = N and/or ozone factors used in the current study; "Monitoring" refers to sites without treatments, or where only control treatment data were used. Coordinates are presented approximately for sites where the landowner may be sensitive about revealing the site location.

Site	Country	Long.	Lat.	Alt.	Precip.	Temp.	Vegetation	Factors (N or O_3)
AlpFlix	Switzerland	9.650	46.533	2000	1300	1.1	Grassland	N, O3
Clocaenog	UK	-3.465	53.055	492	995	7.5	Heathland	Monitoring
Gårdsjön	Sweden	12.500	58.050	130	685	9.1	Conifer Forest	N
Glensaugh	UK	-2.6	56.9	300	1530	7.8	Grassland (Moorland)	Monitoring
Grizedale	UK	-3.0	54.3	115	1920	9.6	Broadleaf Forest	Monitoring
Kiskunsag	Hungary	19.417	46.867	108	572	10.5	Steppe / Broadleaf Forest	Monitoring
Klausen	Austria	16.048	48.121	515	768	7.6	Broadleaf Forest	Monitoring
Ladybower	UK	-1.8	53.4	265	1265	10.5	Coniferous forest	Monitoring
Llyn Brianne	UK	-3.7	52.1	450	2020	10.1	Coniferous forest	Monitoring
Montseny	Spain	2.358	41.779	720	870	9.5	Heathland / Broadleaf Forest	Monitoring
Moor House	UK	-2.4	54.7	540	1930	6.1	Grassland (Moorland)	Monitoring
Oldebroek	Netherlands	5.917	52.400	25	940	10.8	Heathland	Monitoring
Solling	Germany	9.500	51.667	508	1100	7.3	Coniferous forest	Monitoring
Sourhope	UK	-2.2	55.5	495	1280	7.7	Grassland	Monitoring
Whim	UK	-3.272	55.766	288	1090	7.7	Bog	N

Figure 3. Locations of monitoring and experimental sites used for testing the MADOC model.

4. Results:

4.1 Results of leaf-scale (DO3SE) modelling

The Bangor experimental dataset provides an excellent set of data with which to develop and test the A_n-g_{sto} DO$_3$SE model. The Bangor experiments were conducted on birch grown over two years under conditions of variable N and O_3 concentration. Throughout this period leaf level physiological measurements were made which have provided data to parameterise the A_n-g_{sto} DO$_3$SE model.

The Bangor data provides a good dataset to evaluate the DO_3SE Tleaf module with Tair and Tleaf data being collected with all physiological measurements that are made. Across the high and low N and O_3 treatments, the difference between modelled T_{leaf} and observed T_{air} (T_{leaf} -T_{air}) ranged from 4.8 to -1.1°C. A comparison of the modelled and observed T_{leaf} is shown in **Figure *4*** for the low O_3 and N treatments (there were only very minimal differences (less than 0.3°C) between N and O_3 treatments).

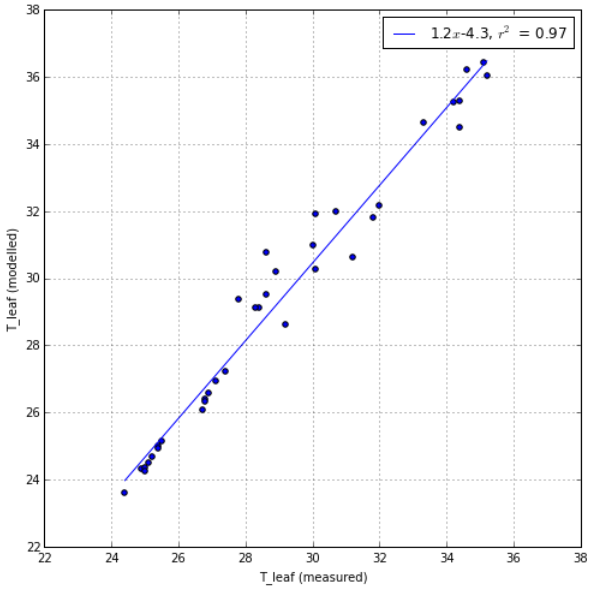

Figure 4. Comparison of observed ("measured") and simulated ("modelled") T_{leaf} (based on observed T_{air}) for the Bangor birch dataset at low O_3 concentration and low N deposition.

These comparisons show that the new T_{leaf} module is capable of simulating the difference between T_{leaf} and T_{air} with a reasonable level of accuracy.

As described in section 3.2 one difficulty in applying the Vcmax O_3 damage module is its parameterisation. It was possible to overcome this by calibrating the model to the observed values of Vcmax that were collected for Birch over the growing season. This calibration selected the most appropriate value for the co-efficient that related Fst to a change in Vcmax to give an end of season Vcmax value that most closely fitted the measured data (**Figure *5***). **Figure *5*** shows the variation in Vcmax that the model simulates using two different 'y' thresholds (1 (red line) and 2 (blue line) nmol O_3 m^{-2} PLA s^{-1}) over the growing season. The measured Vcmax values to which the model has been calibrated are shown as blue dots (mean values) and green crosses (individual values). The four plots show both high and low leaf N levels (N- and N+ respectively) and high and low ozone fumigation levels (O_3- and O_3+ respectively). The model is parameterised for high and low N by selecting an appropriate start of growing season Vcmax value. Similar methods are used for the data collected from Curno which also collected A/Ci and A/Q curves allowing the calibration of Vcmax over the growing season (data not shown).

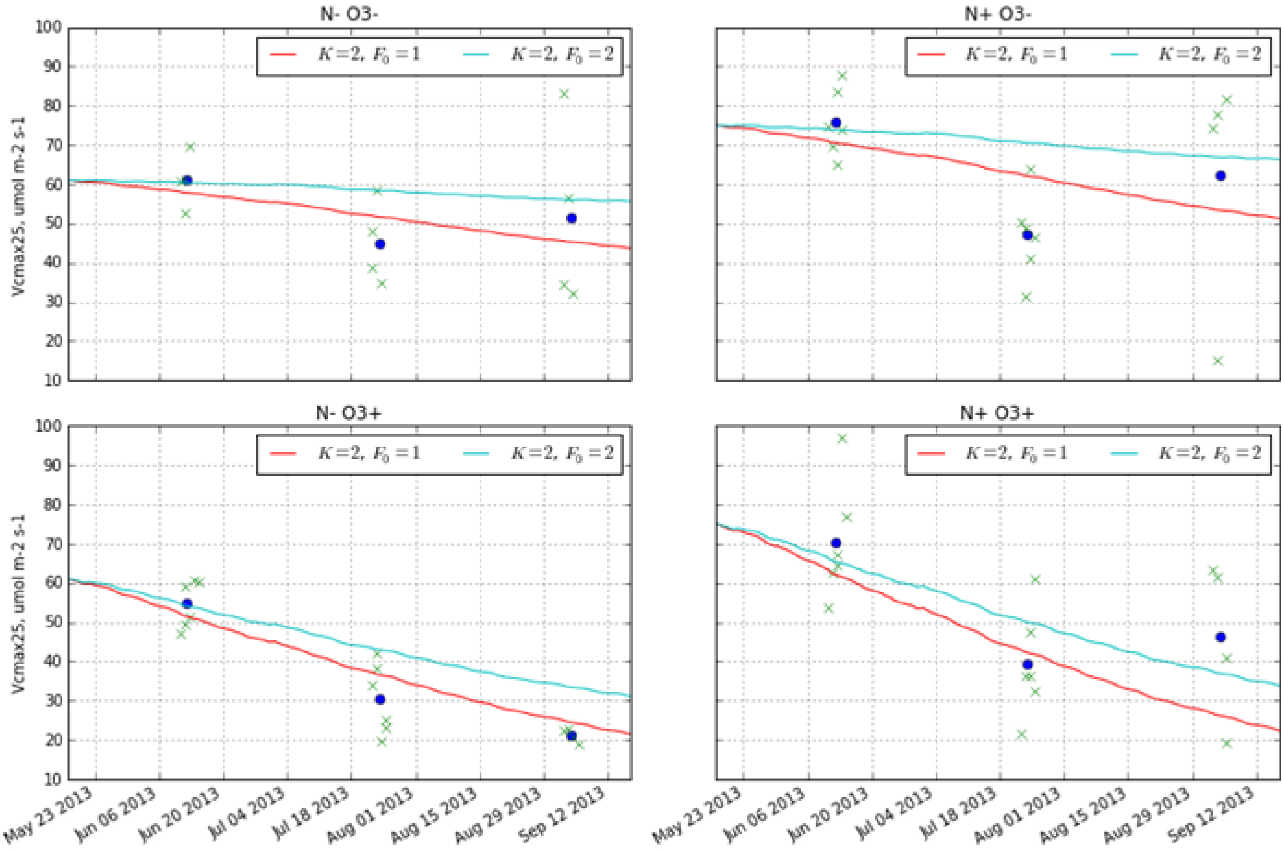

Figure 5. The DO_3SE A_n-g_{sto} models simulation of Vcmax over the course of the growing season compared to observations made for Birch grown in the Bangor solardomes. Simulations are made for high and low conditions of both O_3 and leaf N (see test for further description).

Evaluation of this new version of the DO_3SE A_n-g_{sto} model suggests the model is capable of simulating these variables within the range of observed values (see WP4 report for further details). **Figure *6*** shows simulations of A_n and g_{sto} made at two different N levels. This is important since it gives an indication of how these physiological variables (that will determine carbon assimilation and therefore end of season biomass) respond. In these simulations there are only differences in the variables during the day light period and they do not translate into substantial differences in either A_n or Fst. There is a systematic bias with higher N levels leading to higher A_n and Fst values.

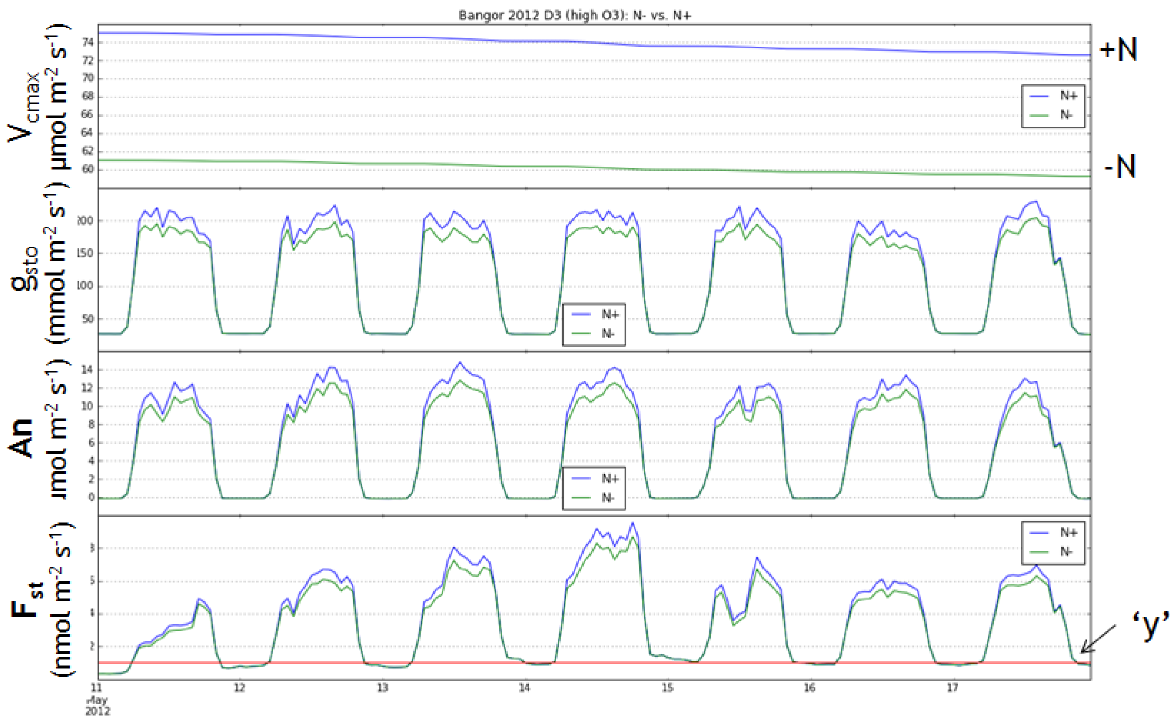

Figure 6. Simulations of photosynthesis and stomatal conductance in comparison to observations made on Birch from the Bangor solardome experiment.

The effect of this on biomass is useful to explore further. Higher A_n will see more carbon laid down whilst higher Fst will see more O_3 damage so it is interesting to see whether N causes a net increase or decrease in biomass (which will depend on the strength of the An *vs* Fst-O_3 damage response). **Figure *7*** shows simulations of end of season C assimilation using the An-gsto DO$_3$SE model to produce estimates of net primary productivity (NPP) for the living biomass and POD using a y threshold of 1 (POD_1) for the Birch trees performed in the Bangor experiment. This shows that for the same POD the biomass response is rather similar, however there is small tendency for higher N treated plants to be less affected by O_3 than their lower N treated counterparts.

Application of this model in a 'real world' setting will be interesting to perform to see how the dynamics in the leaf physiological variables changes over the course of a growing season and how this influences NPP. This will be particularly interesting since in a real world situation, O_3 concentrations will be episodic in nature (in contrast to the steady O_3 fumigation received in the experimental study) which would allow the modelled Vcmax to recover and hence alter the seasonal dynamics of A_n, g_{sto} and F_{st} in relation to leaf N levels.

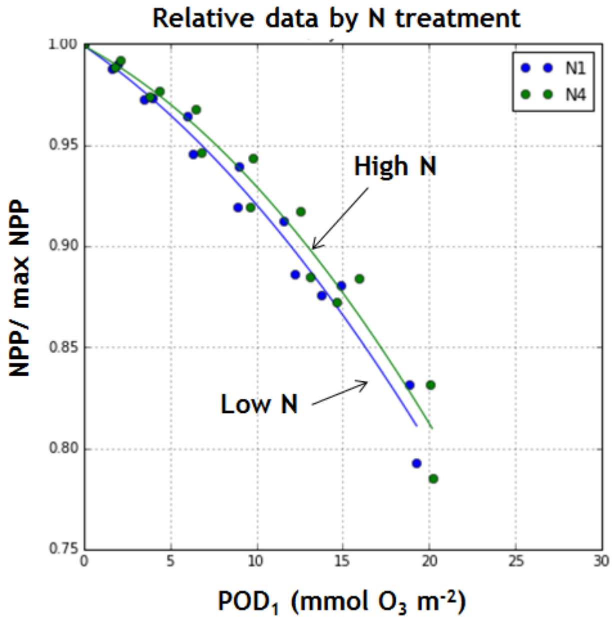

Figure 7. An-gsto DO$_3$SE model simulations of end of season relative NPP against POD$_1$ for the low and high N treatments applied to Birch trees fumigated with ozone in the Bangor solardomes.

The following key tasks have been achieved:

1. A mechanism to incorporate an instantaneous O_3 damage function has been developed and incorporated into the A_n-g_{sto} DO$_3$SE model. This mechanism is able to assess the combined effect of O_3 dose and N deposition (through a relationship with leaf N) and represents a step-change in our ability to model the effects that pollutants have in combination on biomass.
2. This new DO$_3$SE A_n-g_{sto} model has calibrated against experimental data collected for birch trees in the Bangor solardomes (see WP10 for further details). The model was found to be capable of simulating realistic ranges of key leaf physiological variables (i.e. A_n, g_{sto}).
3. The capability of the A_n-g_{sto} model to predict NPP has also been demonstrated. Results suggest that higher leaf N may reduce the damaging effect of O_3 though further analysis is necessary.

4.2 Results of ecosystem-scale (MADOC) modelling

The MADOC model successfully reproduced the magnitude and trends of soil solution concentrations of major ions that were observed at a set of long-term monitoring sites, in response to trends in N and S deposition (Figure 8). Data on ecosystem responses to ozone and N exposure were very limited, which inevitably restricted the testing that could be done on these aspects of the model. The ozone treatment imposed on the CLIMAITE experiment at Brandbjerg in Denmark was on single shoots and for a very limited period, so did not provide usable test data. The only source of ecosystem-level data on effects of ozone-N interactions was the Alp Flix experiment on alpine grassland in Switzerland, which included two levels of both ozone exposure and N deposition (Figure 9a). The experimental results showed a significant increase in NPP with N addition, but there no significant response of NPP to increased ozone exposure. The temporal changes in NPP predicted by setting up MADOC for each of the treatments reproduced the observed response to N, but also suggested that there would be a response to ozone. However this simulated ozone response was not large, and simulations were broadly consistent with the observations.

An experiment at Whim in the UK also provided useful test data for comparison with model predictions of the effects of different N deposition rates and forms. Different N forms, and the counterions with which ammonium and nitrate were added, are expected to have different effects on soil pH and therefore on the dissolution of potentially-dissolved organic carbon (Rowe et al., 2014).

These was reflected to an extent in observed fluxes of dissolved organic carbon (DOC), with an increase in DOC flux in the (alkalising) sodium nitrate treatment, and a decrease in DOC flux in the (acidifying) ammonium chloride treatment (Figure 9b). The MADOC simulations overestimated the responses in comparison to observations, but simulated responses were in the expected directions.

Another useful site for testing MADOC model performance was the set of catchments at Gårdsjön, Sweden, which were subjected to N addition and removal (via catchment roofing and substitution of artificial ‘clean’ rain) treatments. Detailed and long-term measurements related to C and N cycling are shown in Figure 10, along with MADOC model predictions. The model was reasonably successful in reproducing the direction of changes in mineral N and total soil C/N, and performed well at predicting trends in dissolved organic carbon (DOC) and dissolved organic nitrogen (DON). Concentrations of DOC greatly affect water treatment costs, and DON flux is a major route for N loss from ecosystems.

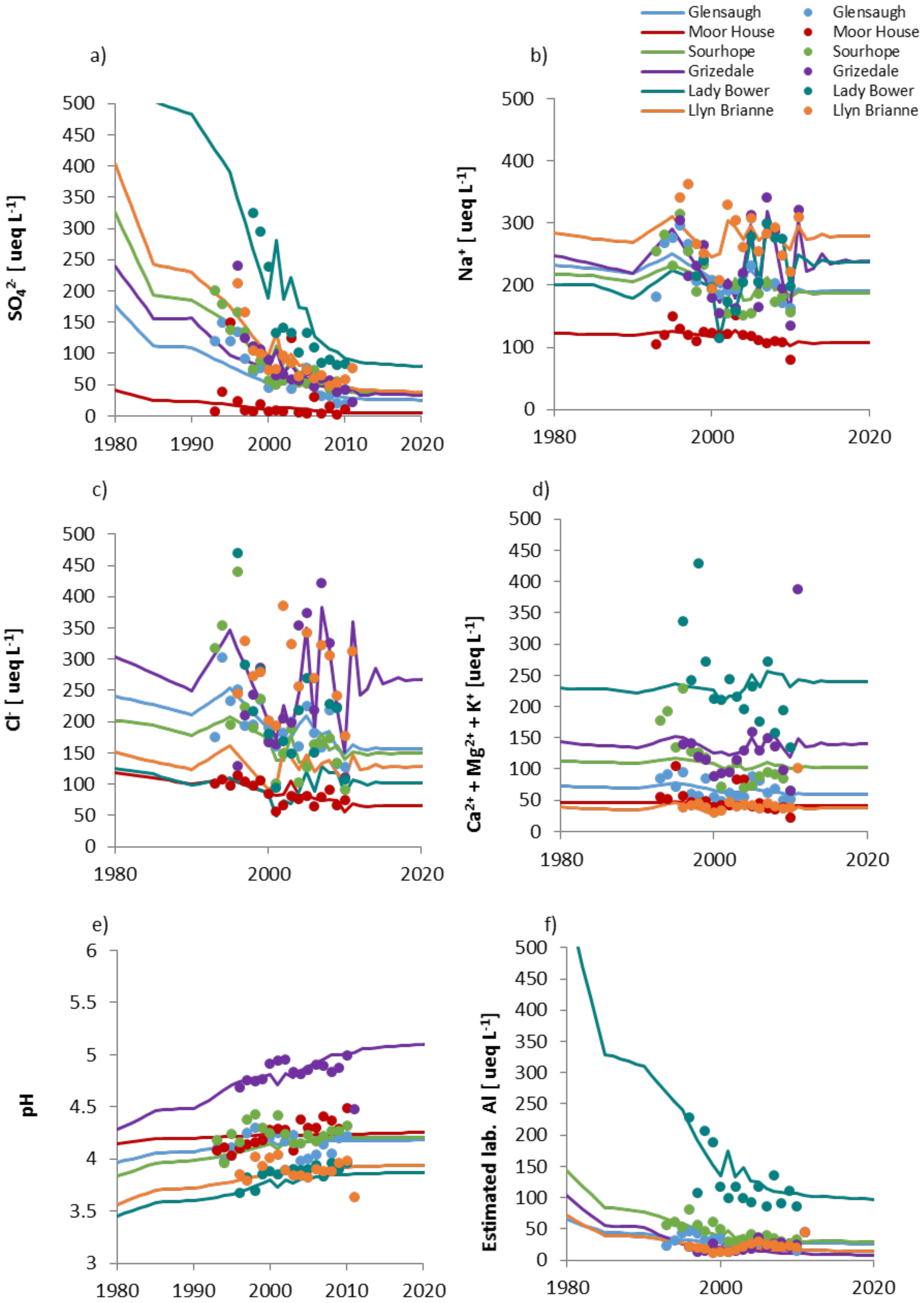

Figure 8. Observed annual average concentrations of major ions in soil lysimeters at six long-term monitoring sites (symbols), and equivalent results simulated by the MADOC model (lines).

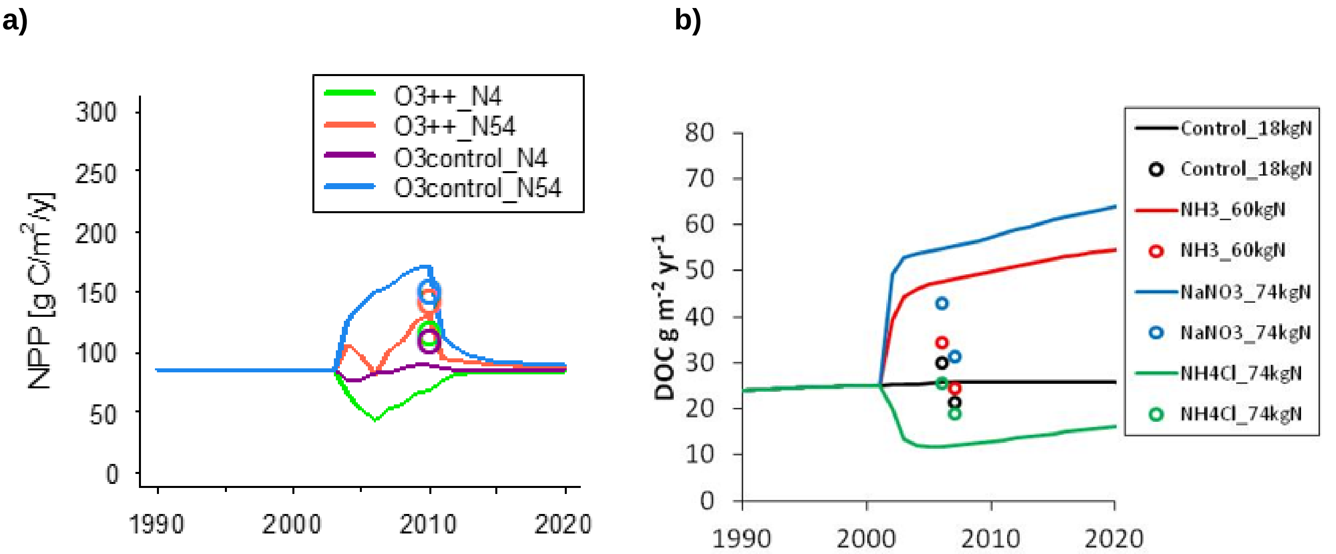

Figure 9. a) Observed effects (symbols) of two levels of ozone exposure (++ = elevated; and control) and two levels of nitrogen deposition (N4 = background deposition of 4 kg N ha^{-1} yr^{-1}; N54 = total deposition of 54 kg N ha^{-1} yr^{-1}) on net primary plant productivity (NPP) in alpine grassland at the Alp Flix site, and equivalent results simulated by the MADOC model (lines). b) Observed effects (symbols) of exposure to different rates and forms of N (Control = background deposition of 18 kg N ha^{-1} yr^{-1}; NH3 = additional deposition of dry ammonia, estimated to be 60 kg N ha^{-1} yr^{-1}; NaNO3 = sodium nitrate added to give a total rate of 74 kg N ha^{-1} yr^{-1}; NH4Cl = ammonium chloride added to give a total rate of 74 kg N ha^{-1} yr^{-1}) on leaching flux of dissolved organic carbon at the Whim site, and equivalent results simulated by the MADOC model (lines).

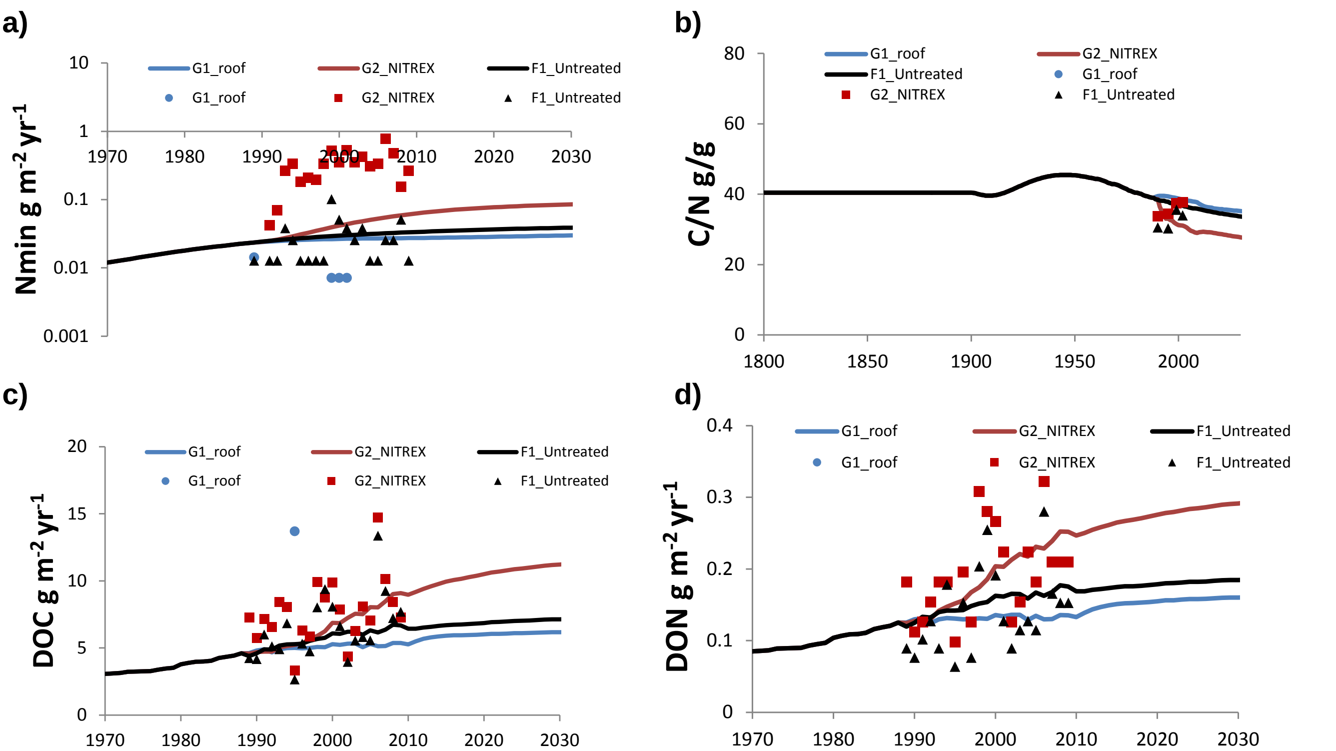

Figure 10. Observed effects (symbols) of three rain chemistry treatments at the Gårdsjön site: G1 roof (cleaned rain; blue); G2 Nitrex (nitrogen addition; red) and F1 Untreated (untreated; black), and equivalent results simulated by the MADOC model (lines): a) mineral N leaching flux; b) soil total carbon / nitrogen ratio; c) dissolved organic carbon (DOC) leaching flux; and d) dissolved organic nitrogen (DON) leaching flux.

The MADOC model has mainly been tested against either long-term monitoring data or data from N addition experiments. The single test against an ozone exposure experiment, in which observed effects of ozone were minimal, does not greatly increase confidence in the simulations of ozone effects and ozone-N interactions. However, the ozone responses introduced in the new version of MADOC are based on empirically-derived functions, and are consistent with evidence from *ex-situ* experiments. Given the paucity of empirical data on the ecosystem effects of ozone-N interactions, simulated responses to are the best available basis for assessing these effects.

The effects of ozone on NPP and on leaf senescence can be expected to affect N cycling within ecosystems, as well as other important ecosystem processes and functions. These effects were explored using sensitivity analyses in which the simulated levels of exposure to ozone and N were varied separately (Figure 11). In these simulated responses, increasing amounts of N clearly increased NPP, whereas ozone exposure decreased NPP. Ozone caused a greater proportional decrease in NPP with larger amounts of N. Carbon storage in soil was largely determined by plant productivity and followed a similar pattern. Nitrogen leaching also clearly increased in line with increased N deposition, but was also increased at greater ozone concentrations. This was partly due to a reduction in plant N uptake caused by smaller N demand from ozone-affected vegetation, and partly due to the greater N concentration in senescing leaves resulting from ozone damage.

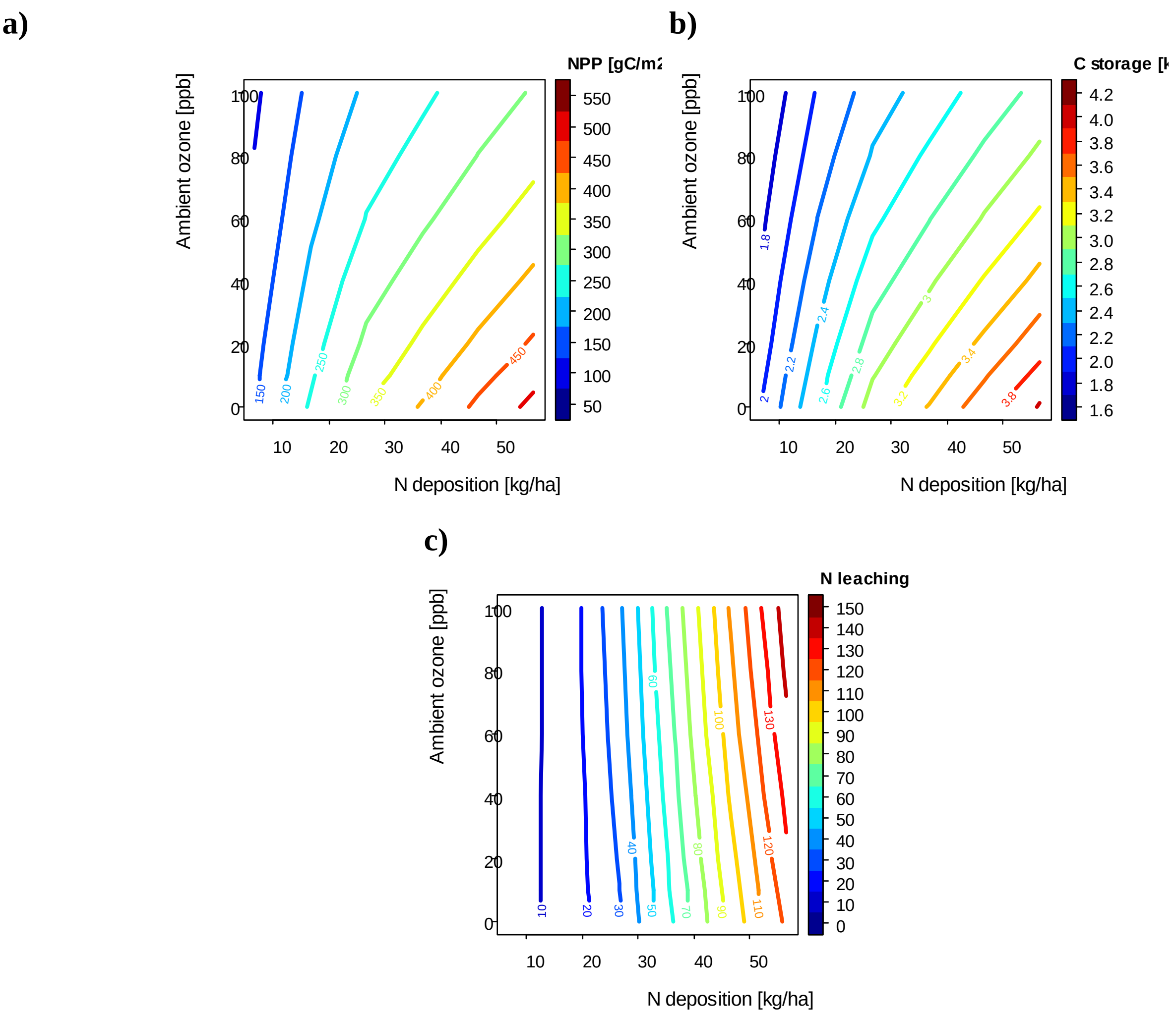

Figure 11. Effects of variation in N deposition rate and ambient ozone concentration (both treatments imposed from 2020) at a broadleaf forest site in the UK, Grizedale, on ecosystem-scale properties in 2100: a) net primary production (NPP, g C m^{-2} yr^{-1}); b) carbon stored in soil (g C m^{-2}); and c) N leaching (total mineral N concentration in leachate, µeq L^{-1}).

Overall, the ecosystem effects of ozone and N can be viewed mainly as contrasting effects of a toxic compound (ozone) and a fertilising element (N). Increases in plant productivity driven by N pollution will be beneficial for crop and forest production, and may also lead to the storage of more C in soil. The latter has benefits in terms of reducing net greenhouse gas emissions, and arguably increases soil 'quality', e.g. by buffering nutrient and cation availability, and by improving soil structure and aeration (Bhogal et al., 2008). However, the fact that N often has a 'fertilising' effect does not mean that the consequences of N deposition are all beneficial for people. The leaching of N has important implications for water quality and human health, and has an acidifying effect on soil. In many habitats there is an inverse relationship between plant productivity and biodiversity value – for example, the diversity of plant species (particularly the more distinctive and scarce species) tends to be less in fertile agricultural pastures than in less-productive grassland. For these reasons, the uncontrolled addition of N to the European landscape through increased atmospheric deposition is usually considered to be polluting.

An interesting effect that emerged from the study is the suggestion that ozone decreases ecosystem-scale nitrogen use-efficiency, both by reducing demand for N and by increasing the concentration of N in plant litter. Extra losses of N caused by ozone are likely to be environmentally harmful, whether these leave the system as leached nitrate or as gaseous losses of ammonia or nitrous oxide.

5. Milestones achieved:

M56 (due Month 6, 31/03/2012) Identification of priorities for model development. Completed on time.

M57 (due Month 12, 30/09/2012) Collation of preliminary data from experimental sites for initial model application. Completed on time.

M58 (due Month 18, 31/03/2013) Initial application and testing of integrated models. Completed 05/04/2013, as described in Deliverable 13.2 report.

M59 (due Month 24, 30/09/2013) Update of experimental datasets, completed testing of site-based and regional-scale models. Completed 31/03/2015, as described in current report.

6. Deviations and reasons:

Initial deviations were minor, but the current report has been considerably delayed. Completing the collation of data was delayed due to the identification of additional sites, and of new data that had not yet been included in the NITROEUROPE or ECLAIRE databases. The finalisation of an ozone-responsive version of the MADOC model was delayed due to the need to incorporate response functions derived from the data-mining exercise. These functions did not become available until June 2014. Lastly, the process of setting up and testing the models was more time-consuming than anticipated. However, considerable improvements have been to the DO_3SE and MADOC models. A publication describing the improvements to DO_3SE is currently in preparation. The MADOC model has been published in a peer-reviewed journal, and results of the final testing round will shortly be submitted for peer-review.

7. Publications:

Rowe EC, Sawicka K & Evans (2013) MADOC – update on progress. Presentation at ECLAIRE conference, Zagreb, Croatia, 22-24 October 2013.

Rowe EC, Sawicka K & Evans (2013) MADOC – ozone response functions and sensitivity analyses. Presentation at ECLAIRE conference, Zagreb, Croatia, 22-24 October 2013.

Rowe EC (2013) Biodiversity endpoints. Presentation at ECLAIRE conference, Zagreb, Croatia, 22-24 October 2013.

Emberson LD, Bueker P, Briolat A. (2013) DO_3SE – update on progress. Presentation at ECLAIRE conference, Zagreb, Croatia, 22-24 October 2013.

Emberson LD, Bueker P, Briolat A. (2013) DO_3SE – Using DO_3SE as an analytical tool for experimental studies. Presentation at ECLAIRE conference, Zagreb, Croatia, 22-24 October 2013.

Rowe EC, E Tipping, Davies J, Monteith DT & Evans CD (2014) Towards an understanding of feedbacks between plant productivity, acidity and dissolved organic matter. Oral presentation, European Geosciences Union conference, Vienna, Austria, 28 April - 2 May 2014.

Rowe EC, Tipping E, Posch M, Oulehle F, Cooper DM, Jones TG, Burden A, Hall J & Evans CD (2014) Predicting nitrogen and acidity effects on long-term dynamics of dissolved organic matter. *Environmental Pollution* 184: 271-282.

Emberson LD, Bueker P, Briolat A. (2014) The use of DO_3SE in seasonal crop forecasting. Meeting at JRC, ISPRA. Italy. Nov 2014.

Evans C, Hayes F, Sawicka K, Mills G & Rowe E (2014) Ecosystem responses to nitrogen and ozone simulated by MADOC. Presentation at ECLAIRE conference, Budapest, Hungary, 29 Sept - 2 Oct 2014.

Rowe E, Sawicka K, Hayes F & Evans C (2014) MADOC. Presentation at ECLAIRE conference, Budapest, Hungary, 29 Sept - 2 Oct 2014.

Rowe E, Hayes F, Sawicka K, Mills G & Evans C (2014) Modelling ozone impacts in the UK and elsewhere. Oral presentation, Joint Expert Group on Dynamic Modelling (15th Meeting), Sitges, Spain, 28-30 October 2014.

Rowe EC (2015) Humus and humility in ecosystem model design. Abstract for European Geosciences Union conference, Vienna, Austria, 13-16 April 2015.

Rowe EC, Hayes F, Sawicka K, Mills G, Jones L, Moldan F, Sereina B, van Dijk N & Evans C (2015) Ecosystem-scale trade-offs between impacts of ozone and reactive nitrogen. Abstract for European Geosciences Union conference, Vienna, Austria, 13-16 April 2015.

Emberson LD, Bueker P, Briolat A. (*in prep*.). The incorporation of multiple stresses (O3 and N) on plant growth using process based methods within the DO_3SE model. *Global Change Biology*.

Rowe EC, Sawicka K Hayes F, Mills G, Albert KR, Bassin S, Sheppard LJ & Evans CD (*in prep.*) Predicting integrated effects of nitrogen and ozone on plant productivity and carbon storage. *Environmental Pollution*.

Sawicka K, Rowe EC, Monteith DT, Vanguelova E, Wade AJ, Clark JM (*in prep.*) Modelling past, current and future trends in soil water dissolved organic carbon. *Science of the Total Environment*.

8. Meetings:

- ECLAIRE conference, Zagreb, Croatia, 22-24 October 2013. Development of MADOC presented.
- European Geosciences Union conference, Vienna, Austria, 28 April - 2 May 2014. Development of MADOC presented.
- ECLAIRE conference, Budapest, Hungary, 29 Sept - 2 Oct 2014. Development of and results from ozone-sensitive version of MADOC presented.
- 15th Meeting of the Joint Expert Group on Dynamic Modelling under the Working Group on Effects, Sitges, Spain, 28-30 October 2014. Development of and results from ozone-sensitive version of MADOC presented.

9. List of Documents/Annexes:

None.

References

Alonso, R., Elvira, S., Sanz, M.J., Gerosa, G., Emberson, L.D., Bermejo, V., Gimeno, B.S., 2008. Sensitivity analysis of a parameterization of the stomatal component of the DO3SE model for Quercus ilex to estimate ozone fluxes. Environmental Pollution 155, 473-480.

Ashmore, M.R., Buker, P., Emberson, L.D., Terry, A.C., Toet, S., 2007. Modelling stomatal ozone flux and deposition to grassland communities across Europe. Environmental Pollution 146, 659-670.

Ball, J.T., Woodrow, I.E., Berry, J.A., 1987. A model predicting stomatal conductance and its contribution to the control of photosynthesis under different environmental conditions., in: Biggens, J. (Ed.), Progress in photosynthesis research, Vol IV. Dordrecht: Martinus Nijhoff.

Bhogal, A., Boucard, T., Chambers, B.J., Nicholson, F.A., Parkinson, R., 2008. Road testing of 'trigger values' for assessing site specific soil quality. Phase 2 - Other soil quality indicators. UK Environment Agency. Science report SC050054SR2. https://www.gov.uk/government/uploads/system/uploads/attachment_data/file/291143/scho1008bosv-e-e.pdf, p. 68.

Bonten, L.T.C., Posch, M., Reinds, G.J., 2010. The VSD+ soil acidification model - model description and user manual. Alterra and Coordination Centre for Effects.

Büker, P., Morrissey, T., Briolat, A., Falk, R., Simpson, D., Tuovinen, J.P., Alonso, R., Barth, S., Baumgarten, M., Grulke, N., Karlsson, P.E., King, J., Lagergren, F., Matyssek, R., Nunn, A., Ogaya, R., Penuelas, J., Rhea, L., Schaub, M., Uddling, J., Werner, W., Emberson, L.D., 2012. DO3SE modelling of soil moisture to determine ozone flux to forest trees. Atmospheric Chemistry and Physics 12, 5537-5562.

Butler, A., 2010. The GBMOVE ensemble (MultiMOVE): A technical summary. . Biomathematics & Statistics Scotland, Edinburgh. Report to Centre for Ecology & Hydrology.

Campbell, G.S., Norman, J.M., 1998. An Introduction to Environmental Biophysics. Springer-Verlag, New York.

Emberson, L.D., Ashmore, M.R., Cambridge, H.M., Simpson, D., Tuovinen, J.P., 2000. Modelling stomatal ozone flux across Europe. Environmental Pollution 109, 403-413.

Emberson, L.D., Ashmore, M.R., Simpson, D., Tuovinen, J.P., Cambridge, H.M., 2001a. Modelling and mapping ozone deposition in Europe. Water Air and Soil Pollution 130, 577-582.

Emberson, L.D., Buker, P., Ashmore, M.R., 2007. Assessing the risk caused by ground level ozone to European forest trees: A case study in pine, beech and oak across different climate regions. Environmental Pollution 147, 454-466.

Emberson, L.D., Simpson, D., Tuovinen, J.-P., Ashmore, M.R., Cambridge, H.M., 2001b. Towards a model of ozone deposition and stomatal uptake over Europe. Norwegian Meteorological Institute, Oslo, EMEP MSC-W Note 6/2000., p. 57.

Farquhar, G.D., von Caemmerer, S., Berry, J.A., 1980. A biochemical model of photosynthetic CO2 assimilation in leaves of C3 species. Planta 149, 78–90.

Kinose, Y., Azuchi, F., Uehara, Y., Kanomata, T., Kobayashi, A., Yamaguchi, M., Izuta, T., 2014. Modeling of stomatal conductance to estimate stomatal ozone uptake by Fagus crenata, Quercus serrata, Quercus mongolica var. crispula and Betula platyphylla. Environmental Pollution 194, 235-245.

Mills, G., Pleijel, H., Braun, S., Buker, P., Bermejo, V., Calvo, E., Danielsson, H., Emberson, L., Fernandez, I.G., Grunhage, L., Harmens, H., Hayes, F., Karlsson, P.E., Simpson, D., 2011. New stomatal flux-based critical levels for ozone effects on vegetation. Atmospheric Environment 45, 5064-5068.

Posch, M., Reinds, G.J., 2009. A very simple dynamic soil acidification model for scenario analyses and target load calculations. Environmental Modelling & Software 24, 329-340.

Rowe, E.C., Hayes, F., Sawicka, K., Mills, G., Bassin, S., Sheppard, L., Moldan, F., Evans, C.D., in prep. Predicting integrated effects of nitrogen and ozone on plant productivity and carbon storage. Environmental Pollution.

Rowe, E.C., Tipping, E., Posch, M., Oulehle, F., Cooper, D.M., Jones, T.G., Burden, A., Monteith, D.T., Hall, J., Evans, C.D., 2014. Predicting nitrogen and acidity effects on long-term dynamics of dissolved organic matter. Environmental Pollution 184, 271-282.

Sawicka, K., Rowe, E.C., Evans, C.D., Monteith, D.T., Vanguelova, E., Wade, A.J., Clark, J.M., in prep. Modelling past, current and future trends in soil water dissolved organic carbon. Science of the Total Environment.

Tipping, E., Rowe, E.C., Evans, C.D., Mills, R.T.E., Emmett, B.A., Chaplow, J.S., Hall, J.R., 2012. N14C: a plant-soil nitrogen and carbon cycling model to simulate terrestial ecosystem responses to atmospheric nitrogen deposition. Ecological Modelling 247, 11-26.