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D5.3 Future evolution of the produced fertilisers effectiveness

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Abstract

In this deliverable (D5.3) entitled Future evolution of the produced fertilizers effectiveness, the BBFs performance is studied under different climatic scenarios. To develop effective management strategies, in-depth evaluations of BBFs nutrient value and environmental performance under both average weather conditions and future climatic scenarios across Europe has been carried out. This provides an overview of expected values as well as temporal and spatial variability in BBFs performance, both within and beyond Europe. Additionally, this deliverable offers initial insights into potential effects under projected climate change scenarios.

For this purpose, two process-oriented models have been studied: DNDC for soil carbon-nitrogen dynamics and DSSAT/CROPGRO for broccoli biomass production. Harmonized field and ecotron trials in Belgium, Estonia, Norway, Spain, and France applied BBFs and a mineral control at 120 kg N ha^{-1}, generating comprehensive soil, crop, and weather datasets for model calibration. Site-specific DNDC tuning achieved strong fits for aboveground biomass and yield ($R^2 \geq 0.84$) but revealed shortcomings in soil moisture dynamics and NO_3^-/NH_4^+ partitioning. DSSAT calibration delivered satisfactory biomass predictions (RSR < 0.50) in Spain and Norway. Under future climate scenarios (+3.5 °C warming; CO_2 from 550 to 775 ppm), simulations show that warming accelerates BBF nutrient mineralization (Q_{10} effect), closing the yield gap with mineral fertilizers, while elevated CO_2 further enhances yield only when nitrogen supply and sink capacity remain unsaturated. Key recommendations include refining DNDC's irrigation and microbial-activity parameters and extending DSSAT to represent BBF biostimulant mechanisms—such as enhanced root growth and accelerated nutrient uptake—to improve predictions of next-generation fertilizers under climate change.

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Glossary

BBF: Biobased fertiliser

BP: Bokashi pellet

CAT1: Protein fraction

D: Deliverable

D: Deliverable

DM: Dry matter

DNDC: Denitrification-decomposition model

DSSAT: Decision support system for agrotechnology transfer

FER3: NPK solution with amino acids

FER5': Bio stimulant coming from microalgae

FMP: Fish mix pelleted fertiliser

FSP: Fish sludge pelleted fertiliser

GENCALC : Genetic Coefficient Calculator in the DSSAT suite

WFPS: Water filled pore space

WP: Work Package

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1 Introduction

To meet the food demands of a growing human population, future agricultural production must become more efficient and environmentally sustainable. Since the development of the Haber-Bosch process for producing mineral nitrogen fertilizers, their use and dependence have risen significantly, leading to increased crop yields. However, the Haber-Bosch synthesis is highly energy-intensive and has a considerable climate impact due to its reliance on fossil fuels. An alternative to mineral N fertilizers could be the repurpose of underutilized organic materials to create biobased fertilizers (BBFs). These BBFs are defined as materials or products derived from biological sources that contain bioavailable plant nutrients suitable for crop fertilization (Wester-Larsen et al., 2022). Given their relatively recent introduction, the efficiency of these novel BBFs and their potential to replace mineral N fertilizers produced through the Haber-Bosch method remain largely unexplored. Notably, aquaculture generates substantial amounts of animal by-products not intended for human consumption, along with other waste, which must be managed properly to reduce potential health risks.

Cabbage (*Brassica oleracea* L.) is a crop with high nitrogen demands and ranks as the third most important vegetable group in Europe. Ensuring sufficient cabbage production requires a thorough understanding of the interactions between crop growth, environmental conditions, and nutrient requirements that affect yield and quality. Among brassica crops, broccoli (*Brassica oleracea* L. var. *italica*) stands out for its adaptability to cool-season production and represents a significant share of the total brassica vegetable yield. Given that field experiments can be labour-intensive, costly, and time-consuming, process-oriented crop simulation models offer a valuable alternative for simulating crop growth and predicting yield potential.

Several crop growth simulation models are widely recognized and used by researchers worldwide. Among them, the CROPGRO model, integrated into the Decision Support System for Agrotechnology Transfer (DSSAT), stands out. Originally developed for legume crops, CROPGRO can simulate crop responses to various fertilizers based on climatic, soil, and environmental conditions. Another widely used model is the denitrification-decomposition (DNDC) model, a process-oriented simulation tool focused on soil carbon and nitrogen biogeochemistry. The DNDC model is designed to estimate the impacts of climate change, land use, agricultural management practices, soil properties, and atmospheric nitrogen deposition on soil carbon and nitrogen dynamics.

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Fertilizer application must be adjusted according to yield potential, crop nutrient requirements, and environmental factors, such as soil type and climatic conditions.

Bio-based products can significantly contribute to soil fertility and plant nutrition. WP5 aims develop in-depth evaluations of nutrient value and environmental performance of BBFs developed in WP3 and WP4 under different conditions as BBFs effect is not always as predictable as that of mineral fertilisers.

Specific objectives:

- Conduct *in situ* validation of the agronomic and environmental performance of bio-based fertilizers under contrasting environmental conditions across Europe.
- Adapt a simulation model to assess the agronomic and environmental performance of bio-based fertilizers under different climate and soil conditions.

The DNDC model is a process-based simulation tool for analysing carbon and nitrogen biogeochemistry in agricultural ecosystems. It is used to predict crop yield, carbon sequestration, nitrate leaching, and emissions of carbon and nitrogen gases. The model operates in two modes: site and regional, allowing users to manage input data for specific locations or broader regions (DNDC, 2012).

Climate, soil chemical and physical properties, vegetation cover, and management practices are main drivers for the DNDC model. It consists of two main components: the first predicts soil temperature, moisture, pH, redox potential, and substrate concentration profiles. Additionally, plant growth with water and N-uptake as well as decomposition of organic matter more specifically fresh litter partitioning, microbial assimilation, SOC turnover, and CO_2 production is modelled in the first component. The second component forecasts both gaseous emissions and nutrient leaching from plant-soil systems. The model accounts for processes like nitrification, denitrification, and fermentation, influenced by soil conditions such as temperature, moisture, and pH. It uses an "anaerobic balloon" scheme to predict soil aeration and substrate allocation, affecting nitrogen transformations and gas emissions. After harvest, crop residues contribute to soil organic matter (SOM) dynamics, which are modelled through various decomposition rates and pools. The role of plant growth in regulating soil C, N, and water regimes, which again are affecting soil processes, is emphasized in the model.

The model integrates classical scientific principles and empirical data to simulate complex biogeochemical cycles. Accurate input data for the ecological drivers and other parameters are crucial for successful simulations, as detailed in the User's Guide and case studies. Users can for example modify crop parameters, such as maximal

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biomass production, biomass fraction of grain (fruit, florets), leaf, and stem with corresponding C/N ratios and more, to simulate growth influenced by temperature, nitrogen uptake, and water stress.

Over a course of years different versions of the DNDC have been developed to suit different ecosystems (Forest-DNDC, Forest-DNDC-Tropica), specific crops (DNDC-Rice, DNDC-CSW), regionalised for different areas of the world (NZ-DNDC, UK-DNDC), or modularised (Mobile-DNDC, Landscape-DNDC) (Gilhespy et al., 2014).

Development of the DNDC model to improve soil hydrology and incorporate mechanistic tile drainage was performed on two experimental sites in Canada and USA for a duration of five years. The study showed that DNDC was able to capture the observed differences in water and N losses after incorporation of the Root Zone Water Quality Model (Smith et al., 2020). In contrast, Kröbel et al. (2010) cautioned about using the DNDC model without site-specific testing as it failed to capture the soil water dynamics in a floodplain soil.

Use of the version of DNDC adopted to high latitudes where energy exchange within soil-snow-vegetation-atmosphere system was explicitly modelled lead to satisfactory capture of observed impacts of the manipulations in soil environments on C gas fluxes (Deng et al., 2015).

Importance of correct model parametrization was further highlighted in a study of 10 corn-soybean rotation filed experiment in Illinois, USA. The initial DNDC negative modelling efficiency values obtained using the default parameter values were substantially improved with parameter calibration resulting in modelling efficiency ranging 0.25 – 0.85 (Tonitto et al., 2007).

The DNDC is often used for field-scale and regional-scale applications, making it suitable for assessing the long-term impacts of agricultural management practices on soil and environmental quality. Additional model parametrization would be beneficial to accurately capture short-term dynamics.

Dubache et al. (2019) found that the standard DNDC model was insufficient in accurately simulating nitrogen dynamics, indicating a need for updating the model. This led to the development of an improved version, DNDC95_NH_3, which aims to address the identified shortcomings. Additionally, the DNDC95 may not represent the most optimal version for accurately modelling bio-based fertilizers. Our findings underscore the necessity for developing a specialized DNDC module that can precisely parameterize these products.

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A newer version of the DNDC model and automated adjustment of model parameters to improve the model's performance and predictive capabilities may be advantageous. For example, Bhattarai et al. (2022) integrated the DNDCv.CAN with an inverse model, PEST at a source code level. They found that automated parameter calibration was timesaving, however automatic calibration must be verified with values that make sense in the real world.

The aim of this work was to model the future effectiveness of the biobased fertilisers using the base DNDC model version 9.5.

To do so, the first step is to accurately model todays situation. For those BBFs where the field trials were satisfactory modelled for at least some of the parameters, modelling of the future effect/nutrient loss were performed.

2 Materials and methods

Within the Sea2Land project, the DSSATS and DNDC models were applied to five experimental sites, located in different European biogeographical regions. The experimental setup and the sampling / monitoring strategy were harmonised to the highest extent possible.

The datasets collected at each experimental site for the negative control treatment were used for initial model parameterization. As a next step, both models were calibrated against the reference data, up to availability. The calibrated model parameters were then applied to the different BBFs to investigate their effect on soil nitrogen dynamics and gaseous emissions from the soil-plant system.

To continue, we will clarify the two terms used in the context of modelling. Model parameterization refers to the process of assigning values to the model's parameters based on prior knowledge, literature, or measured data. These parameters define the physical and biological characteristics of the system being modelled. In contrast, model calibration involves adjusting certain parameters within plausible ranges to improve the agreement between model outputs and observed data. While parameterization sets the foundation for the model, calibration fine-tunes it to better reflect site-specific conditions and observed dynamics.

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2.1 Field experiments and data collection

The data sets used for model evaluation were derived from field experiments carried out in 2023 in Belgium, Estonia, Norway and Spain and in 2024 in France and in Spain. The Belgian field experiment was conducted in Upigny, Belgium (50.57163, 4.87223) at the research station of BRIOAA (Belgian Research Institute of Organic Agriculture and Agroecology). The Norwegian field experiment was located at research station NIBIO Apelsvoll (60°42 10°52). The Estonian field experiment was carried out in Jõgeva, Estonia (58° 45' 47.22"N, 26° 24' 14.40"E). The French field experiment was carried out in Assat, in south-west of France, close to Pyrenees. The Spanish field experiments were carried out in Zamudio (Bizkaia, the Basque Country) at NEIKER facilities (430 17' 24''N, 20 52' 15'' W) during two consecutive years in the same field. Three common fertilizers were tested in each field trial, plus one or two locally decided and one positive control. The three common fertilizers were FSP from GRÖNN, solid biobased fertilizer (fish sludge pellet), CAT1 from CATAR, solid biobased fertilizer (protein fraction) and FER3 from FERTINAGRO liquid biobased fertilizer (NPK solution with amino acids).

The five experimental sites involved in this study were in Belgium, Estonia, France, Norway, and Spain; and the field experiments used for modelling soil nitrogen dynamics were performed in 2023, 2023, 2024, 2023, and 2024. respectively. Daily meteorological data were recorded at meteorological stations situated nearby the experimental sites. Figure 1. presents the recorded data for wind speed, solar radiation, daily average temperature, and precipitation. Additionally, soil temperature and soil water content were monitored at some of the stations.

In Norway, meteorological data, soil temperature and soil moisture content were measured at the NIBIO meteorological station, located nearby the experimental site (Agrometeorology Norway, lmt.nibio.no, Apelsvoll, 01.01.2023-31.12.2023) in hourly resolution at 20 cm depth.

At the Jogeva experimental site in Estonia, Soil Scout, a continuous soil monitoring system, was installed at the same time as plants were transplanted. The weather data were collected from the weather station at the experimental site.

Weather data for the experimental sites in Upigny, Belgium; Zamudio, Spain; and Assat, France were acquired from nearby weather stations.

Additionally, soil moisture in all five countries was assessed throughout the growing season using gravimetric sampling as well. Soil samples were collected at regular intervals from

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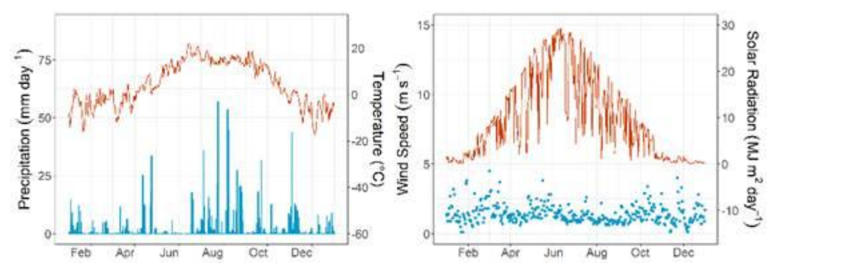
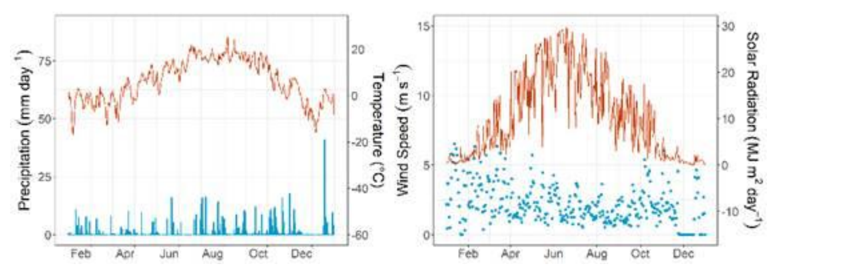
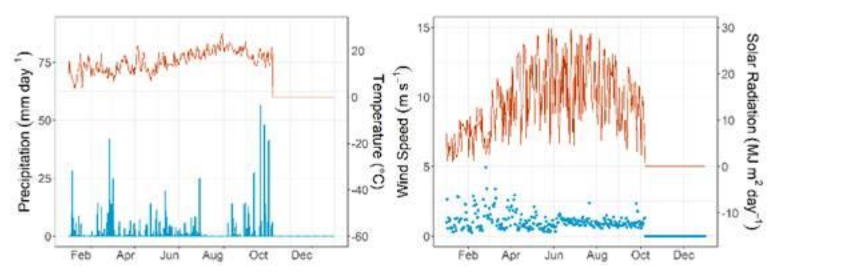
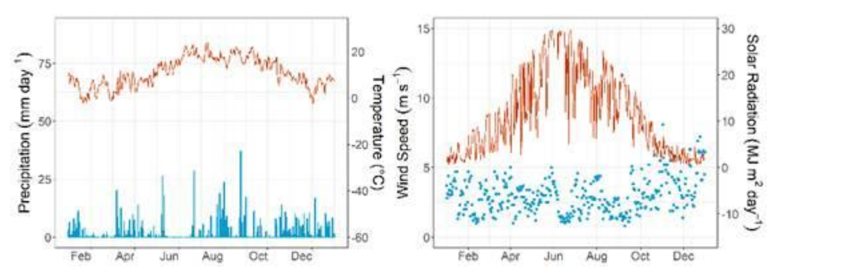
the field and immediately sealed to prevent moisture loss. The gravimetric water content (GWC) was determined by weighing the fresh soil samples, drying them at 105 °C for 24 hours, and then reweighing them. The GWC was calculated as the mass of water lost during drying divided by the dry mass of the soil.

To convert gravimetric water content to volumetric water content (Θ), GWC was multiplied by the soil bulk density. Soil bulk density was determined by collecting undisturbed soil cores and calculating the ratio of dry soil mass to the volume of the core.

Norway	
Estonia	
Spain	
Belgium	

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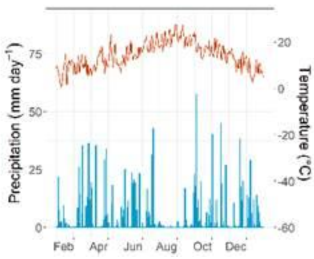
France



Extreme weather ECOTRON

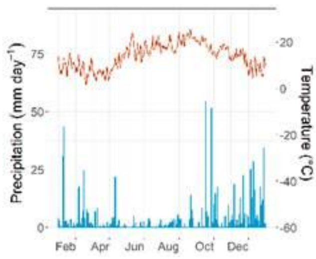


Figure 1. Daily precipitation sum, average air temperature, solar radiation, and wind measured at the experimental sites in different countries during the study period.

Broccoli was selected as the test plant because it is a vegetable commonly grown in all five countries. The transplanting and harvest dates, along with the characteristic meteorological conditions during the growing season, are provided in Table 1.

Table 1. Weather conditions during the growing season, crop transplanting and harvesting dates at the different experimental sites.

	Tmax °C	Tmin °C	Tav °C	Precipitation mm	Transplanting date	Harvest date
Norway 23	29.0	2.5	15.8	387.1	31.05.	15.08.
Norway 24						
Spain 24	29.9	2.6	13.7	154.8	19.03.	28.05.
Spain 23						
France	37.4	4.4	19.3	394.2	23.07.	20.10.
Estonia	30.0	1.7	16.6	132.6	05.06.	04.08.
Belgium	31.1	4.6	17.1	263.1	04.05.	22.08.

Field management practices, including soil tillage, fertilization and irrigation are described in Deliverable 5.1. At each experimental site, soil and plant samples were collected in a harmonized way for describing soil properties as well as initial soil nutrient status of the topsoil and plant properties at different plant development stages. The sampling procedure and the measurement methods are described in Deliverable 5.1. Soil characteristics, determined from soil samples taken from the 0-10 cm layer are given in Table 2.

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Table 2. The characteristics of the soil evaluated for the upper 0-10 cm layer across all five experimental sites.

Site	Soil textural class	Clay fraction	pH	C (%)	N (%)	C/N	Organic C (%)	Bulk density (g/cm^3)	NH_4-N (mg N kg^{-1})	NO_3-N (mg N kg^{-1})
Norway	Loam	0.19	6.15	2.34	0.23	10.17	2.34	1.32	4.04	5.62
Spain	Silt loam	0.20	7.30	1.52	0.15	10.41	1.54	1.15	1.30	49.70
France	Silt loam	0.20	6.67	2.70	0.20	13.65	2.70	1.32	0.9	21.4
Estonia	Silt loam	0.14	6.33	1.86	0.17	11.10	1.86	1.06	0.76	14.12
Belgium	Silt loam	0.21	7.31	1.36	0.13	10.16	1.38	1.37	3.41	4.10

Soil texture (sand, silt and clay content) was determined and used to classify the soil textural classes according to the USDA soil textural classification.

In the case of DNDC we selected four treatments (unfertilized control – **CON0**, CATAR-Atlantic Sea – **CAT1**, Fish NIBIO-North Sea – **FSP**, and FERTINAGRO-Cantabrian Sea – **FER3**) applied in all partner countries to model the soil nitrogen dynamics. In the case of DSSAT 5 treatments were used (unfertilized control – **CON0**, mineral fertilization-**CON+** CATAR-Atlantic Sea – **CAT1**, Fish NIBIO-North Sea – **FSP**, and FERTINAGRO-Cantabrian Sea – **FER3**)The amount of fertilizer was calculated to correspond to 120 kg N ha^{-1} application rate. Characterisation of the bio-based fertilizers is given in the chapter D6.1.

Soil samples were collected prior to broccoli plant transplantation as well as during growing season, and soil NH_4-N and NO_3-N was measured. Sample processing and chemical analysis described in more detail in the chapter D6.3.

Soil moisture that was measured in the disturbed soil samples was multiplied with soil bulk density to get the volumetric fraction of water filed pores (wfps).

Within the framework of the DSSAT (Decision Support System for Agrotechnology Transfer) model, the incorporation of supplementary agronomic data is required. This includes: • Phenological observations at key intervals—specifically on days 0, 7, 14, and 21 following planting—to track crop development stages • Documentation of field operations, such as planting, irrigation, fertilization, and tillage, along with their respective execution dates • Records of phytosanitary interventions, detailing the types of treatments applied (e.g., pesticide or fungicide applications), product specifications, and application dates.

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All data processing and calculations were performed using the R statistical software environment (R Core Team, 2024).

The model's performance relative to the observed data was evaluated using the Nash-Sutcliffe Efficiency (NSE) (as cited in: Moriasi et al. (2015) and the coefficient of determination (R^2). These metrics were applied to continuous measurements (Tsoil and θ). NSE values range from negative infinity to 1. A perfect model fit to the observed data yields an NSE of 1, indicating a complete match between simulated and observed values. An NSE of 0 suggests that the model predictions are as accurate as simply using the mean of the observed data, while negative values indicate that the mean of the observed data provides better predictions than the model.

Additionally, for the comparison of the simulated crop yields and field observations, RMSE-observation standard deviation ratio (RSR) was used to assess coincidence between simulated and observed values (Equation1). RSR below 50% is considered as very good (Moriasi et al., 2007).

$$\mathrm{RSR} = \frac{RMSE}{STDEV_i} = \frac{\sqrt{\sum_i^n (O_i - S_i)^2}}{\sqrt{\sum_i^n (O_i - O_{avg})^2}}$$

Equation 1.

Relative change was calculated as the ratio of the actual change in a value to a reference value (unfertilized treatment) (Equation 2).

$$\text{relative change}(v_{ref}, v) = \frac{\text{actual change}}{\text{reference value}} = \frac{\Delta v}{v_{ref}} = \frac{\Delta v}{v_{ref}} - 1$$

Equation 2.

To evaluate the performance of the crop yield and soil NO^3-N and NH^4-N concentration models, the coefficient of determination (R^2) was used as a measure of goodness-of-fit. R^2 quantifies the proportion of variance in the observed data that is explained by the model, with values closer to 1 indicating a better fit. This metric was calculated for each model to assess its predictive accuracy and reliability.

3 DNDC Model

3.1 Model parametrization

Model parameters not available from direct measurements (sub-chapter 2.1) were either estimated or set based on literature data. Alternatively, the model's default values were used during the initial parameter setup.

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In this sub-chapter we focus on the data, collected from the experimental sites, which were further used for parameterising and calibrating the DNDC model. The most important input and reference data, as well as model parameters for the model, are described in Table 2.

Table 3. Input data and model parameters, used for setting up and calibrating the DNDC model.

Data type	Parameter code	Parameter name	Resolution	Type	Source
Meteorological	Max T	Max air temperature	daily	Driving variables	Meteorological station nearby the experimental plots Input files
	Min T	Min air temperature			
	Prec	Daily precipitation sum			
	WindSpeed	Wind speed			
	Rad	Solar radiation			
	Hum	Humidity			
Soil	**Texture**	**Soil textural class**	**constant**	**Model parameter**	**Measured from topsoil samples, values in Table 2**
	Clay fraction	Soil clay fraction			
	Bulk density	Soil bulk density			
	θ_FC	Field capacity			Estimated as described in sub-chapter 2.2, values in Table 4
	θ_WP	Wilting point			
	Ksat	Saturated hydraulic conductivity			
	Porosity	Fraction of soil pores			
	Soil pH	Soil pH			Measured from topsoil samples, values in Table 2
	NO_3 - N	Initial value for soil nitrate		Initial condition	
	NH_4 - N	Initial value for soil ammonium			
	SOC	Initial value for soil organic carbon			
	NO_3 - N	Soil nitrate concentration	5-6 occasions	Reference data	Measured; data used for evaluation
	NH_4 - N	Soil ammonium concentration.			
	Θ	Soil water content			
Crop		Max. yield	constant	Model parameter	Measured; data used for calibration
		Biomass fraction			
		C/N ratio			
		Thermal degree days for maturity			
		Optimum temperature			
Management practice		Tillage	constant	Model parameter	Experiment setup
		Irrigation			
		Fertilization/Manure Amendment			

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Parameterising fertilizers (BBFs)

As the applied fertilizers are bio-based products with considerable amount of organic matter, the "Manure Amendment" input interface was used for parametrisation of BBFs. The DNDC allows user to choose one of the following manure types 1 – farmyard manure, 2 – green manure, 3 – straw, 4 – slurry animal waste, 5 – compost, 6 – bean cake, 7 – human waste, 8 – poultry waste, 9 – sewage sludge, and 10 – meat or blood meal. Due to the low dry matter content, the liquid BBF FER3 was parametrised as type 4. For the dry CAT1 and pelleted FSP, type 8 was selected. Organic C, organic N as well as NH_4-N and NO_3-N were set to correspond to fertilizer characteristics and application rates (Table 4). Application date and method were set to correspond to management practice described in D5.1.

Table 4. DNDC model fertilizer parameters.

	CAT1	FSP	FER3
Manure type	8 - poultry waste	8 - poultry waste	4 - slurry animal waste
Solid C/N ratio	6.11	6.35	2.67
Organic C (kg C ha^{-1})	733	758	320
Organic N (kg N ha^{-1})	119.95	119.46	119.85
$NH4^+$ (kg N ha^{-1})	0.535	1.202	5.785
$NO3^-$ (kg N ha^{-1})	0.002	0.002	0.002

Crop properties

For the selection of appropriate method for calculating soil hydraulic properties, the inbuilt (default) DNDC plant parameters for perennial grass were used. This was necessary to accurately represent the plant cover at the meteorological station where the soil moisture sensors were located. The default values for perennial grass cover are max biomass production 186.66 kg C ha^{-1} y^{-1}, biomass fraction 0.02 grain and 0.7 leaves and stems, biomass C/N ratio 35, thermal degree days for maturity 2000, water demand 200 g water g^{-1} dry matter, N fixation1.5, and optimum temperature 21°C.

For the soil N dynamics measured at the experimental sites, the default model parameters for the broccoli crop were adjusted to align with those measured during the experiment as will be discussed in chapter 4.1. Crop planting and harvest dates, field management, and irrigation details are provided in the field experiment section. Broccoli plants were transplanted according to standard management practices. Soil samples

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were collected during vegetational season, and broccoli was harvested at maturity. Plants were processed and analysed as described in D5.1.

Soil properties

Accurate simulation of soil temperature and soil water content dynamics is crucial to effectively model the components of the soil nutrient balance (e.g., soil nutrient content, emission, leaching, etc.). The DNDC model calculates soil water content based on soil physical and hydraulic properties. These properties - including field capacity, porosity, wilting point, and hydraulic conductivity - play a crucial role in soil hydrological calculations and are often identified as the most important parameters during soil hydrological model sensitivity analyses.

For the selection of the optimal method for derivation of missing soil hydraulic parameters we used Norwegian data sourced from an onsite weather station with a continuous soil moisture monitoring under a permanent grass cover. We compared the measured soil water content dynamics with the those, calculated by the DNDC model when implementing soil hydraulic parameters, estimated using i) national data (Riley, 1996) and ii) a European database (euptfv2)(Szabó et al., 2021). Both methods require input parameters such as soil sand, silt, clay, and organic matter contents, as well as soil bulk density (Table 2). Additionally, euptfv2 incorporates soil pH into the calculations.

The Nash-Sutcliffe Efficiency (NSE) calculated for the measured and simulated soil water contents was 0.516 when using the euptfv2 method, indicating good model performance, and 0.014 for the Riley method, referring to a very poor model performance. These results indicate that the euptfv2 method, developed for the whole Europe can give good, and even better results than the national estimation methods and can be used for all the pilot fields of this study. Therefore, we derived the soil hydraulic properties using the euptfv2 functions for further analyses.

Table 4. Soil hydraulic properties derived using updated European hydraulic pedotransfer functions (euptfv2)

	Longitude	**Latitude**	**Field capacity at -100 cm matric potential head (cm^3 cm−3)**	**Wilting point at - 15.000 cm matric potential head (cm^3 cm^{-3})**	**Saturated hydraulic conductivity (m h^{-1})**	**Water content at saturation (cm^3 cm^{-3})**
Belgium	4.87223	50.57163	0.36	0.15	0.014	0.49
Estonia	26.403889	58.763056	0.43	0.11	0.050	0.50
France	0.299167	43.25	0.40	0.16	0.008	0.56
Norway	10.86952	60.70024	0.36	0.15	0.015	0.48
Spain	2.870833	43.29	0.38	0.15	0.026	0.54

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Initial model performance assessment

A perennial grass crop from the model database was utilized to assess the model performance, using both measured soil parameters and those obtained through euptfv2. The modelled and observed topsoil temperature and water content for the data obtained from the Norwegian weather station are shown in Figure 2. The model could capture changes in soil temperature for both winter and summer periods, resulting in an NSE of 0.925. The NSE calculated for the measured and simulated soil water contents was 0.516.

Figure 2. Simulated and measured soil temperature at 10 cm depth and soil water content during 2023.

The graphical evaluation of the measured and observed soil water content dynamics indicates that the model performance cannot be assessed during periods when the soil is frozen. In the case of the DNDC model, the simulated soil water content remained at field capacity (initial water content) during winter and early spring, assuming that all the water is in the liquid phase. In contrast, soil moisture sensors measure only the liquid phase of water in the soil, meaning that the observed values in Figure 2. do not account for the frozen water present in the soil.

Even though the DNDC interface indicated the existence of a "Drainage efficiency" parameter, there is no such parameter in the model input files. This parameter might be

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tested still or could be available in the commercial version of the model. In our case, it could not be included in the sensitivity analyses.

The DNDC modelled soil temperature and water content appeared to be the most sensitive against the following soil parameters: soil bulk density, wilting point and soil field capacity.

We also experienced some strange model "behaviour" during the calibration procedure of hydrological sub-routine, as the model completely disregarded the irrigation amounts set in the input files. Even when very high irrigation amounts were given, they did not have any influence on the simulated soil moisture contents. As a solution, the irrigation amounts were added to the precipitation records to ensure the correct water input in the model.

Parameter sensitivity test for "Depth of water retention layer" (tested range 1 - 9.99 m) and "Drainage efficiency" (tested range 0 – 1) parameters showed no effect of these parameters.

3.2 Calibration of the DNDC model

Model crop parameters were adjusted site-specifically by calibrating the modelled biomass yield against the measured total broccoli biomass yield.

For each output variable, preliminary sensitivity analyses were manually performed to identify the parameters with the highest impact on the model output in focus. As the next step, the selected parameters were adjusted to achieve an acceptable match between the measured and simulated values.

Crop parameters collected during the experiment (as described in Chapter 2.2) were used as baselines for calibrating the crop parameters. This adjustment was necessary because the default broccoli plant parameters were suited to plants grown in entirely different climates. Broccoli thrives in mild temperatures, so the DNDC default value for crop optimal temperature of 25°C was changed to 15°C. Furthermore, higher temperatures would have an adverse effect on broccoli yield. Longer periods with air temperature above 20°C contribute to lower yields (Kałużewicz et al., 2012), so any higher temperature than 20°C would not be considered as the optimal temperature for a broccoli plant.

The model was not sensitive to changes of "crop water demand parameter". As the default value was within the reasonable range, this parameter was not tested further. "Thermal time for maturity" (°Cday) was range tested with respect to obtained yields

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both in fertilized and unfertilized treatments and the value that fitted best to observed data coincided with the values found in literature (Dufault, 1997; Tan et al., 2000).

To establish the appropriate biomass yield and C/N ratio for the broccoli crop, we systematically tested the DNDC model outcomes over the entire realistic range of these parameter values. The manual calibration results indicated a different value for Estonia compared to other regions (Table 5). This difference corresponds with the specific variety of broccoli used in Estonia (Cézar), as opposed to the Parthenon variety used in the other countries.

The biomass of the broccoli was divided into two fractions, commercial yield (defined as heads with a diameter above 8 cm) and leaves plus stems including heads with a diameter under 8 cm. The model does not define what would be considered as a commercial yield for broccoli plants so we tested a range of values found in literature (Bowen et al., 1999),(Irsan & Riyanto, 2021), with respect to measured biomass yield in both fertilized and unfertilized treatments. The carbon to nitrogen ratio (C/N) was measured in our experiment and was used as a guiding point for our calibration.

Table 5. Parameter input for the crop.

Crop parameter		Thermal degree days for maturity (°Cday)	Biomass production commercial yield (kg C ha^{-1} year^{-1})	Biomass fraction commercial yield	Biomass fraction stalks and leaves	C/N commercial yield	C/N stalks and leaves
DNDC default value for broccoli		1800	1200	0.3	0.54	10	14.7
Range tested		600-1800	600-1200	0.1-0.3	0.54-0.84	10-20	10-45
Chosen value	Norway	1200	1200	0.2	0.7	15	30
	Estonia	1200	950	0.15	0.8	15	43
	Belgium	1200	1200	0.2	0.7	10	25
	France	1200	1200	0.2	0.7	10	10
	Spain	1200	1200	0.2	0.7	10	10

* Root biomass has not been measured in this study. The measured total biomass and marketable yield (grain in the DNDC model) values have been updated with the values found in the literature. We calibrated the model parameters to ensure best fit to the measured total biomass (marketable yield plus biomass of stalks, leaves and unmarketable yield). The goodness-of-fit for each selected crop parameter combination was evaluated using the determination coefficient (R^2) for simulated and observed total aboveground broccoli biomass yield.

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Certain parameters were not evaluated during the model calibration for various reasons. Specifically, we used the default value for "plant water demand" due to the absence of reference values in literature, thereby preventing us from establishing a test range for sensitivity analyses.

3.3 DNDC modelling results

3.3.1 Norway

In Norway the simulated aboveground crop biomass yield in kg C ha^{-1} per year was 1616 in the unfertilized treatment (CON0) and 2733 (CAT1), 2710 (FSP), and 3211 (FER3) in the fertilized treatments. The corresponding measured biomass yields were 1743.1(CON0), 2765.0 (CAT1), 2259.3 (FSP), and 3334.4 (FER3) kg C ha^{-1} per year. For the comparison of simulated and observed yield, the R^2 and the RSR was 0.84 and 0.41, respectively, both conceived as very good (Moriasi et al., 2015; Moriasi et al., 2007).

The DNDC model did however demonstrate a limited ability to capture soil moisture dynamics when comparing the simulated data with soil moisture data obtained from disturbed soil samples (Figure 3).

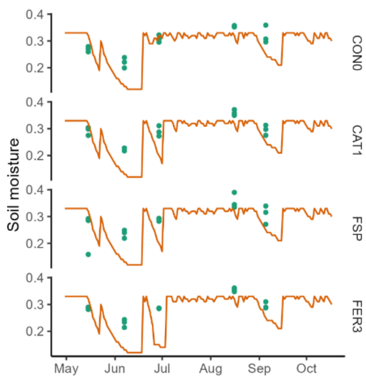

Figure 3. Measured (dots) and simulated soil moisture at a depth of 10 cm (line) during the growing season is presented as a fraction of water-filled pores (wfps) for the data collected at the Apelsvoll experimental site in Norway.

Also, the prediction of soil NH_4-N and NO_3-N concentrations was not satisfactory with $R^2 = 0.50$ and $R^2 = 0.35$, $p < 0.01$ in both cases (Figure 5).

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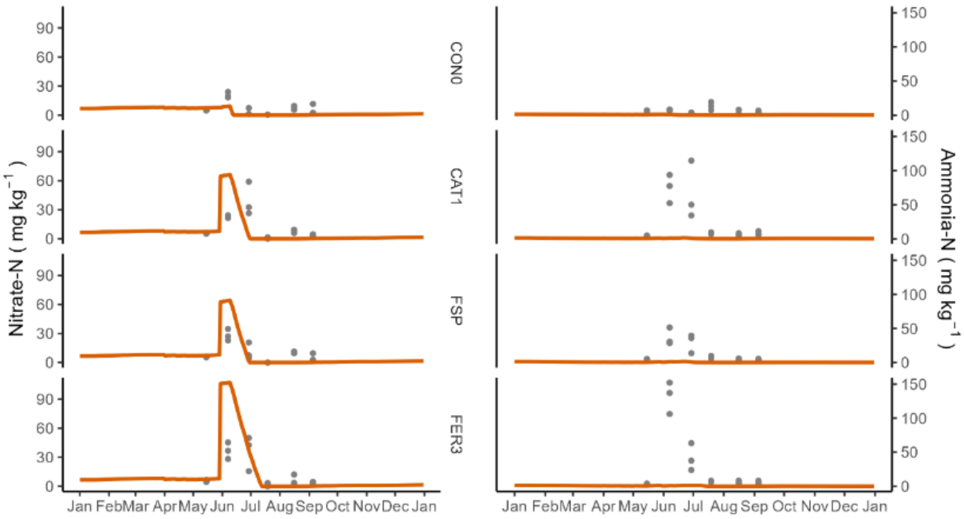

Figure 4. A comparison of the measured concentrations of soil NO_3-N and NH_4-N at the Apelsvoll experimental site, and the simulated values produced by the DNDC model, which was calibrated specifically for this site, at a depth of 0-10 cm.

The inadequate model performance with respect to the soil N dynamics could be partially explained with the DNDC microbial activity parameter limitation, which influences the distribution between soil NO_3-N and NH_4-N pools (Figure 4). The only way to increase simulated soil NH_4-N levels is to set microbial activity to 0. However, this approach is ineffective because it results in much lower soil NO_3-N levels than those observed, and it is unreasonable to assume there was no microbial activity in the soil. No intermediate distribution was available in the DNDC model used in this project.

Further refinement of the microbial activity parameter within the DNDC code might improve model performance. When the microbial activity parameter is set to 1, the applied NH_4-N pool is immediately added to NO_3-N pool, while setting it to 0 shifts the balance to NH-4 side, meaning that NO_3-N is added to NH_4-N pool.

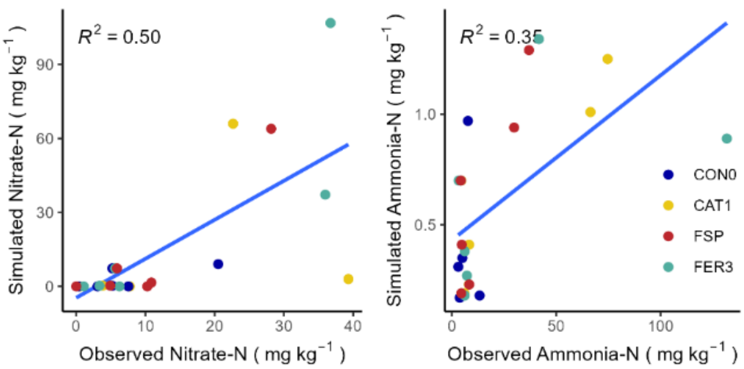

Figure 5. Comparison of measured and modelled concentrations of soil NO_3-N and NH_4-N at a depth of 0-10 cm for the Apelsvoll experimental site.

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The DNDC model more accurately captured the soil mineral nitrogen content, represented as the sum of soil NO_3-N and NH_4-N, with an R^2 value of 0.73 and $p < 0.01$ (Figure 6). There is a good agreement between simulated and measured SMN.

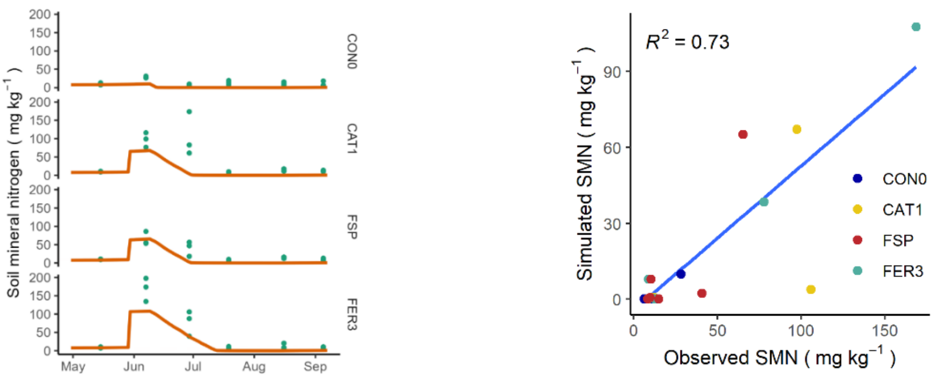

Figure 6. Comparison of measured (dots) and simulated (line) soil mineral nitrogen (as a sum of NO_3-N and NH_4-N) at 10 cm dept plotted as a function of time on the left-hand side figure for the Apelsvoll experimental site.

A relative change of soil NO_3-N and NH_4-N with unfertilized treatment (CON0) set as a baseline or reference value is shown in Figure 7. Both simulated and observed values indicated a higher mineral nitrogen availability early in the season under FER3 treatment compared to FSP and CAT1. Soil N content was higher in all fertilized treatments compared to unfertilized plots.

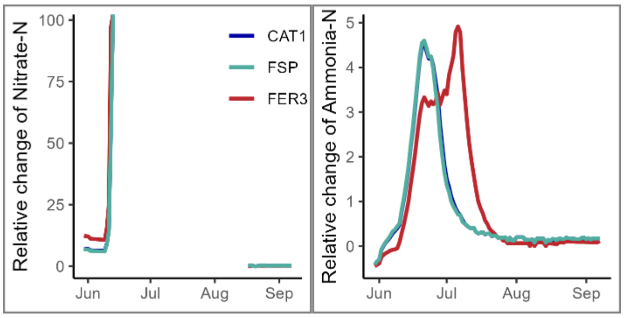

Figure 7. Comparison of the dynamics of relative changes in soil NO_3-N and NH_4-N content for the three BBFs, calculated with the unfertilized treatment set as the reference value at Apelsvoll experimental site.

The nitrogen gas fluxes were not directly measured during the field experiments. Therefore, the values simulated by the DNDC model could only indicate a trend of N dynamic (Table 6). The model indicated a potentially higher N leaching and N-gasses volatilization in FER3 compared to CAT1 and FSP, but lower CO_2 emissions which were

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461.1, 587.2 (0.27), 693.4 (0.50) and 700.2 (0.52) kg C ha^{-1} per year for CON, FER3, CAT1 and FSP respectively (relative change given in brackets).

Table 6. Simulated N fluxes for the Apelsvoll experimental site in Norway. Relative change, expressed as a fraction rather than a percent, calculated with respect to unfertilized treatments.

	CON	FER3		CAT1		FSP	
	N (kg N ha^{-1}y^{-1})	N (kg N ha^{-1}y^{-1})	Relative change	N (kg N ha^{-1}y^{-1})	Relative change	N (kg N ha^{-1}y^{-1})	Relative change
Soil N leaching	2.99	7.29	1.44	4.53	0.52	4.44	0.48
Crop N uptake from soil	65.96	161.09	1.44	128.82	0.95	127.25	0.93
NH3 volatilization	0.58	1.38	1.38	1.24	1.14	1.24	1.14
N2O	0.08	0.2	1.50	0.14	0.75	0.14	0.75
NO	0.01	0.28	27.00	0.17	16.00	0.17	16.00

3.3.2 Extreme weather scenario

For the extreme weather conditions the simulation of yields, soil moisture, nitrogen dynamics, and N-gas emissions used an extreme climate scenario from the ECOTRON experiment (Deliverable 5.2). Main characteristics of the simulated weather conditions is higher mean temperature (15.4 °C) with intense rain/drought events (Figure 1). The DNDC simulation relied on mean temperature and precipitation data used in ECOTRON experiment, while CO_2 was kept at the DNDC default value (350 ppm) initially.

The simulated aboveground crop biomass yield for extreme weather in kg C ha^{-1} per year were 2071 (CON0), 2625 (CAT1), 2625(FSP), and 2620(FER3). Compared to the simulated yield in 2023, the model indicates a change of +28 % (CON0), -18 % (FER3), -4 % (CAT1) and -3 % (FSP).

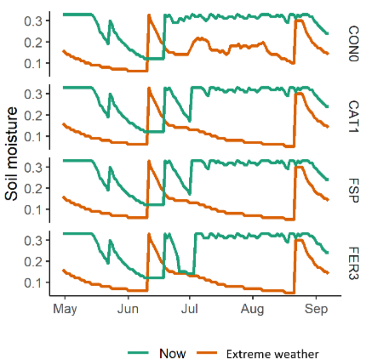

Figure 8. Simulated soil moisture expressed as fraction of water filled pores for year 2023 (green), and extreme weather scenario used for the ECOTRON experiment (red) for the Apelsvoll experimental site.

Soil moisture content under simulated extreme weather conditions was lower than the predicted values based on measured climate data. Higher temperatures may have promoted organic matter mineralization, leading to higher yields in the CON0 treatment.

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The amounts of mineralized N changed from 39.8, 48.2, 48.5, and 43.6 kg N ha^{-1} as simulated for the measured weather conditions for the CON0, CAT1, FSP, and FER3 treatments respectively; to 91.1, 96.2, 96.5, and 91.1 kg N ha^{-1} for the same treatments simulated using extreme weather data.

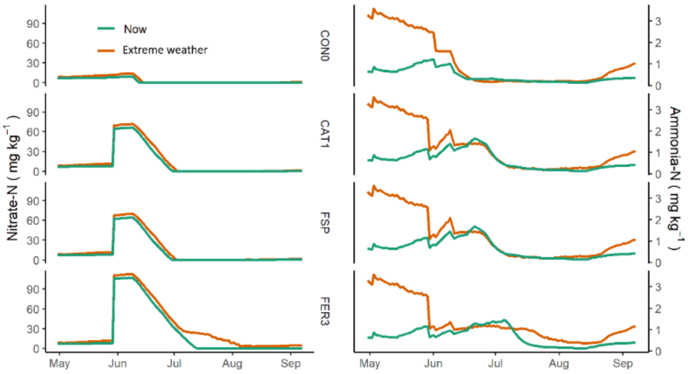

Figure 9. A comparison of soil nitrate and ammonia dynamics simulated using the weather data obtained from the weather station at Apelsvoll experimental site and using the extreme weather data.

Here must be noted that the scale for the simulated NH_4-N values (0-3 mg N kg^{-1} dry weight), measured weather conditions at the experimental site and hypothetical extreme weather obtained from the ECOTRON experiment, is not the same as the scale used for the figure showing measured soil NH4-N vs simulated for the same period (0-150 mg N kg^{-1} dry weight) (Figure 9).

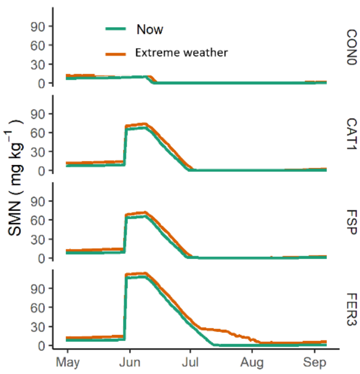

Figure 10. Simulated soil mineral nitrogen obtained using the weather data collected at the Apelsvoll experimental site in Norway compared with simulated values produced using the extreme weather data.

A comparison of the simulated values for soil mineral nitrogen concentration indicated an increase in concentration under extreme weather conditions (Figure 10).

Simulated CO_2 emissions under extreme weather conditions were higher than simulated values obtained using the measured weather data for all treatments resulting in an

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increase of 166% CON0 (127.6 kg C $ha^{-1}y^{-1}$), 120% FER3 (1290.6 kg C $ha^{-1}y^{-1}$), 102% CAT1 (1401.9 kg C $ha^{-1}y^{-1}$) and 101% FSP (1409.1 kg C $ha^{-1}y^{-1}$).

The model indicated an increase in soil N leaching and emissions of NH_3, N_2O and NO under higher temperatures and extreme precipitation distribution in comparison to the simulated values obtained using the weather data collected at the experimental site (Table 7). The greatest change was in the unfertilized treatment. There was a reduction in simulated crop N uptake for the three fertilized treatments under extreme weather conditions in comparison to the simulated values for the measured weather conditions. This corresponds with the reduction in crop yield for the three BBFs caused by higher temperatures and longer periods without precipitation under extreme weather scenario. The opposite was observed for the unfertilized treatment.

Table 7. Simulated nitrogen fluxes in Norway utilizing ECOTRON extreme weather data. The relative change compared to the simulated gas fluxes for the year 2023 expressed as a fraction rather than a percentage.

	CON0		FER3		CAT1		FSP	
	Losses (kg N $ha^{-1}y^{-1}$)	Change	Losses (kg N $ha^{-1}y^{-1}$)	Change	Losses (kg N $ha^{-1}y^{-1}$)	Change	Losses (kg N $ha^{-1}y^{-1}$)	Change
Leaching	5.10	0.71	11.72	0.61	7.28	0.61	7.17	0.61
Crop uptake	85.01	0.29	123.40	-0.23	123.69	-0.04	123.70	-0.03
NH_3	2.96	4.10	4.44	2.22	3.96	2.19	3.95	2.19
N_2O	0.37	3.63	0.82	3.10	0.54	2.86	0.54	2.86
NO	0.06	5.00	0.32	0.14	0.21	0.24	0.20	0.18

In the subsequent simulation, an elevated atmospheric CO_2 concentration (775 ppm compared to the default value of 350 ppm in the DNDC model) was introduced alongside extreme temperature and precipitation conditions.

The simulated aboveground crop biomass yield for extreme weather conditions in kg C ha^{-1} per year were 2330 (CON0), 3872 (CAT1), 3847 (FSP), and 4383 (FER3). All treatments showed higher simulated yields for extreme weather with elevated CO_2 compared to 2023, with positive change of 44 % (CON0), 36 % (FER3), 42 % (CAT1) and 42 % (FSP).

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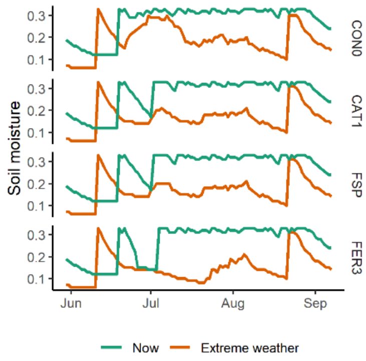

Figure 11. Simulated soil moisture expressed as fraction of water filled pores for year 2023 (green), and extreme weather scenario including elevated atmospheric CO_2 level (red) obtained using model calibrated to Apelsvoll data.

With increased atmospheric CO_2 the DNDC model does not seem to penalise the simulated crop biomass yield despite very low soil moisture content (Figure 11). An increase in total crop biomass yield does not necessarily mean an increase in commercial product yield.

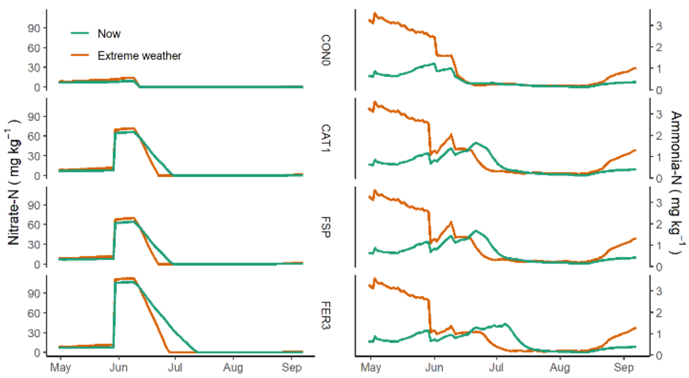

Figure 12. Comparison of soil nitrate and ammonia dynamics simulated with current and extreme weather conditions including elevated CO_2 obtained using the DNDC model calibrated to Apelsvoll data.

With increased atmospheric CO_2 levels and subsequently higher simulated yields, simulated soil NO_3-N concentration dropped more rapidly under extreme climate conditions in comparison to the one obtained using the present weather data (Figure 12). Soil NH_4-N concentration was higher under extreme weather conditions. Overall, simulated total soil mineral concentration followed the soil NO_3-N concentration, and it was lower under extreme weather (Figure 13).

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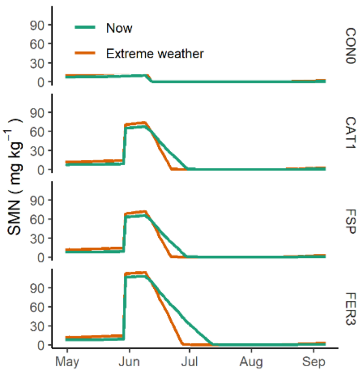

Figure 13. Comparison of simulated soil mineral nitrogen obtained using the weather data collected at the Apelsvoll experimental site in Norway compared with simulated values produced using the extreme weather data, including elevated CO_2 as a driver for the model.

Increased temperature, more extreme precipitation distribution and increased atmospheric CO_2 concentration resulted in an increase of simulated CO_2 emissions of 178% CON0 (1284.1 kg C $ha^{-1}y^{-1}$), 151% FER3 (1473.3 kg C $ha^{-1}y^{-1}$), 133% CAT1 (1616.8 kg C $ha^{-1}y^{-1}$) and 132% FSP (1625.1 kg C $ha^{-1}y^{-1}$) in comparison to the simulated values obtained using the measured weather data.

Table 8. Simulated nitrogen fluxes in Norway utilizing ECOTRON extreme weather data and elevated CO_2 concentration. The relative change compared to the simulated gas fluxes for the year 2023 expressed as a fraction rather than a percentage.

	CON0		FER3		CAT1		FSP	
	Losses (kg N $ha^{-1}y^{-1}$)	Change	Losses (kg N $ha^{-1}y^{-1}$)	Change	Losses (kg N $ha^{-1}y^{-1}$)	Change	Losses (kg N $ha^{-1}y^{-1}$)	Change
Leaching	5.07	0.70	6.36	-0.13	6.00	0.32	5.98	1.35
Crop uptake	87.37	0.32	182.67	0.13	149.58	0.16	147.96	1.16
NH_3	2.97	4.12	3.52	1.55	3.62	1.92	3.62	2.92
N_2O	0.37	3.63	0.41	1.05	0.42	2.00	0.42	3.00
NO	0.06	5.00	0.29	0.04	0.20	0.18	0.19	1.12

The amounts of mineralized N changed from 39.8, 48.2, 48.5, and 43.6 kg N ha^{-1} as simulated for the measured weather conditions for the CON0, CAT1, FSP, and FER3 treatments respectively; to 93.8, 103.1, 103.5, and 95.7 kg N ha^{-1} for the same treatments simulated using extreme weather data.

Relative change of the simulated emission of N gasses was lower under extreme weather condition with elevated atmospheric CO_2 concentration for FER3 and CAT1, but not FSP (Table 7 and Table 8). Relative change of the simulated emission for control treatment remained approximately the same under both atmospheric CO_2 concentrations.

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3.3.3 Estonia

In Estonia the simulated aboveground crop biomass yield in kg C ha^{-1} per year were 2378 (CON0), 3292 (CAT1), 3273 (FSP), and 3679 (FER3), while measured biomass yield in kg C ha^{-1} per year was 2769.0 (CON0), 3535.3 (CAT1), 3282.7 (FSP), and 3663.7 (FER3). The fit between observed and simulated values was very good (R^2 of 0.94 and RSR of 0.67).

In Estonia, soil moisture was measured both by a continuous soil monitoring system (Soil Scout soil sensor), and by calculations based on disturbed soil samples (as for the other countries). There was a discrepancy between the data from these two sources. The cause of the difference between the two figures is not fully understood. The implementation of a continuous soil moisture monitoring system may offer advantages over measuring soil moisture in disturbed soil samples for verification of simulated data. Both datasets are shown in Figure 14, along with the modelled soil moisture content. Soil Scout data corresponded with the simulated values better than the data for soil moisture measured in disturbed soil samples on sampling dates. However, there was a poor correlation of observed and simulated values NSE and R^2 of -2.23 and 0.07 ($p<0.01$) when the Soil Scout data was compared to simulated as continuous values measured throughout the growing season.

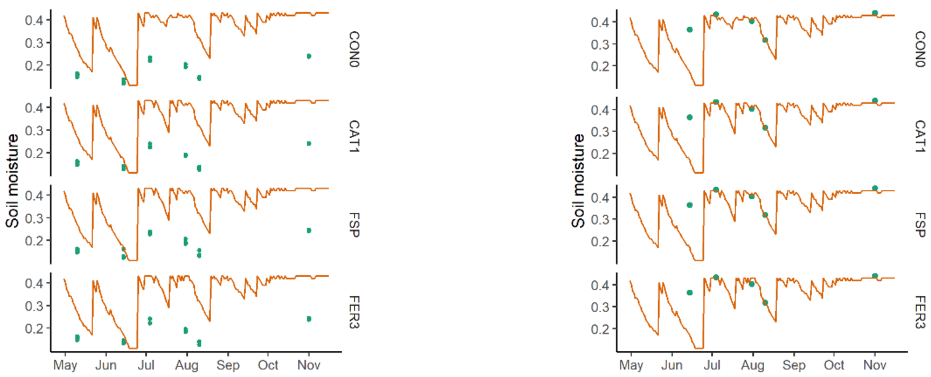

Figure 14. Comparison of soil moisture as a fraction of water filed pores at 10 cm depth. The dots in the figure on the left-hand side represent values measured in the field. Soil moisture in the figure on the right-hand side represented with dots was measured in the experimental field using Soil Scout soil sensor system.

The model captured soil NO_3-N dynamics well ($R^2 = 0.91$, $p < 0.01$), but it failed in case of NH_4-N (Figure 15 and Figure 16). The model was not satisfactory ($R^2 = 0.41$, $p < 0.01$) due to the DNDC microbial activity parameter constraints.

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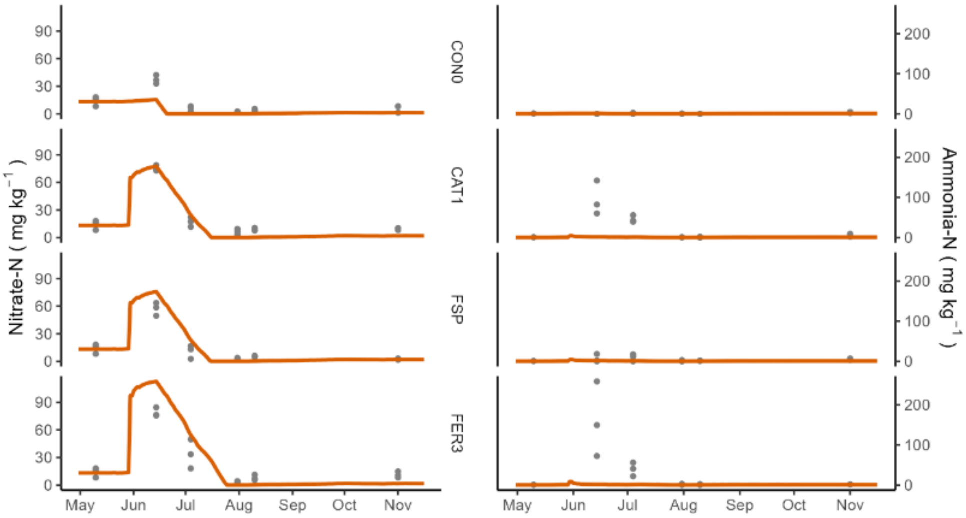

Figure 15. A comparison of the measured concentrations of soil NO_3-N and NH_4-N at the Jogeva experimental site, and the simulated values produced by the DNDC model, which was calibrated specifically for this site, at a depth of 0-10 cm

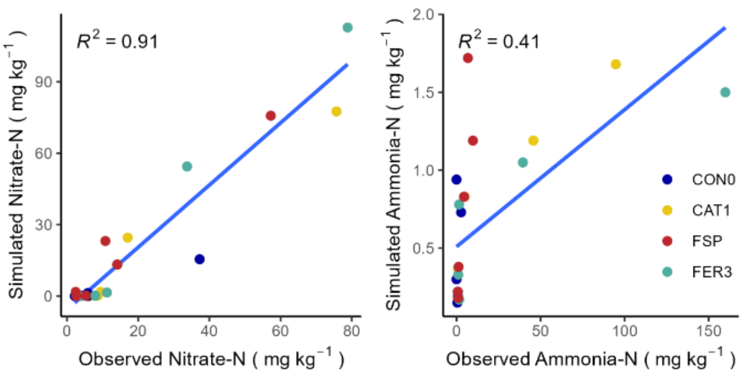

Figure 16. Comparison of observed and simulated soil NO_3-N and NH_4-N concentrations in the 0-10 cm topsoil layer at the Jogeva site.

The site-specifically calibrated DNDC model performed well with respect to the soil mineral nitrogen calculated as a sum of NO_3-N and NH_4-N ($R^2 = 0.87$, $p < 0.01$) (Figure 17).

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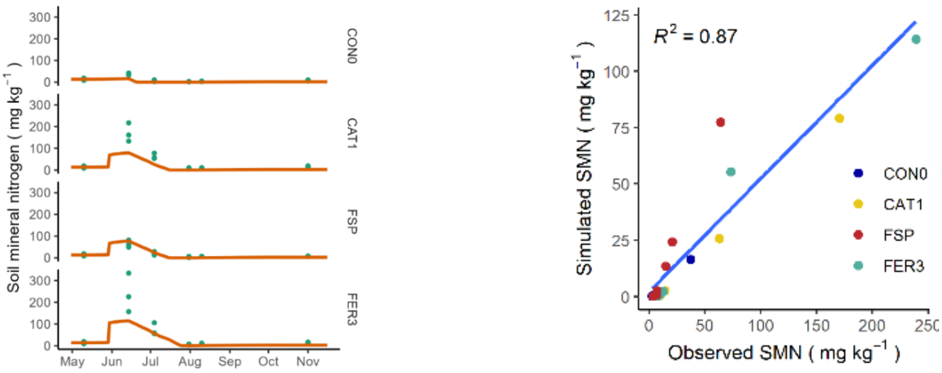

Figure 17. Comparison of measured (dots) and simulated (line) soil mineral nitrogen (as a sum of NO_3-N and NH_4-N) at 10 cm dept plotted as a function of time on the left-hand side figure for the Jogeva experimental site.

The model also indicates a higher SMN content in FER3 compared to other BBFs when the unfertilized treatment was set as reference value (Figure 18). This was more apparent early in the season. Similarly, the highest modelled emissions of N gases were for FER 3 (Table 9).

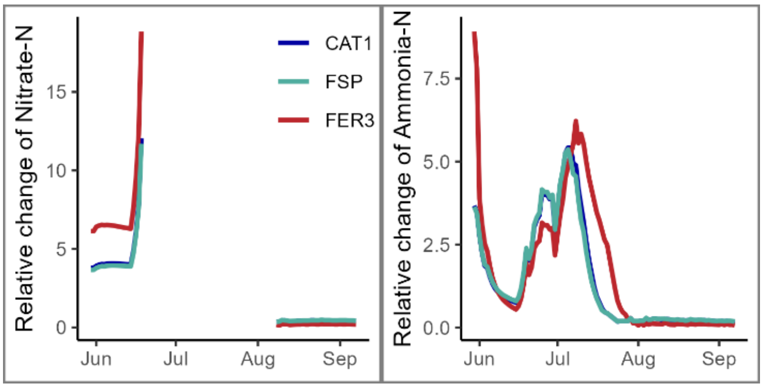

Figure 18. Soil N dynamics from fertilization date with respect to unfertilized treatment

Simulated soil CO_2 emissions for CON, FER3, CAT1 and FSP were 379.3, 466.1, 582.6 and 589.6 kg C ha^{-1}y^{-1} respectively. The model indicated an increase in simulated CO_2 emission for FER3, CAT1 and FSP of 23%, 54% and 55% with respect to unfertilized treatment.

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Table 9. DNDC model simulated N fluxes using the data collected at the Jogeva experimental site, Estonia. Relative change with respect to the unfertilized treatment expressed as a fraction.

	CON	FER3		CAT1		FSP	
	N (kg N $ha^{-1}y^{-1}$)	N (kg N $ha^{-1}y^{-1}$)	Relative change	N (kg N $ha^{-1}y^{-1}$)	Relative change	N (kg N $ha^{-1}y^{-1}$)	Relative change
Soil N leaching	5.08	16.2	3.19	11.3	2.22	11.09	2.18
Crop N uptake from soil	62.5	150.74	2.41	124.55	1.99	123.27	1.97
NH_3 volatilization	0.85	3.75	4.41	2.98	3.51	2.93	3.45
N_2O	0.05	0.09	1.80	0.09	1.80	0.09	1.80
NO	0.05	0.19	19.00	0.14	14.00	0.13	13.00

3.3.3.1 Extreme weather scenario

To examine one of the potential future scenarios, extreme weather conditions with a higher mean temperature of 15.4°C and more intense rain/drought events employed for the ECOTRON experiment were utilized as input for the Jogeva model. The DNDC model showed a decrease in yield compared to simulated yields obtained using measured weather data: CON0 decreased by 7.1% to 2029 kg C $ha^{-1}y^{-1}$, FER3 simulated biomass yield decreased by 13.7% to 3175 kg C $ha^{-1}y^{-1}$, CAT1 decreased by 3.5% to 3176 kg C $ha^{-1}y^{-1}$, and FSP decreased by 3% to 3176 kg C $ha^{-1}y^{-1}$. The simulated loss of yield may be attributed to lower soil moisture under simulated extreme weather conditions (Figure 19).

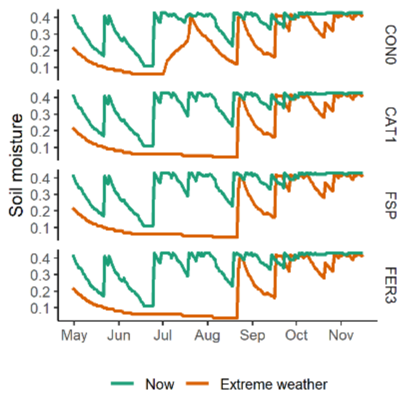

Figure 19. Simulated soil moisture in fraction of water filed pores for the Jogeva experimental field in Estonia. Simulated data for the experimental year 2023 (green), and extreme weather scenario used for the ECOTRON experiment (red).

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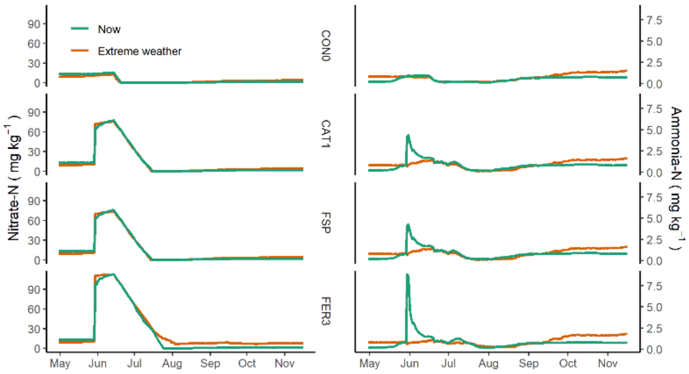

Figure 20. A comparison of soil nitrate and ammonia dynamics simulated with weather data measured at the Jogeva experimental site and simulated using the extreme weather scenario.

There is a close match in simulated soil NO_3-N concentrations for both weather datasets (collected at the experimental site and extreme weather scenario) (Figure 20). Simulated soil NH_4-N for the measured weather data was higher in comparison to the one obtained using the extreme weather scenario. Simulated soil mineral nitrogen concentration was similar for both weather datasets.

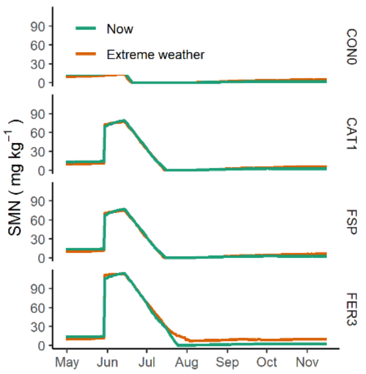

Figure 21. Simulated soil mineral nitrogen as a sum of NO_3-N and NH_4-N for the Jogeva experimental site in Estonia. Simulated data for the experimental year 2023 (green), and extreme weather scenario (red).

The DNDC model indicated an increase of CO_2 emissions under extreme weather conditions of 69% for CON0 (640.4 kg C $ha^{-1}y^{-1}$), 49% for FER3 (696.5 kg C $ha^{-1}y^{-1}$), 39% for CAT1 (811.2 kg C $ha^{-1}y^{-1}$) and 39% for FSP (818.6 kg C $ha^{-1}y^{-1}$).

Reduced simulated crop N-uptake corresponds with the reduced simulated crop biomass yield under extreme weather scenario in reference to simulated values obtained using the measured weather data at the Jogeva experimental site. The model indicates a reduction in NH_3 volatilization under extreme weather for all three BBFs.

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Table 10. Simulated gas fluxes in Estonia using the extreme weather scenario, relative change with respect to the simulated gas fluxes for 2023 given as a fraction.

	CON		FER3		CAT1		FSP	
	N (kg N $ha^{-1}y^{-1}$)	Relative to 2023	N (kg N $ha^{-1}y^{-1}$)	Relative to 2023	N (kg N $ha^{-1}y^{-1}$)	Relative to 2023	N (kg N $ha^{-1}y^{-1}$)	Relative to 2023
Soil N leaching	18.60	2.66	35.12	1.17	22.23	0.97	21.81	0.97
Crop N uptake	58.15	-0.07	116.56	-0.23	116.59	-0.06	116.60	-0.05
NH_3 volatilization	1.67	0.96	2.56	-0.32	2.70	-0.09	2.71	-0.08
N_2O	0.24	3.80	0.50	4.56	0.31	2.44	0.31	2.44
NO	0.04	3.00	0.30	0.58	0.21	0.50	0.20	0.54

The amounts of mineralized N changed from 31.3, 39.8, 40.2, and 34.2 kg N $ha^{-1}y^{-1}$ as simulated for the measured weather conditions for the CON0, CAT1, FSP, and FER3 treatments respectively; to 60.1, 41.2, 40.8, and 48.0 kg N $ha^{-1}y^{-1}$ for the same treatments simulated using extreme weather data.

When the extreme weather scenario with elevated temperatures (mean temperature 15.4 °C) and more intense rain/drought events was supplemented with increased atmospheric CO_2 (775 ppm) the simulated aboveground crop biomass yields in kg C $ha^{-1}y^{-1}$ were 2387 (CON0), 4759 (CAT1), 4736 (FSP), and 5240 (FER3) indicating an increase in biomass yields of 0.3%, 44%, 44%, and 42% compared to simulated values using the measured weather data in 2023.

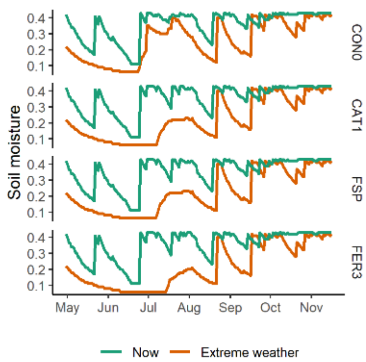

Figure 22. Simulated soil moisture expressed as a fraction of water filled pores for year 2023 (green), and for extreme weather scenario that includes an increase of atmospheric CO_2 concentration to 775 ppm (red) for the Jogeva experimental site.

Despite very low soil moisture (Figure 22), the DNDC model does not reduce crop yield when atmospheric CO_2 levels are set to 775 ppm. However, these modelling results may not accurately reflect real-world conditions.

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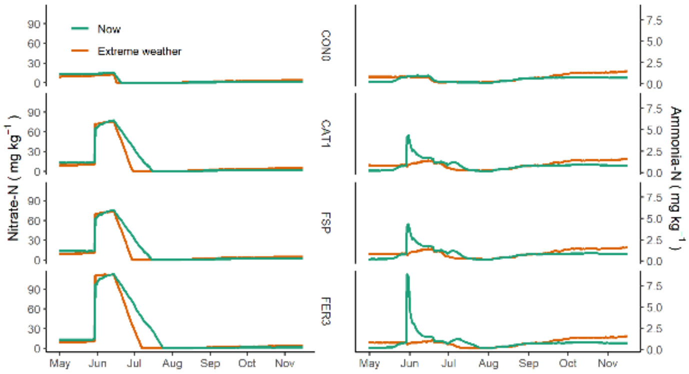

Figure 23. A comparison of soil nitrate and ammonia dynamics simulated with weather data measured at the Jogeva experimental site and simulated using the extreme weather scenario with elevated atmospheric CO_2.

Visual inspection of the simulated soil NO_3-N and NH_4-N dynamics indicates that there was a more rapid decrease of the two parameters shortly after fertilizer application under extreme weather scenario in comparison to recorded weather conditions when an increase in atmospheric CO_2 was included in the model (Figure 23).

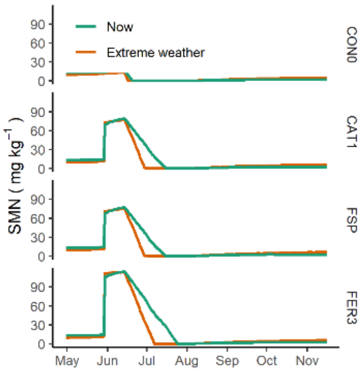

Figure 24. Simulated soil mineral nitrogen obtained using the weather data collected at the Jogeva experimental site in Estonia compared with simulated values produced using the extreme weather data that include increased atmospheric CO_2 concentration.

Simulated soil mineral nitrogen decreased more rapidly under extreme weather scenario shortly after fertilizer application (Figure 24).

The DNDC model indicated an increase of CO_2 emissions under extreme weather conditions of 73% for CON0 (654.4 kg C $ha^{-1}y^{-1}$), 67% for FER3 (779.0 kg C $ha^{-1}y^{-1}$), 57% for CAT1 (917.4 kg C $ha^{-1}y^{-1}$) and 57% for FSP (925.7 kg C $ha^{-1}y^{-1}$) for higher atmospheric CO_2 concentrations. These values are higher than the ones obtained using the extreme weather scenario and the default atmospheric CO_2 concentration.

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Table 11. Simulated gas fluxes at Jogeva experimental site in Estonia using the extreme weather scenario and increased atmospheric CO_2 concentration. Relative change with respect to the simulated gas fluxes for 2023 given as a fraction.

	CON0		FER3		CAT1		FSP	
	N (kg N $ha^{-1}y^{-1}$)	Change	N (kg N $ha^{-1}y^{-1}$)	Change	N (kg N $ha^{-1}y^{-1}$)	Change	N (kg N $ha^{-1}y^{-1}$)	Change
Soil N Leaching	18.56	2.65	20.5	0.27	20.12	0.78	20.11	0.81
Crop N uptake	59.07	-0.05	157.73	0.05	127.19	0.02	125.74	0.02
NH_3	1.67	0.96	2.19	-0.42	2.51	-0.16	2.53	-0.14
N_2O	0.23	3.60	0.3	2.33	0.3	2.33	0.3	2.33
NO	0.04	3.00	0.28	0.47	0.2	0.43	0.19	0.46

The amounts of mineralized N changed from 31.3, 39.8, 40.2, and 34.2 kg N $ha^{-1}y^{-1}$ as simulated for the measured weather conditions for the CON0, CAT1, FSP, and FER3 treatments respectively: to 50.9, 60.7, 61.1, and 53.5 kg N $ha^{-1}y^{-1}$ for the same treatments simulated for the extreme weather data and elevated atmospheric CO_2 concentration.

3.3.4 Belgium

At harvest time, most broccoli plants had heads larger than 8 cm in diameter, meeting the commercial yield criteria. However, many were flowering and thus not viable commercially. For biomass calculation however, all plants reaching maturity were considered viable.

Weather data for the field experiment was collected on-site. Since DNDC input needs year-round data, additional weather information was obtained from a nearby station.

The simulated aboveground crop biomass yields for the the DNDC model calibrated using the data collected at the Upigny experimental site in Belgium, were 1114 (CON0), 2235 (CAT1), 2219 (FSP), and 2562 (FER3) kg C $ha^{-1}y^{-1}$. The corresponding measured crop biomass yields were 1144 (CON0), 1485 (CAT1), 1322 (FSP), and 1560 (FER3) kg C $ha^{-1}y^{-1}$. The coefficient of determination between simulated and observed broccoli biomass yields ($R2 = 0.85$, $p<0.01$) was very good according to Moriasi et al. (2015). However, the RMSE-observation standard deviation ratio ($RSR = 4.81$) was unsatisfactory based on Moriasi et al. (2007). Despite numerous calibration efforts, the RSR remained unsatisfactorily high, suggesting that the model failed to adequately fit the data. Our attempt to introduce a correction factor for yields to improve the model's predictive capability was ineffective.

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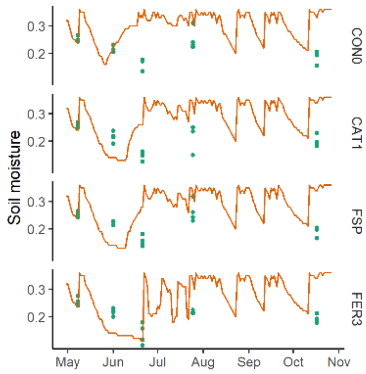

Figure 25. Measured (dots) and simulated soil moisture at a depth of 10 cm (line) during the growing season is presented as a fraction of water-filled pores (wfps) for the data collected at the Upigny experimental site in Belgium.

There was a substantial discrepancy in the observed and simulated soil moisture content (Figure 25).

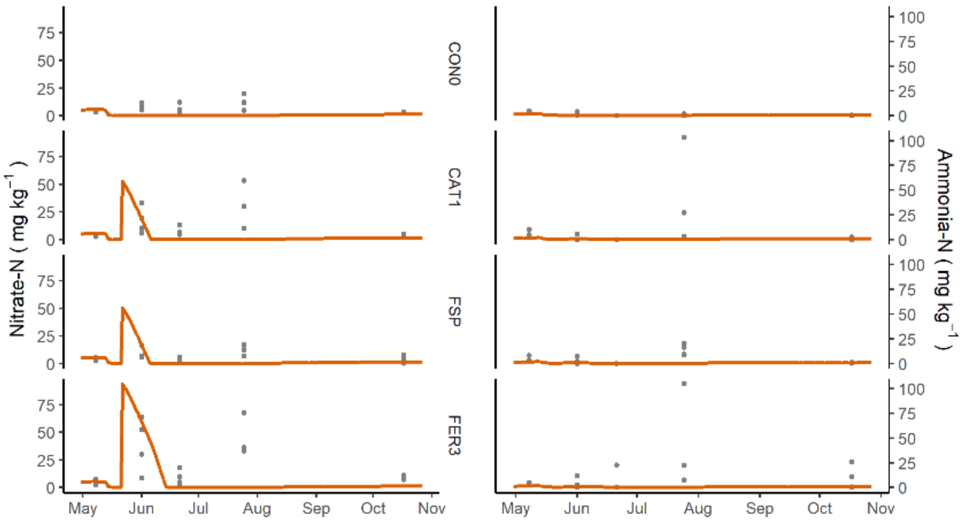

Figure 26. A comparison of the measured concentrations of soil NO_3-N and NH_4-N at the Upigny experimental site, and the simulated values produced by the DNDC model, which was calibrated specifically for this site, at a depth of 0-10 cm.

Our model underperformed with respect to soil NO_3-N and NH_4-N concentration, with $R^2 = 0.20$ ($p = 0.046$) and $R^2 = 0.08$ ($p = 0.23$) for the two parameters, respectively (Figure 26 and Figure 27).

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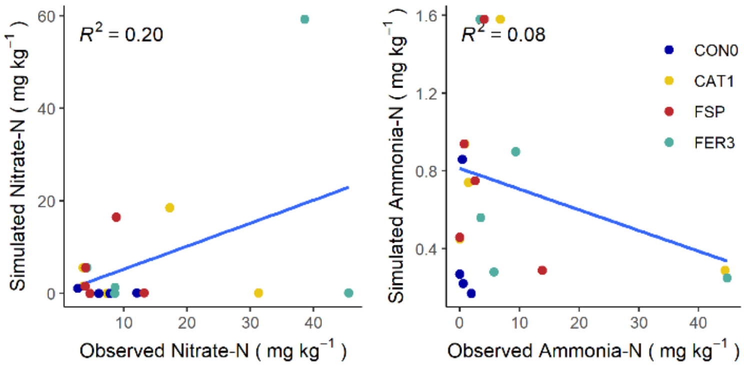

Figure 27. Comparison of measured and modeled concentrations of soil NO_3-N and NH_4-N at a depth of 0-10 cm for the Upigny experimental site

There was a poor correlation between observed and simulated soil mineral nitrogen content (R^2 = 0.04, p = 0.09) for the model calibrated for the Upigny experimental site.

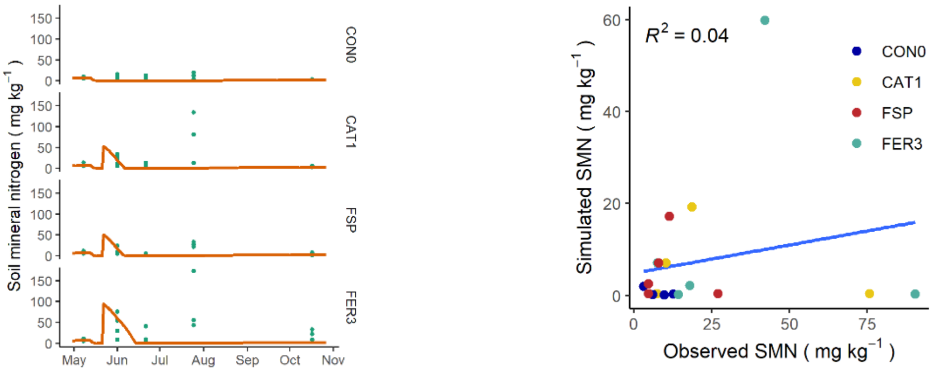

Figure 28. Comparison of measured (dots) and simulated (line) soil mineral nitrogen (as a sum of NO_3-N and NH_4-N) at 10 cm dept plotted as a function of time on the left-hand side figure for the Upigny experimental site.

The simulated soil NO_3-N concentration for the control treatment decreased to zero immediately after transplanting, making it impossible to calculate the relative change during the growing period. After the harvest, the value gradually increased. A comparison of the simulated NO_3-N concentrations later in the season demonstrated that the availability of simulated soil NO_3-N is greater for the CTA1 and FSP treatments compared to the FER3 treatment (Figure 29).

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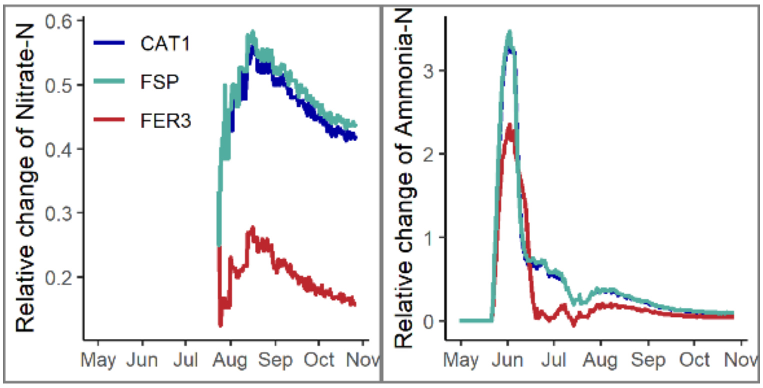

Figure 29. Comparison of the dynamics of relative changes in soil NO_3-N and NH_4-N content for the three BBFs, calculated with the unfertilized treatment set as the reference value at Upigny experimental site.

Simulated soil CO_2 emissions for CON, FER3, CAT1 and FSP were 538.5, 673.7, 809.7 and 817.4 kg C ha^{-1}y^{-1} respectively. The model indicated an increase in simulated CO_2 emissions for FER3, CAT1 and FSP of 25%, 50% and 52% with respect to unfertilized treatment. Simulated crop N uptake from soil was higher for the fertilized treatments, along with the loss of N gases through volatilization (Table 12).

Table 12. DNDC model simulated N fluxes using the data collected at the Upigny experimental site, Belgium. Relative change with respect to the unfertilized treatment expressed as a fraction.

	CON0	**FER3**		**CAT1**		**FSP**	
	N **(kg N ha^{-1}y^{-1})**	N **(kg N ha^{-1}y^{-1})**	Relative change	N **(kg N ha^{-1}y^{-1})**	Relative change	N **(kg N ha^{-1}y^{-1})**	Relative change
Soil leaching	2.75	2.79	0.01	2.84	0.03	2.84	0.03
Crop N uptake from soil	56.84	152.12	1.68	118.79	1.09	117.16	1.06
NH_3 volatilization	2.12	2.95	0.39	3.31	0.56	3.32	0.57
N_2O	0.05	0.07	0.40	0.06	0.20	0.06	0.20
NO	0.01	0.21	20.00	0.12	11.00	0.12	11.00

Given the identified constraints and uncertainties affecting the model's predictive capability, we find its application to extreme weather scenario modelling unjustifiable. Therefore, we will not utilize this model for such projections.

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3.3.5 Spain

The field experiment was conducted in two consecutive years (2023-2024). As described in the D5.1, plant damage caused loss of yield in 2023. Therefore, data from the trial in 2024 was used for modelling of soil nitrogen dynamics. FER3 was applied differently in 2024 compared to the previous year and all other countries. It was used as a bio stimulant supplemented with mineral fertilizer, and therefore not included the DNDC model based on the Spanish data.

The parameter calibration procedure resulted in simulated crop biomass yields of 1603, 2209, and 2192 kg C $ha^{-1}y^{-1}$ for the CON0, CAT1, and FSP treatments, respectively. The discrepancy between simulated and observed crop biomass yields, which were 790 (CON0), 1504 (CAT1), and 1760 (FSP) kg C $ha^{-1}y^{-1}$, was narrowed by multiplying the observed crop yields with correction factor 2. For the corrected values the R^2 and RSR between simulated and observed broccoli biomass yields was 0.92 ($p < 0.01$) and 0.56, respectively, which are considered as good.

A notable difference was observed between the measured soil moisture and the simulated values (Figure 30). Several factors could account for this. The soil parameters may need further calibration, the weather data obtained from a nearby weather station might not precisely represent the actual conditions at the experimental site or there could have been some moisture loss from the soil samples before measuring the weight.

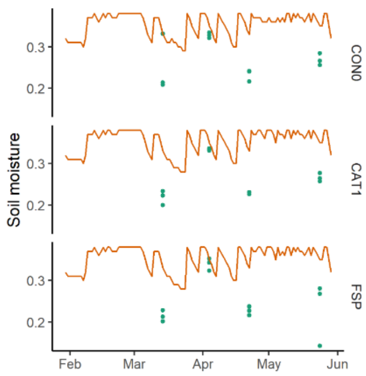

Figure 30. Measured (dots) and simulated soil moisture at a depth of 10 cm (line) during the growing season is presented as a fraction of water-filled pores (wfps) for the data collected at the Zamudio experimental site in Spain.

The model reasonably represented the measured soil NO_3-N data (R^2 of 0.60 and $p < 0.01$), but it did not perform as well for NH_4-N ($R^2 = 0.43$, $p = 0.03$, Figure 31, Figure 32). The post-harvest soil NO_3-N concentration was lower compared to pre-transplantation levels (observed and simulated). This indicates that the crop absorbed both the NO_3-N present

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in the BBFs and the amount mineralized during the growing period by the harvest time, along with depleting the soil NO_3-N pool.

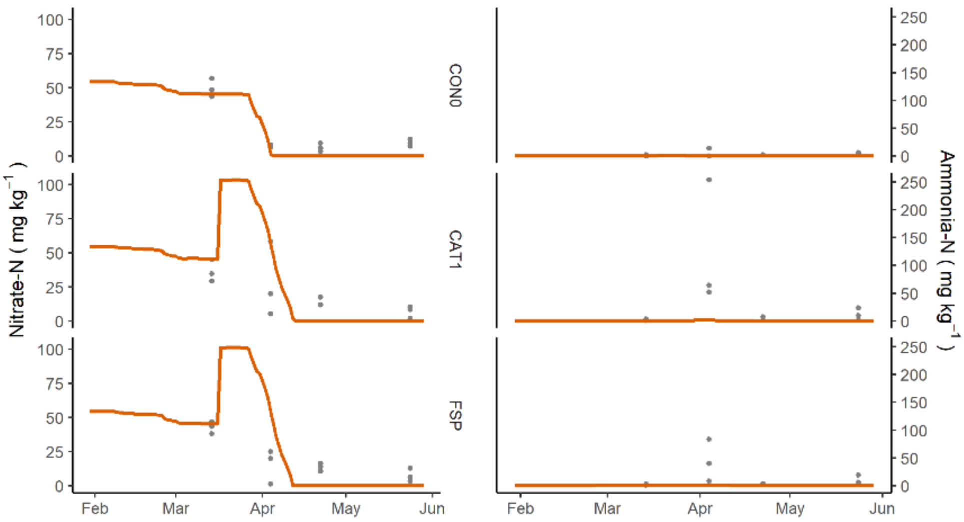

Figure 31. A comparison of the measured concentrations of soil NO_3-N and NH_4-N at the Zamudio experimental site, and the simulated values produced by the DNDC model, which was calibrated specifically for this site, at a depth of 0-10 cm.

Simulated NO_3-N or the unfertilized treatment (CON0) was rapidly decreased to zero from transplantation date (Figure 31), and did not rise again until well after simulated harvest. A rapid decrease of soil NO_3-N concentration right after transplantation was observed for CAT1 and FSP as well.

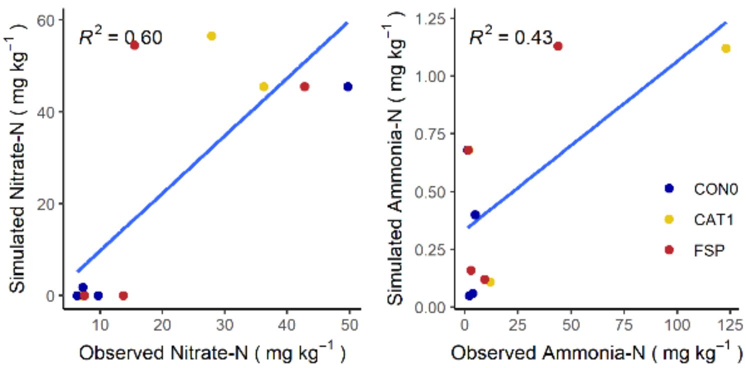

Figure 32. Comparison of measured and modelled concentrations of soil NO_3-N and NH_4-N at a depth of 0-10 cm for the Zamudio experimental site.

The model showed a good fit for total soil mineral nitrogen ($R^2 = 0.58$, $p < 0.01$, Figure 33). By the harvest time both observed and simulated soil mineral nitrogen pools were depleted.

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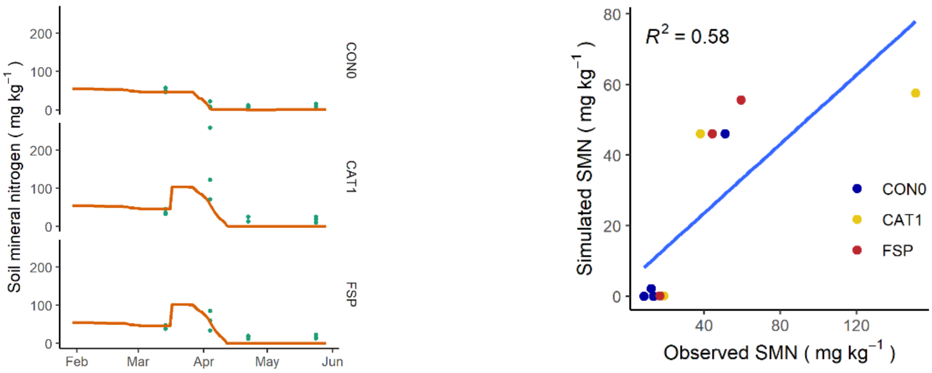

Figure 33. Comparison of measured (dots) and simulated (line) soil mineral nitrogen (as a sum of NO_3-N and NH_4-N) at 10 cm dept plotted as a function of time on the left-hand side figure for the Zamudio experimental site.

There was no substantial difference between simulated relative NO_3-N and NH_4-N between CAT1 and FSP (Figure 34).

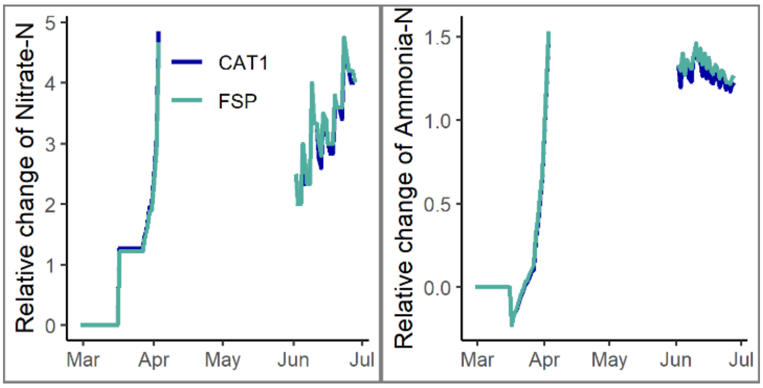

Figure 34. Comparison of the dynamics of relative changes in soil NO3-N and NH4-N content for the three BBFs, calculated with the unfertilized treatment set as the reference value at Zamudio experimental site.

Simulated soil CO_2 emissions for CON, CAT1 and FSP were 687.7, 873.4 and 879.8 kg C ha^{-1}y^{-1} respectively. The model indicated an increase in simulated CO_2 emission for CAT1 and FSP of 27% and 28% with respect to unfertilized treatment. Simulated N fluxes were similar for the two BBFs with respect to unfertilized treatment CON0 (Table13).

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Table 13. Simulated N fluxes for the Zamudio experimental site in Spain. Relative change, expressed as a fraction rather than a percent, calculated with respect to unfertilized treatments.

	CON	CAT1		FSP	
	N (kg N $ha^{-1}y^{-1}$)	N (kg N $ha^{-1}y^{-1}$)	Relative change	N (kg N $ha^{-1}y^{-1}$)	Relative change
Soil N leaching	33.14	34.58	1.04	34.53	1.04
Crop N uptake from soil	178.56	239.70	1.34	237.94	1.33
NH_3 volatilization	1.16	2.78	2.40	2.82	2.43
N_2O	0.16	0.21	1.31	0.21	1.31
NO	0.01	0.18	18.00	0.18	18.00

3.3.6 France

As described in D5.1, the field experiment failed in 2023, so data collected in 2024 was used for the DNDC. The weather data at the experimental site showed irregularities in wind speed, with average speeds sometimes higher than maximum speeds (e.g., on 18/01/24, an average of 243.4 km/h vs. a maximum of 38.6 km/h). As a result, only T max, T min, precipitation, and radiation were used as driving factors for the DNDC model, whereas other countries included wind speed and humidity as well.

The DNDC automatically changes soil hydraulic conductivity obtained using euptf2 (0.008 m h^{-1}) and replaces it with 0.015 m h^{-1}. This could not be overwritten.

Simulated crop biomass yields were 933, 1519, 1510, and 1747 kg C $ha^{-1}y^{-1}$ for the CON0, CAT1, FSP, and FER3 treatments, respectively. Despite testing multiple parameter values and combinations during the calibration procedure, a substantial discrepancy remained between the simulated and observed crop yields, which were 263 (CON0), 421 (CAT1), 549 (FSP), and 648 (FER3) kg C $ha^{-1}y^{-1}$. This discrepancy was significantly reduced by applying a correction factor of 3.5 to the observed values. For the corrected values the R^2 and RSR between simulated and observed broccoli biomass yields was 0.86 ($p < 0.01$) and 0.66, respectively, which are considered as good.

The poor match between observed and simulated soil moisture (Figure 35) values may be partially due to the DNDC not allowing changes in soil hydraulic conductivity parameter beyond built-in values, but other factors may contribute to the explanation as well. Further calibration of soil parameters, improved sample collection and processing, and continuous measurement of the weather data at the experimental site could help reduce the discrepancy between observed and simulated values.

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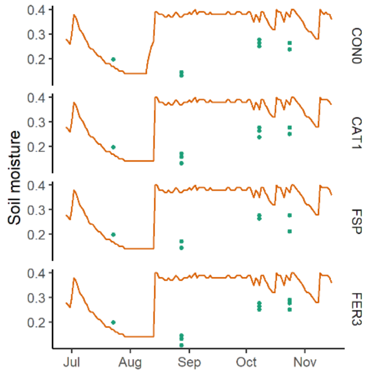

Figure 35. Measured (dots) and simulated soil moisture at a depth of 10 cm (line) during the growing season is presented as a fraction of water-filled pores (WFPS) for the data collected at the Assat experimental site in France.

The model fit to the data was poor for soil NO_3-N and NH_4-N as well, with R^2 of 0.05 (p = 0.386) and 0.11 (p = 0.216) for the two parameters respectively (Figure 36 and Figure 37). There was also a substantial discrepancy between observed and simulated values for the soil mineral nitrogen concentration (R2 = 0.04, p = 0.246, Figure 38).

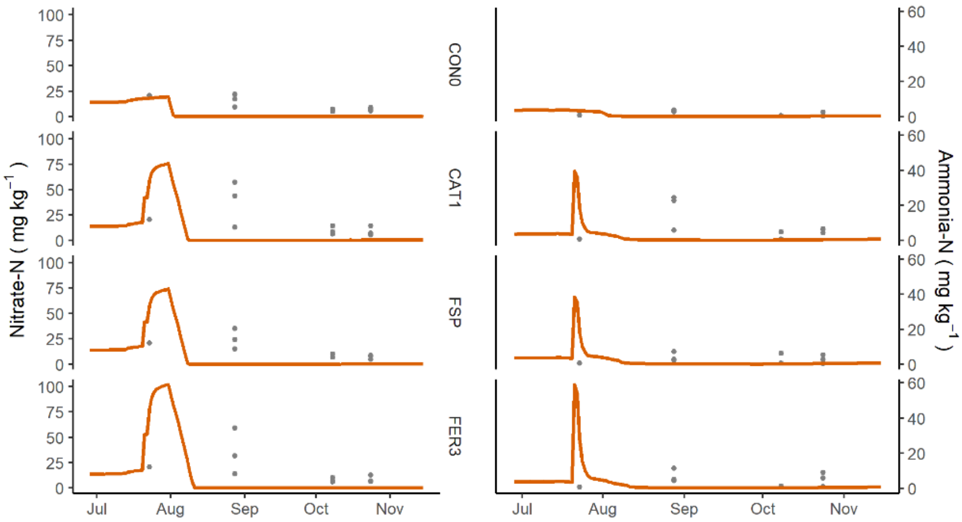

Figure 36. A comparison of the measured concentrations of soil NO_3-N and NH_4-N at the Assat experimental site, and the simulated values produced by the DNDC model, which was calibrated specifically for this site, at a depth of 0-10 cm

The simulated NH_4-N concentration peak observed in the fertilized treatments (Figure 36) within the model calibrated to the Assat dataset represents an anomaly when compared to the corresponding data (Figure 4, Figure 15, Figure 26, Figure 31) for other countries. All parameters, except the choice of climate data type, were identical or were calibrated using the same methodology across all countries. As explained, climate data type 2 used for the Assat dataset includes maximum temperature (T max), minimum temperature (T

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min), precipitation, and radiation. In contrast, climate data type 5 used for the other datasets also includes wind speed and humidity.

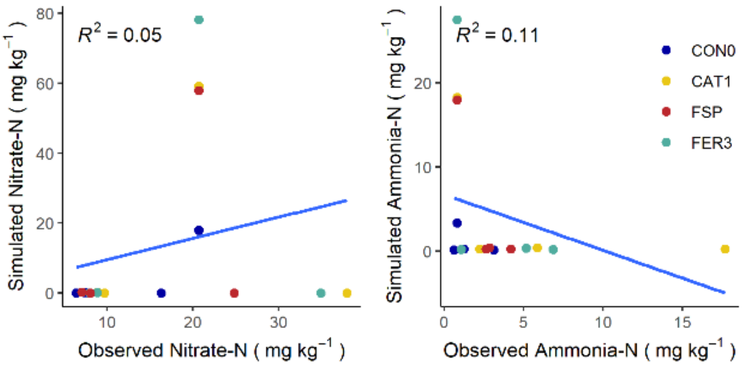

Figure 37. Comparison of measured and modeled concentrations of soil NO_3-N and NH_4-N at a depth of 0-10 cm for the Assat experimental site.

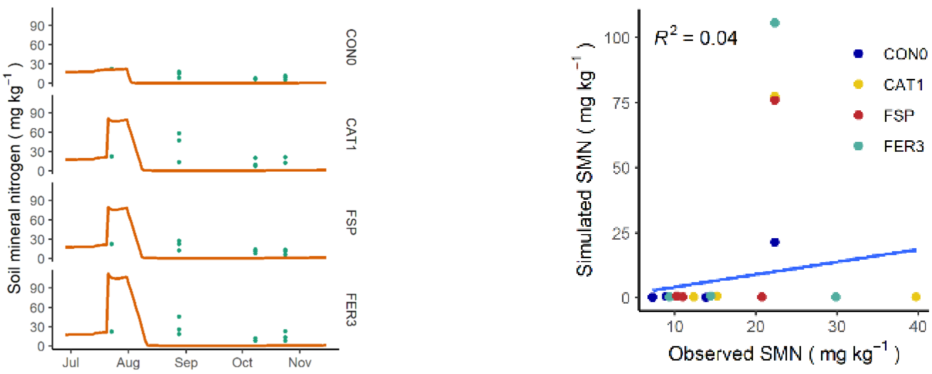

Figure 38. Comparison of measured (dots) and simulated (line) soil mineral nitrogen (as a sum of NO_3-N and NH_4-N) at 10 cm dept plotted as a function of time on the left-hand side figure for the Assat experimental site.

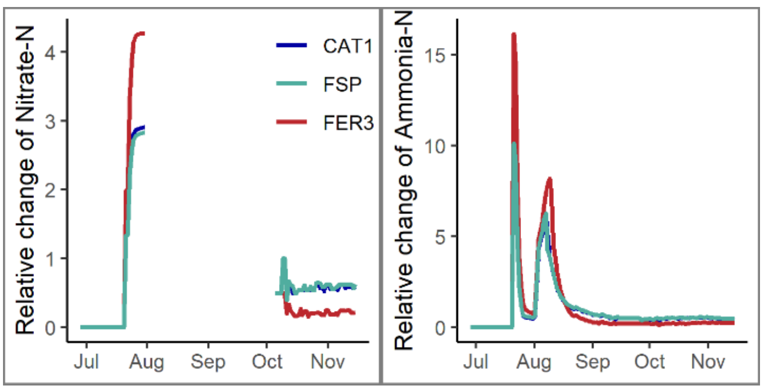

Figure 39. Comparison of the dynamics of relative changes in soil NO_3-N and NH_4-N content for the three BBFs, calculated with the unfertilized treatment set as the reference value at Assat experimental site.

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Simulated soil CO_2 emissions for CON, FER3, CAT1 and FSP were 1047.9, 1238.4, 1328.6 and 1333.4 kg C $ha^{-1}y^{-1}$ respectively. The model indicated an increase in simulated CO_2 emission for FER3, CAT1 and FSP of 18%, 27% and 27% with respect to unfertilized treatment.

Table 14. Simulated N fluxes for the Assat experimental site in France. Relative change, expressed as a fraction rather than a percent, calculated with respect to unfertilized treatments.

	CON	FER3		CAT1		FSP	
	N (kg N $ha^{-1}y^{-1}$)	N (kg N $ha^{-1}y^{-1}$)	Relative change	N (kg N $ha^{-1}y^{-1}$)	Relative change	N (kg N $ha^{-1}y^{-1}$)	Relative change
Soil N leaching	28.76	28.82	0.00	28.83	0.00	28.83	0.00
Crop N uptake from soil	102.09	193.03	0.89	168.8	0.65	167.8	0.64
NH_3 volatilization	2.53	17.84	6.05	13.27	4.25	12.98	4.13
N2O	0.93	0.95	0.02	0.95	0.02	0.95	0.02
NO	0.07	0.33	3.71	0.24	2.43	0.24	2.43

Given the identified constraints and uncertainties affecting the model's predictive capability, we find its application to extreme weather scenario modelling unjustifiable. Therefore, we will not utilize this model for such projections.

3.4 Summary for all five countries

Norway showed relatively good agreement between simulated and measured biomass yields. Soil moisture data were collected from a local meteorological station, and while nitrogen dynamics were modelled with limited accuracy, the overall performance was more consistent than in other sites. The availability of high-resolution climate and soil data contributes positively to the model's reliability.

The DNDC model performed well in simulating soil nitrogen dynamics in Estonia. However, soil moisture simulations were more challenging, showing significant deviations from measured values. The site benefited from continuous soil monitoring using the Soil Scout system, which provided high-resolution data.

Calibration efforts did not improve model predictive accuracy in Belgium. Simulated biomass values were consistently higher than observed ones. Soil moisture simulations were also inaccurate, and nitrogen dynamics were poorly captured, with low correlation between simulated and measured nitrate and ammonium levels.

Spain demonstrated strong performance in biomass modelling after correction, with good alignment between simulated and observed values. Nitrogen dynamics were

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evaluated for CAT1 and FSP due to different fertilizer application, and the model fitted the measured soil NO_3-N data. However, like in the other countries, model performance with respect to soil moisture remained a challenge.

France experienced substantial discrepancies in both biomass and nitrogen simulations. Although the biomass fit improved after applying a correction factor, the nitrogen dynamics remained poorly modelled. The DNDC model struggled with soil moisture simulations, partly due to limitations in adjusting hydraulic conductivity parameters. Additionally, the site used a different climate data format, which may have influenced model performance.

In summary, while all sites faced difficulties with soil moisture simulation, the DNDC model's ability to simulate nitrogen dynamics and biomass yield varied. Estonia and Norway showed relatively better performance in biomass and nitrogen modelling, There is a need for improved calibration and parameter flexibility in the DNDC model to accurately describe the data collected at Belgium, Spain and France.

Across all five countries, the DNDC model consistently simulated a rapid post-fertilization increase in NO_3-N followed by a seasonal decline, with variations in magnitude and timing influenced by initial soil conditions, fertilizer type, and local climate. Overall, simulated soil NO3-N after fertilization was higher for FER3 compared to both CAT1 and FSP. Spain and Estonia showed the most pronounced NO_3-N fluctuations, while Belgium exhibited the most stable profile. These findings underscore the importance of site-specific calibration and management strategies to optimize nitrogen use efficiency and minimize environmental losses. Both simulated and empirical data demonstrate that post-harvest soil NO3-N levels are reduced in comparison to the levels recorded prior to fertilization and plant transplantation.

The DNDC model simulations under measured weather conditions reveal clear trends in nitrogen gas emissions across the five experimental sites. Fertilized treatments consistently resulted in higher emissions of NH_3, N_2O, and NO, with the highest values observed in Estonia and Norway. Spain showed moderate emissions, while France and Belgium presented challenges in model reliability.

The DNDC model simulations conducted for Apelsvoll in Norway and Jogeva in Estonia aimed to assess the impacts of extreme weather conditions—characterized by elevated temperatures, increased drought and rainfall variability, and higher atmospheric CO_2 concentrations—on crop productivity, nitrogen dynamics, and greenhouse gas emissions.

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In Norway, the simulations revealed that elevated CO_2 levels significantly boosted aboveground biomass across all treatments, with increases ranging from 36% to 44%. However, this productivity gain came with trade-offs. Soil nitrate levels declined more rapidly after fertilization, while ammonium concentrations rose under extreme conditions. Overall, the total soil mineral nitrogen pool was reduced. Greenhouse gas emissions, particularly CO_2 and N_2O, surged under these scenarios, with CO_2 emissions increasing by up to 178% in unfertilized plots. Nitrogen leaching also intensified, especially in fertilized treatments, indicating a potential risk to water quality.

In Estonia, the response to extreme weather was more nuanced. While elevated CO_2 helped maintain or slightly increase biomass yields in fertilized treatments, yields declined when CO_2 was not elevated. Soil nitrogen dynamics mirrored those observed in Norway, with faster depletion of nitrate and ammonium under stress conditions. The model performed well in simulating nitrate dynamics but struggled with ammonium and soil moisture. CO_2 emissions rose across all treatments, though less dramatically than in Norway, and ammonia volatilization actually decreased. Nitrous oxide and nitric oxide emissions increased, particularly in unfertilized plots, suggesting a shift in nitrogen loss pathways.

The application of the DNDC model across diverse agroecosystems revealed several critical challenges that influenced the accuracy and reliability of the simulations. One of the foremost issues was the parameterization and calibration of the model. While some parameters could be derived from direct measurements, many had to be estimated from literature or default values, introducing uncertainty.

Another challenge was the quality and completeness of input data, particularly meteorological variables. The model's sensitivity to such inputs underscores the importance of comprehensive and high-resolution environmental data for accurate simulations.

Moreover, the model structure itself posed limitations. The DNDC version used (v9.5) lacked certain functionalities needed to simulate the behavior of bio-based fertilizers (BBFs) with sufficient precision. The findings suggest that a specialized DNDC module tailored to BBFs would be necessary to enhance model performance.

Finally, despite harmonized experimental protocols, site-specific variability in soil properties, climate, and management practices introduced additional complexity. While the model performed well in some locations (e.g., Norway), it failed to replicate observed patterns in others (e.g., France and Belgium), even after extensive calibration.

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This variability emphasizes the need for localized model adjustments and possibly the integration of automated calibration tools, such as PEST, to improve predictive accuracy.

In summary, the modelling exercise highlighted the DNDC model's potential, but also its limitations when applied to short-term, site-specific studies involving novel fertilizer types. Addressing these challenges will require both technical improvements to the model and enhanced data collection strategies.

4 DSSAT and CROPGRO

4.1 Model description

The Decision Support System for Agrotechnology Transfer (DSSAT) was originally developed by an international network of scientists collaborating in the International Benchmark Sites Network for Agrotechnology Transfer project. Its goal was to facilitate the application of crop models using a systems approach to agronomic research. The system was initially motivated by the need to integrate knowledge about soil, climate, crops, and management to improve decision-making when transferring production technology across locations with differing soil and climate conditions. DSSAT consists of a collection of independent programs that work together, with crop simulation models at its core. It includes databases that describe weather, soil, experimental conditions, measurements, and genotype information, enabling the application of models to various scenarios. The software assists users in preparing these databases and comparing simulated results with observations to either build confidence in the models or identify the need for modifications to enhance accuracy.

The CROPGRO model, embedded in DSSAT, was originally designed to simulate the growth of legume crops. Based on climatic, soil, and environmental conditions, CROPGRO can simulate crop responses to different fertilizers. Its generic framework allows the integration of other crops, including cabbage. However, the CROPGRO cabbage model in DSSAT has only been calibrated under tropical Hawaiian climate conditions for the cabbage cultivar Tastie and under temperate European climate conditions for the cultivar Kalorama. So far, no calibration has been conducted for broccoli.

DSSAT supports simulation for more than 40 crops, including essential staples such as maize, wheat, rice, and soybean, allowing for broad agricultural research and application. Its Cropping System Model (CSM) employs a modular framework with distinct, interchangeable components for soil, weather, crop growth, and management.

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This structure facilitates easy updates, integration of new scientific advances, and model customization and it can be used for analysing climate change

4.2 Parametrization and Calibration DSSAT

The data collected from field trials need to be adapted into three DSSAT file types: *agronomic management files containing* agricultural practices; *soil files*, containing soil property data; and *observed data files* which include agronomic records necessary for comparison with model-simulated outputs. Additionally, meteorological data for each experimental site and year (including station details) were formatted to comply with DSSAT's weather data structure.

DSSAT provides dedicated tools for creating each file type. Soil, weather, and observational data are entered using the SBuild, Weatherman, and ATCreate applications, respectively (Jones *et al*. 2003). Agronomic management data are input through XBuild- it is a tool within the DSSAT model suite that helps users set up and manage crop simulation experiments. It provides a menu-driven interface to describe key components of an agricultural experiment-, which also allows for defining the structure of the experiments to be simulated. This includes linking plots, soil types, weather stations, cultivars, sowing, fertilization, and tillage practices previously loaded into XBuild or other tools. XBuild also enables the user to adjust simulation criteria—such as toggling modules or selecting between submodel options for specific processes. Furthermore, it includes an interface to implement controlled environmental modifications over defined timeframes by systematically altering daily values of selected meteorological variables. This feature enables sensitivity analysis of weather variables including temperature, solar radiation, relative humidity, wind speed, precipitation, and atmospheric CO_2 concentration.

Calibration process is summarized in figure 40

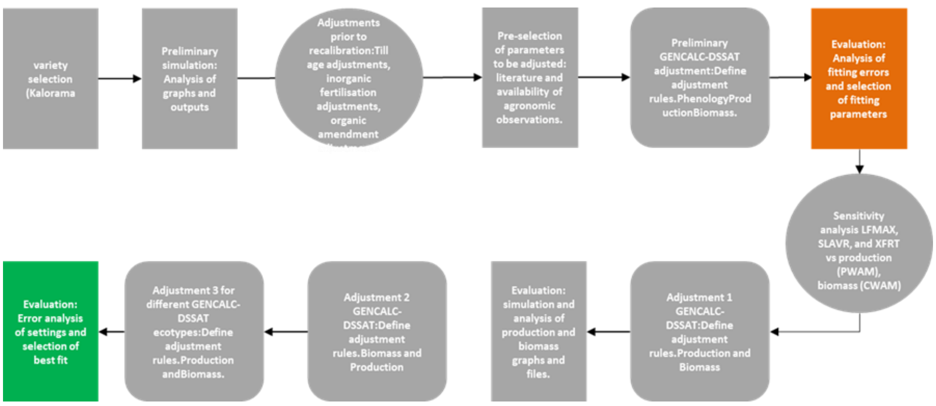

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Figure 40. Scheme of DSSAT calibration process

Calibration of the DSSAT broccoli model began with a thorough review of existing DSSAT applications to Brassica crops. Finding only one relevant study—Übelhör et al. (2015), which provided a database of genetic coefficients for cauliflower—we adopted their "Kalorama" entry from the cultivar (.CUL) file as our starting point. Using DSSAT's CROPGRO submodel, which organizes genetic parameters into cultivar, ecotype, and species files, we defined each trial in XBUILD and ran the corresponding simulations. By comparing DSSAT's numerical and graphical outputs with our observed agronomic data, we quantified initial discrepancies and then refined the genetic coefficients in successive iterations. This cycle of simulation, comparison, and adjustment continued until model predictions aligned closely with field measurements.

DSSAT's GENCALC tool (Genetic Coefficient Calculator in the DSSAT suite). It helps to estimate the cultivar-specific parameters that drive crop development and yield in the DSSAT models) was then used for parameter calibration. Prior to using GENCALC, candidate parameters were selected for adjustment:

SLAVR: specific leaf area under standard conditions.

LFMAX: maximum photosynthesis rate at 30 °C, 35 ppm CO_2, and high radiation.

XFRT: maximum fraction of daily growth allocated to seed or reproductive structures (in the case of broccoli, the harvested head).

These parameters align with observed productivity metrics—namely, dry above-ground biomass and dry head weight—entered into the agronomic record files.

Both the parameter selection and calibration rules (e.g., matching parameters to observations, iterative adjustment protocols) were implemented within GENCALC. Although ecotype parameters cannot be adjusted directly in GENCALC, cultivar values can be associated with different ecotypes. Accordingly, calibrations were performed for each ecotype present in the DSSAT database, based on the parameters adjusted in the first phase. This resulted in a two-step calibration process: first, using the Kalorama cultivar and ecotype; and second, applying the tuned parameters to other ecotypes.

Calibration was also supported by a prior sensitivity analysis, conducted with DSSAT's built-in tool, to identify suitable starting values for genetic parameters.

This calibration process used trials conducted in Norway and Spain in 2023 (for the Parthenon variety) and Estonia in 2023 (for the Cezar variety). In both the Norway and

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Spain cases, one treatment was excluded from calibration due to inconsistent production and biomass data. The rest of the countries were not considered due to an inconsistency of data.

During the calibration process it has been found that DSSAT is able to simulate satisfactorily the accumulation of aboveground biomass throughout the crop cycle. There seems to be an important problem related to the simulation of phenological development. The maturity of the crop, understood as the moment when the seeds contained in the fruit have completed their development, does not coincide with the maturity from a productive point of view (broccoli heads with adequate size before the inflorescences start to elongate). This generates mismatches as the DSSAT model engine for cauliflower (broccoli) simulation is CROPGRO which is designed to simulate pea-type legumes. So, the harvestable product is understood as pods. The date of harvesting determines the yield, that is considered the heads, (PWAMS) to a large extent, because of this phenological mismatch.

The experiments carried out include treatments with experimental organic amendments that probably have biostimulant properties that condition the growth and development of the crop. Such effects are not simulated by DSSAT. To simulate this type of effect, it would be necessary to carry out a more detailed study of these effects, to unravel the biochemical and biophysical mechanisms on which they are based and to modify the equations governing the model (in this case DSSAT) to include this type of effect.

Once the calibration process was completed, simulations of temperature increase and CO2 concentration increase scenarios were carried out, using the experiments included in the calibration as a reference.

4.3 DSSAT Modelling results

As previously indicated, the calibration of the DSSAT model was conducted exclusively using datasets from Norway and Spain for the Parthenon variety, and from Estonia for the Cezar variety. This selection was driven by the inconsistency and unreliability observed in the data from France and Belgium, which were excluded from the calibration process due to quality concerns as some essential data as phenological status observations required by DSSAT were missing, those datasets had to be excluded from the analysis.

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4.3.1 Spain -Norway results

4.3.1.1 Calibration results

The decision to integrate datasets from Spain and Norway jointly is based on the premise that combining data from agroclimatic distinct regions enhances the model's ability to simulate crop production across a wider range of environmental conditions. This diversity strengthens the robustness and transferability of the calibration outcomes.

It is important to emphasize that the volume and heterogeneity of input data directly influence simulation accuracy—the broader and richer the dataset, the more precise and generalizable the model's predictive capabilities become.

As detailed in the Methods section, model performance was assessed using the Root Mean Square Error (RMSE) and the RMSE-to-standard-deviation ratio (RSR). The RMSE—defined as the square root of the average of squared residuals—estimates the sample standard deviation of those residuals, thereby quantifying the mean magnitude of prediction errors in the response variable's units.

RSR is defined as the quotient of the model's root mean square error (RMSE) and the sample standard deviation of the observed values:

Interpretation of RSR coefficient (Moriasi *et al*., 2007):

RSR ≤ 0.50 → very good

0.50 < RSR ≤ 0.60 → good

0.60 < RSR ≤ 0.70 → satisfactory

RSR > 0.70 → unsatisfactory

Figures 41 and 42 present the calibration outputs for the Parthenon cultivar derived from experimental field trials conducted in Spain and Norway.

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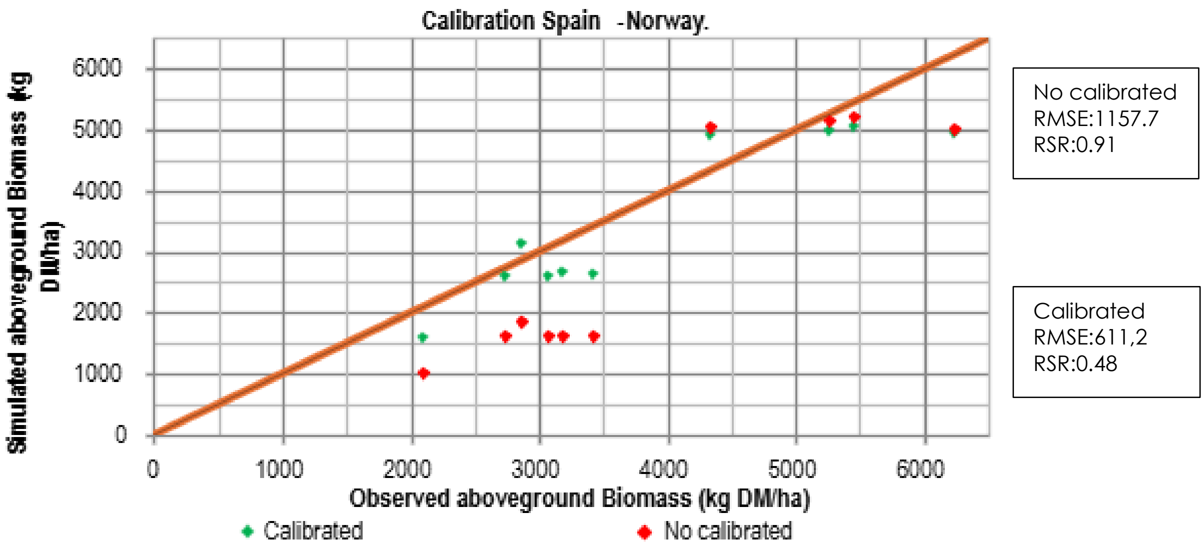

Figure 41 A comparison of the measured aboveground biomass in Spain and Norway experimental sites, and the simulated values produced by the DSSAT model, which was calibrated specifically for these sites.

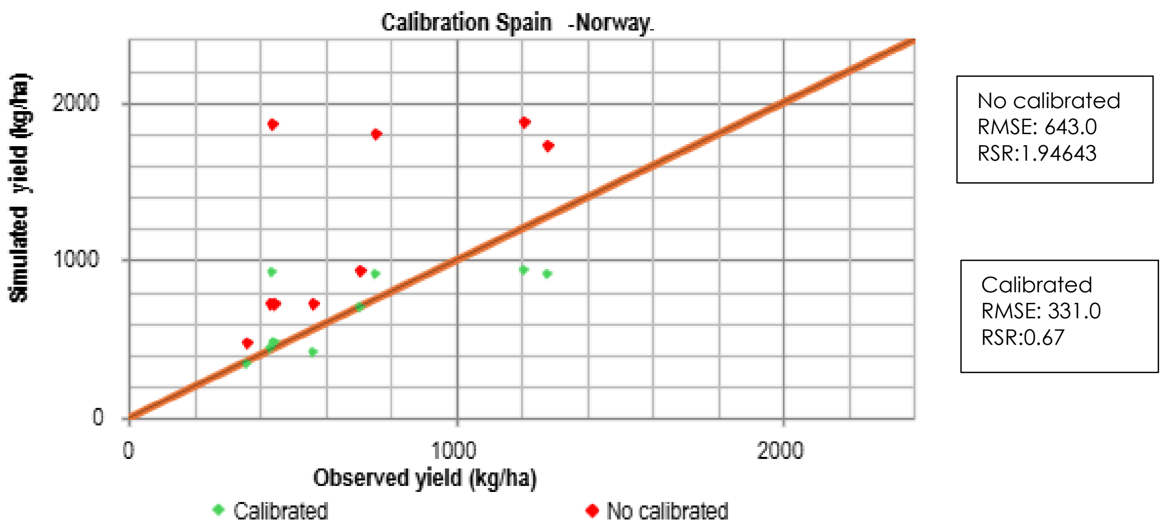

Figure 42 A comparison of the measured yield in Spain and Norway experimental sites, and the simulated values produced by the DSSAT model, which was calibrated specifically for these sites.

It can be observed that for the Parthenon cultivar under Spanish and Norwegian conditions, calibration reduced the RSR to 0.48 and the RMSE to 611,2 kg DM ha^{-1}, indicating that the DSSAT model accurately reproduces aboveground biomass. This level of agreement shows that the model's crop-growth processes are well parameterized for these environments. The consistent underestimation across trials reveals a systematic bias

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rather than random error, making it straightforward to correct with a simple linear adjustment. Introducing a correction factor (e.g. multiplying simulated biomass by a scalar >1) could align predictions with observed values without overhauling the model structure. However, such post hoc adjustments should be validated across multiple seasons and management regimes to ensure they do not mask deeper parameter misspecifications.

On the contrary, yield (broccoli heads), although calibration markedly enhances the accuracy of yield predictions, shown elevated RSR values and increased residual variance. This likely stems from simplifications in the flower-number algorithm that overlook variability in head size and kernel count, as well as from under-representing dynamic nutrient stress during critical phenological stages. Model accuracy could be enhanced by refining the genetic coefficients that govern biomass partitioning between reproductive and vegetative tissues, and by integrating detailed head-count measurements to better constrain the yield sub-models. Enhancing these modules will not only reduce RMSE and RSR for yield but also strengthen confidence in the model's utility for scenario analysis and decision support.

4.3.1.2 Modellization Results

Following the completion of the DSSAT model calibration phase, simulations were conducted to assess crop response under projected climate change conditions. These scenarios incorporated incremental increases in ambient temperature and elevated atmospheric CO_2 concentrations to evaluate potential impacts on both marketable yield and aboveground biomass accumulation.

The simulations were executed in three regional groupings:

- Spain and Norway:

  Although calibration was performed jointly for the Spanish and Norwegian sites, scenario simulations were run separately for each region, since their historic temperature baselines and projected warming increments differ.

- Estonia, modelled independently based on calibration data for the *Cezar* variety, which exhibits distinct growth and productivity dynamics compared to *Parthenon*.

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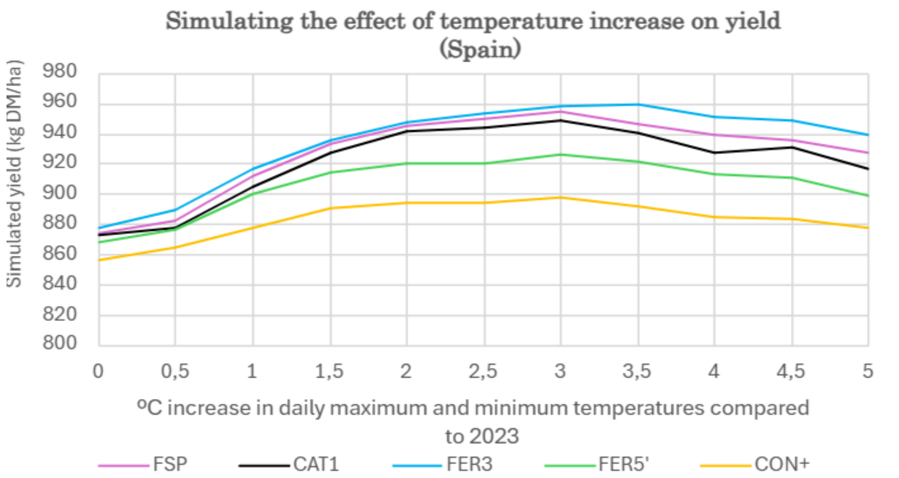
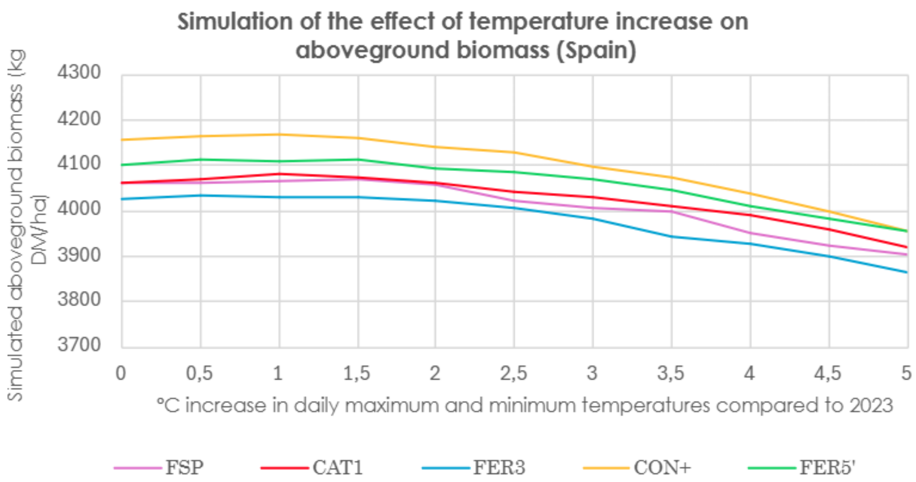
This dual-variety structure was chosen to capture varietal differences in phenological sensitivity and productivity under stress, enabling a comparative analysis of genotype-by-environment interactions under future climate conditions

4.3.1.2.1 Spain

Figures 43 and 44 illustrate the modelled impact of rising temperatures on broccoli, showing how incremental warming affects both yield (Figure 43) and total aboveground biomass (Figure 44).



Figures 43. Simulation of T increase on Broccoli Yield. Spain



Figures 44. Simulation of T increase on Broccoli abovergound biomass. Spain

Figure 43 illustrates that increasing average temperatures have a positive influence on yield, leading to greater total head biomass production. This favourable effect persists up to a simulated average temperature increase of 3.5°C. Given that the basal

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temperature used in the simulation is those temperatures recorded during field trial (average 19° but with maximum of 32°), this results in a projected average of 22,5 C with maximums of 35°. Beyond this threshold, yield begins to decline, as the temperature surpasses the optimal range for broccoli cultivation. This observation aligns with findings reported by Siomos *et al.* 2022, which also emphasize the sensitivity of broccoli to elevated temperatures and the potential negative impact on head formation and quality.

All bio-based fertilizers (BBFs) followed a similar trend for this parameter, yet those formulations with higher organic matter or biostimulant effect consistently showed a marginally greater boost in production. This suggests that elevating the organic fraction in fertilizer not only supplies nutrients directly but also enhances soil structure and microbial activity, leading to improved crop performance (Deliverable 6.3).

Similarly, Figure 44 shows that rising temperatures lead to a reduction in total aboveground biomass. The same effect is recorded for all the treatments.

Regarding to increase of CO_2, the response of yield and aboveground biomass is presented in figures 45 and 46 below

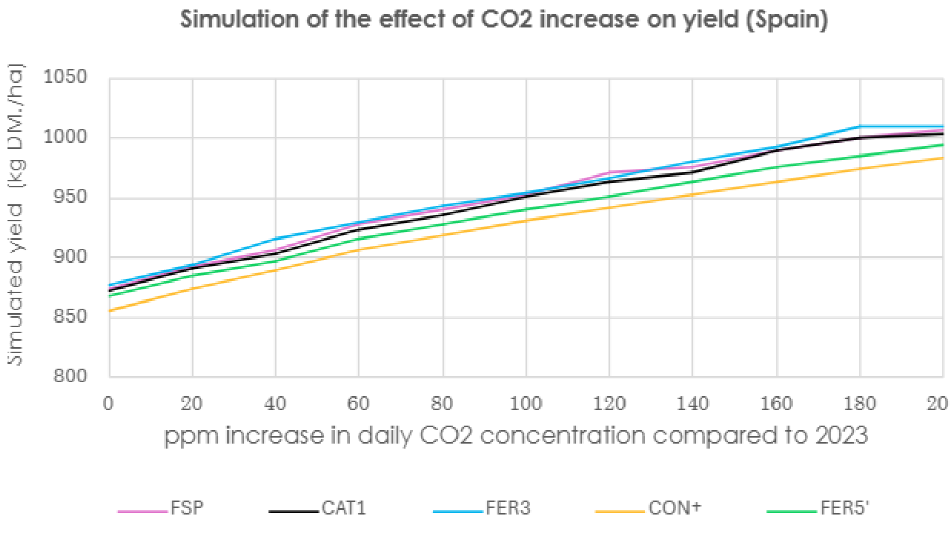

Figure 45. Simulation of effect of CO_2 increase on Broccoli yield (Spain)

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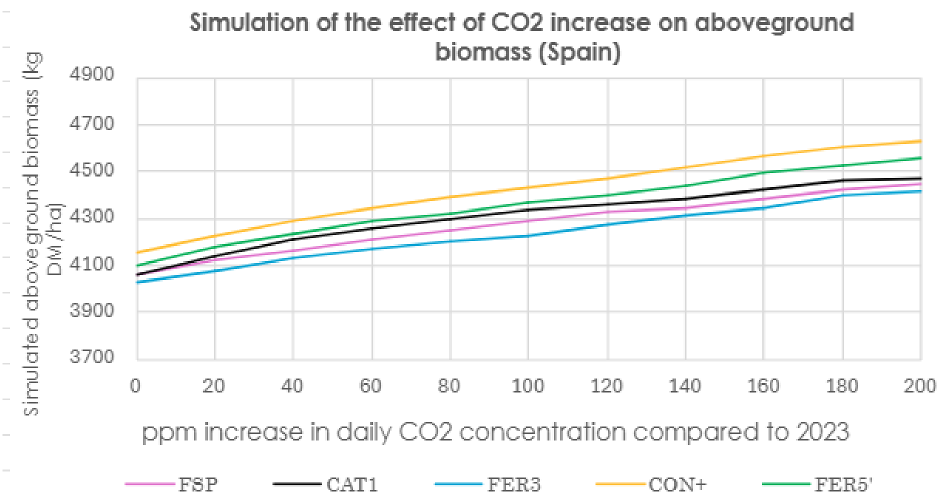

Figure 46. Simulation of effect of CO_2 increase on Broccoli aboveground biomass (Spain)

When atmospheric CO_2 is increased in 20 ppm steps—up to 200 ppm above the 2023 baseline (420 ppm) —both yield and aboveground biomass rise uniformly across all BBF treatments. This response is uniform regardless of the bio-based fertilizer used, indicating that BBF type has no impact on this parameter. This agrees with Liu et Zhou (2007) that found that under controlled-environment chambers, +200 ppm CO_2 enhanced head weight by 12–15 % when N was non-limiting.

This agrees with the results in the Ecotron trial (Deliverable5.2) where was demonstrated the feasibility of BBFs as agronomically performant alternatives to mineral fertiliser, with most BBFs achieving yields comparable to yields under synthetic fertiliser, particularly under the future climate scenario.

4.3.1.2.2 Norway

In the case of Norway, effect of temperature increase is shown in figure 47 and 48

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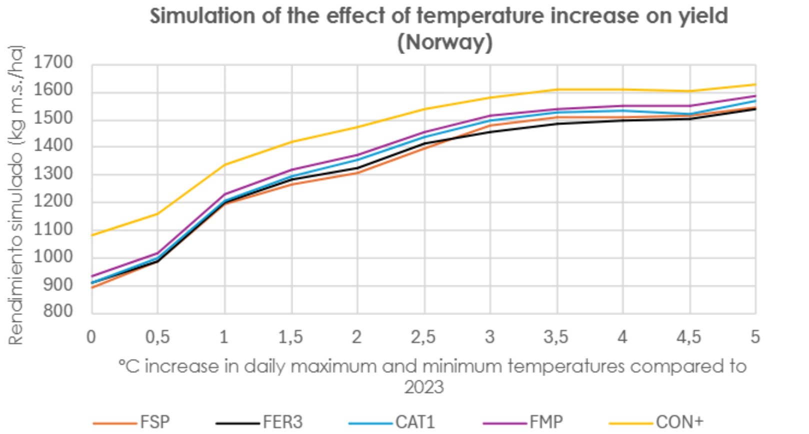

Figure 47. Simulation of effect of T° increase on Broccoli yield (Norway)

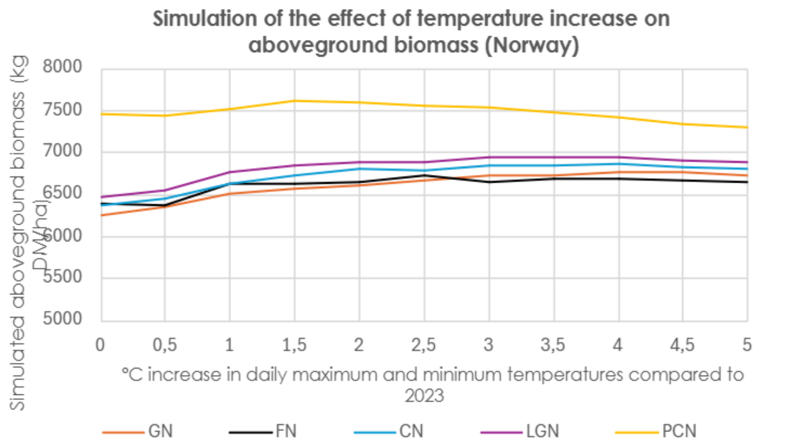

Figure 48. Simulation of effect of T° increase on Broccoli aboveground biomass (Norway)

In the Norway simulation, rising temperatures produce a continuously positive effect on yield—unlike the Spanish trial. This divergence reflects each country's 2023 baseline: Norway's average was just 16.5 °C (max 29 °C), so a +3.5 °C increase brings the mean to 20 °C and the peak to 32.5 °C. Because these values stay within broccoli's optimal 15–21 °C window, yields are not affected

When it comes to yield, mineral fertilisation outperformed bio-based fertilisers (BBF) by up to 28% at lower temperatures, reducing to a 5% advantage as temperatures increased.

In the Norway simulation, aboveground biomass remained unchanged as temperatures rose. This contrasts with the Spanish trial, where warmer conditions drove measurable losses in biomass,

Regarding CO_2 concentrations it can be registered increment of 4 % in yield and a 6% in aboveground biomass related to the CO2 increase as it is shown in figure 49 and 50

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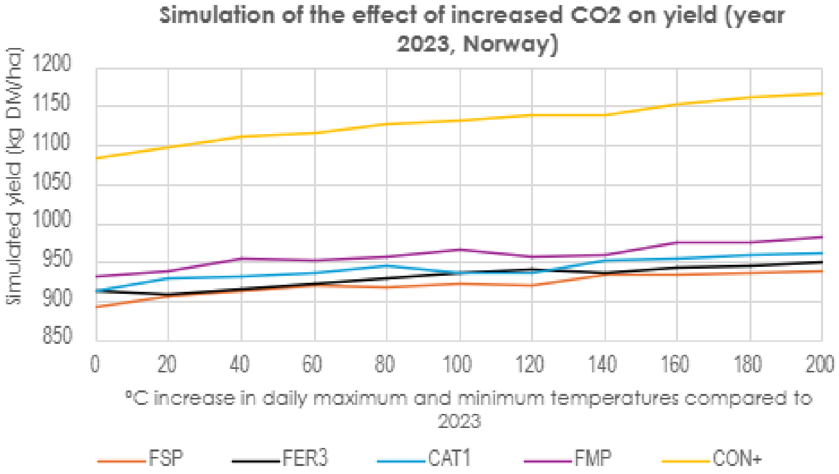

Figure 49. Simulation of effect of CO_2 increase on Broccoli yield (Norway)

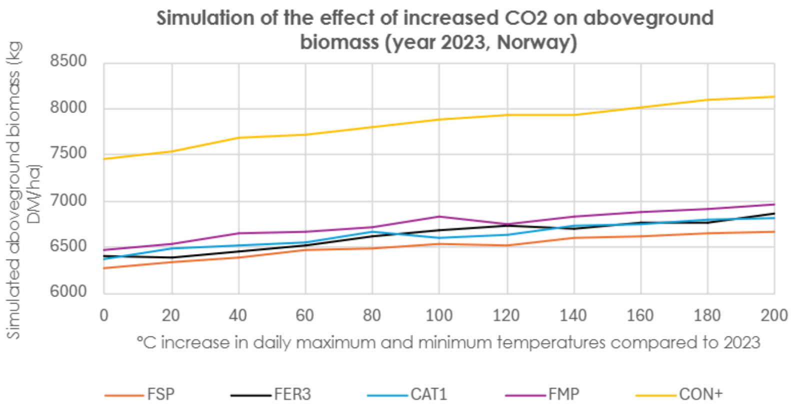

Figure 50. Simulation of effect of CO_2 increase on Broccoli aboveground biomass (Norway)

Together, these findings hint that under future climate scenarios—where both temperature and CO_2 rise—BBFs may close the performance gap with synthetic fertilizers. Warmer conditions can accelerate the mineralization of organic matter in BBFs, releasing nutrients more rapidly and bringing their agronomic results closer to those of mineral

4.3.2 Estonia results

4.3.2.1 Calibration results

Calibration for yield and aboveground biomass are presented in figures 51 and 52

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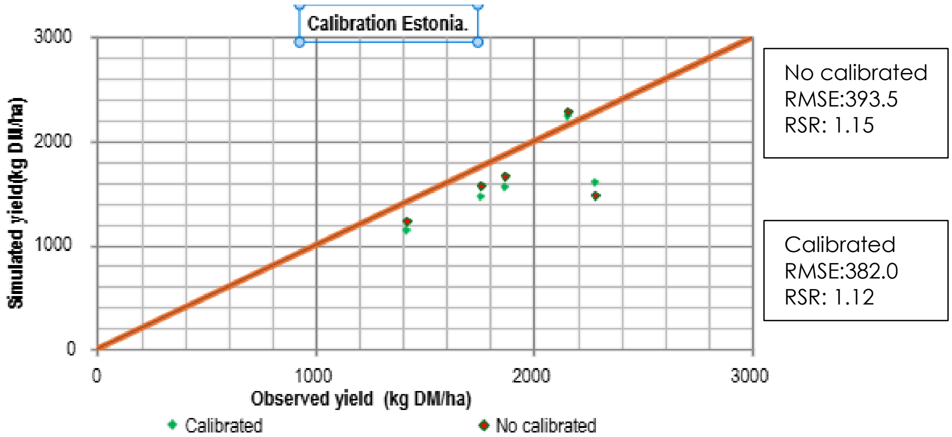

Figure 51 A comparison of the measured yield in Estonia experimental site, and the simulated values produced by the DSSAT model, which was calibrated specifically for this site.

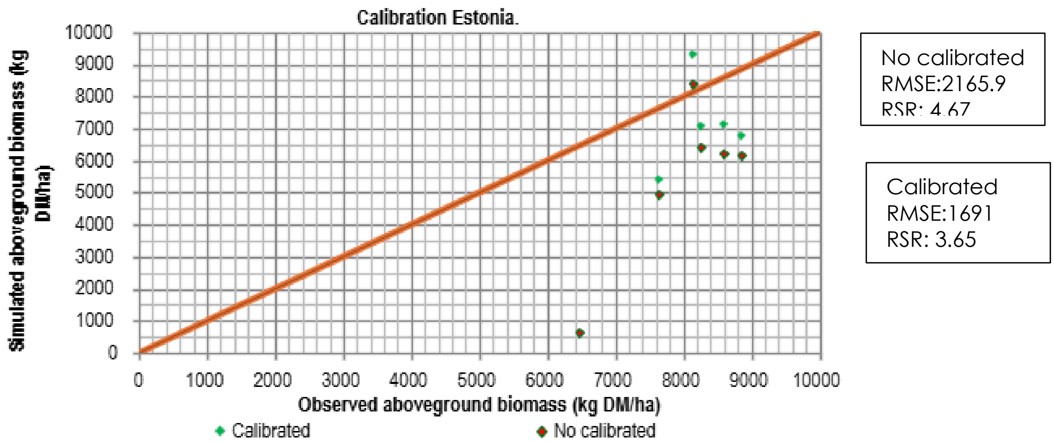

Figure 52 A comparison of the measured aboveground in Estonia experimental site, and the simulated values produced by the DSSAT model, which was calibrated specifically for this site.

In it can be seen the comparison of simulated an observed values for aboveground biomass and yield. he differences in calibration accuracy could be due to the smaller dataset used for Cezar compared to the more comprehensive Norwegian and Spanish trials

In contrast, the simulation accuracy for Estonia, calibrated separately for the Cezar variety, exhibits comparatively lower reliability. This may be attributed to narrower environmental representation, lower data variability, or varietal-specific model constraints. Despite these discrepancies, the variable yield stands out as the most robust and consistent output.

Anyway, the model was run for future conditions related to temperature and CO_2 concentrations, results are presented in the next section

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4.3.2.2 Modellization Results

After calibrating the model and accounting for its uncertainty, we simulated yield and aboveground biomass; the results are shown in Figures 53 and 54.

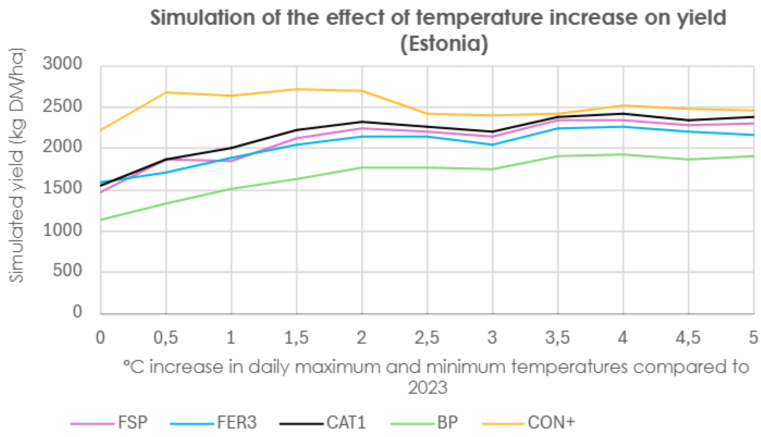

Figure 53. Simulation of effect of T° increase on Broccoli yield (Estonia)

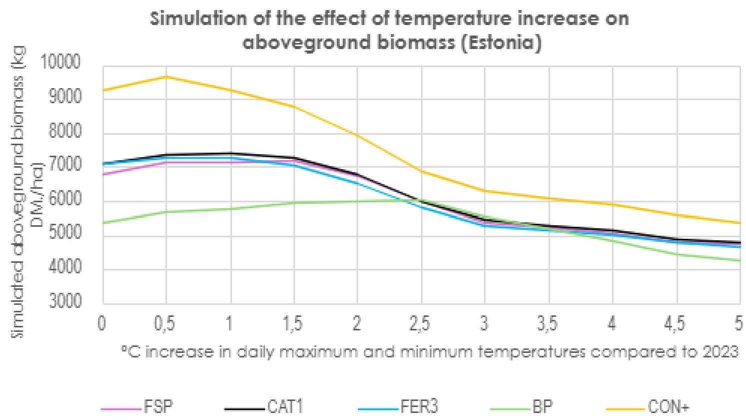

Figure 54. Simulation of effect of T° increase on Broccoli aboveground biomass (Estonia)

As shown in Figures 53 and 54, warming up to +3.5°C above the baseline enhances yield while reducing total aboveground biomass. This pattern reflects a shift in dry-matter partitioning toward reproductive organs at the expense of vegetative tissues. Interestingly, as temperatures rise, the yield responses to mineral fertilizers and bio-based fertilizers converge, indicating that warmer conditions tend to equalize their agronomic performance.

This convergence in performance happens because higher temperatures boost microbial activity and accelerate the mineralization of organic matter in BBFs, releasing nutrients almost as quickly as mineral fertilizers. Thanks to the Q_{10} effect—where every 10 °C rise roughly doubles microbial reaction rates—a 3.5 °C increase can speed N, P and K mineralization by about 20–30 % (Curtin et al. 2012). As a result, nutrients convert more

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rapidly into plant-available forms, narrowing the gap between supply and uptake. At the same time, warmer soils stimulate root growth and nutrient absorption, allowing broccoli plants to take up these freshly released nutrients nearly as efficiently as they would from synthetic salts. Under these conditions, BBFs can achieve yields similar to mineral fertilizers.

Regarding to CO2 increase, no effect of elevated CO_2 on either yield or aboveground biomass was observed (Figures 55 and 56). This contrasts with the CO_2 fertilization responses reported for Spain and Norway, where significant increases in both variables were documented.

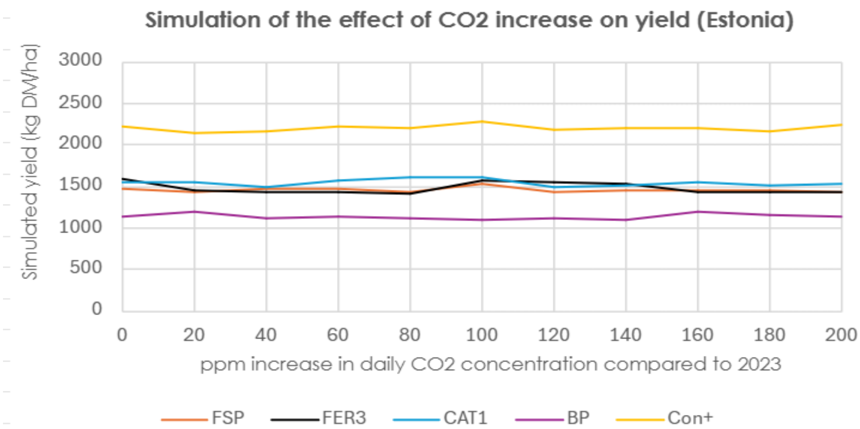

Figure 55. Simulation of effect of CO_2 increase on Broccoli yield (Estonia)

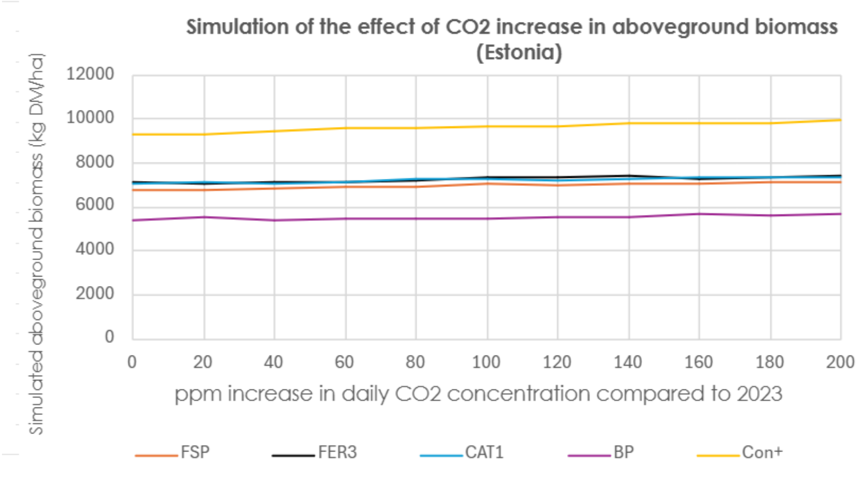

Figure 56. Simulation of effect of CO_2 increase on Broccoli aboveground biomass (Estonia)

The lack of response to increased CO_2, which normally enhances plant growth, may be due to both genetic limitations of the cultivar and insufficient nitrogen availability in relation to the high production in Estonia, much higher than in Spain and Norway. At the applied N levels (≈120 kg N ha^{-1}), there is still scope for additional CO_2 to increase yield

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and biomass in Spain and Norway, whereas in Estonia the cultivars have already reached their maximum growth potential and do not respond to CO_2 enrichment.

5 Conclusions

Related to Models

The application of the models across diverse agroecosystems revealed several critical challenges that influenced the accuracy and reliability of the simulations. One of the foremost issues was the parameterization and calibration of the model. While some parameters could be derived from direct measurements, many had to be estimated from literature or default values, introducing uncertainty.

Another challenge was the quality and completeness of input data. The models' sensitivity to such inputs underscores the importance of comprehensive and high-resolution environmental and management data for accurate simulations.

Moreover, the model structure itself posed limitations. The DNDC version used (v9.5) lacked certain functionalities needed to simulate the behaviour of bio-based fertilizers (BBFs) with sufficient precision. The findings suggest that a specialized DNDC module tailored to BBFs would be necessary to enhance model performance. Similar constraints affect DSSAT as well: it was designed for conventional fertilizers and struggles to represent next-generation biostimulants, since key processes—enhanced root growth, altered hormone signaling, and accelerated nutrient uptake—are not currently parameterized.

In summary, the modelling exercise highlighted the moddels' potential, but also its limitations when applied to short-term, site-specific studies involving novel fertilizer types. Addressing these challenges will require both technical improvements to the model and enhanced data collection strategies.

Related to results in future scenarios

Given the inherent uncertainties in the modelling, these conclusions should be interpreted with caution, even though the observed trends are coherent and plausible.

It seems that BBFs supply plant-available nutrients comparably to mineral N under current fertilisation rates, often achieving 90–100 % of mineral-fertiliser yields in Spain and Norway.

In cooler climates (e.g., Norway), BBFs initially lag behind mineral fertilisers at low temperatures but converge in performance as warming accelerates organic-matter mineralisation. Under moderate warming (+3.5 °C), It seems that the BBFs benefit from

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enhanced microbial activity (Q_{10} effect), releasing nutrients 20–30 % faster and narrowing the yield gap with synthetic fertilisers.

Elevated CO_2 boosts BBF-driven growth only when N supply and sink capacity are not already saturated; in high-yielding systems (e.g., Estonia at ≈ 120 kg N ha^{-1}, 8 Mg ha^{-1} biomass) no additional CO_2 response was observed.

DNDC simulations capture BBF nitrogen dynamics and show higher early-season mineral N peaks for liquid formulations (FER3) but highlight limitations in microbial-activity partitioning and irrigation handling that affect long-term N flux predictions.

Overall, BBFs represent agronomically viable alternatives to mineral N, especially under future warming scenarios, but both modelling frameworks need improvement to fully characterise their dynamic nutrient release for biobased fertilisers and biostimulant modes of action

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