

Formatvorlagendefinition: Überschrift 3: Einzug: Links:
0 cm, Hängend: 1.27 cm, Keine Aufzählungen oder
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1 Regional Assessment and Uncertainty Analysis of Carbon and Nitrogen Balances at
2 cropland scale using the ecosystem model LandscapeDNDC

3
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14

15 Abstract

16 The assessment of cropland carbon and nitrogen (C & N) balances play a key role to identify
17 cost effective mitigation measures to combat climate change and reduce environmental
18 pollution. In this paper, a biogeochemical modelling approach is adopted to assess all C & N
19 fluxes in a regional cropland ecosystem of Thessaly, Greece. Additionally, the estimation and
20 quantification of the modelling uncertainty in the regional inventory are realized through the
21 propagation of parameter distributions through the model leading to result distributions for
22 modelling estimations. The model was applied on a regional dataset of approximately 1000
23 polygons deploying model initializations and crop rotations for the 5 major crop cultivations
24 and for a timespan of 8 years. The full statistical analysis on modelling results ([including the](#)
25 [uncertainty ranges given as ± values](#)) yields for the C balance carbon input fluxes into the soil
26 of 12.4 ± 1.4 tons C ha⁻¹ yr⁻¹ and output fluxes of 11.9 ± 1.3 tons C ha⁻¹ yr⁻¹, with a resulting
27 average carbon sequestration of 0.5 ± 0.3 tons C ha⁻¹ yr⁻¹. The averaged N influx was $212.3 \pm$
28 9.1 kg N ha⁻¹ yr⁻¹ while outfluxes were estimated on average of 198.3 ± 11.2 kg N ha⁻¹ yr⁻¹. The
29 net N accumulation into the soil nitrogen pools was estimated to 14.0 ± 2.1 kg N ha⁻¹ yr⁻¹. The
30 N outflux consist of gaseous N fluxes composed by N₂O emissions 2.6 ± 0.8 kg N₂O-N ha⁻¹ yr⁻¹
31 ¹, NO emissions of 3.2 ± 1.5 kg NO-N ha⁻¹ yr⁻¹, N₂ emissions 15.5 ± 7.0 kg N₂-N ha⁻¹ yr⁻¹ and
32 NH₃ emissions of 34.0 ± 6.7 kg NH₃-N ha⁻¹ yr⁻¹, as well as aquatic N fluxes (only nitrate leaching
33 into surface waters) of 14.1 ± 4.5 kg NO₃-N ha⁻¹ yr⁻¹, N fluxes of N removed from the fields in
34 yields, straw and feed of 128.8 ± 8.5 kg N ha⁻¹ yr⁻¹.

35

36 KEYWORDS: greenhouse emissions, ecosystem modelling, cropland carbon and nitrogen
37 balance, inventory, Thessaly region, LandscapeDNDC

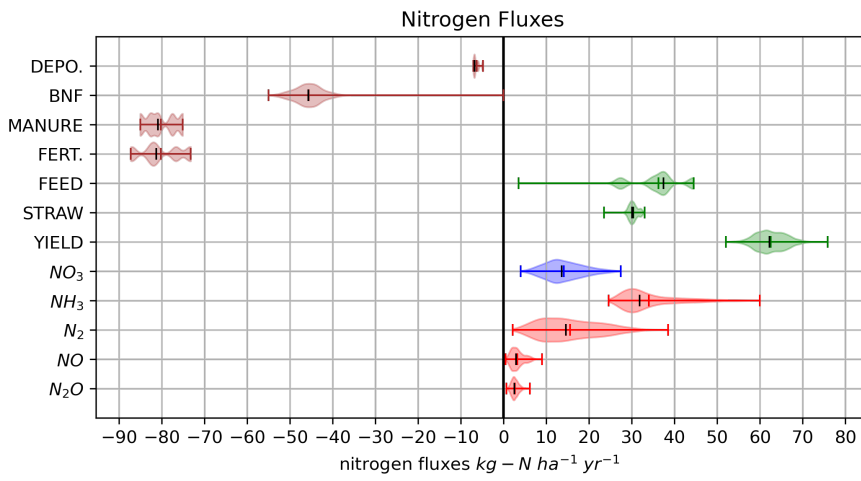
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41 Graphical abstract: Result distributions of all nitrogen fluxes with means and medians

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45 1 Introduction

46 Food security as well as the agricultural productivity depend to a major extent on the applied
47 nitrogen (N) fertilizers ([Klatt et al., 2015a](#)). Worldwide, the N fertilizer use for the years 1960 to
48 2005 has increased from 30 to 154 million tons ([IFADATA, 2015](#)). In Europe, the increase of
49 yields in arable land and grassland systems was 45-70% since 1950 ([EFMA, 2009](#)) due to the
50 agricultural production systems intensification. Excessive use of N fertilizers, though
51 beneficially affecting the yield, could cause a harmful impact to the environment, e.g. increased
52 gaseous emissions and aquatic fluxes of nitrous oxide (N₂O) to the atmosphere and leaching
53 of nitrate (NO₃) into water bodies ([Erisman et al., 2011](#); [Galloway et al., 2013](#); [Kim et al., 2015](#)).
54 The N₂O poses a twofold environmental threat. From the one hand, it is a strong greenhouse
55 gas with a warming potential of 300 times greater (in a 100-year time period) than carbon
56 dioxide (CO₂) and from the other hand, it is a major driver of ozone depletion in stratosphere
57 ([Ravishankara et al., 2009](#)). The fertilizer use aiming at the increase of the agricultural
58 production is the most crucial anthropogenic source of atmospheric N₂O, which at present
59 contributes for approximately 45% of total anthropogenic N₂O emissions on a global scale
60 ([Jones et al., 2014](#)). Because of the global population growth and thus a growing food and
61 feed demand ([Godfray et al., 2010](#)), the fertilizer use will probably increase. Consequently, the
62 prediction of the current business-as-usual scenarios show doubled anthropogenic N₂O
63 emissions by the year 2050 ([Davidson and Kanter, 2014](#)). The European countries have
64 recently set up bilateral agreements in order to reduce N₂O emissions from cultivated crop
65 lands ([EU-Commission, 2014](#)). Similarly, the European Nitrates Directive ([EU-Commission,](#)
66 [2019](#); [Musacchio et al., 2020](#)) aims at NO₃ leaching reduction to water bodies to avoid both an
67 increase of eutrophication ([Camargo and Alonso, 2006](#)) and drinking water pollution. Because
68 of the hazardous N₂O and NO₃ effects, agricultural systems are necessary to be evaluated for
69 their profitability and productivity as well as for their impacts to the environment.
70 The N₂O and NO₃ production and consumption in agricultural lands are regulated to a large
71 extent by N plant uptake and, also, the microbial processes of denitrification and nitrification
72 ([Butterbach-Bahl et al., 2013](#)). The factors controlling both the microbial metabolism and plant

73 N uptake are a) soil conditions ([Butterbach-Bahl et al., 2013](#)) and b) cultivation management
74 practices e.g. crop rotation, fertilizing amount and timing, and ploughing ([Smith et al., 2008](#)).
75 In order to reach a minimization of the environmental footprint of agricultural production while
76 securing the global food security ([Garnett et al., 2013](#)), it is mandatory to tighten the N cycling
77 on intensified agricultural systems e.g., by harmonizing N demand of crops with soil N
78 availability by N fertilization.

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79 [Full nitrogen balance inventories provide a comprehensive understanding of the different N](#)
80 [input and output fluxes within an arable system to the scientific community, farmers and policy](#)
81 [makers. The assessment of the N balance is essential to optimize nitrogen use and production](#)
82 [and minimize environmental impact and pollution. Especially policy making and regulatory](#)
83 [bodies require accurate and robust information on all different nitrogen fluxes to develop](#)
84 [effective strategies in agricultural N management. Up to now, our understanding of N cycling](#)
85 [in arable land lacks observations of the full N balance as only few studies tried to quantify the](#)
86 [total N balance of agricultural systems, e.g. \(\[Zisti-Schlingmann et al., 2020\]\(#\)\) using stable](#)
87 [isotope techniques or \(\[Schroeck et al., 2019\]\(#\)\) using process based modelling.](#)

88 [A recent opinion paper by a large group of leading scientists \[Grosz et al., \\(2023\\)\]\(#\) in the field of](#)
89 [process based ecosystem modelling identified the lack of knowledge on the full N balance and](#)
90 [“the scarcity of complete modeled N balances in the literature stems from the reluctance of the](#)
91 [scientific community to support the publication of unvalidated modeled results, especially given](#)
92 [that the simulation results of these neglected N pools and fluxes may be unrealistic. This this](#)
93 [self-censorship of authors has resulted in a missed opportunity to share knowledge and](#)
94 [improve our understanding of modeled processes.”](#)

95 [Grosz et al., \(2023\) conclude that “including the entire N balance and related should become](#)
96 [standard when publishing the results of N model studies.” Grosz et al., \(2023\) emphasize that](#)
97 [this would allow to assess the robustness of modelled N fluxes and full N balances, and to](#)
98 [illustrate the diversity and uncertainty of the different process based modeling approaches,](#)
99 [e.g. modelling denitrification processes in soils.](#)

102 In this analysis, the process-based bio-geochemical model LandscapeDNDC (Haas et al.,
 103 2013) was applied to the agricultural cropland systems in the region of Thessaly (Greece). The
 104 objective of our study was threefold:

105 i) Assesing and reporting the cropland C and N balance including all associated
 106 fluxes such as e.g. CO₂, N₂O and NH₃ emissions, NO₃ leaching as well as the soil
 107 carbon stock changes as demanded by Grosz et al., (2023),

108 ii) Increasing the robustness and trustworthiness of the balance modelling by
 109 assesing and quantifying the modelling uncertainty of the simulated C and N
 110 balance and flux estimations as requested before by the IPCC (IPCC, 2019)

111 iii) Presenting a regional uncertainty assessment methodology for C and N cycling to
 112 advance the balance modelling by propagating 500 joint parameter and input data
 113 distributions through the model (each representing a full regional C and N balance
 114 inventory simulation) yielding regional result distributions for any modelling
 115 estimations.

117 2 Material and Methods

118 2.1 Model description

119 LandscapeDNDC is a modular process-based ecosystem model for simulating the bio-
 120 geochemical change of C and N in croplands, forest and grassland systems at both site and
 121 regional scale. The modules combined are about plant growth, micro-meteorology, water
 122 cycling, physico-chemical-plant and microbial C and N cycling and exchange processes with
 123 atmosphere and hydrosphere of terrestrial ecosystems. LandscapeDNDC is a generality of the
 124 plant development and soil biogeochemistry of the agricultural DNDC and Forest-DNDC (Li,
 125 2000). There is a successful application of earlier model versions in a number of studies, e.g.
 126 water balance (Grote et al., 2009; Holst et al., 2010), plant growth (Cameron et al., 2013;
 127 Werner et al., 2012), NO₃ leaching (Kim et al., 2015; Thomas et al., 2016) and soil respiration
 128 and gas emission trace (Chirinda et al., 2011; Kraus et al., 2014; Molina-Herrera et al., 2015).

hat gelöscht: A number of environmental/ecosystem models have been developed and used to describe the structure of multiple biogeochemical

hat gelöscht: processes (Wainwright and Mulligan, 2004.). For the estimation/quantification of the GHGs emissions from different agroecosystems, modelling approaches are constantly gaining ground due to the in-situ data limitation (field campaign and laboratory costs) and the variation in spatial and temporal scales. The simulated results may, also, have uncertainties resulting from different sources, which can be, though, quantified increasing the accuracy of the estimates. Mechanistic models integrating relevant processes, which simulate agricultural production, and, also, reactive N losses to the environment are valuable tools to infer practices for a sustainable agriculture. In recent years, process-based biogeochemical models such as e.g. DNDC (Li, 2000), DAYCENT (Parton et al., 1998), ECOSSE (Bell et al., 2012) and CERES-EGC (Gabrielle et al., 2006) have proven their applicability to simulate N₂O emissions and NO₃ leaching from various land uses. Despite the fact that their accuracy is being assessed against in-situ data, few studies are reported to use sensitivity and uncertainty analyses in total N and C cycling simulation by process-based models (Verbeek et al., 2006).¶

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hat gelöscht: iii) to demonstrate the feasibility and robustness of a regional uncertainty assessment methodology for C and N cycling

166 For the initialization of LandscapeDNDC physical and chemical site-specific soil profile
167 information is used (specified for different soil depths): Soil organic carbon (SOC) and nitrogen
168 (SON) content, soil texture (clay, sand and silt content), of the plant growth and soil
169 biogeochemistry, bulk density, pH value, saturated hydraulic conductivity, field capacity and
170 wilting point. Daily or hourly climate data of air temperature (max, min and average), N
171 deposition, precipitation, and atmospheric CO₂ concentration are used in LandscapeDNDC in
172 combination with agricultural management practices e.g. crop planting and harvesting,
173 fertilizing (synthetic and organic) or feed cutting and tilling are used to drive LandscapeDNDC
174 simulations. Regarding fertilization management three types of mineral fertilizers, i.e. urea,
175 compound fertilizers based on NH₄ and NO₃ as well as organic amendments, i.e. green
176 manure, farmyard manure, slurry, straw, bean cake and compost are currently considered.
177 The growth of crops and grasses is similar to the DNDC approach using two major parameters
178 that describe seasonal plant development (cumulative temperature degrees days) and
179 maximum reachable biomass under optimum conditions ([Li, 2000](#)) while daily growth
180 limitations due to water and nutrient availability are considered. Model parameters describing
181 soil and vegetation characteristics are obtained from an external parameter library. In
182 LandscapeDNDC, the parameterization of the main cultivated commodity crops in Europe
183 occurs by default parameter sets representing an average plant type while process parameter
184 values for micro-meteorology, water cycle and bio-geochemical processes were obtained from
185 previous validation studies, e.g. ([Klatt et al., 2015a](#); [Molina-Herrera et al., 2016](#); [Rahn et al.,](#)
186 [2012](#)) proving that the LandscapeDNDC model could be universally applicable for similar
187 conditions.

188 For all simulations in the current study, site-specific crop parameterizations were derived in a
189 preceding analysis of various site scale simulations and validations of yield characteristics
190 across the region. An overview of the crops cultivated at the different study sites and detailed
191 information on specific crop rotations used to simulate crop growth are provided in Table A2
192 (supplementary material).

193 2.2 Case study description and input data

194 The region of Thessaly is located in Central Greece covering a total area of 14 000 Km², where
195 5000 Km² is lowland and approx. 2300 Km² and 6500 Km² are semi-mountainous and
196 mountainous land respectively. The plain of Thessaly is considered to be among the largest
197 agricultural land of the country ([Kalivas et al., 2001](#)) accounting for almost 410 000 ha, of which
198 about 370 000 ha is arable land where almost 80% is covered by annual and 10% by perennial
199 crops (ELSTAT, 2012). The crop/plant production of the region is around 14.2% (ELSTAT,
200 2012) of the total production of the country (2nd in Greece).

201 Soil input data for the region was available from the European Project Nitro Europe IP ([Sutton
202 et al., 2013](#)) based on the European Soil Database ([ESDB v2.0, 2004](#)) containing, soil type
203 and soil profile description of bulk density, SOC content, texture (sand, silt clay), pH value,
204 stone fraction, saturated hydraulic conductivity, wilting point and water-holding capacity in
205 various soil strata ([Cameron et al., 2013](#)). A regional soil dataset for the area of interest
206 contained about 1500 spatial polygons out of which approximately 1000 covered the cultivated
207 cropland that was finally simulated. The climate data for the regional simulations was derived
208 at polygon level from gridded ERA5 climate data for Greece.

209 2.3 Agricultural Management and model input data processing

210 The total cultivated area and the respective yields for the years 2010 to 2016, used in the
211 current analysis were obtained from the Hellenic Statistical Authority (ELSTAT). Moreover,
212 data associated with the animal capital for the respective years was also provided (ELSTAT)
213 in order to estimate the annual manure production distributed in the region however no data is
214 available on whether and how much of the manure is used in croplands. For the water
215 management, the percentage of irrigated and non-irrigated land (estimated to almost 50% for
216 each case) was also given (ELSTAT) while indicative sets of irrigation management data were
217 acquired through the River Basin Management Plans of the Special Secretariat for Water,
218 Ministry of Environment and Energy ([YPEKA, Portmann et al., 2010](#)). The irrigation water
219 volumes were estimated based on the crops needs and the minimum and maximum quantities

220 necessary according to literature while using upscaling tools to get the regional values. The
 221 fertilization data sets were provided by Fertilizer Producers and Merchandiser Association
 222 (FPMA) for the recent years (2010-2016) and are equated to the annual consumed quantities
 223 on a national level, scaled down to a regional level based on crop pattern in the Region of
 224 Thessaly cultivated land.

225 In this study, the five main crops maize, wheat, clover, cotton and barley were considered,
 226 covering the majority of the cultivated arable land in the region (over 95%) while the remaining
 227 cropland was included acquiring the final corrected land/crop coverage. In [Table 1](#), the resulting
 228 crop rotation scenarios (R1 - R5) are presented for the evaluation period 2012 - 2016. Note,
 229 each rotation sequence (R1 – R5) is shifted in time such that for each year, each crop appears
 230 exactly in one rotation. Based on the crop cover contribution in each simulated year the crop
 231 rotation contribution factors were estimated and are summarized in [Table 2](#). The management
 232 practices were based on the general agricultural practices applied in the region and information
 233 provided by farmers.

hat gelöscht: Table 1

hat gelöscht: Table 2

235 *Table 1. Summary of the crop rotation scenarios (R1- R5) for the region of Thessaly. The crop abbreviations corn,*
 236 *wiwh, clover, cott and wbar refer to maize (food corn and silage maize), winter wheat, clover (legume feed crops*
 237 *s.a. alfalfa or vetch), cotton and winter barley respectively.*

year	R1	R2	R3	R4	R5
2012	clover	cotton	wbar	corn	wiwh
2013	cotton	wbar	corn	wiwh	clover
2014	wbar	corn	wiwh	clover	cotton
2015	corn	wiwh	clover	cotton	wbar
2016	wiwh	clover	cotton	wbar	corn

238
 239 *Table 2. Crop cultivation area contribution per year to the aggregation of the five rotations; data constant across*
 240 *the region of Thessaly*

Crop Rotation Contribution [% / 100]					
Years	R1	R2	R3	R4	R5
2012	0.15	0.15	0.45	0.11	0.14
2013	0.13	0.29	0.09	0.10	0.39

2014	0.29	0.13	0.10	0.35	0.12
2015	0.15	0.11	0.43	0.16	0.16
2016	0.10	0.36	0.14	0.14	0.25

243

244

245 2.4 Uncertainty analysis

246 As stated in the IPCC 2006 guidelines and updated in 2019, the assessment of uncertainty is
 247 considered a major and crucial/mandatory component when compiling regional or national
 248 GHG emission inventories ([Larocque et al., 2008](#)). The difference in scale in which the model
 249 is used results in divergent errors of the C and N dynamics prediction across different climate
 250 zones and scales. Thus, uncertainty analysis is a crucial step towards a higher quality decision
 251 making process. The sources of uncertainty can vary and are related to a) the initial conditions
 252 (starting values), b) the drivers (e.g. climate and crop management data), c) the conceptual
 253 model uncertainty and d) the parameter uncertainty of the various processes ([Refsgaard et al.,](#)
 254 [2007](#); [Wang and Chen, 2012](#)).

255 [Santabárbara, \(2019\)](#) performed a Bayesian Model Calibration and Uncertainty Analysis using
 256 a Monte Carlo Markov Chain (MCMC) approach targeting uncertainties associated to the data
 257 (bulk density, SOC, pH, clay content) of the initial soil conditions, drivers (cropland
 258 management such as fertilization/manure rates & timing, harvest & seeding timing, tillage
 259 timing) and bio-geochemical process parameterizations.

260 In order to identify the most sensitive process parameters with a reduced number of model
 261 simulations, the Morris method ([Morris, 1991](#)) obtains a hierarchy of parameters influence on
 262 a given output (gaseous N fluxes) and evaluates whether a non-linearity exists or not. ([Morris,](#)
 263 [1991](#)) proposed that this order can be assessed through the statistical analysis of the changes
 264 in the model output, produced by the "one-step-at-a-time" changes in "n" number of proposed
 265 parameters. Incremental steps of each parameter range, lead to identifying which ones have
 266 substantial influences over the concerned results, without neglecting that some effects could

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267 cancel each other ([Saltelli et al., 2000](#)), leading to the identification of the 24 most sensitive
268 process parameters ([Houska et al., 2017](#); [Myrqiotis et al., 2018b](#)).

269

270 Metropolis – Hastings algorithm

271 The Markov Chain Monte Carlo (MCMC) Metropolis–Hastings algorithm results in numerous
272 parameter sets that approximate the posterior joint parameter distribution by performing a
273 random walk through the space of joint parameter values. This probability evaluation of the
274 data obtained from each step leads to the update of the initial uniform parameter distributions.
275 Bayes' formula relating conditional probabilities may become a powerful and practical
276 computational tool when combined with Markov chain processes and Monte Carlo methods,
277 so-called Markov Chain Monte Carlo (MCMC). A Markov chain is a special type of discrete
278 stochastic processes wherein the probability of an event depends only on the event that
279 immediately precedes it. Integrating parameters (θ) and observation data (D) into Bayes' rule
280 results in the formula:

281

$$P(\theta|D) = \frac{P(D|\theta) * P(\theta)}{P(D)} \quad 2.1$$

282 where $P(D|\theta)$, the probability of the data, is used to obtain the probability of these parameters
283 updated by the data: $P(\theta|D)$ where the evidence is computed as:

284

$$P(D) = \int \text{likelihood} \cdot \text{prior} \cdot d\theta \quad 2.2$$

285 where $P(D)$ can be numerically approximated with the aforementioned MCMC method ([Robert
286 and Casella, 2011](#)).

287 The method uses prior knowledge concerning the sources of the model uncertainty to obtain
288 a narrowed posterior distribution for each one of the sources. By propagating the parameter
289 distributions through the model, the overall uncertainty in the model results can be quantified.

290 [In a previous study by Santabárbara, \(2019\), an extensive sensitivity analysis on all soil bio-](#)
291 [geochemical process parameters, soil initial data and arable management data was performed](#)
292 [identifying the 24 most sensitive process parameters \(listed in supplementary material\), the](#)
293 [most sensitive soil initial data \(soil profile data on bulk density, soil organic carbon content, pH](#)
294 [value\) and the most sensitive management information \(fertilization and manure N rates, tilling](#)
295 [depth\) to aquatic and gaseous N fluxes from arable soils. This was digested in the MCMC](#)
296 [simulation sampling a combination of 24 parameter values, 3 values of soil initial data and 3](#)
297 [management information. The sampling of the soil initial data as well as the management data](#)
298 [was performed as perturbations to the existing data: For each quantity, a perturbation was](#)
299 [sampled individually and applied to all corresponding values in the soil profile or to all years in](#)
300 [the management description. The MCMC simulation performed by Santabárbara, \(2019\)](#)
301 [simulated more than 100 000 iterations for various arable sites until the MCMC simulation](#)
302 [converged towards a stable combined posterior distribution of parameter values and soil and](#)
303 [management input data perturbations.](#) In the current analysis, we have sampled 500 joint
304 parameter / input data perturbation sets from the posterior distributions as reported by
305 Santabárbara, (2019) and we deployed them in simulations (propagation through the model)
306 for the regional inventory leading to 500 inventory simulations. A statistical analysis was,
307 afterwards, applied to estimate the updated regional and temporal result distributions.

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309 2.5 Statistical methods and data aggregation

310 Regional result aggregation

311 One full regional inventory simulation consists of 10 individual inventory simulations: Five (5)
312 different crop rotations for irrigated and rain feed conditions were simulated in parallel (see
313 section 2.3). The results of the crop rotations were aggregated according to the crop shares
314 per year (see Table 2) accounting for all effects of the different crops cultivated in the region
315 for irrigated and rain feed conditions. The final inventory simulation results were obtained by
316 considering irrigated versus rain feed water management. The final inventory contains

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323 simulation results aggregated to area weighted yearly means across the total simulation
324 domain accounting for the cropland area of each polygon.

325

326 Uncertainty quantification and statistical analysis

327 A regional aggregation was performed for all 500 uncertainty simulations. All the uncertainty
328 results were finally reported via statistical measures evaluating the 500 regional uncertainty
329 simulation runs reporting mean values, standard deviation, medians and the 25 and 75
330 interquartile ranges (IQR, Q25 to Q75).

331

332 3 Results Analysis and Evaluation

333 The simulation time span was from 2009 to 2016, while the years 2009 – 2011 were used as
334 spin-up to get all soil C and N pools into equilibrium after the initialization. Therefore, reported
335 simulation results are limited to years 2012 - 2016. The assessment of the regional C and N
336 balances (CB and NB) were obtained - as a consequence of the uncertainty quantification -
337 resulting in distributions and therefore reported by statistical measures such as mean/median
338 or interquartile ranges of the uncertainty ensemble.

339

340 3.1 Regional yield simulations and validation

341 The evaluation of the model performance in estimating the NB and CB components was
342 analyzed based on the comparison of the simulated yield values with the observed yield data
343 provided by the Hellenic Statistical Authority (ELSTAT), averaged for the total simulated
344 period.

345

346 Crop yields and feed production

347 For model validation, datasets of crop yields from Hellenic Statistical Authority (ELSTAT) were
 348 used. [Table 3](#), summarizes the aggregated regional crop yields for all the simulated years and
 349 the respective mean, median and standard deviation values resulted from the statistical
 350 analysis of the simulation results together with the observed yield and feed production provided
 351 by the Hellenic Statistical Authority (ELSTAT). Simulated yields consist for cotton of the cotton
 352 bolls, clover feed is the total cutting and harvested above ground biomass, for wheat and barley
 353 is the grain yield and for maize is accounted grain ear and the stems. Based on the
 354 observations, maize appears to be the dominant crop with an average yield of 12 tons ha⁻¹,
 355 followed by clover product of 8.4 tons ha⁻¹. The rest of the three crop yields appear to be in the
 356 same order of magnitude from 3.3 up to 3.4 tons ha⁻¹.

hat gelöscht: Table 3

357

358 *Table 3. Simulated and observed yields and feed production [tons dry matter ha⁻¹] in the region of Thessaly. All*
 359 *results are based on statistical aggregation across all polygons, rotations, years and finally across all 500 UA*
 360 *inventory simulations. The observed values of dry matter (DM) are provided by the Hellenic Statistical Authority.*

Simulated crop yield and feed distributions [tons dry matter ha ⁻¹]				Observed [tons dry matter ha ⁻¹]
Crops	Median	Mean	standard deviation	Mean
Cotton	3.5	3.3	0.8	3.3
Clover	9.8	9.6	0.6	8.4
Wheat	3.9	3.6	0.9	3.4
Barley	4.7	4.5	1.0	3.3
Maize ¹⁾	10.2	9.9	1.4	12.0

361 ¹⁾ Observation data for maize did not distinguish between food corn and silage maize.

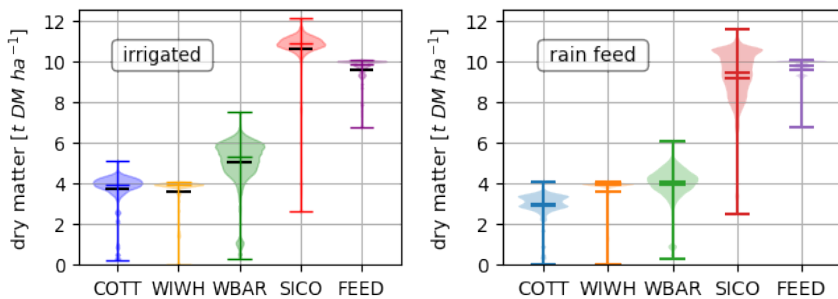
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363 Additionally, the simulated average yield of cotton was estimated to 3.3 ± 0.8 tons DM ha⁻¹,
 364 wheat to 3.6 ± 0.9 tons DM ha⁻¹, barley 4.5 ± 1 tons DM ha⁻¹, maize 9.9 ± 1.4 tons DM ha⁻¹. As
 365 for the feed, the clover was estimated to 9.6 ± 0.6 tons DM ha⁻¹. The average nitrogen use
 366 efficiency (NUE) across time and space is 63.29%.

367

369 [Figure 1](#), presents the uncertainties of the simulated crop yield across the whole evaluation
 370 time span 2012 -2016 both in irrigated and rain feed conditions. As shown, corn shows a much
 371 more narrow distribution with a higher median for the irrigated scenario compared to the rain
 372 feed while shows the same extreme value variations. To the contrary, winter barley has a wider
 373 distribution and slightly higher median for the irrigated scenario and, also, a wider extreme
 374 value variation. As for cotton, the distribution appears to be bimodal for the rain feed scenario
 375 in which the median is also lower than the one in the irrigated case. In addition, the extreme
 376 value variation is wider in the latter case. Finally, for the example of winter wheat irrigated and
 377 rain feed scenarios reach the same results.

378



379

380 *Figure 1. Simulated crop yield uncertainties across the evaluation time span 2012 - 2016 for irrigated and rain feed*
 381 *conditions. Horizontal lines indicate median, mean, maximum and minimum values of the distributions.*

382

383 3.2 Regional Carbon and Nitrogen Balance

384 Carbon Balance (CB)

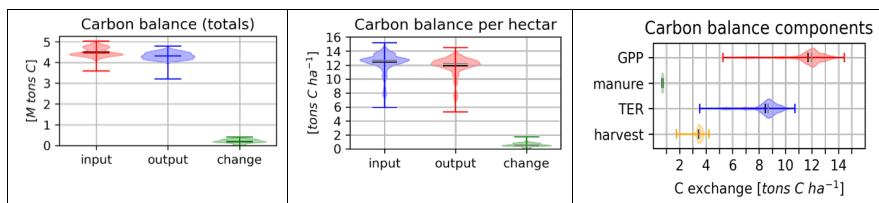
385 For the CB, [Figure 2](#), presents average C input fluxes into the soil of 12.4 ± 1.4 tons C ha⁻¹ yr⁻¹
 386 ¹ (with inter quartile ranges (IQR) from Q25 to Q75 of 12.1 to 13.2 tons C ha⁻¹ yr⁻¹) and output
 387 fluxes of 11.9 ± 1.3 tons C ha⁻¹ yr⁻¹ with IQR from 11.6 to 12.7 tons C ha⁻¹ yr⁻¹. The resulting
 388 carbon sequestration was estimated to 0.5 ± 0.3 tons C ha⁻¹ yr⁻¹ with IQR from 0.4 to 0.7 tons
 389 C ha⁻¹ yr⁻¹ (data summarized in [Table 4](#)).

hat gelöscht: Figure 1

hat gelöscht: Figure 2

hat gelöscht: Table 4

393



394 Figure 2. Carbon balance for cropland cultivation for the region of Thessaly: a) Total carbon balance of cropland
 395 soils in mio. tons C, b) averaged Carbon Balance in tons C ha⁻¹ and c) averaged fluxes across the region and the
 396 years 2012-2016. (Positive change equals soil C sequestration).

397

398 The input fluxes consist of annual gross primary productivity (GPP) of 11.7 ± 1.4 tons C ha⁻¹
 399 yr⁻¹ with IQR from 11.4 to 12.4 tons C ha⁻¹ yr⁻¹ and carbon applied to soils in manure estimated
 400 by 0.7 ± 0.001 tons C ha⁻¹ yr⁻¹ (see Table 4). This compares on the other hand to respirative
 401 carbon fluxes from the soil to the atmosphere (TER) of 8.5 ± 1.1 tons C ha⁻¹ yr⁻¹ with IQR from
 402 8.2 to 9.1 tons C ha⁻¹ yr⁻¹ and carbon fluxes via exported crop yields and feed (including all
 403 straws and removed crop residues) of 3.4 ± 0.3 tons C ha⁻¹ yr⁻¹ with IQR from 3.4 to 3.6 tons
 404 C ha⁻¹ yr⁻¹. The aggregation of the carbon fluxes to the regional level of approx. 360 000 ha of
 405 cropland results in 4.25 ± 0.20 M tons C yr⁻¹ by GPP, 0.25 ± 0.01 M tons C yr⁻¹ carbon influx
 406 via organic fertilizers compared to 3.08 ± 2.97 M t C yr⁻¹ TER and 1.24 ± 0.05 M t C yr⁻¹ carbon
 407 exports via crop yields and feed production leading to a net carbon sequestration of 0.5 ± 0.3
 408 M tons C ha⁻¹ yr⁻¹ with IQR from 0.4 to 0.7 M tons C ha⁻¹ yr⁻¹ (M tons C as Million tons carbon).
 409

hat gelöscht: Table 4

410 Table 4. **Carbon Balance** (per hectare) Assessment and Uncertainty Analysis of the of cropland cultivation at the
 411 region of Thessaly, Greece. ¹⁾ mean; ²⁾ standard deviation; ³⁾ median; Interquartile ranges: ⁴⁾ Q25: 25 quartile, ⁵⁾
 412 Q75: 75 quartile are applied across the 500 values for the quantities in this table; ⁶⁾ C-Inputs as the sum of the
 413 absolute values of all the input fluxes of the 500 simulations; ⁷⁾ C-Outputs as the sum of the absolute values of all
 414 the output fluxes of the 500 simulations; ⁸⁾ SOC-changes as the difference between the input and output fluxes of
 415 each of the 500 simulations.

	Mean ¹⁾	Std ²⁾	Median ³⁾	Q25 ⁴⁾	Q75 ⁵⁾
	[tons C ha ⁻¹ yr ⁻¹]	[tons C ha ⁻¹ yr ⁻¹]	[tons C ha ⁻¹ yr ⁻¹]	[tons C ha ⁻¹ yr ⁻¹]	[tons C ha ⁻¹ yr ⁻¹]
C-Inputs ⁶⁾	12.4	1.4	12.7	12.1	13.2

C-Outputs ⁷⁾	11.9	1.3	12.2	11.6	12.7
SOC-changes ⁸⁾	0.5	0.3	0.5	0.4	0.7
Input fluxes					
GPP	11.7	1.4	12.0	11.4	12.4
C in manure	0.7	0.0	0.7	0.7	0.7
Output fluxes					
TER	8.5	1.1	8.7	8.2	9.1
Biomass export	3.4	0.3	3.5	3.4	3.6

417

418 Nitrogen balance (NB)

419 In [Figure 3](#), the assessment of the distribution of the NB with the in- and out-fluxes is presented.

hat gelöscht: Figure 3

420 The averaged nitrogen influx (represented by the uncertainty ensemble mean) per hectare was

hat gelöscht:

421 estimated to $212.3 \pm 9.1 \text{ kg N ha}^{-1} \text{ yr}^{-1}$ with IQR from 203.3 to 220.0 $\text{kg N ha}^{-1} \text{ yr}^{-1}$ while nitrogen

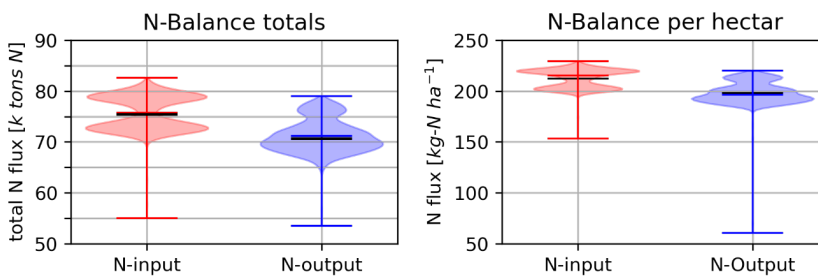
422 out-fluxes were estimated in average to $198.3 \pm 11.2 \text{ kg N ha}^{-1} \text{ yr}^{-1}$ with IQR from 191.4 to

423 $204.0 \text{ kg N ha}^{-1} \text{ yr}^{-1}$ ([Figure 3](#)) leading to a net N accumulation in the soil of $14.0 \pm 2.1 \text{ kg N ha}^{-1}$

hat gelöscht: Figure 3

424 yr^{-1} with IQR from 11.9 to 16.0 $\text{kg N ha}^{-1} \text{ yr}^{-1}$.

425



426

427 *Figure 3. Nitrogen balance for cropland cultivation for the region of Thessaly; a) Total NB in k-tons N and b)*
 428 *averaged NB in kg N ha^{-1} ; Data averaged for the years 2012-2016. Horizontal lines indicate mean (red), median*
 429 *and minimum and maximum of the distribution.*

430

434 Table 5. Nitrogen Balance (per hectare). Summary of the Assessment and Uncertainty Analysis of the **NB Fluxes**
 435 (per hectare) of cropland cultivation of the region of Thessaly, Greece. ¹⁾ N-Inputs as the sum of the absolute values
 436 of all input fluxes of the 500 simulations; ²⁾ N-Outputs as the sum of the absolute values of all the output fluxes of
 437 the 500 simulations; ³⁾ N-stock-changes as the difference between the input and output fluxes of each of the 500
 438 simulations; ⁴⁾ Gaseous emissions are the sum of N₂O, NO, N₂ and NH₃ fluxes; ⁵⁾ Aquatic flux is nitrate leaching
 439 (NO₃).

	Mean	Std	Median	Q25	Q75
	[kg N ha ⁻¹ yr ⁻¹]	[kg N ha ⁻¹ yr ⁻¹]	[kg N ha ⁻¹ yr ⁻¹]	[kg N ha ⁻¹ yr ⁻¹]	[kg N ha ⁻¹ yr ⁻¹]
N-Inputs ¹⁾	212.3	9.1	215.2	203.3	220.0
N-Outputs ²⁾	198.3	11.2	196.4	191.4	204.0
N-stock-changes ³⁾	13.8	2.1	13.7	14.5	12.5
Input fluxes					
N deposition	6.3	0.8	6.8	6.0	6.8
Bio. N fixation	45.6	4.3	45.7	43.7	47.7
N in min. fertilizer	80.2	4.8	81.3	76.6	82.7
N in organic fertilizer	80.2	3.6	80.9	77.5	82.7
Output fluxes					
Gaseous emissions ⁴⁾	55.4	8.8	55.1	48.9	61.6
N ₂ O	2.6	0.8	2.5	2.1	3.1
NO	3.2	1.5	2.9	2.0	4.1
N ₂	15.5	7.0	14.6	9.9	20.7
NH ₃	34.0	6.7	31.8	29.3	36.9
Aquatic fluxes ⁵⁾					
NO ₃ leaching	14.1	4.5	13.6	11.0	17.0

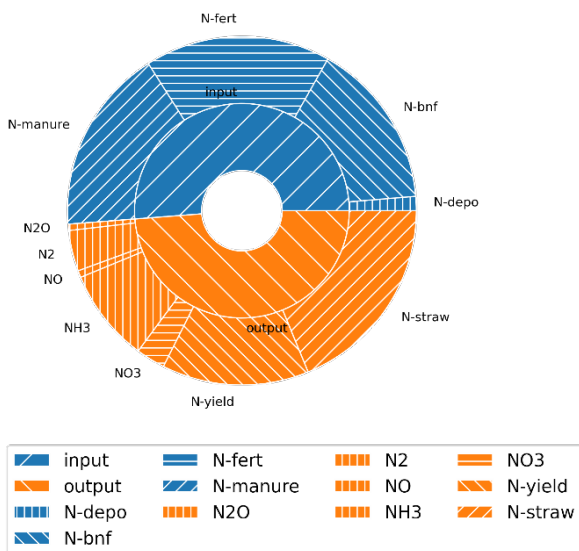
440
 441 The N influx was composed by the input of synthetic fertilizer of 80.2 ± 4.8 kg N ha⁻¹ yr⁻¹ (IQR
 442 76.6 to 82.7) and organic fertilizer of 80.2 ± 3.6 kg N ha⁻¹ yr⁻¹ (IQR from 77.5 to 82.7), followed
 443 by the biological nitrogen fixation (BNF) via legumes estimated as 45.6 ± 4.3 kg N ha⁻¹ yr⁻¹ (IQR
 444 from 43.7 to 47.7) and nitrogen deposition of 6.3 ± 0.8 kg N ha⁻¹ yr⁻¹ (IQR from 6.0 to 6.8). Thus,
 445 almost 75% of the nitrogen input influx is related to the fertilization (mineral and organic) whilst
 446 the minor part that corresponds to nitrogen fixation and deposition approximates to 25%.

447 The N outflux consist of gaseous N fluxes of $55.4 \pm 8.8 \text{ kg N ha}^{-1} \text{ yr}^{-1}$ (IQR from 48.9 to 61.6),
 448 aquatic N fluxes (only nitrate leaching into surface waters was considered) of $14.1 \pm 4.5 \text{ kg N}$
 449 $\text{ha}^{-1} \text{ yr}^{-1}$ (IQR from 11.0 to 17.0), N fluxes by removed N in yields, straw and feed of $128.8 \pm$
 450 $8.5 \text{ kg N ha}^{-1} \text{ yr}^{-1}$ (IQR of 125.2 to 131.7) (see [Figure 4](#), and [Table 5](#)). Based on the
 451 aforementioned results all gaseous and aquatic N-fluxes correspond to about 28% and 7% of
 452 the N output flux respectively, while the far largest N output flux was N removed in yields, straw
 453 and feed representing almost 65% of the N outflux ([Figure 4](#)).

hat gelöscht: Figure 4

hat gelöscht: Table 5

hat gelöscht: Figure 4



454

455 *Figure 4. Averaged annual nitrogen balance (inner ring of the pie diagram) and their decomposition into the various*
 456 *components of the N fluxes (outer ring of the pie diagram); (all data summarized in [Table 5](#)).*

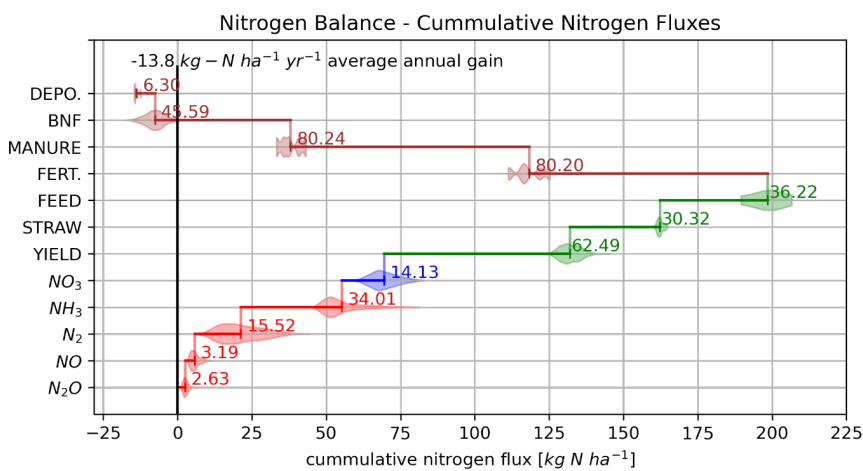
hat gelöscht: Table 5

457

458 The simulated gaseous fluxes were composed of N_2O emissions estimated to $2.6 \pm 0.8 \text{ kg}$
 459 $\text{N}_2\text{O-N ha}^{-1} \text{ yr}^{-1}$ (IQR from 2.1 to 3.1), NO emissions of $3.2 \pm 1.5 \text{ kg NO-N ha}^{-1} \text{ yr}^{-1}$ (IQR from
 460 2.0 to 4.1), N_2 emissions $15.5 \pm 7.0 \text{ kg N}_2\text{-N ha}^{-1} \text{ yr}^{-1}$ (IQR range from 9.9 to 20.7) and NH_3
 461 emissions of $34.0 \pm 6.7 \text{ kg NH}_3\text{-N ha}^{-1} \text{ yr}^{-1}$ (IQR from 29.3 to 36.9). Ammonia volatilization
 462 represents the largest share (61.48%) of gaseous N losses, with highest densities in the
 463 emission distribution between approx. 25 and 35 kg N ha^{-1} , followed by di-nitrogen losses

468 (28.03%) of gaseous N losses, with a much wider emission variability in the distribution,
 469 followed by NO_3 (5.79%) and N_2O (4.7%). [Figure 5](#) shows the overall NB in a waterfall diagram
 470 adding up cumulative all in- and out-fluxes illustrating the uncertainty distribution of each flux
 471 contributions. The waterfall diagram illustrates the overall outcome of the NB, a N accumulation
 472 into the soil as the difference between all out-fluxes minus all in-fluxes.
 473

hat gelöscht: Figure 5



474
 475 *Figure 5. Waterfall representation of the result distributions of the different Nitrogen in- and outfluxes of the cropland*
 476 *cultivation in Thessaly. Vertical lines in the distributions indicate mean values of the corresponding N-flux. Red*
 477 *colors indicate gaseous outfluxes, blue aquatic fluxes, green biomass yield and feed production outfluxes and brown*
 478 *color indicates N influxes such as synth. N-fertilizer, N-Manure, biological N fixation (BNF) and N deposition. The*
 479 *Resulting N sink of the Nitrogen Balance (based on distribution means) is $-13.8 \text{ kg N ha}^{-1} \text{ yr}^{-1}$. (Negative value*
 480 *indicates flux into the soil).*

481
 482 Nitrate leaching mean estimates were $14.1 \pm 4.5 \text{ kg NO}_3\text{-N ha}^{-1} \text{ yr}^{-1}$ (IQR from 11.0 to 17.0)
 483 with a bell-shaped distribution.
 484 Total yield and biomass (straw and feed) N export fluxes were $62.4 \pm 4.4 \text{ kg N ha}^{-1} \text{ yr}^{-1}$ with
 485 uncertainty ranges from 59.9 to 65.1 consisting of yield N exports (grains and cotton balls) of
 486 $30.3 \pm 1.7 \text{ kg N ha}^{-1} \text{ yr}^{-1}$ (IQR from 29.6 to 30.9) and for straw and feed N exports of 36.1 ± 6.0
 487 $\text{kg N ha}^{-1} \text{ yr}^{-1}$ (IQR from 34.9 to 37.6). The result distributions for yield N are well bell shaped,

489 for feed biomass N very moderate bell shaped and well distributed within the bounds and for
 490 straw N very sharp within a comparable small interval.

491 [Figure 5](#), illustrates the cumulative nitrogen fluxes composing the NB as a waterfall diagram
 492 considering the mean of each component. The NB results in a net N sink of 13.8 kg N ha⁻¹ yr⁻¹
 493 ¹ (see result distribution in [Figure 6](#)) for the region corresponding to an annual carbon
 494 sequestration of approx. 0.5 tons C ha⁻¹ yr⁻¹ as depicted in [Figure 2](#), b) (see also the annual
 495 dynamics of the topsoil (30 cm) soil organic carbon and nitrogen distributions in [Figure 8](#)).

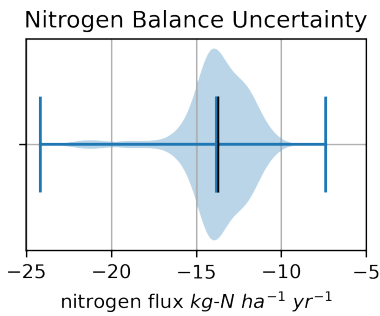
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496



497

498 *Figure 6. Distribution of the overall Nitrogen Balance of the cropland cultivation in Thessaly: Statistical analysis*
 499 *across all 500 individual NB results of the inventory simulations (mean 13.8 kg N ha⁻¹ yr⁻¹, median 13.7 kg N ha⁻¹*
 500 *yr⁻¹) corresponding to the Carbon balance in [Figure 2](#).*

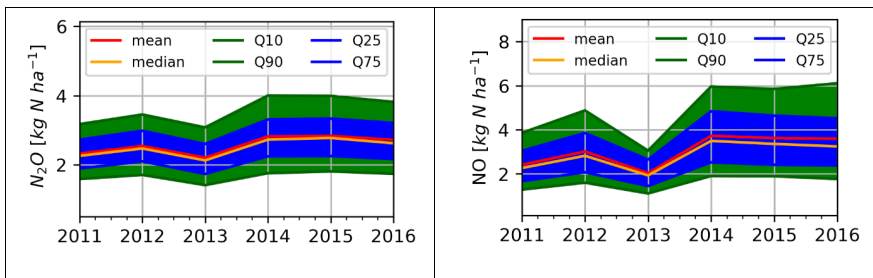
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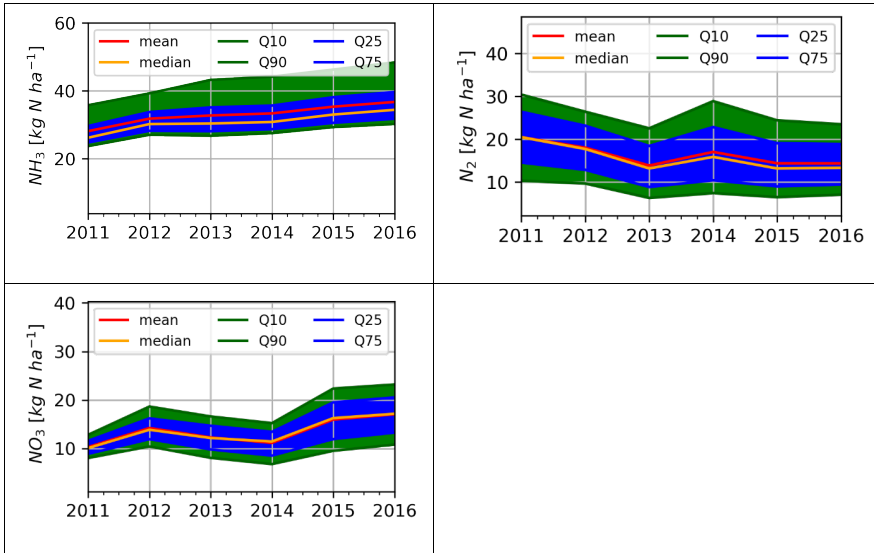
501

502 [Figure 7](#), and [Figure 8](#), show the dynamics of the annual distribution of the gaseous and aquatic
 503 outfluxes as well as the dynamics of the annual distributions of the top soil (30 cm) soil organic
 504 carbon and nitrogen pools for the evaluation period 2011 – 2016.

hat gelöscht: Figure 7

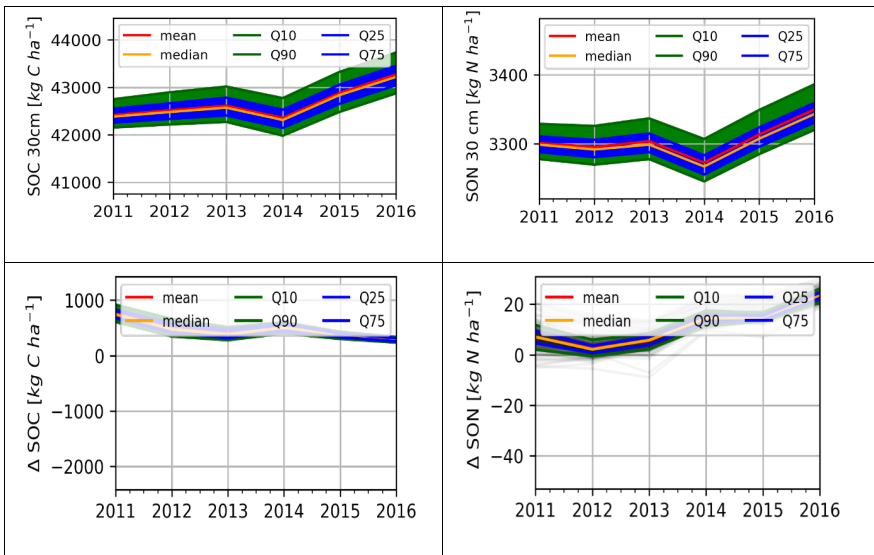
hat gelöscht: Figure 8





512 Figure 7. Annual dynamics of the uncertainty distributions of the gaseous (subfigure a) to d) and aquatic (subfigure
 513 e)) N outfluxes 2011 – 2016. Uncertainty bandwidth (blue band) defined as the range between the q25 and the q75
 514 quartile, green band (Q10. to Q90 interval) indicating the variance of the fluxes neglecting the outliers of the
 515 distribution.

516



517 Figure 8. Annual dynamics of the uncertainty distributions of the soil carbon (subfigure a)) and soil organic nitrogen
518 (subfigure b)) and the corresponding dynamics of the uncertainty distributions of the annual change rates of the
519 total soil carbon and nitrogen pools (subfigures c) and d)) respectively.

520 4 Discussion.

521 In this study, [following the recommendation of Grosz et al., \(2023\)](#), an assessment of the
522 [combined](#) full C and N balance of a regional cropland agroecosystem is reported for the first
523 time using inventory simulations with a process-based ecosystem model. [The additional](#)
524 [quantification of the associated modelling uncertainty of the balance simulations increase the](#)
525 [trustworthiness of the study.](#)

526 Up to present, process-based modelling studies mainly focus on single site applications e.g.
527 Daycent: [\(del Grosso et al., 2005; Gurung et al., 2020\)](#), APSIM: [\(Vogeler et al., 2013\)](#), CERES-
528 EGC: [\(Dambreville et al., 2008; Gabrielle et al., 2006; Heinen, 2006; Hénault et al., 2005\)](#),
529 CERES-Wheat: [\(Mavromatis, 2016\)](#), DNDC: [\(Li, 2000\)](#), LandscapeDNDC: [\(Haas et al., 2013;](#)
530 [Klatt et al., 2015a; Molina-Herrera et al., 2016; Zhang et al., 2015\)](#). Fewer studies deploy
531 models on the regional to national [\(del Grosso et al., 2005; Kim et al., 2015; Klatt et al., 2015a\)](#)
532 or continental to global scale [\(del Grosso et al., 2009; Franke et al., 2020; Jägermeyr et al.,](#)
533 [2021; Smerald et al., 2022; Thompson et al., 2019\)](#). All of these studies [are subject to criticism](#)
534 [stated by Grosz et al., \(2023\) as they are reporting](#), in general [only](#) one specific or a few
535 components of the carbon or nitrogen cycle such as e.g. soil carbon stocks or N₂O emissions,
536 [lacking any information on the full C and N balance.](#)

537 There are [only a](#) very few cases where an attempt for regional estimation of the NB has been
538 made. [The study reported by Schroeck et al., \(2019\) is the only previous attempt fulfilling the](#)
539 [requirements of Grosz et al., \(2023\) in reporting](#), the [full](#) NB for a large alpine watershed in the
540 Austrian Alps characterized by arable production in the low-lying areas and grassland in the
541 mountains [using a process based model](#). In addition, [Lee et al., \(2020\)](#) tried to estimate
542 nitrogen balances in Switzerland alternating the cropping systems or management practices.
543 There were, also, cases where the regional NB was estimated with the use of nitrogen balance
544 equations [\(He et al., 2018\)](#). [Recently, Zistl-Schlingmann et al., \(2020\) assessed the full N](#)
545 [balance of alpine grasslands using the ¹⁵N stable isotope techniques.](#)

hat gelöscht: Simulating the N and C budgets is helpful for the understanding/explanation of the pattern how nutrients are being supplied from the soil to crop as well as the pathways of the excess gaseous and aquatic excess nitrogen fluxes. In this way, improvements on the agricultural practices e.g. N fertilization strategy could be accomplished to sustain agricultural output and minimize environmental harm.

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558 In order to achieve a more concrete and complete analysis of the CB and NB that could be
 559 used for future policy development, an uncertainty analysis is considered as
 560 necessary/mandatory. The IPCC guidelines demand for UNFCCC reporting the uncertainty
 561 quantification of any reported inventory study (IPCC Updated guidelines 2019). Recent
 562 publications have reported the deployment of different methods to assess and quantify the
 563 various sources of uncertainty in ecosystem modelling. (Klatt et al., 2015b) published a study
 564 on the impact of parameter uncertainty on N₂O emissions and NO₃ leaching on the regional
 565 scale. (Houska et al., 2017) deployed the GLUE method (Generalized Likelihood Uncertainty
 566 Estimation) for the LandscapeDNDC model on a grassland site, other studies such as
 567 (Lehuger et al., 2009a; Li et al., 2015; Myrgiotis et al., 2018a) used the Bayesian Model
 568 Calibration and Uncertainty Assessment approach, which has been used in the current study
 569 as well.

571 4.1 Yield and feed Production

572 LandscapeDNDC was validated in a study by Molina-Herrera et al., (2016) on cropland and
 573 grassland sites across Europe reporting good agreement in reproducing observed above
 574 ground biomass and yield estimates. Similar model performance for the cultivation of
 575 commodity crops was reported by (Kasper et al., 2019; Klatt et al., 2015a; Molina-Herrera et
 576 al., 2017; R. J. Petersen et al., 2021).
 577 Voloudakis et al., (2015) simulated cotton production in seven different areas of Greece
 578 applying the AquaCrop. Iyra and Loukas, (2021) used REPIC model to estimate the crop
 579 growth/yield production of several crops in the Basin of Almyros, Thessaly. The simulated
 580 results were approximately 11 tons ha⁻¹ clover, 3.3/3.5 tons ha⁻¹ cereals/wheat, 3.8 tons ha⁻¹
 581 cotton and 9 tons ha⁻¹ maize, being well compared to the results of our research shown in
 582 Table 3. The simulated results presented in our study are in line with the results by Voloudakis
 583 et al., (2015) simulating cotton production in seven different areas of Greece applying the
 584 AquaCrop model. Similar results were reported by (Tsakmakis et al., 2019).

- hat gelöscht:** s
- hat gelöscht:** A number of studies including crop yields estimates under different environmental conditions and crop management options have been published.
- hat gelöscht:** reported validation results deploying LandscapeDNDC
- hat gelöscht:** . The study reported
- hat gelöscht:** leading to a high trustworthiness of model results
- hat formatiert:** Schriftfarbe: Rot, Durchgestrichen
- hat gelöscht:** model for future climate scenarios. The model was calibrated and the
- hat gelöscht:** results were validated with data sets acquired for years 2006 and 2005/2007 respectively from a site experiment conducted in the area of Karditsa, Thessaly. The observed and simulated results presented in the study were well matched and in line with the results Voloudakis et al., (2015) simulated cotton production in seven different areas of Greece applying the AquaCrop presented in our study
- hat gelöscht:** with averaged yields of 3.65 tons ha⁻¹ (mean 3.3 tons ha⁻¹ and median 3.5 tons ha⁻¹). ¶
- Formatiert:** Tabstopps: Nicht an 1.11 cm + 1.43 cm
- hat gelöscht:** the
- hat gelöscht:** current
- hat gelöscht:** Table 3
- hat gelöscht:** ¶
- hat gelöscht:** The application of AquaCrop in the cotton cultivation of the research of Tsakmakis et al., (2019)., proved the accurate estimation of the cotton yield when using the default set of parameters in both
- hat gelöscht:** cases of growing degree days (GDD) and calendar days (CD) modes for a site in Northern Greece. For the year of 2015 the harvested seed cotton yield was 3.974 tons ha⁻¹ ± 0.45 and 3.35 tons ha⁻¹ ± 0.397 in 2016 with a slight overestimation of 0.018 tons ha⁻¹ and 0.026 tons ha⁻¹ while in 2016 there
- hat gelöscht:** was a marginal underestimation by 0.06 tons ha⁻¹ and 0.046 tons ha⁻¹ for the respective aforementioned cases. The model did not perform well when the parameter sets were altered based on other studies (García-Vila et al., 2009).
- hat formatiert:** Schriftfarbe: Schwarz, Englisch (Vereinigtes Königreich)

625 There are few cases in literature concerning yield simulations on a European level. Based on
626 the yield datasets of FAO and EUROSTAT, [Ciais et al., \(2010a\)](#) estimated mean crop yields
627 for the period 1990–1999 at the scale of EU-25 as 6.1 (FAO) and 5.3 (EUROSTAT) tons DM
628 $\text{ha}^{-1} \text{yr}^{-1}$, respectively, which corresponds well to results of our study. [Haas et al., \(2022\)](#)
629 estimated with a model ensemble mean for crop yields for EU-27 of 4.41 ± 1.85 tons DM ha^{-1}
630 yr^{-1} for the period 1990–1999. [Lugato et al., \(2018\)](#) estimated cropland yield projections of
631 4.34 tons DM $\text{ha}^{-1} \text{yr}^{-1}$ (mean), ranging from 3.69 to 4.90 tons DM $\text{ha}^{-1} \text{yr}^{-1}$ with the DayCent
632 model for EU-27, comparable to the 6.18 tons DM $\text{ha}^{-1} \text{yr}^{-1}$ average simulated crop yields of
633 this study. The simulated yields in the current study vary from 3.3 to 9.9 tons DM $\text{ha}^{-1} \text{yr}^{-1}$ for
634 the cases of cotton and maize respectively.

635 Higher yield estimates for the region of Thessaly in this study are certainly due to the inclusion
636 of the legume feed crops in the rotations. This argument is supported by a recent meta-analysis
637 by [Lu, 2020](#) that concluded that on average yield increases of 5.0 to 25% can be expected
638 for various conditions if residues are completely returned to the field as compared to no-residue
639 return systems. Similar results were reported by [Fuchs et al., \(2020\)](#) and [Barneze et al., \(2020\)](#).
640 [Following the recommendations of Grosz et al., \(2023\), our study has reported transparently](#)
641 [all major C & N fluxes for the region as being simulated by the model. In our study, we have](#)
642 [not calibrated the model against any observations, therefore all simulation results will be](#)
643 [discussed versus other modelling results available. As up to now, there is only one comparable](#)
644 [modelling study available in literature reporting and discussing the total N balance of a site or](#)
645 [region, which we have used to compare our N balance against.](#)

646

647 [4.2](#) Carbon and Nitrogen Balance:

648 [Full N balance](#)

649 [At present, the studies of Schroeck et al., \(2019\) and Lee et al., \(2020\) are the only to be found](#)
650 [by Web of Science under the search key words “nitrogen AND balance AND process AND](#)
651 [based AND modelling” reporting a compilation of the nitrogen balance and all associated N](#)

652 [fluxes for a site or region applying a process-based ecosystem model as demanded by Gosz](#)
653 [et al \(2023\).](#)

654 [Leip et al., \(2011\)](#) reported the first nitrogen balance for Europe following a mixed approach
655 [combining the CAPRI \(Common Agricultural Policy Regionalised Impact\) model \(a global](#)
656 [economic model for agriculture\) with different approaches estimating various nitrogen fluxes](#)
657 [in arable land cultivation, but the approach lacks the explicit quantification of the different](#)
658 [gaseous N fluxes. The study of Schroeck et al., \(2019\) overcame this hurdle and applied the](#)
659 [process-based ecosystem model LandscapeDNDC to estimate the full regional nitrogen](#)
660 [budgets including all fluxes of different ecosystems \(cropland, grassland and pastures\) and](#)
661 [climatic zones of a water shed in Austria. That has been the first attempt estimating and](#)
662 [reporting all the N fluxes possible as demanded by Gosz et al \(2023\).](#)

663 [The N balance estimate in Schroeck et al., \(2019\) for a catchment in Austria and the N balance](#)
664 [reported in our study compares very well despite the inherent differences in land management](#)
665 [and N inputs. As highlighted by Grosz et al., \(2023\), such intercomparisons demonstrate the](#)
666 [different model behaviours when applied to different ecosystem. In our study, we see the](#)
667 [partitioning of the N outfluxes from our arable system in similar shares as reported by Schroeck](#)
668 [et al., \(2019\) for the arable land.](#)

669 [The N₂O estimate in Schroeck et al., \(2019\) and the current study is of a comparable level. We](#)
670 [estimated N₂O emissions of 2.6 kg N ha⁻¹ yr⁻¹ while Schroeck et al., \(2019\) reports 1.51 kg N](#)
671 [ha⁻¹ yr⁻¹, about 40% lower. The NO fluxes differ significantly since we reported a mean value](#)
672 [of 3.2 kg NO-N ha⁻¹ yr⁻¹ while Schroeck et al., \(2019\) reports 0.08 kg NO-N ha⁻¹ yr⁻¹. This is](#)
673 [on one hand related to some recent model advances, which have been made during this study,](#)
674 [which elevated the NO production in LandscapeDNDC \(Molina-Herrera et al., 2017\) and on](#)
675 [the other hand due to the high share of organic N fertilization in our study fostering NO](#)
676 [emissions. Ammonia volatilization differs substantially between the two studies, while our study](#)
677 [reports 34 kg NH₃-N ha⁻¹ yr⁻¹, Schroeck et al., \(2019\) reported moderate emissions of 0.23 kg](#)
678 [NH₃-N ha⁻¹ yr⁻¹. The strong NH₃ volatilization in our study is mostly driven by the high pH-](#)
679 [values of the soils in the region of Thessaly \(pH values from 6.5 to 8.2 with a considerable](#)

680 [spatial variation, Greek Soil Map, 2015](#)) and the comparable high manure inputs into the arable
681 [system in our study, while in the research of Schroeck et al., \(2019\)](#) the manure was preferably
682 [applied only to the grassland systems and mineral fertilizers to the arable land. Concerning](#)
683 [the NO₃, Schroeck et al., \(2019\)](#) reported 45.3 kg NO₃-N ha⁻¹ yr⁻¹ which was 3 times higher
684 [compared to this study \(14.1 kg N ha⁻¹ yr⁻¹\) considering the N-input of approximately 160 kg](#)
685 [and 212.3 kg N ha⁻¹ yr⁻¹ respectively. Even though 50 % of the arable land in our study was](#)
686 [irrigated, the resulting water percolation rates in our study were by far lower than the](#)
687 [percolation simulated in the study of Schroeck et al., \(2019\) as the Austrian pre-alpine](#)
688 [catchment received nearly double annual precipitation.](#)

689 [The N balance modelling study of Lee et al., \(2020\)](#) was estimating for Switzerland a national
690 [cropland N balance using an upscaling method based on process-based site simulations with](#)
691 [the DayCent model differentiating the management of the considered cropping systems e.g.](#)
692 [fertilizer rates, tillage or land cover change. The study reported for conventional cultivations](#)
693 [\(averaged across 20 years\) yield related N outfluxes accounting for about 60%, NO₃ leaching](#)
694 [36.1% and gaseous N emissions 4.1% of the total N outputs. Lee et al., \(2020\)](#) did not report
695 [the different gaseous N fluxes, even though the DayCent model must have simulated all of](#)
696 [them. Although the yield related N outflux is in accordance with our result of 64.95% there](#)
697 [seems to be a discrepancy in the reported gaseous and aquatic N fluxes contribution, as we](#)
698 [report 27.94% for gaseous and 7.11% for NO₃ leaching in our study. As demanded by Gosz](#)
699 [et al \(2023\) we can elaborate different preferences in simulated N outflux partitioning \(36%](#)
700 [NO₃ and 4% gaseous losses for DayCent versus 7% NO₃ and 28% gaseous losses for](#)
701 [LandscapeDNDC\) due to the different simulation models, regionalization and upscaling](#)
702 [approaches as well as due to the different soil, climatic and management conditions included](#)
703 [in the respective studies.](#)

704 [Velthof et al., \(2009\)](#) used the MITTERA-EUROPE model/method, based on the concoction of
705 [GAINS and CAPRI models, to estimate N fluxes of European soils on NUTS2 scale with the](#)
706 [use of European datasets and literature coefficients, where the fertilizer application and](#)
707 [management was similar to our methodology. The average N Input-Output balance was](#)

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708 [calculated as 117 kg N ha⁻¹ yr⁻¹ composed by manure of 49 kg N ha⁻¹ yr⁻¹, synthetic fertilizer of](#)
709 [58 kg N ha⁻¹ yr⁻¹ \(in the current study for both cases 80.2 kg N ha⁻¹ yr⁻¹\), biological nitrogen](#)
710 [fixation of 2 kg N ha⁻¹ yr⁻¹ \(our research 45.6 kg N ha⁻¹ yr⁻¹\) and N deposition of 7 kg N ha⁻¹](#)
711 [\(current study 6.3 kg N ha⁻¹ yr⁻¹\). In contrast to our study the reported output fluxes for NH₃ of](#)
712 [8 kg NH₃-N ha⁻¹ yr⁻¹, N₂O of 2 kg N₂O-N ha⁻¹ yr⁻¹, NO_x of 2 kg NO_x-N ha⁻¹ yr⁻¹, N₂ of 51 kg N₂-N](#)
713 [ha⁻¹ yr⁻¹ and NO₃ leaching of 7 kg NO₃-N ha⁻¹ yr⁻¹ while the differences with the results presented](#)
714 [in our study are NH₃ of 34.0 kg NH₃-N ha⁻¹ yr⁻¹, N₂O of 2.6 kg N₂O-N ha⁻¹ yr⁻¹, NO_x of 3.2 kg](#)
715 [NO_x-N ha⁻¹ yr⁻¹, N₂ of 15.5 kg N₂-N ha⁻¹ yr⁻¹ and NO₃ leaching of 14.1 kg NO₃-N ha⁻¹ yr⁻¹.](#)
716 [Additionally, the yield output is estimated as 48 kg N ha⁻¹ yr⁻¹. Again, we see a different](#)
717 [preference in N outflux partitioning towards large shares in gaseous N fluxes versus small NO₃](#)
718 [leaching shares and the difference with the results presented in our study are related to the](#)
719 [different input data used for initialization and driving of the model, based on regional statistics](#)
720 [and the use of a biogeochemical model versus emission factor approaches.](#)
721 [He et al., \(2018\) assessed the soil N balance for a time span between 1984 to 2014 based on](#)
722 [the N budget equations \(N input – N output\) using multiple coefficients from literature in order](#)
723 [to estimate the nitrogen input and output fluxes of six grouped regions in China. The used](#)
724 [datasets were acquired from national Authorities and include cropping land and yields,](#)
725 [synthetic fertilizers, animal heads, soil types etc. The N synthetic fertilizer input is in average](#)
726 [182.4 kg N ha⁻¹ and the organic fertilizer of 97.3 kg N ha⁻¹, N fixation is estimated as 16.8 kg](#)
727 [N ha⁻¹ and the atmospheric deposition as 22 kg N ha⁻¹. Almost half of the total averaged N](#)
728 [output losses, 48.9%, was attributed to crop uptake while the respective gaseous losses were](#)
729 [N₂ 19.9%, volatilized NH₃ 17.3%, N₂O 1.2% and NO 0.7%. As for the NO₃ leaching share was](#)
730 [5.8% of the total output N fluxes. These reported N outflux proportions comparable well to our](#)
731 [study. The differences in the N uptake data remain and are mainly due to the differences in](#)
732 [the crops and management.](#)
733 [As reported in OECD \(OECD, 2020\) the net averaged nitrogen balance of the area of our study](#)
734 [is 11.6 kg N ha⁻¹ yr⁻¹ input to the soil which corresponds very well to the simulated mean](#)
735 [nitrogen balance as an in-flux of 13.8 kg N ha⁻¹ yr⁻¹ \(IQR 11.9 to 16.0\) into the soil.](#)

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736 [So far, the discussion of the presented N balance and N out fluxes compares well to most of](#)
737 [the available studies reporting N balances while one modelling study report different N outflux](#)
738 [partitioning between gaseous and NO₃ leaching fluxes. For more detailed intercomparison on](#)
739 [the overall quality of our C and N fluxes we aim to compare our results versus various studies](#)
740 [addressing individual components of the C and N balance and associated fluxes.](#)

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741 **SOC stocks**

hat gelöscht: ¶

742 [Haas et al., \(2022\)](#) reported results of a European inventory simulation of soil carbon stocks
743 and N₂O emissions using a model ensemble. The study deployed in a baseline simulation
744 across EU-27 a similar residues management as compared to our study resulting in very stable
745 carbon stock dynamics over a long period (1950-2100). In this study, the estimated carbon
746 sequestration of 0.5 (UA mean and median) ± 0.3 tons C ha⁻¹ yr⁻¹ is mainly caused by the
747 inclusion of legume feed crops within the crop rotation leading to increased litter production
748 and C input into the soil ([Barneze et al., 2020](#); [Fuchs et al., 2020](#); [K. Petersen et al., 2021](#)).
749 [Haas et al., \(2022\)](#) reported a management scenario with 100% of crop litter remaining on the
750 field leading to averaged C-sequestration rates of over 1 ton C ha⁻¹ yr⁻¹ across EU-27. As the
751 residues management in this study is between the baseline and buried scenario of [Haas et al.,](#)
752 [\(2022\)](#), our results compare well to results reported in this study.

753 Other [modelling](#) studies such as ([Lugato et al., 2014](#)) reported C sequestration rates for the
754 conversion of cropland into grassland ranging between 0.4 and 0.8 tons C ha⁻¹ yr⁻¹. [Lugato et](#)
755 [al., \(2014\)](#) reported averaged SOC change rates for a cereal straw incorporation scenario for
756 EU-27 of 0.1 tons C ha⁻¹ yr⁻¹ (estimates from 2000 to 2020).

757 [The SOC dynamics reported in this study show a stable carbon dynamic in the soil within the](#)
758 [simulation time span \(2009 - 2014\) with only three years of model spin-up. The initialization of](#)
759 [the various carbon pools with the SOC data from the soil database is balanced by the average](#)
760 [litter production of the deployed crop rotations. The SOC increase in 2015 and 2016 is due to](#)
761 [climatic conditions and higher litter inputs simulated by the model.](#)

hat gelöscht: The Mediterranean agroecosystems show a winter/summer rainfall and soil cover variation,

hat gelöscht: spatial diversity, and the longest continuous settlement and dense cultivation by man (Yaalon, 1997). Based on the Greek National Map of SOC (2020) by Triantakonstantis and Detsikas, (2021), SOC values for the region of Thessaly vary from 22.95 to 86.97 tons ha⁻¹ with the lower values in the main plain

hat gelöscht: of the region and higher values in the croplands closer to the mountainous areas. Comparing these maps with SOC map of the 30cm topsoil of our story, we clearly see similar patterns, which relate to the similarity of SOC data used to initialize the region in LandscapeDND. C.

778 N₂O emissions

779 This study reported estimates of N₂O emissions of 2.6 ± 0.8 kg N₂O-N ha⁻¹ yr⁻¹ (IQR from 2.1
780 to 3.1) for a mixed crop / legume feed crop rotation, which were well above the estimates
781 resulting from IPCC Tier I direct emission factors. IPCC would lead to 1.6 kg N₂O-N ha⁻¹ yr⁻¹
782 when applying 30pprox.. 160 kg N ha⁻¹ yr⁻¹. The higher N₂O emission strength of the modelling
783 is likely to result from emission peaks after irrigation due to low anaerobicity (Grosz et al.,
784 2023; Janz et al., 2022). Cayuela et al., (2017), conducted a meta-analysis of the direct N₂O
785 emissions for a number of cropping systems for the Mediterranean climate where the emission
786 factors (Efs) were altered under different fertilization and irrigation conditions. Higher
787 fertilization rates led to higher Efs (0.82% less than the 1% of IPCC). Additionally, irrigated and
788 intensively cultivated crops had higher Efs than rainfed (up to 0.91% dependent on the
789 irrigation method). The relatively high EF of maize in this study could be possibly attributed to
790 the irrigation without the application of water-saving methods and the on average higher N
791 application rates.

792 The LandscapedNDC validation study of Molina-Herrera et al., (2016) reported for the Italian
793 site Borgo Cioffi (Mediterranean climate, Ranucci et al., (2011) annual N₂O emissions of 2.49
794 kg N₂O-N ha⁻¹ yr⁻¹ while two sites in southern France showed annual N₂O emissions from 0.52
795 to 3.34 kg N₂O-N ha⁻¹ yr⁻¹. N₂O emission estimates of our study were higher than results
796 reported by Haas et al., (2022) using a multi model ensemble estimating average soil N₂O
797 emissions from European (EU-27) cropping systems for the period 1980–1999 of 1.46 ± 1.30
798 kg N₂O-N ha⁻¹ yr⁻¹ under conventional (*Baseline*) management and comparable average N
799 input. Klatt et al., (2015a) reported for an inventory (Saxony, Germany) mean N₂O emission
800 of 1.43 ± 1.25 kg N₂O-N ha⁻¹ yr⁻¹.

801 Overall, the reported N₂O flux component of our study compares well to the findings
802 reported in literature. As criticised by Grosz et al. (2023), many studies only focus on the
803 performance of the models in simulating N₂O emissions and the models were even
804 calibrated for this purpose. Without reporting all the other N fluxes from the models, this

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hat formatiert: Schriftfarbe: Schwarz, Englisch
(Vereinigtes Königreich)

hat verschoben (Einfügung) [1]

hat gelöscht: (

hat formatiert: Schriftfarbe: Schwarz, Englisch
(Vereinigtes Königreich)

hat gelöscht:

hat gelöscht: (Cayuela et al., 2017)

hat gelöscht: ¶ ... [1]

hat gelöscht: Leip et al., (2011)

hat gelöscht: applied the DNDC–Europe model across
EU-25 reporting averaged N₂O emissions of 1.8 kg
N₂O-N ha⁻¹ yr⁻¹, while on basis of UNFCC reporting and
a fuzzy logic model

hat gelöscht: Ciais et al., (2010b)

hat gelöscht: estimated average N₂O emissions from
EU-27 croplands at 1.46 ± 0.22 kg N₂O-N ha⁻¹ yr⁻¹. ¶

hat gelöscht: using a very similar uncertainty
quantification approach...

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821 [focusing and calibration for only one quantity can easily lead to inaccuracies for other](#)
822 [components of the N cycle as they may not be checked for consistency anymore.](#)
823 [Janz et al., \(2022\)](#)[Janz et al., \(2022\)](#),
824 Nitrate leaching

825 This study reported average NO₃ leaching fluxes (only nitrate leaching into surface waters) of
826 14.1 ± 4.5 kg NO₃-N ha⁻¹ yr⁻¹. [Reported nitrate leaching observations for the region or Greece](#)
827 [could not be found in literature](#) estimated the NO₃ leaching with the use of four different models
828 [with varying values from 5 to 40 kg NO₃-N ha⁻¹ yr⁻¹ for the area of our study. These high values](#)
829 [could be explained by the fact that it corresponds both to groundwater and runoff.](#) [Molina-](#)
830 [Herrera et al., \(2016\)](#) reported for the LandscapeDNDC validation study cropland nitrate
831 leaching fluxes of approx. 7 to 88 kg NO₃-N ha⁻¹ yr⁻¹. In addition, in the research of [Molina-](#)
832 [Herrera et al., \(2017\)](#) the described NO₃ leaching results varied from 13 to 8 kg NO₃-N ha⁻¹ yr⁻¹
833 ¹ [showing higher values in regards to the precipitation and fertigation. The most comparable](#)
834 [site Borgo Cioffi resulted in a comparable annual NO₃ leaching flux of 18.62 kg NO₃-N ha⁻¹ yr⁻¹](#)
835 ¹ [Klatt et al., \(2015b\)](#) reported in an uncertainty assessment for a regional inventory (Saxony,
836 Germany) leaching rates of 29.32 ± 9.97 kg NO₃-N ha⁻¹ yr⁻¹ for a wheat-barley-rapeseed
837 rotation simulated by the LandscapeDNDC model. The agricultural system and management
838 regime is comparable; higher NO₃ leaching rates were most likely due to high N fertilization
839 rates [in combination](#) with higher annual precipitation in the region leading to more intense
840 percolation and therefore to stronger leaching of available NO₃ while in our study the
841 fertilization regime was more lean, such that soil nutrient competition was higher and available
842 nitrate was more likely to be immobilized by plant uptake. [Myrgiotis et al., \(2019\)](#) reported in a
843 [similar assessment NO₃ leaching factor \(LF\) mean for their region of 14% \(±7 %\), in](#)
844 [comparison we report mean NO₃ leaching factor of 7%.](#)
845
846

hat nach oben verschoben [1]: Cayuela et al., (2017) conducted a meta-analysis of the direct N₂O emissions for a number of cropping systems for the Mediterranean climate where the emission factors (EFs) were altered under different fertilization and irrigation conditions. Higher fertilization rates led to higher EFs (0.82% less than the 1% of IPCC). Additionally, irrigated and intensively cultivated crops had higher EFs than rainfed (up to 0.91% dependent on the irrigation method). The relatively high EF of maize in this study could be possibly attributed to the irrigation without the application of water-saving methods and the on average higher N application rates (Cayuela et al., 2017). ¶

hat gelöscht: As discussed by

hat gelöscht: Haas et al., (2022)

hat gelöscht: and

hat gelöscht: Janz et al., (2022)

hat gelöscht: , increased N₂O emissions can be seen after the addition of crop residues and may be attributed to a stimulation of denitrification activity by the added substrate and the creation of anaerobic microsites by increased soil respiration. ¶

Arable land cultivation in Thessaly does not experience strong winter frost and severe soil freezing such that N₂O freeze-thaw emissions as

hat gelöscht: reported by Wagner-Riddle et al., (2017) or del Grosso et al., (2022) do not play any role in the N budget.

hat gelöscht: ¶

The N₂O estimations related to livestock presented in the study of Sidropoulos and Tsilingiridis, (2009) va

hat gelöscht: ried in a range of 0.74 to 4.33 kt N₂O, with an average of 2.84 kt N₂O depended on the average values of emission factors used (for the year 2005). The estimates were based on the emission factors of IPCC guidelines and the number of animal heads were derived from the data sets acquired fr... [2]

hat gelöscht: Cayuela et al., (2017)

hat gelöscht: (Cayuela et al., 2017)

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hat verschoben (Einfügung) [2]

hat gelöscht: . de Vries et al., (2011)

hat gelöscht:

hat gelöscht: reported

hat gelöscht: from 2009 to 2012

hat gelöscht: .

hat nach oben verschoben [2]: de Vries et al., (2011) estimated the NO₃ leaching with the use of four different

hat gelöscht: de Vries et al., (2011)

hat gelöscht: er

hat gelöscht: (up to 150 kg N) compared

hat gelöscht: (up to average of 80 kg N input)

hat gelöscht: ¶

912 NO emissions

913 In the current study, the model estimated NO emissions were in average 3.2 ± 1.5 kg NO-N
914 $\text{ha}^{-1} \text{yr}^{-1}$. [Butterbach-Bahl et al., \(2009\)](#) performed the very first European inventory of soil NO
915 emissions using a modified version of DNDC reporting low NO emission rates mostly below 2
916 kg NO-N $\text{ha}^{-1} \text{yr}^{-1}$. [Molina-Herrera et al., \(2017\)](#) recently reported a full NO emission inventory
917 for the State of Saxony Germany compiling annual NO emissions from agricultural soils
918 ranging from 0.19 to 6.7 kg NO-N $\text{ha}^{-1} \text{yr}^{-1}$ simulated by LandscapeDNDC. The study reported
919 the model performance on simulating soil NO emissions on more than 20 different sites. The
920 study of [Schroeck et al., \(2019\)](#) reported for a regional inventory of arable soils in Austria
921 simulated by LandscapeDNDC annual NO emissions of 1.0–1.5 kg NO-N ha^{-1} (for the year
922 2000), while empirical approaches such as [Stehfest and Bouwman, \(2006\)](#) estimated emission
923 of similar magnitude. [Zhang et al., \(2015\)](#) reported in a model inter-comparison and validation
924 study of NO and N₂O fluxes including three ecosystem models, consistent simulation results
925 for the LandscapeDNDC model with NO emission strengths of cropland soils were between 1
926 and 3 kg NO-N $\text{ha}^{-1} \text{yr}^{-1}$ across the sites.

927

928 NH₃ emissions

929 [Schroeck et al., \(2019\)](#) stated that validation studies of NH₃ volatilization for any
930 biogeochemical model were very rarely reported in literature, mainly due to the complexity and
931 a lack of flux observations at spatial and temporal high resolution.

932 In our study [we estimate](#) soil NH₃ emissions of 34.0 ± 6.7 kg NH₃-N $\text{ha}^{-1} \text{yr}^{-1}$. High NH₃
933 volatilization and emission rates can be explained by the predominating neutral to basal soils
934 conditions (pH values of 7 and above) in the study region favouring the Henry NH₄/NH₃
935 equilibrium towards higher NH₃ gases enabling ammonia to diffuse out of the soil into the free
936 atmosphere.

hat gelöscht: the assessment of

938 The IPCC emission factor (EF) method for NH₃ volatilization reports estimates of 20% of N
939 input into the soil to be volatilized as NH₃. For our study, IPCC methodology for NH₃ would
940 lead to 32 kg NH₃-N ha⁻¹ yr⁻¹, which is well in line with the simulated result.

941 Sidiropoulos and Tsilingiridis, (2009) estimated a national livestock originated NH₃ emission
942 corresponding to approx. 22 kg ha⁻¹ yr⁻¹ for the region of Thessaly.

943 There is a number of national NH₃ inventories which could be considered detailed and well-
944 studied like the ones in Denmark, Netherlands, Europe, UK and US. In Denmark, (Geels et al.,
945 2012) used the DAMOS model to estimate the Danish NH₃ emissions (crop, grass and manure
946 manipulation) where the values ranged in the 5 regions under study from a very small quantity
947 to 17.4 kg NH₃-N ha⁻¹ yr⁻¹.

948 As discussed by Sutton et al., (2013) the majority of the NH₃ emissions come as a result of the
949 agricultural production and are considerably impacted by climate influence. In the case of NH₃
950 volatilization, it could almost double every 5°C temperature given certain complex
951 thermodynamics dissociation and solubility, whilst soil NH₃ emission is influenced by the
952 available water quantity allowing the NH_x dissolution and use by microbial organisms, which is
953 afterwards leading to decomposition.

954
955

956 4.3 Uncertainty Analysis and Quantification

957 Santabárbara, (2019) used the MCMC algorithm to estimate the joint parameter distribution of
958 the fundamental bio-geochemical process parameters in LandscapeDNDC when simulation
959 soil C and N fluxes. Propagating these joint parameter distributions through the model (by
960 sampling 500 joint parameter distributions and performing inventory simulations with each
961 parameter set with the model) for estimating the regional C and N fluxes was leading to various
962 distributions for any model result on the regional scale. Statistical analysis calculating mean,
963 median as well as the interquartile range (Q25 to Q75) determines best estimates and the
964 uncertainty range of any model output on the regional scale, demonstrating the superiority of

- hat gelöscht: 16 ...2 kg NH₃-N ha⁻¹ yr⁻¹, which is approximately half the emission strength of the...e (... [3])
- hat gelöscht: value of about 40 kt NH₃ yr⁻¹ of the t (... [4])
- hat gelöscht: Ramanantenasoa et al., (2018)
- hat gelöscht: compared two methods (... [5])
- hat gelöscht: . In the case of the Netherlands
- hat gelöscht: (Velthof et al., 2012)
- hat gelöscht: , a method was applied based on the (... [6])
- hat gelöscht: de Vries et al., (2011)
- hat gelöscht: used four N budget models of varyin (... [7])
- hat gelöscht: Full N balance ¶ (... [8])
- hat gelöscht: Schroeck et al., (2019)
- hat gelöscht: and
- hat gelöscht: Lee et al., (2020)
- hat gelöscht: are the only to be found by Web (... [9])
- hat gelöscht: Leip et al., (2011)
- hat gelöscht: reported the first nitrogen balan (... [10])
- hat gelöscht: Schroeck et al., (2019)
- hat gelöscht: overcame this hurdle and applie (... [11])
- hat gelöscht: Ogle and Paustian, (2005)
- hat gelöscht: .¶ (... [12])
- hat gelöscht: Schroeck et al., (2019)
- hat gelöscht: and the current study is of a (... [13])
- hat gelöscht: Schroeck et al., (2019)
- hat gelöscht: reports 1.51 kg N ha⁻¹ yr⁻¹ lower (... [14])
- hat gelöscht: Schroeck et al., (2019)
- hat gelöscht: reports 0.08 kg NO-N ha⁻¹ yr⁻¹. (... [15])
- hat gelöscht: Molina-Herrera et al., 2017
- hat gelöscht:). Ammonia volatilization differs, (... [16])
- hat gelöscht: Schroeck et al., (2019)
- hat gelöscht: moderate emissions of 0.23 kg h (... [17])
- hat gelöscht: Schroeck et al., (2019)
- hat gelöscht: the manure was preferably appli (... [18])
- hat gelöscht: Lee et al., (2020)
- hat gelöscht: is estimating for Switzerland a n (... [19])
- hat gelöscht: Velthof et al., (2009)
- hat gelöscht: used the MITTERA-EUROPE (... [20])
- hat gelöscht: He et al., (2018)
- hat gelöscht: assessed the soil N balance for (... [21])
- hat gelöscht: Myrriotis et al., (2019)
- hat gelöscht: reported a N₂O emission factor (... [22])
- hat gelöscht: (OECD Nutrient Balance, 2020)
- hat gelöscht: the averaged nitrogen input rate (... [23])
- hat gelöscht: T...he MCMC algorithm to was use (... [25])
- hat formatiert (... [24])

1424 the method for assessing any ecosystem response by modelling instead of reporting single
1425 results. This is a novel approach, that to our knowledge has not been reported before in
1426 literature for the [full](#) carbon and nitrogen balance and neither been applied to regional
1427 simulations by any process-based model.

1428 In this study, the estimated UA mean and median of the carbon sequestration of 0.5 ± 0.3 tons
1429 $C\ ha^{-1}\ yr^{-1}$ is associated with an uncertainty range from 0.4 to 0.7 tons $C\ ha^{-1}\ yr^{-1}$ which
1430 compares well to the spatial uncertainty of C-sequestration in the study of [Haas et al., \(2022\)](#).

1431 The approach used in this study enabled to assess the carbon and nitrogen balance of the
1432 [Lehuger et al., \(2009b\)](#) used the Bayesian calibration method for the enhancement of the
1433 CERES-EGC model parameterization (reduction of the apriori parameter distribution) as well
1434 as quantification of the uncertainty of the simulated N_2O emissions in different sites. The
1435 estimated fluxes of the different sites resulted in a range between 0.088 to 3.672 $kg\ N_2O-N\ ha^{-1}\ yr^{-1}$
1436 with values for the q05 quantile of 0.066 to 0.115 $kg\ N_2O-N\ ha^{-1}\ yr^{-1}$ and for the Q95
1437 quantile from 1.676 to 5.874 $kg\ N_2O-N\ ha^{-1}\ yr^{-1}$ with an averaged value of 1.04 $kg\ N_2O-N\ ha^{-1}\ yr^{-1}$
1438 which is lower than the result of the current study but still in the same order of magnitude.

1439 [Klatt et al., \(2015b\)](#) quantified a parameter-induced uncertainty analysis on the regional scale
1440 applying the [same process](#) model for simulating N_2O emission and NO_3 leaching inventories
1441 similar to our study. The region was represented by 4000 polygons of arable land (state of
1442 Saxony, Germany) for crop rotations of barley, wheat and rapeseed [while climatic conditions](#)

1443 [differ](#). The results of [Klatt et al., \(2015b\)](#) display a likelihood range of 50% (the IQR range
1444 between Q25 and Q75) for N_2O emissions from 0.46 to 2.05 $kg\ N_2O-N\ ha^{-1}\ yr^{-1}$ which is in

1445 good comparison to our results of 2.1 to 3.1 $kg\ N_2O-N\ ha^{-1}\ yr^{-1}$. The average N_2O emissions
1446 are 1.43 $kg\ N_2O-N\ ha^{-1}\ yr^{-1}$ comparable to the result of our study (mean: 2.6 and median: 2.5
1447 $kg\ N_2O-N\ ha^{-1}\ yr^{-1}$ across approx. 1000 polygons). As for leached NO_3 , [Klatt et al., \(2015b\)](#)
1448 reported leaching rates of mean value: 29 $kg\ NO_3-N\ ha^{-1}\ yr^{-1}$, (IQR from 24.5 to 36.0), which
1449 is higher compared to the results of our study: Mean: 14.1 $kg\ NO_3-N\ ha^{-1}\ yr^{-1}$, median: 13.6
1450 $kg\ NO_3-N\ ha^{-1}\ yr^{-1}$ (IQR from 11 to 17). [Despite the difference in climatic and soil conditions,](#)

hat gelöscht: cropland ecosystems including an assessment of the prediction uncertainty. [¶](#)
[van Oijen et al., \(2005\)](#)

hat gelöscht: used the Bayesian calibration method to acquire the parameter posterior probability distribution to sample from, for simulation of the model results.

hat gelöscht: LandscapeDNDC

hat gelöscht: The investigated model parameter related uncertainties give a high confidence for the parameter use in our research.

hat gelöscht: direct

1462 [both uncertainty analysis studies reported similar regional estimates and uncertainty ranges](#)
1463 [for N₂O emissions and NO₃ leaching.](#)
1464 [Butterbach-Bahl et al., \(2022\)](#) reported the influence of management uncertainties for
1465 compiling national inventories of CH₄ and N₂O emission from various rice cultivation systems
1466 in Vietnam. The study applied a sampling technique varying model input data within a given
1467 range and [analysing](#) the influence on the assessed CH₄ and N₂O emission strengths. As the
1468 underlying cropland systems were fundamentally different, the assessed uncertainty ranges
1469 were comparable and the study is supporting our approach to focus on reporting uncertainty
1470 ranges rather than single values.

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hat gelöscht: analyzing

1471 5 Conclusion

1472 In this research, we presented for the first time a regional inventory of the full carbon and
1473 nitrogen balance including all sub-components of these fluxes simulated by a process-based
1474 model. Additionally, the study has fulfilled the demand to report always the associated
1475 uncertainties for any modelling results being published in literature. This supports the
1476 trustworthiness of the reported results [for](#) the C and N balances.

hat gelöscht: The current study postulates a novel approach to report regional scale C and N fluxes from process-based models to become the standard reporting method fulfilling the long-time demanded reporting requirements of the IPCC (IPCC Guidelines and IPCC 2019 updates on Guidelines). Additionally, instead of focusing only on topics limited to soil carbon stocks dynamics or greenhouse gas emissions, we propose the report of the full C and N balance including all components of the various fluxes e.g. gaseous and/or aquatic being available by the individual process-based models. This constitutes an effective method to assess the environmental impact of the crop production on a national scale, therefore optimize the farming practices, and suggest possible solution for sustainable agriculture development. ¶

1477 [Comparing the modelled N balance with a similar approach modelling the full N balance with](#)
1478 [all associated fluxes for a catchment in pre-alpine Austria leads to the conclusion, that](#)
1479 [especially the partitioning the N outflux into the different N flux components is more inherent](#)
1480 [to the LandscapeDNDC model itself used in both studies than induced by the two very different](#)
1481 [agricultural and climatical systems. Nevertheless, specific N outfluxes between the two studies](#)
1482 [show large differences \(e.g. NH₃ volatilization\), which is purely caused by model processes](#)
1483 [due to different soil PH values. Comparing to a less granular and detailed study of the N](#)
1484 [balance for Switzerland gives a first impressions of the differences to be expected in modelling](#)
1485 [the arable N balance with various different models. The discussion of such results will become](#)

hat gelöscht: . The LandscapeDNDC model is applied in the region of Thessaly after using the MCMC Bayesian calibration method against soil, daily climatic and crop management regional datasets. The main scope/goal was the assessment of the total C and N balance that enhance the efforts towards the understanding of the cropland system and the respective interactions with

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hat gelöscht: Observed GHG emission datasets are scarce if not unavailable. Thus, the modelled yield results were evaluated/validated against the observed values of crop yields provided by the Hellenic Statistical Authority and showed a good fit for almost all simulated crops except for the case of maize where there was a slight underestimation.

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1522 [more lively and maybe controversial as soon as more comparable studies using different](#)
1523 [models become available.](#)

1524 In addition, a full uncertainty analysis is presented based on the Metropolis-Hastings algorithm
1525 where a parameter subset and input data [perturbation](#) was sampled and simulated, resulting in
1526 [various probability density functions \(PDF\)](#) for each one of the N and C balance fluxes building
1527 a full uncertainty analysis of the modelled results. This helps to build trustworthiness in
1528 modelling assessments and estimates [of the balances as well as of the model behaviour.](#)

1529 [As demanded by the nitrogen modelling community,](#) all of the above constitute the novelty of
1530 the conducted research that could be [seen as a prototype to analyse and report N cycling in](#)
1531 [agro-ecosystems in the future.](#)

hat gelöscht: e

hat gelöscht: in 500 iterations

hat gelöscht: a final

hat gelöscht: A

hat gelöscht: further elaborated by a number of proposed mitigation measures, which could help in the abatement of the GHG emissions and N fluxes from crop/agricultural land.

1533 6 Acknowledgements

1534 The author Odysseas Sifounakis received a Ph.D. research scholarship from Alexandros S.
1535 Onassis Public Benefit Foundation, Greece, part of which is the research presented in the
1536 current publication.

1537

1538 7 Code/Data availability

1539 The LandscapeDNDC model source code is available via Butterbach-Bahl, Klaus; Grote,
1540 Rüdiger; Haas, Edwin; et al. (2021): LandscapeDNDC (v1.30.4). Karlsruhe Institute of
1541 Technology (KIT). DOI: 10.35097/438

1542 All publication results (tables and data for figures) will be made available in the supplementary
1543 material associated with this paper.

1544

1545

1554 8 Author contributions

1555 Mr. Odysseas Sifounakis has conceived and designed the analysis and collected the data. He,
1556 also, performed the analysis and wrote the paper.

1557 Dr. Edwin Haas conducted research and wrote the paper.

1558 Prof. Dr. Klaus Butterbach-Bahl substantially contributed to research planning, manuscript
1559 writing and editing and, also, provided funding opportunities.

1560 Prof. Dr. Maria P. Papadopoulou substantially contributed to research planning, manuscript
1561 writing and editing, and provided funding opportunities.

1562

1563 9 Competing interests

1564 All authors have reviewed and accepted the submitted version and declare no conflicts of
1565 interest related to this publication.

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1931 11 Appendix

1932 11.1 Material and Methods

1933 **Sensitivity Index**

1934 In the first step, the Sensitivity Index algorithm (SI) (Pannell, 1997) was calculated for all
1935 process parameters by splitting the parameter ranges into 10 equidistant values from minimum
1936 to maximum and by rating SI values:

1937
$$SI = \frac{CUM_{max} - CUM_{min}}{CUM_{max}}$$

1938 where CUM_{max} and CUM_{min} are the maximum and minimum cumulative results of 10
1939 simulations. High SI values explain a high sensitivity of the underlying parameter with respect
1940 to the model results, whereas low values or even zero indicates low or no sensitivity.

1941

1942 11.2 Results

1943 *Table A 1. Observed yield rates in the region of Thessaly. Cotton yields are the cotton bolls, clover feed is the total*
1944 *harvested above ground biomass, for wheat and barley it is the grain yield, maize is accounted grain ear and the*
1945 *stems Source ELSTAT.*

Crop Yields [tons dry matter ha ⁻¹]						
Crops	2012	2013	2014	2015	2016	Mean
Cotton	2.7	3.6	3.5	3.4	3.3	3.3
Clover	8.6	8.9	8.7	7.9	7.7	8.4
Wheat	3.3	3.3	3.3	3.7	3.6	3.4
Barley	3.2	3.2	3.2	3.5	3.5	3.3
Maize	10.9	12.1	12.3	12.7	12.1	12.0

1946

1947 *Table A 2. Crop rotation scenarios (R1 – R5) for the region of Thessaly where the crop abbreviations corn, wiwh,*
1948 *perg, cott and wbar refer to maize, winter wheat, clover (legume feed crops s.a. alfalfa or vetch), cotton and winter*
1949 *barley respectively.*

years	R1	R2	R3	R4	R5
2010	corn	wiwh	perg	cott	wbar
2011	wiwh	perg	cott	wbar	corn
2012	perg	cott	wbar	corn	wiwh
2013	cott	wbar	corn	wiwh	perg

2014	wbar	corn	wiwh	perg	cott
2015	corn	wiwh	perg	cott	wbar
2016	wiwh	perg	cott	wbar	corn

1950

1951 *Table A 3. Carbon Balance (totals) Summary of the Assessment and Uncertainty Analysis of the of cropland*
 1952 *cultivation of the region of Thessaly, Greece, GPP gross primary productivity, TER terrestrial ecosystem respiration,*
 1953 *Biomass export includes all C in yield, straw and feed exported from the fields, 360000 ha cropland.*

	Mean	Std	Median	Q25	Q75
	[mio. tons C yr ⁻¹]	[mio. tons C yr ⁻¹]	[mio. tons C yr ⁻¹]	[mio. tons C yr ⁻¹]	[mio. tons C yr ⁻¹]
C-Inputs	4.51	0.20	4.45	4.36	4.69
C-Outputs	4.32	0.17	4.31	4.19	4.45
SOC-changes	0.19	0.11	0.20	0.14	0.27
Input fluxes					
GPP	4.25	0.20	4.21	4.11	4.42
C in manure	0.25	0.01	0.26	0.25	0.26
Output fluxes					
TER	3.08	0.16	3.06	2.97	3.20
Biomass export	1.24	0.05	1.24	1.21	1.27

1954

1955 *Table A 4 Nitrogen balance (totals) Summary of the Assessment and Uncertainty Analysis of the total Nitrogen*
 1956 *Balance of cropland cultivation of the region of Thessaly, Greece.*

	Mean	Std	Median	Q25	Q75
	[kt-N yr ⁻¹]	[kt-N yr ⁻¹]	[kt-N yr ⁻¹]	[kt-N yr ⁻¹]	[kt-N yr ⁻¹]
N-Inputs	76.5	3.2	77.8	73.3	79.1
N-Outputs	71.7	3.2	71.2	69.4	73.7
N-stock-changes	4.8	0.0	6.6	3.9	5.4
Input fluxes					
N deposition	2.0	0.3	2.1	1.9	2.1
Bio. N fixation	16.7	1.6	16.7	15.9	17.5
N in min. fertilizer	28.9	1.7	29.3	27.6	29.8
N in organic fertilizer	28.9	1.3	29.2	27.9	29.8

Output fluxes					
Gaseous emissions ¹⁾	21.2	3.1	21.1	18.9	23.4
N ₂ O	0.9	0.3	0.9	0.7	1.1
NO	1.1	0.5	1.0	0.7	1.4
N ₂	4.9	2.4	4.5	2.9	6.6
NH ₃	14.3	2.6	13.5	12.5	15.6
Aquatic fluxes²⁾					
NO ₃ leaching	3.9	1.3	3.8	3.0	4.7

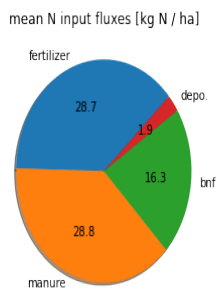
1957 1) Gaseous emissions are the sum of N₂O, NO, N₂ and NH₃ fluxes; 2) Aquatic flux is nitrate leaching (NO₃-)

1958

1959 Table A 5. Total crop yields per cultivar and year.

Crop Yields [tons dry matter]						
Crops	2012	2013	2014	2015	2016	Mean
Cotton	303 676.9	374 424.6	359 806.7	322 292.0	285 780.3	329 196.1
Clover	302 753.2	319 401.7	338 134.6	341 938.4	360 693.9	332 584.4
Wheat	477 700.7	461 875.5	395 902.1	430 014.4	450 254.3	443 149.4
Barley	84 520.8	99 091.8	139 402.9	139 990.8	102 454.7	113 092.2
Maize	332 531.6	431 324.6	377 783.9	351 285.4	334 277.7	365 440.6

1960



1961

1962 Figure 9. Shares of components of the annual nitrogen in- and output fluxes.

1963

1964 Table A 6. Simulated crop yields per cultivar and year for the irrigated land.

Crop Yields [tons dry matter ha ⁻¹]

Crops	Median	Mean	STD
Cotton	4.0	3.7	0.9
Clover	9.8	9.6	0.6
Wheat	3.9	3.6	0.9
Barley	5.3	5.0	1.2
Maize	10.9	10.6	1.3

1965

1966 *Table A 7. Simulated crop yields per cultivar and year for the rain feed land.*

Crop Yields [tons dry matter ha ⁻¹]			
Crops	Median	Mean	STD
Cotton	3.0	2.9	0.7
Clover	9.8	9.6	0.6
Wheat	3.9	3.6	0.9
Barley	4.0	3.9	0.9
Maize	9.5	9.2	1.5

1967

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Seite 33: [5] hat gelöscht Haas, Edwin 17.07.23 16:42:00



Seite 33: [6] hat gelöscht Haas, Edwin 17.07.23 16:44:00



Seite 33: [7] hat gelöscht Haas, Edwin 17.07.23 16:44:00



Seite 33: [8] hat gelöscht Haas, Edwin 17.07.23 14:07:00

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Schriftfarbe: Schwarz, Englisch (Vereinigtes Königreich)

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Seite 33: [25] hat gelöscht Haas, Edwin 17.07.23 16:45:00

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