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Additional Information

1 Improving the modelling and understanding of carbon-nitrogen- 2 water interactions in a semiarid Mediterranean oak forest

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9 Highlights

10 It is important to include carbon measurements in the calibration process

11 The nitrogen plant uptake of additional species may be significant

12 A fixed annual potential uptake may not be appropriate due to seasonality

13 TETIS-CN is an acceptable tool to reproduce the hydrology and biogeochemistry

14 Abstract

15 Mediterranean drylands are often nutrient poor, but parameter requirements of forest
16 ecosystem models are usually high. Therefore, there is a need for developing
17 parsimonious nutrients models. In that sense, this study aims to contribute to a better
18 understanding and modelling of the hydrological and biogeochemical (carbon and
19 nitrogen) cycles and their interactions in semiarid conditions and to test the capability of
20 a new parsimonious model to satisfactorily reproduce them. The proposed model
21 (TETIS-CN) and two additional widely used models were implemented in a *Quercus ilex*
22 forest, and no noteworthy differences were found. Results suggest that: (1) it is important
23 to include carbon observations in the calibration process and to consider all the existing
24 vegetation species in the simulation; (2) a fixed daily potential uptake may not be
25 appropriate to reproduce plant nitrogen uptake; and (3) TETIS-CN, with a lower number
26 of parameters, proved an acceptable tool.

27 **Keywords**

28 Carbon; Nitrogen; Water; Plant-soil interactions; Mediterranean drylands; Quercus ilex

29 **1 Introduction**

30 Precipitation and temperature are the main drivers of ecosystem structure and function,
31 controlling forest stand structure, ecosystem distribution patterns and net primary
32 production at a continental scale (Newman et al., 2006). However, at smaller geographic
33 scales, nutrient availability becomes a limiting factor in many ecosystems (Lozano-
34 García et al., 2016; Newman et al., 2006) and, consequently, ecosystem structure and
35 function usually change along a topographical soil properties gradient (Tateno et al.,
36 2017).

37 Soils in Mediterranean drylands, are often nutrient poor and, as water content is highly
38 variable, nutrient availability is a frequent limiting factor for their ecosystem development
39 (Sardans and Rodà, 2004). In fact, as net primary production responds to water and
40 nutrient addition (Lü et al., 2018; Sardans and Peñuelas, 2013), in semiarid ecosystems
41 it is difficult to know if vegetation growth is controlled by water, nutrient availability or both
42 (Botter et al., 2008). For this reason, models including nutrient cycling are useful tools
43 which allow the analysis of the relationships and behaviour of these ecosystems
44 (Landsberg, 2003), especially in these Mediterranean ecosystems, which stand out in
45 climate change projections as areas where warmer and drier conditions are predicted,
46 leading to more severe and recurrent droughts (Spinoni et al., 2018). Since most of the
47 annual nutrient requirements are supplied from the decomposition of soil organic matter
48 (Aponte et al., 2010) and plant competition increases in resource-limited environments
49 (Calama et al., 2019), changes in forest ecosystem function are expected because of
50 alterations in water, carbon and nitrogen cycles (Dong et al., 2019). Nevertheless, there
51 is a need to develop and test simple nutrient models (Blanco et al., 2005; Zhang et al.,
52 2013).

53 Nitrogen is one of these limiting nutrients in Mediterranean ecosystems, for both
54 photosynthetic capacity and growth (Sardans et al., 2008; Uscola et al., 2017) and,
55 consequently, a better knowledge of its storage and cycling is crucial. However, nitrogen
56 availability is markedly linked to the microbial activity because mineral nitrogen is the
57 result of the microbial decomposition of organic matter, which is also influenced by the
58 C:N ratio of this organic matter (Gleeson et al., 2016; Lucas-Borja et al., 2019; Pastor
59 and Post, 1986). Hence, the carbon and nitrogen cycles are inextricably intertwined,
60 which means that nitrogen models should also include the carbon cycle for a proper
61 modelling. Additionally, soil water content and temperature are the main environmental
62 factors influencing these biogeochemical cycles (Manzoni et al., 2004; Rodrigo et al.,
63 1997), especially in water-limited ecosystems (Wang et al., 2017), where significant
64 interactions between microorganisms and water availability exist (Porporato et al., 2015).
65 A clear example are the wetting and drying cycles, a common characteristic in arid and
66 semiarid climates. This process leads to a fast rewetting in the short term after
67 precipitation stimulating microbial activity, which speeds up decomposition and, as a
68 result, nutrient release (Lado-Monserrat et al., 2014). Thus, daily resolution models with
69 a combined analysis of the water, carbon and nitrogen cycles are necessary for the
70 complete understanding of these terrestrial ecosystems (D'Odorico et al., 2004).
71 Hence, in this article, a new parsimonious model and two existing models of different
72 conceptualization, complexity and purpose, which include the water, carbon and nitrogen
73 cycles, were calibrated using the experimental data recorded in a *Quercus ilex* (holm
74 oak) experimental site under a semiarid climate. The first model is the physically-based
75 model BIOME-BGCMuSo v5.0 (Hidy et al., 2016), which is the modified version of the
76 well-known BIOME-BGC model (Thornton et al., 2002), widely used in natural
77 ecosystems, with an accurate description of the water, carbon and nitrogen cycles and
78 vegetation growth (Chen and Xiao, 2019; Chiesi et al., 2007; Fontes et al., 2010). The
79 second one is the LEACHM model (Hutson, 2003) which is a process-based model
80 developed to simulate water and solute transport in unsaturated or partially saturated

81 agricultural soils and broadly used in agriculture to simulate the nitrogen cycle (Asada et
82 al., 2013; Jung et al., 2010; Wöhling et al., 2013). These two models have been chosen
83 because both include the groundwater transpiration process, necessary in this case
84 study, and particularly, because BIOME-BGCMuSo v5.0 is able to accurately represent
85 tree responses to environmental conditions and LEACHM has an accurate description
86 of soil hydrological and biogeochemical processes. However, these models have high
87 parameter requirements, and consequently it can be challenging to use them in most
88 situations, mainly because the available information is usually limited. Therefore, the
89 third model is a new parsimonious carbon and nitrogen sub-model which has been
90 coupled to the existing conceptual eco-hydrological model TETIS (Pasquato et al., 2015;
91 Ruiz-Pérez et al., 2016) and named TETIS-CN. Parameter requirements of forest
92 ecosystems models, which commonly include nutrient cycles, is usually high (Härkönen
93 et al., 2019), leading to a cumbersome calibration and frequently, to high computational
94 time due to their complex structure (Jin et al., 2016). Consequently, there is a need of
95 developing parsimonious models under the principle that everything should be made as
96 simple as possible, but not simpler (Stocker et al., 2016).

97 Within this framework, this study aims to contribute to a better understanding and
98 modelling of the hydrological and biogeochemical (carbon and nitrogen) cycles and their
99 interactions within the soil-plant continuum in semiarid conditions, and also to test the
100 capability of TETIS-CN to satisfactorily reproduce them.

101 **2 Material and methods**

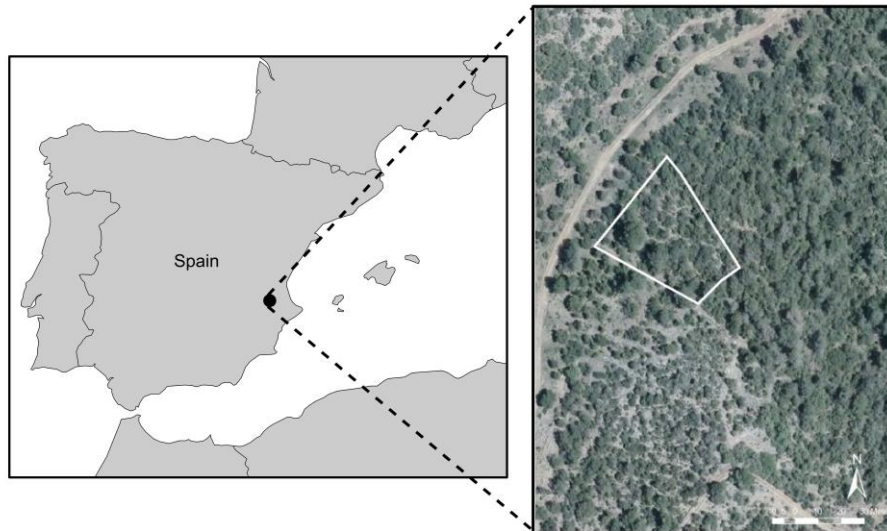
102 2.1 Study area

103 The study area (Fig. 1) is an experimental fenced plot covering 1800 m² located in the
104 public forest *La Hunde*, in east Spain (39°04'29-30" N, 1°14'25-26" W elevation 1,080-
105 1,100 m a.s.l.). The slope of the plot is 31% with NW aspect. Soil in this area is loamy
106 textured with a basic pH, high volumetric content of stones, high calcium carbonate
107 content and a decreasing in depth content of soil organic carbon (Table 1). Soil thickness

108 ranges from 10 to 40 cm, and the parent rock is a karstified Jurassic limestone with
 109 numerous fissures, which were revealed by the boreholes (up to 4 m depth) that were
 110 drilled along the plot (del Campo et al., 2019b). The water table was not found within this
 111 depth, but the parent rock becomes a significant reservoir of deep water (del Campo et
 112 al., 2019b) forming a perched aquifer, very common in Mediterranean catchments
 113 (Medici et al., 2008). According to a close meteorological station (1960-2011), mean
 114 annual precipitation is 466 mm, mean annual temperature is 12.8 °C and mean
 115 Hargreaves reference evapotranspiration is 1200 mm. The climate is classified as
 116 semiarid according to the Köppen climate classification. The forest is a high density
 117 coppice stand of *Quercus ilex* (holm oak) with scarce presence of other species (*Pinus*
 118 *halepensis*, *Quercus faginea*, *Juniperus phoenicea* and *J. oxycedrus*). In May 2012, the
 119 forest structure was characterized. Diameter at basal and breast heights were 10.7 cm
 120 and 7.7 cm respectively, basal area was 5.6 m² ha⁻¹, tree density was 1059/1133 trees
 121 ha⁻¹ (holm oak/all trees) and the averaged Leaf Area Index (LAI), which was seasonally
 122 measured, was 1.13 ± 0.22 m² m⁻² (2012-2016).

Layer	Stoniness (%)	pH	CaCO ₃ (%)	SOC (g kg ⁻¹)	Texture
L Layer	48.4±10.7				
H Layer	59.2±7.1	7.84±0.09	15.3±5.6	131.2±32.0	
0-10 cm	63.9±8.5	8.05±0.11	21.1±6.7	73.2±17.4	44;33;23
10-30 cm	58.6±7.3	8.25±0.12	34.1±6.2	42.3±21.4	57;23;20
30-40 cm	55.5±7.2	8.34±0.04	36.7±1.7	25.1±6.4	48;32;19

123 **Table 1** Soil characteristics of the study site. SOC means soil organic carbon. Soil particle fractions in the
 124 following order: sand, silt and clay (%). (Bautista et al., 2015; del Campo et al., 2018).



125

126 **Figure 1** Location of the experimental plot study site.

127 **2.2 Environmental variables and hydrological field measurements**

128 By means of a central data-logging unit and different instruments connected to it, data
 129 were registered and stored during the observational period, from 01/10/2012 to
 130 26/04/2016. The data-logger was programmed to record all meteorological data and field
 131 measurements every 10 minutes and averaged on a daily basis. Table 2 shows a
 132 summary of the data, while a complete description of the instrumentation and
 133 methodology employed to obtain the data can be found in del Campo et al. (2019a,
 134 2018).

Data	Sensor	Type	Temporal resolution
Precipitation	Davis tipping bucket	Input	Continuously
Air temperature	Decagon Devices T/RH sensor	Input	Every ten minutes
Relative humidity	Decagon Devices T/RH sensor	Input	Every ten minutes
Throughfall	del Campo et al. (2018)	Input	Every ten minutes
Runoff	Diehl Metering Altair v4 volumetric counters	State variable	Every ten minutes
Soil water content	15 FDR probes (EC-5, Decagon Device)	State variable	Every ten minutes
Transpiration	ICT international sap flow sensor	State variable	Every thirty minutes
Field LAI	LAI-2000 sensor	Input	Seasonally
Satellite LAI	Level-4 MODIS global LAI satellite product (NASA, LPDAAC)	Input	Weekly
Mineralization	Resin core method (DiStefano and Gholz, 1986)	State variable	Every two months
Nitrification	Resin core method (DiStefano and Gholz, 1986)	State variable	Every two months

Nitrogen leaching	Resin core method (DiStefano and Gholz, 1986)	State variable	Every two months
NH₄⁺ soil content	Flow injection analyser (FIAStar 5000, Foss Tecator, Höganäs, Sweden)	State variable	Every two months
NO₃⁻ soil content	Flow injection analyser (FIAStar 5000, Foss Tecator, Höganäs, Sweden)	State variable	Every two months
Soil respiration	EGM-4 environmental gas monitor from PP System Company	State variable	Every one or two months

135 **Table 2** Data, sensor employed to record it, type of data and temporal resolution.

136 A Davis tipping bucket rain gauge placed in an open area 20 m away from the plot was
 137 used to continuously measure precipitation, and by means of a Decagon Devices T/RH
 138 sensor placed inside the plot at 2 m height above ground surface, air temperature and
 139 relative humidity were recorded. Throughfall was measured according to the
 140 methodology described in del Campo et al. (2018).

141 Soil water content was measured by means of 15 FDR probes (EC-5, Decagon Device)
 142 installed at 5, 15 and 30 cm depth and the default calibration for mineral soils was used.

143 At the lower boundary of the slope, runoff was measured in two collecting trenches by
 144 means of Diehl Metering Altair v4 volumetric counters.

145 In order to estimate stand transpiration, sap flow velocity was measured through the Heat
 146 Ratio Method (Burgess et al., 2001) in 14 trees, which were divided into 4 different
 147 diametrical classes. One ICT international sap flow sensor was installed in each tree on
 148 the north trunk side at 0.3 - 1.0 m height. These sap flow measurements were upscaled
 149 to stand transpiration accounting for the density of trees and their diameter frequency
 150 distribution.

151 It is worth noting that the impairment between soil water content and transpiration
 152 measurements during the summer months (i.e. transpiration > measured soil water
 153 content changes) suggests that *Q. ilex* has access to subsoil water resources (del
 154 Campo et al., 2019a) and thus, additional groundwater transpiration is considered in this
 155 study (Puertes et al., 2019).

156 LAI was seasonally measured in the field 12 times during the observational period by
157 means of a LAI-2000 sensor, and in order to extend the data series, the estimations from
158 the level-4 MODIS global LEAF Area Index satellite product (NASA, LPDAAC) were used
159 (del Campo et al., 2019a; Puertes et al., 2019).

160 2.3 Carbon and nitrogen field measurements

161 In the case of the carbon and nitrogen field measurements, the observational period only
162 covers the first two hydrological years (01/10/2012 – 30/09/2014). Soil samples were
163 collected from the first 15 cm of soil every two months approximately, and from 9 different
164 sites homogenously distributed inside the plot in order to deal with the common
165 heterogeneity in the spatial distribution of carbon and nitrogen, which is mainly caused
166 by the patchy distribution of vegetation and its variability in life forms (Austin et al., 2004).
167 Mineralization, nitrification and leaching were measured using the resin core method
168 (DiStefano and Gholz, 1986). Soil samples were placed in PVC tubes with resin traps,
169 where they were left incubating (in situ buried cores). Part of the same soil used to fill
170 the tubes was kept refrigerated and transported to the lab where the initial ammonium
171 ($\text{NH}_4^+\text{-N}$) and nitrate ($\text{NO}_3^-\text{-N}$) soil contents were obtained by means of a flow injection
172 analyzer (FIASStar 5000, Foss Tecator, Höganäs, Sweden). The process was repeated
173 approximately every two months, replacing the incubated soil by new soil, and taking it
174 and a sample of the new soil to the lab, where initial (new soil) and final (incubated soil)
175 $\text{NH}_4^+\text{-N}$ and $\text{NO}_3^-\text{-N}$ soil contents were obtained. From the mass balance between the
176 initial and final $\text{NH}_4^+\text{-N}$ and $\text{NO}_3^-\text{-N}$ soil contents, net mineralization and net nitrification
177 accumulated during the incubation period were calculated. The $\text{NH}_4^+\text{-N}$ and $\text{NO}_3^-\text{-N}$
178 accumulated in the deeper resin trap corresponded to the $\text{NH}_4^+\text{-N}$ and $\text{NO}_3^-\text{-N}$
179 accumulated leaching, whilst the initial $\text{NH}_4^+\text{-N}$ and $\text{NO}_3^-\text{-N}$ soil contents corresponded
180 to the punctual $\text{NH}_4^+\text{-N}$ and $\text{NO}_3^-\text{-N}$ observations.

181 An EGM-4 environmental gas monitor from PP System Company was used to obtain the
182 CO_2 efflux (total soil respiration). All the measurements were made at midday, between

183 1100 and 1300 CET and every one or two months on 9 PVC collars (10 cm in diameter
 184 and 5 cm depth) introduced 3 cm into the soil.

185 2.4 Models description

186 The models used in this study are described in the following lines. BIOME-BGCMuSo
 187 and LEACHM are briefly described, while TETIS-CN is described in detail, as it has been
 188 developed during this study. Table 3 shows a comparison between model
 189 characteristics.

	BIOME	LEACHM	TETIS-CN
Hydrological parameters	-	15 + 9 nlayers	21
Carbon and nitrogen parameters	-	19 + 5 nlayers	19
Total number of parameters	194	34 + 14 nlayers	40
Number of layers	10	n (8 herein)	2
Soil water movement	Tipping bucket water balance	Richards' equation	Tipping bucket water balance (4 tanks)
Transpiration	Based on the Penman–Monteith equation using stomatal conductance	Nimah and Hanks (1973)	Multiplicative function relating transpiration and the environmental variables
Dead plant material fractions	5	1	1
Soil organic matter fractions	4	2	2
Inorganic nitrogen fractions	2	2	2
Soil organic matter decomposition	First-order kinetics	First-order kinetics	First-order kinetics
Nitrogen transformations	First-order kinetics	First-order kinetics	First-order kinetics
Nitrogen sorption	Fixed percentage	Linear isotherm	Linear isotherm
Solute movement	Advective movement	Convection-diffusion equation	Advective movement

190 **Table 3** Models characteristics comparison.

191 2.4.1 BIOME-BGCMuSo model

192 The BIOME-BGCMuSo v.5.0 model (Hidy et al., 2016) is the modified version of BIOME-
 193 BGC model (Thornton et al., 2002), hereafter referred as BIOME, which has been widely
 194 used in natural ecosystems (Chen and Xiao, 2019; Chiesi et al., 2007; Fontes et al.,
 195 2010). It is a biogeochemical model with multilayer soil sub-model, which simulates the
 196 storage and flux of water, carbon, and nitrogen between the ecosystem and the

197 atmosphere, and within the components of the terrestrial ecosystem. It uses a scale of 1
198 m², daily meteorological data, site-specific data, ecophysiological data, carbon-dioxide
199 concentration (CO₂) and N-deposition data to simulate the biogeochemical processes of
200 the given biome. The soil profile is divided into 10 layers and the main simulated
201 processes assessed are photosynthesis, allocation, litterfall, carbon, nitrogen and water
202 dynamics in the plant, litter and soil. The model is composed by 60 plant functioning
203 parameters, 24 senescence and soil parameters, 12 growing season parameters, 14 rate
204 scalars, 7 CH₄ parameters and 7 phenological phases, with 11 parameters each (Table
205 A.1).

206 As stated by Hidy et al. (2016), the three most important blocks of the model are the
207 phenological, the carbon flux, and the soil flux block. The phenological block calculates
208 foliage development and therefore affects the accumulation of carbon and nitrogen in
209 leaf, stem (if present), root and consequently the amount of litterfall. In the carbon flux
210 block, gross primary production (GPP) of the biome is calculated using Farquhar's
211 photosynthesis routine (Farquhar et al., 1980) and the enzyme kinetics model based on
212 Woodrow and Berry (1988). Autotrophic respiration is separated into maintenance and
213 growth respirations. In addition to temperature, maintenance respiration is calculated as
214 the function of the nitrogen content of living plant pools, while growth respiration is a fixed
215 proportion of the daily GPP. The soil block describes the decomposition of dead plant
216 material and soil organic matter, nitrogen mineralization and nitrogen balance (Running
217 and Gower, 1991). Dead plant material is partitioned into coarse woody debris and litter,
218 the latter represented by 4 different fractions. Soil organic matter is also divided into four
219 fractions: fast, medium, slow and recalcitrant (humus). Two elements (carbon and
220 nitrogen) represent each fraction and both elements in litter and soil organic matter are
221 transferred into sequentially slower decomposing pools. Organic carbon decomposition
222 is calculated by multiplying the decomposition rate by the carbon content in each pool
223 (i.e. first-order kinetics). Heterotrophic respiration is calculated through the respiration
224 fraction, which is different for each pool. All rates are adjusted based on temperature and

225 soil water content. The soil hydrological calculation can be carried out by using
226 Richards's equation or a "tipping bucket" water balance approach (used in this case
227 study). The model differentiates between soil and groundwater transpiration.

228 2.4.2 LEACHM model

229 The second model employed in this study is the LEACHM model (Hutson, 2003).
230 LEACHM has been broadly used for simulating water and solutes movement in
231 unsaturated soils, mainly in agricultural soils (Asada et al., 2015, 2013; Contreras et al.,
232 2009; Lidón et al., 2013; Nasri et al., 2015). It is a one-dimensional model that divides
233 the soil profile into a user's fixed number of horizontal layers of equal thickness. It
234 employs finite differencing approximation techniques to simulate flow and redistribution
235 of water and solutes; the model homogenously divides the time step and inputs at least
236 into 10-time intervals per day. Its hydrological sub-model is composed of 24 parameters,
237 nine of them defined for each soil layer, and its carbon-nitrogen sub-model is also
238 composed of 24 parameters (Table A.2), five of them defined for each soil layer.
239 Therefore, the model is composed of 48 parameters, but 14 of these parameters are
240 defined for each soil layer, and consequently, increasing the number of layers highly
241 increases the number of parameters to be estimated or calibrated.

242 In order to describe the water flow in the unsaturated zone, LEACHM uses the Richards'
243 equation, in which soil moisture and hydraulic conductivity are related by the equation
244 proposed by Campbell (1974). Runoff estimate is based on the equation proposed by
245 Williams (1991), with the advantage of adjusting the runoff curve number according to
246 the slope. Potential evapotranspiration is split into potential evaporation and potential
247 transpiration according to the plant cover fraction. Actual evaporation is calculated as a
248 function of the potential evaporation and the maximum possible evaporative flux density
249 while actual transpiration is calculated following Nimah and Hanks (1973) as a function
250 of the soil's unsaturated hydraulic properties and the effective water potential gradient at
251 roots-soil interface.

252 Soil organic matter is divided in LEACHM into three different fractions: plant residue
253 (litter), manure (easily degradable) and humus (relatively stable), each one with its
254 corresponding two pools (carbon and nitrogen). Biomass remains an integral part of the
255 plant residue pool. Soil organic matter decomposition is described by first-order kinetics
256 in the carbon pools and nitrogen transformations are given by the C/N ratio of the
257 decomposition products, that in turn, controls net mineralization, that is, the mineral
258 nitrogen released or consumed by the microbial biomass. The synthesis efficiency factor
259 defines the relative production of CO₂ (heterotrophic respiration) and humus, while the
260 humification factor determines the split between humus and biomass. Nitrification,
261 volatilization, and denitrification processes are also modelled by first-order kinetics.
262 Ammonium adsorption and desorption by clay colloids is modelled by a linear sorption
263 isotherm. All transformation equations are corrected accounting for the influence of soil
264 water content and soil temperature (Q₁₀ type function), however, it should be highlighted
265 that an error was found in the code, by which, the temperature correction function was
266 not changing the daily temperature in the case of using the Richards' equation. This error
267 was corrected. Solute transport is modelled following the convection-diffusion equation.
268 Finally, plant nitrogen uptake occurs in the transpiration flux, but if this does not satisfy
269 the requirements (daily potential uptake), a diffusive component for nitrate is considered.
270 In the case of perennial vegetation, a constant daily potential uptake is calculated from
271 the yearly value.

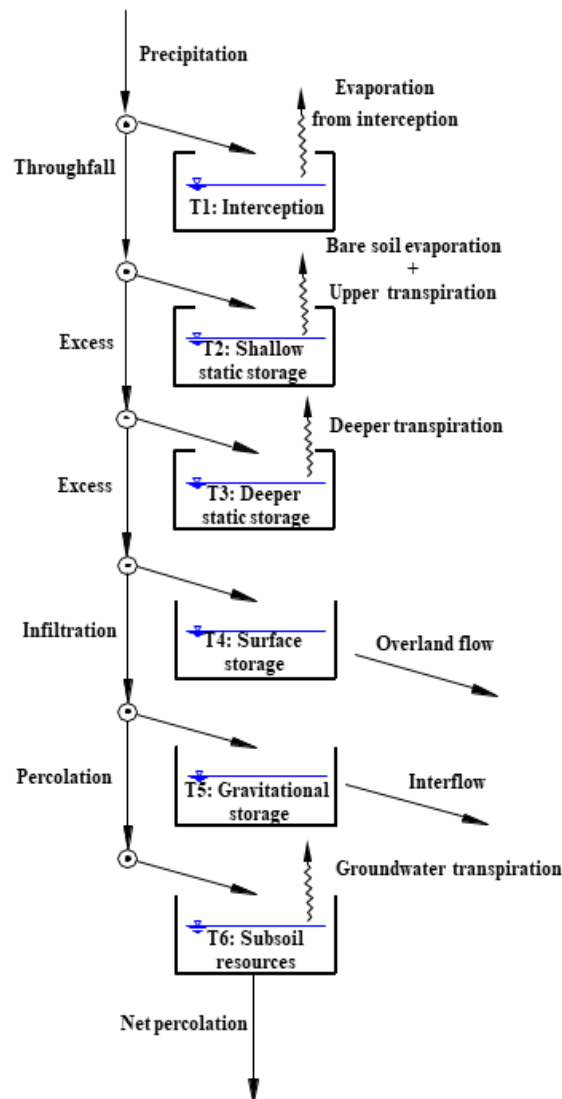
272 Additionally, in this case study, as LEACHM does not simulate plant growth, two new
273 parameters were added to the model with the aim of characterize the plant residue input:
274 a plant death constant (gC m⁻² day⁻¹), which accounts for litterfall and root mortality, and
275 the C/N ratio of the plant residue. Since the rate of added organic matter changes over
276 time, a fixed annual curve based on the measured litterfall curve was considered.

277 2.4.3 TETIS-CN model

278 The TETIS-CN model divides the soil profile into two layers, allows fixing an evaporation
279 depth in this shallow first layer and hence, the evapotranspiration split between bare soil
280 evaporation and transpiration in this first layer, which is necessary in order to properly
281 reproduce nutrient cycles. On the one hand the hydrological sub-model (Pasquato et al.,
282 2015; Ruiz-Pérez et al., 2016) is based on a tank type conceptualization in which water
283 moves downwards as long as the tank outflow capacity is not exceeded (Fig. 2) and is
284 composed of 25 parameters. On the other hand, the new carbon and nitrogen sub-model
285 (Fig. 3) is based on the model proposed by Porporato et al. (2003) because it is already
286 a parsimonious model. It divides soil organic matter into three fractions, which is in good
287 agreement with Batlle-Aguilar et al. (2011) and Jenkinson et al. (1990), who proposed
288 that models should divide soil organic matter at least between two and four fractions to
289 obtain reliable results, while more complex models commonly comprise five (Lardy et al.,
290 2011) or even more, as BIOME. However, this model has been improved, mainly to adapt
291 it to semiarid climates, where temperature and soil water content are the main
292 environmental drivers (Manzoni et al., 2004). Volatilization, denitrification, NH_4^+ sorption
293 and a temperature correction function have been included, and additionally, the soil
294 water correction functions have been improved. Hence, this final carbon-nitrogen sub-
295 model is composed of 19 parameters (Table A.3), leading to a total of 44 parameters
296 and in order to explore the basic mechanisms of the carbon and nitrogen cycles, TETIS-
297 CN was used as simple as possible, keeping its dynamic vegetation sub-model
298 deactivated and introducing as inputs the LAI values simulated by the dynamic
299 vegetation sub-model.

300 The first tank (T1) represents the interception process. Water is stored in this tank
301 depending on its storage capacity and it can only exit by direct evaporation. The next
302 two tanks (T2 and T3) represent the soil static storage. From the shallow layer, water
303 can exit by bare soil evaporation and superficial roots transpiration, while from the
304 underlying layer only transpiration is considered. Tanks T4 and T5 represent the runoff

305 generation, which act as linear storages characterized by residence times. Lastly, as in
 306 this case *Q. ilex* has access to subsoil water resources, the modification introduced by
 307 Puertes et al. (2019) in order to consider groundwater transpiration in this experimental
 308 plot, was used. The modification consists in the introduction of an intermediate tank (T_6)
 309 between the soil and the aquifer from which groundwater transpiration is calculated.
 310 Transpiration and evaporation are calculated using the reference evapotranspiration.
 311 Transpiration is corrected by a water stress factor, the vegetation's LAI, the vegetation
 312 cover fraction and the percentage of roots in each layer, while evaporation is only
 313 corrected by a water stress factor and the vegetation cover factor.



314

315 **Figure 2** Schema of the adapted TETIS-CN hydrological sub-model to the case study.

316 Soil organic matter is divided into three fractions: litter, humus and biomass; each one
 317 represented by two pools (carbon and nitrogen). The mass balance between these pools
 318 is calculated in carbon terms and it is transformed to nitrogen by the C/N ratio of each
 319 fraction. Microbial death, which is recirculated to the litter pool, is represented by a simple
 320 first-order kinetic, without considering soil water content or temperature influence:

$$321 \quad MD = k_{md}C_b \quad Eq(1)$$

322 where MD is microbial death ($\text{gC m}^{-3} \text{ day}^{-1}$), k_{md} is microbial biomass death rate (day^{-1})
 323 and C_b is biomass soil carbon content (gC m^{-3}). However, as soil organic matter
 324 decomposition not only relies on the amount of decomposable material but also on the
 325 microbial activity, soil organic matter decomposition is described by a multiplicative
 326 expression:

$$327 \quad DEC_i = \varphi f(\vartheta) f(t) k_i C_b C_i \quad Eq(2)$$

328 which is still a first-order kinetics, but it includes the influence of the amount of organic
 329 matter and the decomposers (Manzoni and Porporato, 2007). The term φ is a
 330 dimensionless factor which has a value of 1, unless the litter is poor in nitrogen and
 331 immobilization is not enough for the microorganisms, $f(\vartheta)$ and $f(t)$ are terms accounting
 332 for the influence of soil water content and soil temperature, k_i is the decomposition rate
 333 of the litter or hummus soil carbon content ($\text{m}^3 \text{ day}^{-1} \text{ gC}^{-1}$) and C_i is litter or hummus soil
 334 carbon content (gC m^{-3}). Nitrogen net mineralization is controlled by the C/N ratio of the
 335 biomass, which should remain constant. The respiration rate defines the relative
 336 production of CO_2 (heterotrophic respiration) while the humification factor determines the
 337 split between humus and biomass. Nitrification is calculated similarly to decomposition:

$$338 \quad NIT = \varphi f(\vartheta) f(t) k_{nit} C_b NH_4^+_d \quad Eq(3)$$

339 where NIT is nitrification ($\text{gN m}^{-3} \text{ day}^{-1}$), k_{nit} is nitrification rate ($\text{m}^3 \text{ day}^{-1} \text{ gN}^{-1}$) and $NH_4^+_d$
 340 is the dissolved fraction of NH_4^+ -N soil content (gN m^{-3}).

341 Volatilization and denitrification processes are less important at the daily-to-seasonal
 342 time scale in natural soils (Porporato et al., 2003), hence, simple first-order kinetics are
 343 used. Volatilization is calculated as:

$$344 \quad \text{Vol} = f(\vartheta)f(t)k_{vol}NH_4^+ \quad \text{Eq(4)}$$

345 where *Vol* is volatilization (gN m⁻³ day⁻¹) and *k_{vol}* is volatilization rate (day⁻¹). Denitrification
 346 is calculated as:

$$347 \quad \text{De} = f(\vartheta)k_{de}NO_3^- \quad \text{Eq(5)}$$

348 where *De* is denitrification (gN m⁻³ day⁻¹), *k_{de}* is denitrification rate (day⁻¹) and *NO₃⁻* is
 349 *NO₃⁻*-N soil content (gN m⁻³). *NH₄⁺* adsorption and desorption by clay colloids is modelled
 350 in the simplest way, by a linear sorption isotherm:

$$351 \quad c_s = k_d c_L \quad \text{Eq(6)}$$

352 where *k_d* is *NH₄⁺* distribution coefficient (dm³ kg⁻¹), *c_s* is *NH₄⁺*-N concentration in the
 353 sorbed phase (mgN kg⁻¹) and *c_L* is *NH₄⁺*-N concentration in solution (mgN dm⁻³).

354 Nitrogen uptake by vegetation is considered to occur proportionally to the transpiration
 355 flux, and if the nitrogen potential uptake is not accomplished, a diffusive flux is triggered,
 356 which is proportional to the nitrogen content and a diffusion coefficient. A constant daily
 357 potential uptake calculated from the yearly value is considered. *NH₄⁺*-N and *NO₃⁻*-N
 358 leaching is considered to occur proportionally to the percolation flux (i.e. advective
 359 movement). In the case of *NH₄⁺*-N, only the dissolved fraction is considered to be
 360 available for nitrification, volatilization, plant nitrogen uptake and leaching.

361 The function controlling the influence of soil water content on decomposition,
 362 mineralization and nitrification processes is:

$$363 \quad f(\vartheta) = \begin{cases} \vartheta/\vartheta_T & \vartheta < \vartheta_T \\ \vartheta_T/\vartheta & \vartheta \geq \vartheta_T \end{cases} \quad \text{Eq(7)}$$

364 where *ϑ* is soil moisture (cm cm⁻¹) and *ϑ_T* a soil moisture threshold (cm cm⁻¹). Instead of
 365 field capacity, a threshold is used in order to reproduce the pulse dynamics observed in
 366 semiarid environments (Medici et al., 2012). This threshold is included as a parameter in
 367 the model. The function controlling the influence of soil water content on volatilization is:

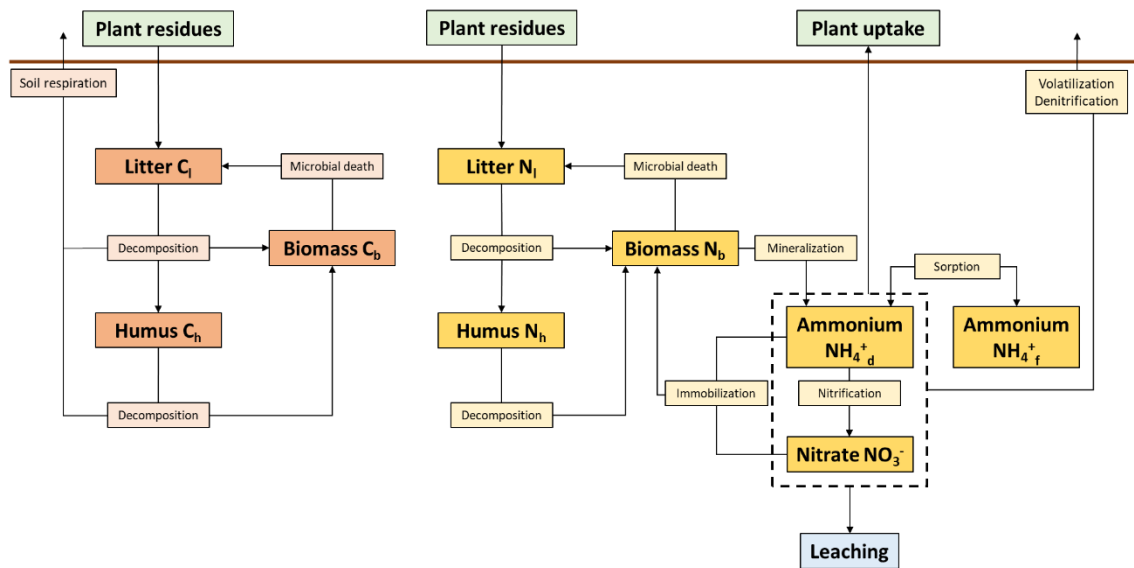
368
$$f(\vartheta) = \begin{cases} \vartheta/\vartheta_T & \vartheta < \vartheta_T \\ 1 & \vartheta \geq \vartheta_T \end{cases} \quad Eq(8)$$

369 and the soil water content correction function for denitrification is:

370
$$f(\vartheta) = \begin{cases} 0 & \vartheta < \vartheta_T \\ 1 & \vartheta \geq \vartheta_T \end{cases} \quad Eq(9)$$

371 The function controlling the influence of temperature is the one proposed by Kätterer and
372 Andrén (2001).

373 Finally, as with LEACHM, in order to characterize the plant residue input, a plant death
374 constant ($gC\ m^{-2}\ day^{-1}$) and its C/N ratio were added as parameters and a fixed annual
375 curve, based on the measured litterfall curve, was also considered.



376 ----->

377 **Figure 3** Schema of the TETIS-CN carbon and nitrogen sub-model.

378 2.5 Model implementation

379 In order to make precise predictions, obtaining the effective parameters through a
380 calibration process is crucial. As models are a simplified representation of the reality,
381 their parameters will be representative of the modelling scale and different to the ones
382 measured in field (Mertens et al., 2005), being their main purpose to compensate for the
383 model structure errors, the spatial and temporal scale effects and the observational
384 errors (Abbaspour et al., 2007; Francés et al., 2007). Consequently, the three models

385 were calibrated and validated using some measurements of the observed state variables
386 and only validated using the remaining measurements.

387 2.5.1 Model evaluation

388 The simulation period included the period with available observations. In the case of the
389 water cycle, from 01/10/2012 to 26/04/2016, including a previous warming-up period
390 (01/08/2012 to 30/09/2012), in which only meteorological data were available. The first
391 two hydrological years were selected to calibrate the hydrology, and the remaining period
392 to validate it. In the case of the carbon and nitrogen cycles, the available observations
393 were from 01/10/2012 to 30/09/2014. The first year was used to calibrate the models,
394 and the second one was used as validation; therefore, as model performance in terms
395 of biogeochemistry was measured during two hydrologically calibrated years, the errors
396 in reproducing the hydrology were not transmitted to the biogeochemical performance of
397 the models. The hydrology was simulated for all the soil profile, however, due to the
398 nitrogen measurements are representative of the first 15 cm of soil, the biogeochemistry
399 was simulated only in these 15 cm of soil in this case study. BIOME and TETIS-CN were
400 directly used with a daily time-step, while LEACHM was used with a 0.05-day time-step,
401 although the output data are expressed daily. They were calibrated and validated using
402 the field measurements of transpiration, soil water content, $\text{NH}_4^+\text{-N}$ soil content, $\text{NO}_3^-\text{-N}$
403 soil content, accumulated net mineralization and accumulated net nitrification. In
404 addition, interception was used in the calibration process in the case of BIOME and
405 TETIS-CN, and the measurements of mineral nitrogen leaching and soil respiration were
406 only used to validate the models.

407 Soil water content measurements were used daily, but transpiration measurements were
408 averaged on a weekly basis. As LEACHM employs weekly reference evapotranspiration
409 and temperature, although the results are daily, it is expected to simply match the weekly
410 transpiration value. Thus in order to compare the models, all were calibrated using
411 weekly transpiration values. Interception data, in the case of BIOME and TETIS-CN,

412 were used accumulated for the whole calibration period with the aim of improving the
413 hydrological annual balance representation. LEACHM does not consider the process of
414 interception, being throughfall the required input. Moreover, LEACHM and TETIS-CN do
415 not calculate autotrophic respiration, therefore, in order to compare the results, the total
416 soil respiration measurements were divided into autotrophic and heterotrophic
417 respiration. According to Hanson et al. (2000), heterotrophic respiration in forests
418 averages 51.4% of total soil respiration (sample of 37 forests), therefore, this value was
419 used. Although soil respiration measurements correspond to the whole soil profile, as
420 microbial biomass content is substantially higher in the surface soil layers (Fierer et al.,
421 2003; Taylor et al., 2002), the calculated heterotrophic respiration can be compared with
422 the results of the models, which correspond to the first 15 cm of soil. However, as it is a
423 transformed variable, it was not used in the calibration process.

424 The performance of the models was measured using the following state variables and
425 goodness-of-fit indices: the Nash and Sutcliffe efficiency index (NS) was used in the case
426 of soil water content (NS_SWC) and transpiration (NS_TR), while the balance error (BE)
427 was used in the case of interception. The Root Mean Squared Error (RMSE) was used
428 to evaluate the performance of the models in terms of NH_4^+ -N soil content (RMSE_ NH_4^+),
429 NO_3^- -N soil content (RMSE_ NO_3^-), accumulated net mineralization (RMSE_Min),
430 accumulated net nitrification (RMSE_Nit), accumulated mineral nitrogen leaching
431 (RMSE_Leach) and heterotrophic respiration (RMSE_Resp).

432 2.5.2 Calibration process

433 In the case of BIOME, an automated model parameter estimation was conducted using
434 PEST (model-independent parameter estimation program) (Doherty, 2007), which has
435 implemented a variant of the Gauss-Marquardt-Levenberg method of nonlinear
436 parameter estimation. PEST minimizes the weighted sum of squared residuals between
437 observed and predicted values of the selected state variables. However, LEACHM and
438 TETIS-CN were calibrated in two different phases. As these models do not explicitly

439 consider vegetation growth, vegetation transpiration is not influenced by nitrogen uptake,
440 and consequently, the inclusion of the carbon and nitrogen to the simulation does not
441 affect the hydrological cycle. Hence, the first phase was the hydrological calibration.
442 Initially, a manual calibration was performed and then an automatic calibration was
443 carried out using the Multiobjective Shuffled Complex Evolution Metropolis (MOSCEM)
444 algorithm (Vrugt et al., 2003), based on the concept of Pareto-optimal solutions. The
445 population size was set to 50.000 and the number of complexes to 200. The compromise
446 solution from the Pareto front was chosen according to the criteria: minimum Euclidean
447 distance calculated using NS_SWC and NS_TR and, a BE less than 40% only in the
448 case of TETIS-CN. A more detailed description of this calibration process can be found
449 in Puertes et al. (2019). Thereafter, the carbon and nitrogen sub-models were calibrated.
450 With LEACHM, as the observed data are scarce, the same mineralization, nitrification
451 and denitrification rates were used for all soil layers (15 cm). An initial manual calibration
452 was done, for which the initial parameters values were found in the literature (Jung et al.,
453 2010; Ramos and Carbonell, 1991; Schmied et al., 2000). Previous experience with the
454 model and field observations were also considered. Later, an automatic calibration was
455 carried out using the MOSCEM algorithm (Vrugt et al., 2003) with a population size of
456 50.000 and 200 complexes. The solution with a smaller value of Euclidean distance,
457 calculated using the RMSE_NH₄⁺, RMSE_NO₃⁻, RMSE_Min and RMSE_Nit, was chosen
458 from the Pareto front as a compromise solution.

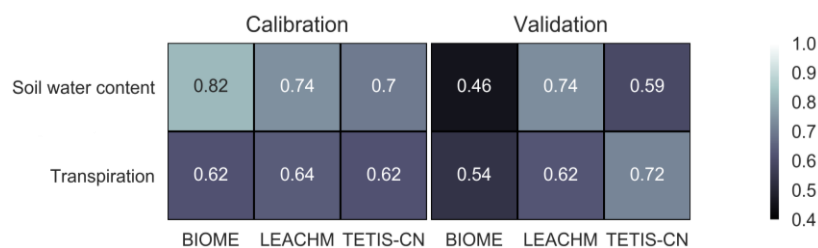
459 The calibration of the TETIS-CN carbon and nitrogen sub-model was similar. A previous
460 manual calibration was carried out, for which the initial values were found in literature
461 (D'Odorico et al., 2003; Manzoni et al., 2004; Manzoni and Porporato, 2007) and taking
462 into account field observations. Then, the automatic calibration using the MOSCEM
463 algorithm (Vrugt et al., 2003) was carried out. In this case, as TETIS-CN is not as time-
464 demanding as LEACHM, the population size was set to 100.000 and the number of
465 complexes to 250. Likewise, the solution with a smaller value of Euclidean distance,

466 calculated using the RMSE_NH₄⁺, RMSE_NO₃⁻, RMSE_Min and RMSE_Nit, was chosen
 467 from the Pareto front as a compromise solution.

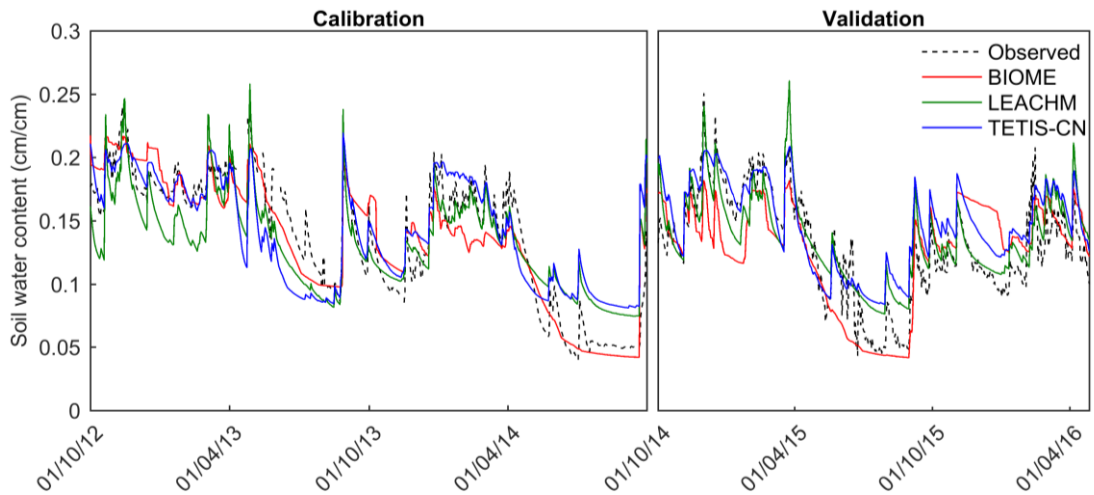
468 3 Results

469 The final parameter values are listed in Table A.1 for BIOME. In the case of LEACHM
 470 and TETIS-CN the hydrological parameters are listed in Puertes et al. (2019) and the
 471 carbon and nitrogen parameters in Table A.2 and Table A.3 respectively.

472 In terms of soil water content (Fig. 4 and Fig. 5), during the calibration period BIOME
 473 showed a very good performance, while LEACHM and TETIS showed a good
 474 performance (Moriasi et al., 2007). Only LEACHM was able to maintain this performance
 475 throughout the validation period, TETIS-CN decreased to a satisfactory performance and
 476 BIOME to an unsatisfactory performance (Moriasi et al., 2007). Conversely, only BIOME
 477 was able to reproduce the low soil water content observed during the warmest and driest
 478 months, from June to September approximately. Neither LEACHM nor TETIS-CN were
 479 able to reproduce this effect and a significant disagreement between observed and
 480 simulated was observed during these months, with a NS index of 0.41 and 0.04
 481 respectively.



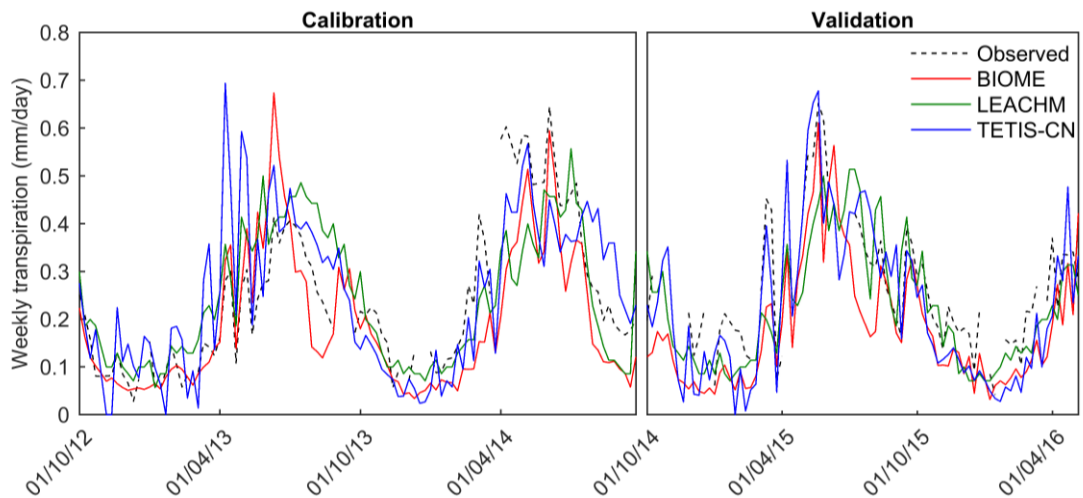
482
 483 **Figure 4** Heatmap representation of soil water content and weekly transpiration NS indices.



484

485 **Figure 5** Observed and simulated soil water content

486 Likewise, the three models reproduced transpiration satisfactorily (Moriassi et al., 2007)
 487 during both, calibration and validation periods (Fig. 4 and Fig. 6). Nonetheless, none was
 488 able to reproduce transpiration during the warmest months (June – September) and
 489 BIOME worsened its performance during the validation period.



490

491 **Figure 6** Observed and simulated transpiration

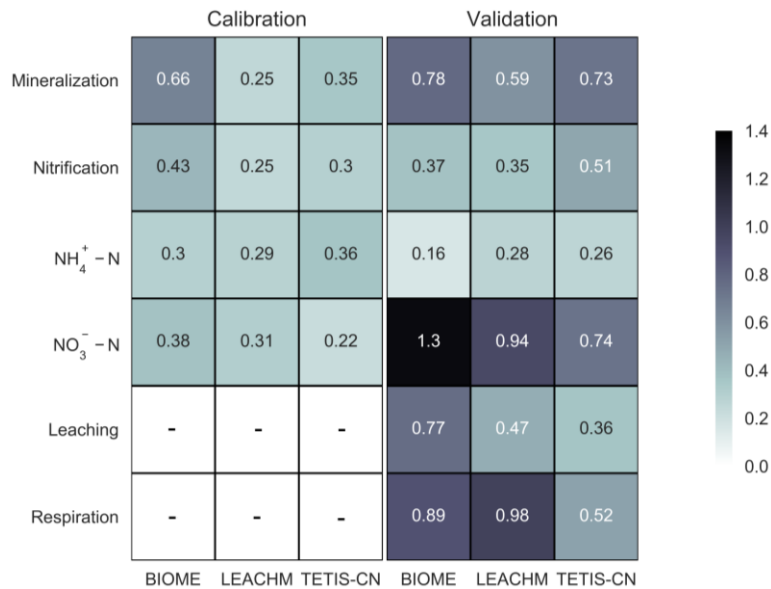
492 Regarding the water balance (Table 4), some differences were found mainly in the soil
 493 evaporation and transpiration results. Both values were lower when using BIOME, which
 494 underestimated total transpiration, leading to a higher percolation value. Nevertheless,
 495 the main differences were found in the evapotranspiration partitioning results of TETIS-
 496 CN, which heavily underestimated interception, leading to high values of soil evaporation
 497 and groundwater transpiration.

Flows (mm)	Obs.	BIOME	LEACHM	TETIS-CN
Precipitation	426.2	426.2	-	426.2
Interception	129.2	129.5	-	81.4
Net precipitation	297.1	296.7	297.1	344.8
Soil evaporation	-	34.4	64.4	118.7
Soil transpiration	-	49.9	68.9	49.6
Groundwater transpiration	-	22.2	21.0	44.2
Total transpiration	101.6	72.1	89.9	93.7
Runoff	4.6	4.0	3.0	0.0
Net percolation	-	188.5	140.8	137.5

498 **Table 4** Mean annual water balances (2012-2015).

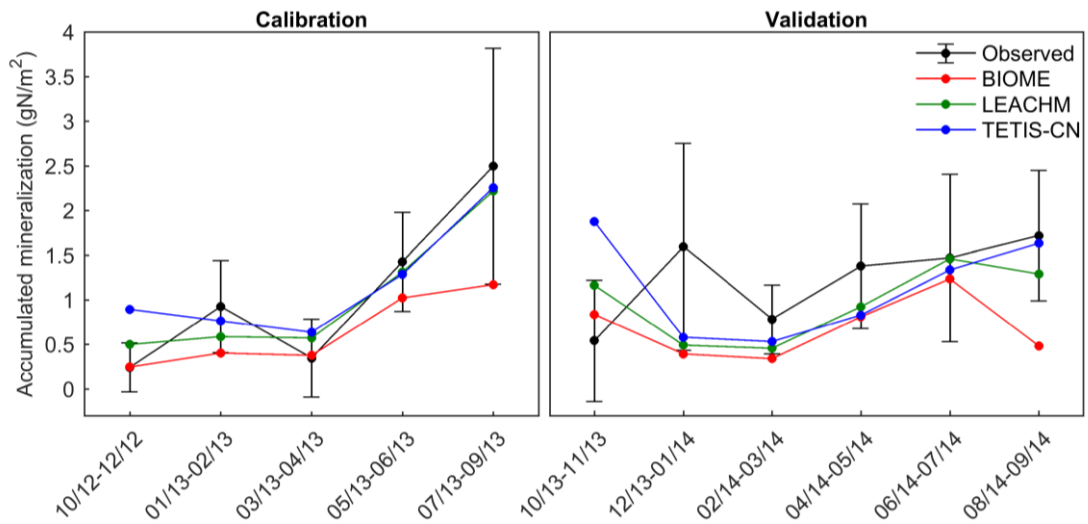
499 On the other hand, the performance of the models in reproducing the carbon and
500 nitrogen field observations after the calibration process was acceptable (Fig. 7).

501 Accumulated mineralization and nitrification were well reproduced taking into account
502 the standard deviation of the measurements (Fig. 8 and Fig. 9). The three models
503 presented almost all simulated values within the limits of the standard deviation;
504 however, BIOME showed mineralization values below the average and both, BIOME and
505 LEACHM had a low temporal variability which led to a low value of dispersion (Fig. 12)
506 in reproducing mineralization and nitrification. TETIS-CN was able to reproduce the
507 observed values and the trend, but it overestimated mineralization and nitrification from
508 October to November, which correspond with the outlier values in Fig. 12.



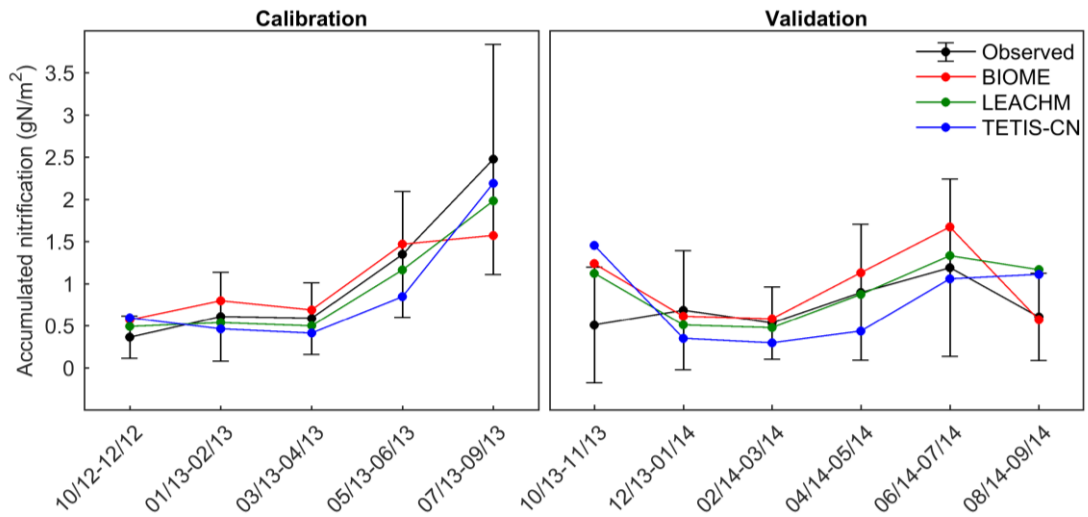
509

510 **Figure 7** Heatmap representation of accumulated net mineralization, accumulated net nitrification, NH₄⁺-N
511 soil content, NO₃⁻-N soil content, accumulated mineral nitrogen leaching and heterotrophic soil respiration
512 RMSE indices.



513

514 **Figure 8** Spatially averaged observed values and simulated values of accumulated mineralization.



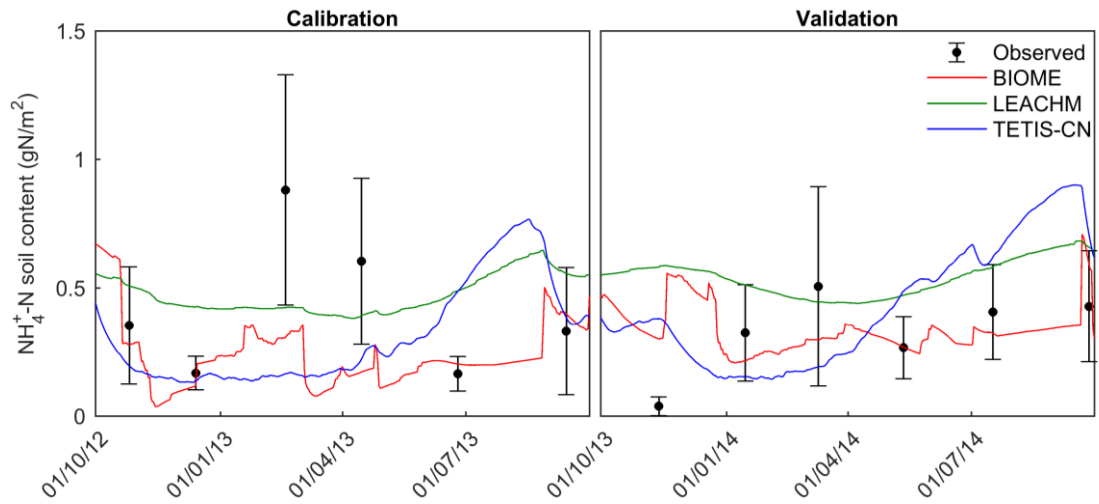
515

516 **Figure 9** Spatially averaged observed values and simulated values of accumulated nitrification.

517 Concerning the NH₄⁺-N soil content, the three models showed an acceptable
 518 performance taking into account the standard deviation of the measurements (Fig. 10).

519 BIOME and LEACHM presented better results, but both were very stable, showing lower
 520 dispersions than the observed one (Fig. 12). TETIS-CN overestimated the NH₄⁺-N soil

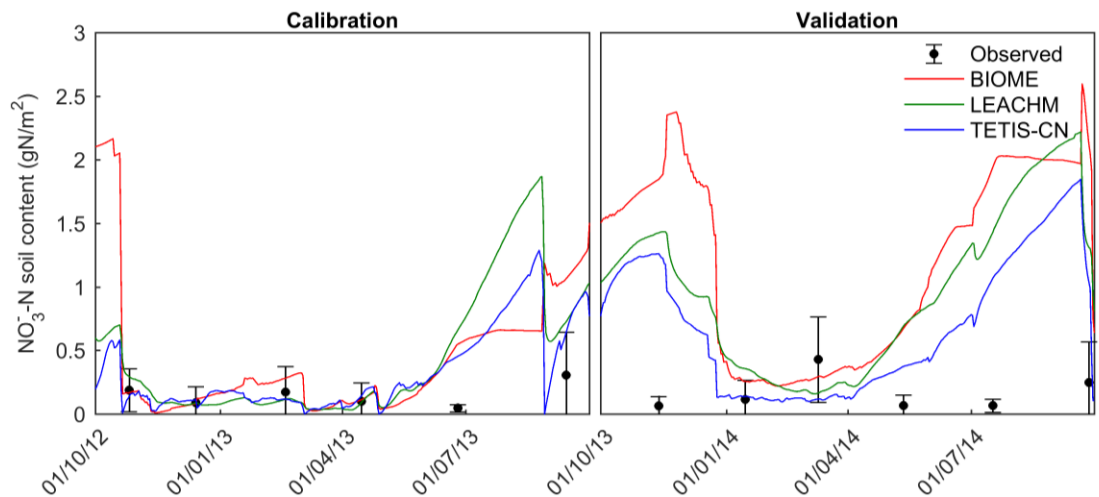
521 content during the warmest months, from June to September, but it was able to maintain
 522 a median and dispersion similar to the observed one (Fig.12).



523

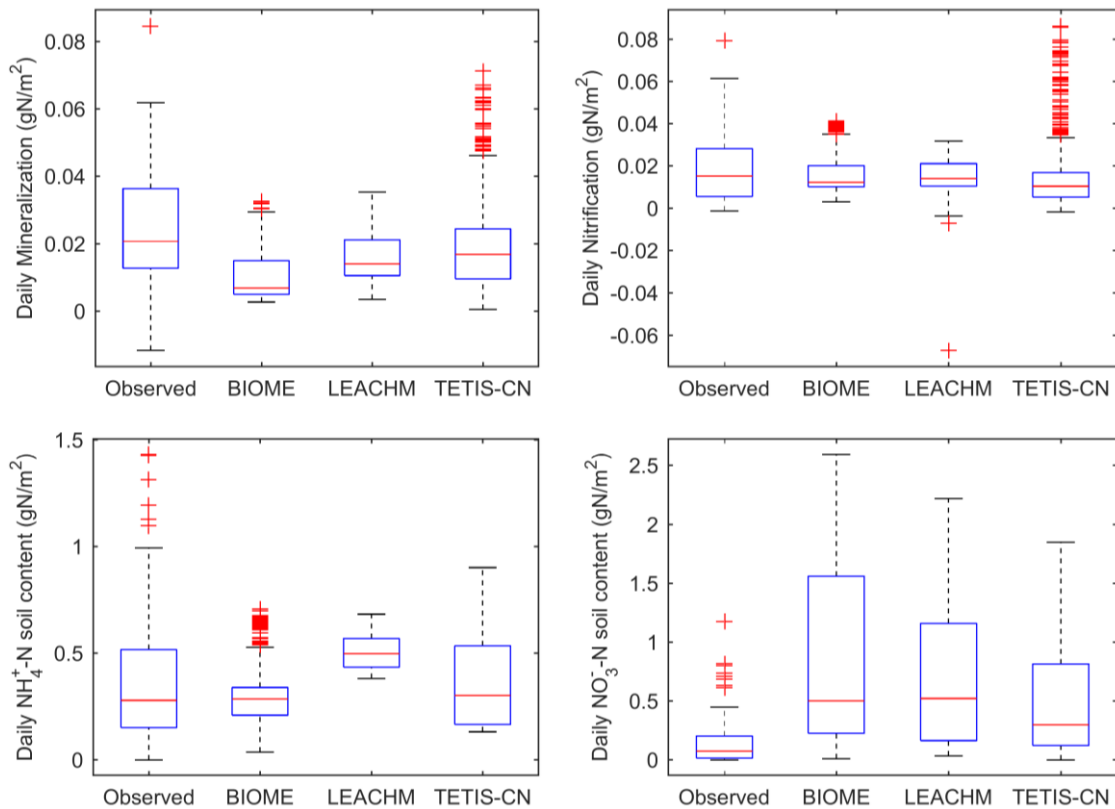
524 **Figure 10** Spatially averaged observed values and simulated values of $\text{NH}_4^+\text{-N}$ soil content

525 In the case of the $\text{NO}_3^-\text{-N}$ soil content, the performance of the models was poor,
 526 especially during the validation period (Fig. 7 and Fig. 11). The maximum simulated
 527 values and the dispersion were well above the observed ones (Fig. 12). Specifically, this
 528 problem was found during the periods with scarce precipitation events (Fig. 11), from
 529 June to November of 2013 and from April to September of 2014 (the 2013-2014
 530 hydrological year was very dry, with a precipitation of 271.1 mm, compared to the 581.2
 531 mm of the 2012-2013 hydrological year). The best results were obtained by TETIS-CN,
 532 but no noteworthy differences were found between the three models.



533

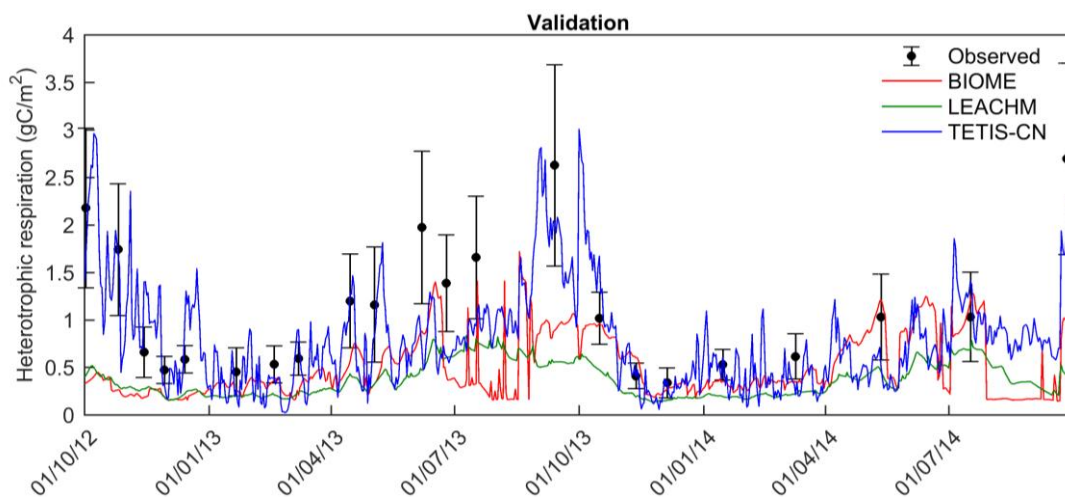
534 **Figure 11** Spatially averaged observed values and simulated values of $\text{NO}_3^-\text{-N}$ soil content



535

536 **Figure 12** Mineralization, nitrification, NH₄⁺-N soil content and NO₃⁻-N soil content box plots of the spatial
 537 and temporal observed values and simulated values.

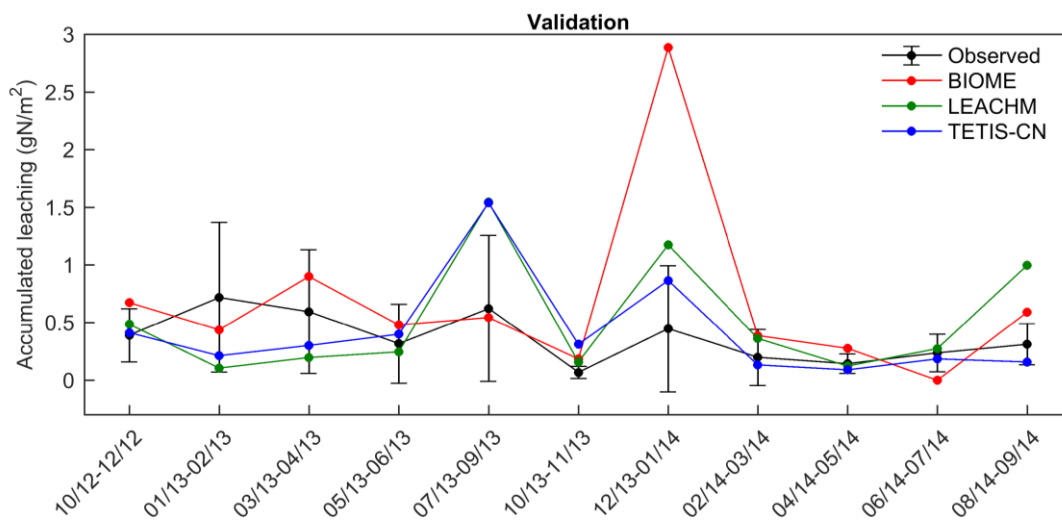
538 Regarding soil respiration, neither BIOME nor LEACHM were able to reproduce the
 539 heterotrophic respiration (Fig. 7). Both models obtained respiration values below the
 540 observed ones and they did not reproduce the trend (Fig. 13).



541

542 **Figure 13** Spatially averaged observed values and simulated values of heterotrophic respiration

543 Accumulated leaching (Fig. 14) was heavily overestimated during the periods with high
 544 precipitation events. Particularly this problem was shown in the case of BIOME, whilst
 545 LEACHM and TETIS-CN showed better results.



546
 547 **Figure 14** Spatially averaged observed values and simulated values of accumulated mineral nitrogen
 548 leaching

549 Finally, some differences were found in the mean annual balances (Table 5). These were
 550 found in the organic carbon plant residue, heterotrophic soil respiration (CO₂ release),
 551 plant uptake and leaching. BIOME and LEACHM obtained lower values of organic
 552 carbon plant residue input and heterotrophic respiration. However, TETIS-CN values of
 553 heterotrophic respiration were closer to the observed ones (Fig. 7 and Fig. 13), according
 554 to the partition between autotrophic and heterotrophic respiration of Hanson et al. (2000).
 555 Moreover, BIOME obtained higher values of leaching and lower values of plant uptake,
 556 but the leaching values of LEACHM and TETIS-CN were closer to the observed ones
 557 (Fig. 7 and Fig. 14).

Fluxes	BIOME	LEACHM	TETIS-CN
Organic carbon plant residue (gC m ⁻²)	152.75	112.95	262.53
Heterotrophic soil respiration (gC m ⁻²)	182.86	135.48	292.21
Organic nitrogen plant residue (gN m ⁻²)	3.28	5.23	9.07
Net mineralization (gN m ⁻²)	3.80	5.77	6.93
Volatilization (gN m ⁻²)	0.00	0.11	0.00
Net nitrification (gN m ⁻²)	5.66	5.34	5.28
Denitrification (gN m ⁻²)	0.33	0.11	0.26
NH ₄ ⁺ -N plant uptake (gN m ⁻²)	0.07	0.07	1.23
NO ₃ ⁻ -N plant uptake (gN m ⁻²)	0.24	1.91	2.23

NH₄⁺-N leaching (gN m⁻²)	1.58	0.07	0.09
NO₃⁻-N leaching (gN m⁻²)	4.36	3.44	3.08

558 **Table 5** Mean annual carbon and nitrogen balances in the first 15 cm of soil (2012-2014)

559 **4 Discussion**

560 Regarding the general water dynamics, BIOME was the only model which heavily
561 worsened its performance during the validation period. This problem may be explained
562 by its high parameter requirements, problem known as model over-parameterization. A
563 simple model may not make the best use of data; nonetheless, a model with a high
564 number of parameters may fit the data in the calibration period accurately and then, have
565 a bad performance in the validation period (Walker et al., 2003). Conversely, simpler
566 models as LEACHM and TETIS-CN were unable to reproduce the soil water content and
567 transpiration during the driest and warmest months (June to September), disagreements
568 that may be explained by their simple representation of transpiration (Puertes et al.,
569 2019). LEACHM uses weekly reference evapotranspiration values, and TETIS-CN only
570 divides the soil into two layers, which may be oversimplified. Moreover, neither LEACHM
571 nor TETIS-CN include the Vapour Pressure Deficit (VPD) influence in the calculation of
572 transpiration and in this case, transpiration was mainly explained by variations in VPD
573 (del Campo et al., 2019a).

574 The main difference regarding the water balance was found in the evapotranspiration
575 partitioning. BIOME and LEACHM reached soil evaporation values close to the range
576 obtained by del Campo et al. (2019a) in this same plot, which was 43-51 mm year⁻¹, and
577 similar groundwater transpiration values, but the 20 mm difference in soil transpiration
578 was substantial. Nevertheless, BIOME underestimated total transpiration in 30 mm
579 approximately, which may be explained by the joint hydrology and biogeochemistry
580 calibration process. In the case of BIOME, the hydrology performance of the model may
581 have been decreased by a better biogeochemistry performance because when more
582 than one objective is included in a calibration process, an improvement in the
583 representation of one causes deterioration in the other one (Vrugt et al., 2003).

584 Conversely, TETIS-CN underestimated interception in almost 50 mm year⁻¹, which led to
585 a very high value of soil evaporation. Its interception modelling is simple and depends
586 on LAI values, which corresponded to corrected satellite LAI values, not being completely
587 representative of the real plot's LAI. As MODIS cell size is 500 m it includes not only the
588 study plot. In contrast, even though LEACHM does not consider vegetation growth, as it
589 does not simulate the process of interception, it did not show this problem. Additionally,
590 TETIS-CN reached a higher value of groundwater transpiration, but the values obtained
591 by the three models were in the range of previous studies developed under semiarid
592 climates (Puertes et al., 2019).

593 In terms of biogeochemistry, the models showed different mean annual values of organic
594 carbon and nitrogen plant residue inputs. BIOME and LEACHM presented a similar value
595 of organic carbon plant residue input, and as in mature natural forests inputs and outputs
596 are generally balanced (Porporato et al., 2003), this value was similar to their
597 heterotrophic soil respiration (CO₂ release). Conversely, TETIS-CN reached higher
598 values, but its heterotrophic soil respiration was closer to the estimated punctual
599 observations, suggesting that BIOME and LEACHM underestimated the organic carbon
600 content of the plant residues, and due to the equilibrium, the heterotrophic soil
601 respiration. This poor performance may be explained by a conceptualization error, a poor
602 description of soil organic matter decomposition or more probably, because no carbon
603 measurement was included in the calibration process. The available observations may
604 not be enough to measure all the characteristics of the system, and thus, their
605 performance may increase if some additional carbon measurements are included as
606 constraints (Uhlenbrook and Sieber, 2005). In fact, in the case of LEACHM, it has been
607 widely used in studies for simulating nitrogen transformation, but these studies rarely
608 consider measured and simulated carbon changes (Mittal et al., 2007) and Asada et al.
609 (2013) modified the model in order to obtain a better description of soil organic matter
610 decomposition. Additionally, as a balanced system, the differences in the organic
611 nitrogen plant residue input between models are associated to the different

612 mineralization values, but these differences were only noteworthy for TETIS-CN from
613 October to November, when mineralization was overestimated. Its correction functions
614 of soil water content and temperature vary in a wider range and consequently, BIOME
615 and LEACHM are more stable. However, in both years 2012 and 2013, during the month
616 of October, the temperature was still elevated, and as it rained, mineralization was
617 overestimated in TETIS-CN.

618 Regarding plant uptake and leaching, the results were very different. Since BIOME
619 includes plant growth, the model simulated root growth towards deep layers (8 m depth),
620 where water was available, reducing the percentage of roots in the first 15 cm of soil and
621 consequently, the nitrogen plant uptake from these soil layers. Conversely, roots depth
622 in LEACHM and TETIS-CN were smaller, being the percentage in these first 15 cm of
623 soil higher. LEACHM potential uptake in the first 15 cm was 26.77 kgN ha⁻¹ year⁻¹, while
624 TETIS-CN was 39.69 kgN ha⁻¹ year⁻¹, resulting in a higher plant uptake and smaller
625 leaching than the other two models. Therefore, all these results suggest that NO₃⁻-N plant
626 uptake could be underestimated, and consequently the models showed a leaching
627 overestimation (Verburg and Johnson, 2001).

628 In line with this, NO₃⁻-N soil content was heavily overestimated during the warm months
629 with scarce precipitation, reinforcing the idea that NO₃⁻-N plant uptake was not properly
630 represented, because nitrification measurements were well represented, which is the
631 only NO₃⁻-N input considered, denitrification is not a noteworthy flux and leaching was
632 overestimated only during these months. Firstly, this can be explained because in this
633 plot, *Q. ilex* coexists with other species, which were not considered in this case study.
634 These nitrogen field measurements are representative of the first 15 cm of soil, and
635 although *Q. faginea* and *P. halepensis* have deeper root systems (Baquedano and
636 Castillo, 2007), it should be highlighted that *J. oxycedrus* and *J. phoenicea* have shallow
637 root systems (Castillo et al., 2002; Gazol et al., 2017), especially the former, which
638 develops most of its roots in the first 15 cm of soil (Castillo et al., 2002). Therefore, the
639 NO₃⁻-N plant uptake by other species, not considered here, may be significant. Secondly,

640 the consideration of a fixed daily potential uptake may have led to an oversimplified
641 representation of the nitrogen plant uptake in the case of LEACHM and TETIS-CN. Due
642 to the seasonal variations of VPD in Mediterranean areas, during the warm periods,
643 which coincides with the growing season, transpiration is higher, especially in spring
644 when soil water is not too limiting (Limousin et al., 2009), and consequently *Q. ilex* NO₃⁻-
645 N plant uptake also changes seasonally (Bonilla and Rodà, 1992). Thus, considering a
646 fixed daily potential uptake may become an error in the conceptualization that could
647 probably be solved coupling the models to a vegetation growth model. However, in spite
648 of considering vegetation growth, BIOME presented the same problem making the first
649 option more probable.

650 **5 Conclusions**

651 In this study, three carbon and nitrogen models, with different conceptualization,
652 complexity and purpose, were calibrated in an experimental *Q. ilex* forest plot, with two
653 objectives. Firstly, contributing to a better understanding and modelling of the
654 hydrological and biogeochemical cycles (carbon and nitrogen) and their interaction within
655 the soil-plant continuum in semiarid conditions, and secondly, testing the capability of a
656 new parsimonious carbon and nitrogen sub-model to satisfactorily reproduce them. In
657 this sense, the three models were able to reproduce the hydrological behaviour of a *Q.*
658 *ilex* forest. However, BIOME presented over-parameterization problems, decreasing its
659 performance during the validation period and TETIS-CN showed a higher dependence
660 of *Q. ilex* on groundwater resources. Due to its simple representation of interception, it
661 was underestimated and soil evaporation was overestimated. Therefore, it is clear this
662 problem could be solved if its vegetation dynamic sub-model is used (i.e., considering
663 the vegetation growth).

664 In terms of biogeochemistry, BIOME and LEACHM showed an underestimation of the
665 organic carbon plant residue input, and consequently also of the heterotrophic soil
666 respiration. This was probably caused because no carbon measurement was included

667 in the calibration process and the available measurements were not enough to measure
668 all the characteristics of the system. Therefore, if no carbon measurement is available
669 the nitrogen performance of these models may be good, but the carbon cycle may not
670 be properly reproduced. In the case of TETIS-CN, the default parameters were able to
671 satisfactorily reproduce the heterotrophic respiration measurements in this case study,
672 but in other applications, it may present this same problem. Regarding to the nitrogen
673 performance of the models, NO₃⁻-N soil content and mineral nitrogen leaching were
674 overestimated, suggesting that NO₃⁻-N plant uptake may be underestimated. This
675 problem may be firstly explained because *Q. ilex* coexists with other species with a
676 different behaviour whose plant uptake may be significant. Secondly, in the case of
677 LEACHM and TETIS-CN, a fixed daily potential uptake may not be appropriate to
678 reproduce plant nitrogen uptake, which presents a clear seasonality. Therefore, it is
679 important to consider all the species, although scarce, and in the case of LEACHM and
680 TETIS-CN, to couple them to a vegetation growth model.

681 Finally, it is worth noting that none of the models stood out from the rest in reproducing
682 the hydrology and the biogeochemistry of this experimental plot. Hence, the similarity
683 between the results demonstrates that TETIS-CN, with a lower number of parameters,
684 is an acceptable tool to be applied to reproduce the carbon and nitrogen dynamics in
685 Mediterranean drylands.

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987

988 **Appendix A.**

Parameter	Units	Value
PLANT FUNCTIONING PARAMETERS		
Transfer growth period as fraction of growing season	Prop.	0.80
Litterfall as fraction of growing season	Prop.	0.80
Base temperature	°C	10
Minimum temperature for growth displayed on current day	°C	0
Optimal1 temperature for growth displayed on current day	°C	11
Optimal2 temperature for growth displayed on current day	°C	28
Maximum temperature for growth displayed on current day	°C	40
Minimum temperature for carbon assimilation displayed on current day	°C	0
Optimal1 temperature for carbon assimilation displayed on current day	°C	12
Optimal2 temperature for carbon assimilation displayed on current day	°C	28
Maximum temperature for carbon assimilation displayed on current day	°C	40
Annual leaf and fine root turnover fraction	yr ⁻¹	0.20
Annual live wood turnover fraction	yr ⁻¹	0.30
Annual whole-plant mortality fraction	yr ⁻¹	0.02
Annual fire mortality fraction	yr ⁻¹	0
C:N of leaves	kgC kgN ⁻¹	37.50

C:N of leaf litter, after retranslocation	kgC kgN ⁻¹	46.50
C:N of fine roots	kgC kgN ⁻¹	43
C:N of fruit	kgC kgN ⁻¹	47
C:N of soft stem	kgC kgN ⁻¹	0.00
C:N of live wood	kgC kgN ⁻¹	73.50
C:N of dead wood	kgC kgN ⁻¹	651
Leaf litter labile proportion	[-]	0.20
Leaf litter cellulose proportion	[-]	0.56
Fine root labile proportion	[-]	0.34
Fine root cellulose proportion	[-]	0.44
Fruit litter labile proportion	[-]	0.30
Fruit litter cellulose proportion	[-]	0.29
Soft stem litter labile proportion	[-]	0.00
Soft stem litter cellulose proportion	[-]	0.00
Dead wood cellulose proportion	[-]	0.75
Canopy water interception coefficient	LAI ⁻¹ d ⁻¹	0.25
Canopy light extinction coefficient	[-]	0.36
Potential radiation use efficiency	g MJ ⁻¹	2
Radiation parameter1 (Jiang et al.2015)	[-]	0.78
Radiation parameter2 (Jiang et al.2015)	[-]	13.60
All-sided to projected leaf area ratio	[-]	2
Ratio of shaded SLA:sunlit SLA	[-]	2
Fraction of leaf N in Rubisco	[-]	1.13e-2
Fraction of leaf N in PEP Carboxylase	[-]	1e-4
Maximum stomatal conductance (projected area basis)	m s ⁻¹	9e-03
Cuticular conductance (projected area basis)	m s ⁻¹	7e-04
Boundary layer conductance (projected area basis)	m s ⁻¹	5e-4
Relative SWC (prop. to FC) to calc. soil moisture limit 1	Prop.	0.35
Relative SWC (prop. to SAT) to calc. soil moisture limit 2	Prop.	0.68
Relative PSI (prop. to FC) to calc. soil moisture limit 1	Prop.	-9999
Relative PSI (prop. to SAT) to calc. soil moisture limit 2	Prop.	-9999
Vapor pressure deficit: start of conductance reduction	Pa	100
Vapor pressure deficit: complete conductance reduction	Pa	800.78
Maximum height of plant	M	8.50
Stem weight at which maximum height attended	kgC m ⁻²	150
Maximum depth of rooting zone	m	8
Root distribution parameter	[-]	54.48
Root length parameter 1 (estimated max root weight)	kgC m ⁻²	0.40
Root length parameter 2 (slope)	Prop.	0.50
Growth respiration per unit of C grown	Prop.	0.40
Maintenance respiration in kgC/day per kg of tissue N	kgC kgN ⁻¹ d ⁻¹	8.8e-2
Theoretical maximum prop. of non-structural and structural carbohydrates	[-]	0.10
Prop. of non-structural carbohydrates available for maintenance respiration	[-]	0.30
Symbiotic + asymbiotic fixation of N	kgN m ⁻² yr ⁻¹	5e-4
SCENESCENCE AND SOIL PARAMETERS		

Maximum senescence mortality coefficient of aboveground plant material	Prop.	0.03
Maximum senescence mortality coefficient of belowground plant material	Prop.	0.03
Maximum senescence mortality coefficient of non-structured plant material	Prop.	0
Effect of extreme high temperature on senescence mortality	Prop.	2
Lower limit extreme high temperature effect on senescence mortality	°C	45
Upper limit extreme high temperature effect on senescence mortality	°C	50
Maximal lifetime of plant tissue	°C	-9999
Turnover rate of wilted standing biomass to litter	Prop.	0.01
Turnover rate of non-woody cut-down biomass to litter	Prop.	0.05
Turnover rate of woody cut-down biomass to litter	Prop.	0.01
Drought tolerance parameter (critical value of DSWS)	Prop.	90
Denitrification rate per g of CO ₂ respiration of SOM	Prop.	0.08
Nitrification coefficient 1	Prop.	0.30
Nitrification coefficient 2	Prop.	0.10
Coefficient of N ₂ O emission of nitrification	Prop.	0.02
Proportion of NH ₄ flux of N-deposition	Prop.	0.80
NH ₄ mobile proportion	Prop.	0.90
NO ₃ mobile proportion	Prop.	1
e-folding depth of decomposition rate's depth scalar	m	10
Fraction of dissolved part of SOIL1 organic matter	Prop.	1e-3
Fraction of dissolved part of SOIL2 organic matter	Prop.	1e-3
Fraction of dissolved part of SOIL3 organic matter	Prop.	1e-3
Fraction of dissolved part of SOIL4 organic matter	Prop.	1e-3
Ratio of bare soil evaporation and pot. evaporation	[-]	10
RATE SCALARS		
Resp. fractions for fluxes between compartments (l1s1)	[-]	0.39
Res. fractions for fluxes between compartments (l2s2)	[-]	0.55
Resp. fractions for fluxes between compartments (l4s3)	[-]	0.29
Resp. fractions for fluxes between compartments (s1s2)	[-]	0.28
Resp. fractions for fluxes between compartments (s2s3)	[-]	0.46
Resp. fractions for fluxes between compartments (s3s4)	[-]	0.55
Rate constant scalar of labile litter pool	[-]	0.70
Rate constant scalar of cellulose litter pool	[-]	0.07
Rate constant scalar of lignin litter pool	[-]	1.40e-2
Rate constant scalar of fast microbial recycling pool	[-]	0.07
Rate constant scalar of medium microbial recycling pool	[-]	1.40e-2
Rate constant scalar of slow microbial recycling pool	[-]	1.40e-3
Rate constant scalar of recalcitrant SOM (humus) pool	[-]	1e-4
Rate constant scalar of physical fragmentation of coarse woody debris	[-]	1e-3
GROWING SEASON PARAMETERS		
Critical amount of snow limiting photosynthesis	kg m ⁻²	5
Limit1 (under:full constrained) of HEATSUM index	°C	20

Limit2 (above:unconstrained) of HEATSUM index	°C	60
Limit1 (under:full constrained) of TMIN index	°C	0
Limit2 (above:unconstrained) of TMIN index	°C	5
Limit1 (above:full constrained) of VPD index	Pa	4000
Limit2 (under:unconstrained) of VPD index	Pa	1000
Limit1 (under:full constrained) of DAYLENGTH index	s	0
Limit2 (above:unconstrained) of DAYLENGTH index	s	0
Moving average (to avoid the effects of extreme events)	day	10
GSI limit1 (greater that limit -> start of vegper)	[-]	0.10
GSI limit2 (less that limit -> end of vegper)	[-]	0.01
CH4 PARAMETERS		
Param1 for CH4 calculations (empirical function of BD)	[-]	212.50
Param2 for CH4 calculations (empirical function of BD)	[-]	1.81
Param1 for CH4 calculations (empirical function of VWC)	[-]	-1.35
Param2 for CH4 calculations (empirical function of VWC)	[-]	0.20
Param3 for CH4 calculations (empirical function of VWC)	[-]	1.78
Param4 for CH4 calculations (empirical function of VWC)	[-]	6.79
Param1 for CH4 calculations (empirical function of Tsoil)	[-]	0.01
PHENOLOGICAL PARAMETERS		
Length of phenophase (growing degree days). Phase 1	°C	500
Length of phenophase (growing degree days). Phase 2	°C	200
Length of phenophase (growing degree days). Phase 3	°C	500
Length of phenophase (growing degree days). Phase 4	°C	200
Length of phenophase (growing degree days). Phase 5	°C	400
Length of phenophase (growing degree days). Phase 6	°C	200
Length of phenophase (growing degree days). Phase 7	°C	100
Leaf allocation. Phase 1 to phase 7	Ratio	0.40
Fine root allocation. Phase 1 to phase 7	Ratio	0.20
Fruit allocation. Phase 1 to phase 7	Ratio	0.20
Soft stem allocation. Phase 1 to phase 7	Ratio	0.00
Live woody stem allocation. Phase 1 to phase 7	Ratio	0.1
Dead woody stem allocation. Phase 1 to phase 7	Ratio	0.00
Live coarse root allocation. Phase 1 to phase 7	Ratio	0.10
Dead coarse root allocation. Phase 1 to phase 7	Ratio	0.00
Canopy average specific leaf area. Phase 1 to phase 7	m ² kgC ⁻¹	9.81
Current growth proportion. Phase 1 to phase 7	Prop.	0.5

989 **Table A.1** BIOME parameter values after the calibration process.

Parameter	Units	Value
Mineral nitrogen fixed	kgN ha ⁻¹ yr ⁻¹	0
Plant death constant	gC m ⁻² d ⁻¹	0.31
Plant residue input C/N ratio	[-]	21.60
Biomass and humus C/N ratio	[-]	14
Synthesis efficiency factor	[-]	0.20
Humification factor	[-]	0.55
Residue mineralization rate (layers 1-3)	day ⁻¹	1.39e-3
Humus mineralization rate (layers 1-3)	day ⁻¹	4.52e-6
Manure mineralization rate (layers 1-3)	day ⁻¹	0.00

NH ₄ ⁺ distribution coefficient	dm ³ kg ⁻¹	6.85
Molecular diffusion coefficient	mm ² day ⁻¹	120
Volatilization rate	day ⁻¹	0.24
Nitrification rate (layers 1-3)	day ⁻¹	7.14e-2
Denitrification rate (layers 1-3)	day ⁻¹	0.57
Plant nitrogen potential uptake	kgN ha ⁻¹ yr ⁻¹	61.84
Base temperature	°C	20
Q ₁₀	[-]	2.22
High end of optimum water content range	[-]	0.08
Lower end of optimum water content	kPa	-162.23
Minimum matric potential for transformation	kPa	-1000
Relative transformation rate at saturation	day ⁻¹	0.6
Urea hydrolysis	day ⁻¹	0.00
Denitrification half-saturation constant	mg l ⁻¹	10
Limiting NO ₃ /NH ₄ ratio in solution for nitrification	[-]	7.40

990 **Table A.2** LEACHM parameter values after the calibration process.

991

Parameter	Units	Value
Plant death constant	gC m ⁻² d ⁻¹	0.72
Plant residue input C/N ratio	[-]	28.94
Humus C/N ratio	[-]	20
Biomass C/N ratio	[-]	8
Respiration rate	[-]	0.6
Humification factor	[-]	0.25
Litter decomposition rate	m ³ d ⁻¹ gC ⁻¹	8.00e-6
Humus decomposition rate	m ³ d ⁻¹ gC ⁻¹	3.55e-7
Microbial biomass death rate	day ⁻¹	2.64e-3
NH ₄ ⁺ distribution coefficient	dm ³ kg ⁻¹	8.89
Volatilization rate	day ⁻¹	1.29e-2
Nitrification rate	m ³ d ⁻¹ gC ⁻¹	2.78e-2
Denitrification rate	day ⁻¹	3.84e-2
Plant nitrogen potential uptake	kgN ha ⁻¹ yr ⁻¹	118.82
Diffusion coefficient	m d ⁻¹	0.33
Soil moisture threshold for soil water content correction function	cm cm ⁻¹	0.19
Maximum temperature difference	°C	1.16
Optimum temperature	°C	30
Minimum temperature	°C	-5

992 **Table A.3** TETIS-CN parameter values after the calibration process.