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# 1 AqYield-N: A simple model to predict 2 nitrogen leaching from crop fields

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## 11 **Abstract**

12 Evaluating and improving cropping systems is essential to reduce nitrate leaching, improve drinking  
13 water quality and prevent eutrophication. Since the intensity of nitrogen (N) leaching varies greatly  
14 spatially and is difficult to measure, crop models are useful tools to quantify the influence of climate, soil  
15 and agricultural practices on N leaching. Our objective was to develop a simple model with low input  
16 data and calibration requirements to predict nitrate leaching from a variety of crop fields over large  
17 areas, such as watersheds, for which data are often limited. The AqYield model is a simple model with  
18 few inputs that has estimated sufficiently well drainage and water flows for several crops and rotations.  
19 Based on this model, we developed AqYield-N, which considers the major N flows in the soil–plant  
20 system, including mineralization, plant uptake and leaching at a daily time step. The present study  
21 presents the development and formalisms of AqYield-N. We developed AqYield-N based on simple and  
22 robust formalisms and low requirements for input data and parameters. As much as possible, we used  
23 equations already published and validated in the scientific literature. We then evaluated AqYield-N using  
24 observed experimental N leaching data. Its estimates were satisfactory for three contrasting  
25 pedoclimatic situations and for various crops and bare soil. Although the model is simple and requires

26 only a few inputs, it was as accurate as more complex crop models widely used and evaluated in the  
27 agronomic literature, such as STICS. The study demonstrated the potential of AqYield-N to estimate the  
28 influence of management practices on N leaching. AqYield-N, whether alone or integrated in larger-scale  
29 modeling approaches, can be used to predict leaching during crop rotations at field and large scale to  
30 evaluate the influence of various agroecological practices on N leaching.

31 **Keywords:** Soil-crop model, N uptake, N mineralization, nitrate, evaluation, model development

## 32 **1 Introduction**

33 Nitrate leaching, which pollutes water, has become a major problem worldwide, mainly due to the  
34 intensification of agricultural production involving the application of nitrogen (N) fertilizers and organic  
35 waste in the past 50 years. Water pollution from agriculture is a significant pressure for rivers, lakes and  
36 coastal water bodies (Taylor et al., 2016). Pollution of groundwater and surface water has consequences  
37 for the health of aquatic ecosystems, biodiversity, human health, water use in industry and agriculture,  
38 and water as a public water supply (Carr and Neary, 2008; Di and Cameron, 2002). Improving cropping  
39 practices to reducing nitrate leaching is essential to improve the quality of drinking water and prevent  
40 eutrophication. Since the intensity of leaching varies greatly spatially, estimates of total N leaching for  
41 large areas of arable land are uncertain. Several factors influence N leaching, such as soil texture,  
42 availability of mineral N in the soil, excess rainfall, crop management and hydrogeological characteristics  
43 (Köhler et al., 2006; Silgram et al., 2008; Singh and Sekhon, 1977).

44 Soil-crop models are useful tools to quantify the influence of climate, soil and agricultural practices on  
45 nitrate leaching (Hoffmann and Johnsson, 1999). These models can be distributed over a large area to  
46 quantify the influence of agricultural practices on nitrate leaching at a large scale (Wagenet and Hutson,  
47 1996). [They can be applied on a small region or watershed of few km<sup>2</sup>, on large watershed of hundreds  
48 of km<sup>2</sup> or a whole country.](#) Linking a soil-crop model to current climates, agricultural soils, cropping  
49 practices and a given agricultural region allows prediction of N leaching at the large scale for current and

50 alternative scenarios of improved agricultural practices, its impact on water quality (Hall et al., 2001) and  
51 the potential of these improved practices to decrease water pollution. Model assessment depends on  
52 the realism of its formalisms, the quality of calibration and the reliability of input data (Loague and  
53 Corwin, 1996). However, the availability of data for calibration or model input is often an obstacle to  
54 applying soil-crop models at a high resolution over large areas (Therond et al., 2009). For regional  
55 assessments, the model must consider large areas that have contrasting soils, climates and management  
56 practices. Estimating the influence of multiple cropping systems and pedoclimatic conditions in a region  
57 requires a robust and generic model that can simulate a variety of crops (e.g. spring and winter cash  
58 crops, cover crops) and crop management practices (e.g. sowing dates, crop rotations). Many crop  
59 models require considerable calibration and many inputs, which can result in a lack of adequate and  
60 sufficient data to run the model at a large scale, such as a region or watershed (Faivre et al., 2004). In  
61 this context, using a simple model with simple formalisms, low input data requirements and as few  
62 parameters as possible, is necessary to accurately estimate leaching at this scale under current  
63 conditions. Since N dispersal in the soil depends strongly on soil water fluxes, one key issue for modeling  
64 N leaching is to estimate these water flows accurately (Addiscott and Wagenet, 1985).

65 The soil-crop model AqYield is a simple and generic model that demonstrated its ability to simulate  
66 dynamic water balance components (soil water content and evapotranspiration) as accurately as a more  
67 complex model for a variety of crop species, crop rotations and management practices (Constantin et al.,  
68 2015; Tribouillois et al., 2018). These two studies demonstrated the model's ability to simulate water  
69 flows with good accuracy, particularly evapotranspiration and water drainage, highlighting the potential  
70 to develop an additional module that estimates nitrate leaching. AqYield has already been applied at the  
71 watershed scale in MAELIA, the integrated simulation platform that can also simulate hydrology  
72 (Therond et al., 2014), since it requires only a few inputs. Crop models can be combined with  
73 hydrological models to study interactions between agricultural practices and the physical characteristics

74 of watersheds (Ferrant et al., 2011; Martin et al., 2016). This combination with hydrological models  
75 enables analysis of impacts of agricultural management on water flows in rivers, levels of pollution and  
76 interactions between water resources in the watershed and irrigation requirements (Cannavo et al.,  
77 2008). Due to its strong parsimony of equations and parameters, it has the advantage of easier  
78 calibration and shorter calculation times and requires only basic input data that are easily collected at a  
79 large scale. These properties also allow to avoid the “black box” effect that results from a lack of  
80 transparent internal structure and a complicated model behavior (Constantin et al., 2015).

81 Our objective was to develop a simple model with low input data and calibration requirements to  
82 estimate nitrate leaching from a variety of crop fields. Considering its simplicity and effectiveness at  
83 simulating water flows, we developed a complementary module for AqYield to estimate leaching at a  
84 large scale, since it is already integrated into the MAELIA simulation platform. This new module can  
85 estimate nitrate leaching within an agricultural region for several types of cropping system options. We  
86 first present the modeling approach, the model structure and the equations for the new formalisms. We  
87 then present results of its evaluation by comparing its leaching estimates to observed leaching data and  
88 to estimates of a more complex soil-crop model, STICS (Brisson et al., 2003).

## 89 **2 Materials and methods**

### 90 **2.1 AqYield overview**

91 The AqYield model is a simple dynamic soil-crop model that estimates water fluxes at the field scale at a  
92 daily time step. It was previously calibrated and evaluated for spring crops with and without irrigation  
93 under various pedoclimatic conditions in southern France (Constantin et al., 2015) and for winter crops,  
94 both separately and in rotations (Tribouillois et al., 2018). Its ability to estimate soil water content  
95 dynamics, water drainage and evapotranspiration under crops or bare soil has been assessed as  
96 satisfactory. The model simulates daily water balance components, phenological stages and annual crop

97 yield. It requires a few inputs: three soil properties (clay content, soil available water capacity and soil  
98 depth), three daily climate features (daily mean temperature, rainfall and reference evapotranspiration)  
99 and the dates of sowing, harvest, irrigation and tillage as well as the amount of irrigation and soil tillage  
100 depth for crop management. Its simplicity comes mainly from not simulating biomass; instead, the  
101 influence of crop development on water fluxes is considered using only a crop coefficient ( $K_c$ ). The  $K_c$   
102 varies according to crop (i.e. phenology, maximum  $K_c$ ) and pedoclimate (i.e. day length, daily mean  
103 temperature and water stress). It influences evaporation and maximum transpiration, which determine  
104 the soil water available for the crop. Soil is represented using a classic tipping-bucket approach and the  
105 concept of available water capacity. Detailed description of equations used in AqYield is provided in  
106 Constantin et al. (2015) and Tribouillois et al. (2018).

## 107 **2.2 Modeling approach used to develop AqYield-N**

108 AqYield-N was based on the functioning of AqYield to estimate N leaching at the field scale at a daily  
109 time step, like for water fluxes. We developed AqYield-N by keeping the same objectives as those of  
110 AqYield: simple formalisms and low requirements for input data and parameters. To obtain an efficient  
111 simple model, we used, as much as possible, equations already published and validated in the scientific  
112 literature. We identified the key processes and most important N inputs, outputs and stocks of the soil-  
113 plant system needed to estimate N leaching: mineral N fertilization and associated N gas losses, N  
114 mineralization from organic residues and soil organic matter, soil mineral N content (SMN) and its  
115 transfer in the soil, crop N uptake and N leaching. Like other models that simulate N leaching,  $N_2O$  and  $N_2$   
116 gas emissions from the soil were not represented, since they represent a negligible loss of N compared  
117 to that lost by leaching (Stenberg et al., 2012; Webb et al., 2000). For example, total  $N_2$  and  $N_2O$  losses  
118 have been estimated at less than  $10 \text{ kg N ha}^{-1} \text{ yr}^{-1}$  for unfertilized crops in a wheat-maize cropping system  
119 (Chen et al., 2019). For N volatilization losses, according to the review of Bussink and Oenema (1998),

120 losses from ammonium nitrate-based fertilizers are generally less than 5% of total N. These authors also  
121 observed that soils and crops are not a major source of NH<sub>3</sub>, with a net loss from crops less than 2 kg NH<sub>3</sub>  
122 ha<sup>-1</sup> yr<sup>-1</sup> in fertilized fields, and even less in unfertilized fields. As a result, these processes were not  
123 included in the AqYield-N module to estimate nitrate leaching.

124 Soil is divided into three successive layers, functioning as a tipping bucket with water and N transfer  
125 downwards. N leaching from fields is the N transfer from the deepest layer.

126 The general approach included four steps:

127 1) We investigated whether the scientific literature contained formalisms that were already  
128 evaluated and published for each key process. The chosen formalisms must be simple, require  
129 few inputs and be generic enough to apply to the wide range of pedoclimatic conditions and  
130 cropping systems.

131 2) When no corresponding formalism was found, we developed simple equations from a more  
132 complex model already evaluated and published in the scientific literature. Since AqYield does not  
133 represent biomass, and we found no formalism linking K<sub>c</sub> and N uptake, we developed equations  
134 for the daily N demand by crops without requiring data on biomass.

135 3) We evaluated AqYield-N's estimates of N leaching under crop fields by comparing them to  
136 observed data on N leaching in a variety of experimental field situations.

137 4) We compared our model to a more complex model already evaluated as accurate for estimating  
138 leaching.

### 139 **2.3 Experimental data for evaluating leaching**

140 We evaluated estimated N leaching by comparing it to data observed from three contrasting  
141 experimental sites in western and northern France that included different crops (Table 1). Kerlavic  
142 (Bretagne) has a humid climate and a large amount of soil organic matter, while Boigneville (Ile-de-

143 France) and Thibie (Champagne-Ardenne) are drier and have less soil organic matter. Thibie has higher  
 144 available water capacity than Boigneville.

145 **Table 1. Description of the three sites whose experimental results were used to evaluate N leaching**  
 146 **estimates of AqYield-N**

Site	Crop	Years	Clay content (%)	AW* capacity (mm)	SOM content (%)	C:N	Bulk density	Rainfall (mm yr <sup>-1</sup> )	Initial SMN (kg N ha <sup>-1</sup> )	Initial AW content (%)	Leaching period measurement
Boigneville	Wheat	3	23	173	2.0	9.5	1.4	643	[51;75]	[24;53]	[Aug-Nov][Nov-Feb]
	Silage maize	4							[32;54]	[77;100]	[Mar-Oct]
Kerlavic	Wheat	3	16	213	4.8	10.7	1.2	1138	[57;73]	[69;100]	[Mar-Aug]
	Italian ryegrass	3							[25;69]	[10;71]	[Aug-Mar]
	Bare soil	3							[26;62]	[2;99]	[Aug-Mar]
Thibie	Wheat	3	9	213	2.6	9.5	1.4	687	[87;108]	[59;85]	[Oct-Feb][Feb-Aug]

147 AW is available water. SOM is soil organic matter. SMN is soil mineral nitrogen. AWC is available water content. Minimum and  
 148 maximum values are given between brackets.

149 In the three experiments, N leaching was measured under two crops (wheat and silage maize) and fallow  
 150 fields with and without a cover crop (Italian ryegrass or bare soil), which represents 19 different  
 151 situations. Some experiments were separated into two leaching periods, resulting in 28 leaching  
 152 situations for model evaluation. Cumulative leaching over a given period was the mean of three  
 153 experimental field replicates. For each site, drained water was measured in lysimeters under soil  
 154 managed in the same way as the fields. For each experimental field, nitrate concentrations were  
 155 measured using porous cups installed 90-110 cm deep (7 porous cups were pooled to make one  
 156 replicate). N leaching was calculated using the trapezoidal method (Lord and Sheperd, 1993), using the  
 157 drainage amount between two measurement dates in the porous cups and the nitrate concentrations on  
 158 the two dates. More details about the sites and the leaching measurements and calculations are  
 159 available in Constantin et al. (2010).

160 Each simulation used to evaluate leaching was initialized between the harvest of the preceding crop and  
 161 sowing of the next one, using the mean SMN and available water content (AWC) measured for a given  
 162 crop (mean of the 3 replicates). The initialization date was always before the start of the leaching



163 measurement period. Depending on the year and crop, initialization conditions and leaching values  
164 differed among years, providing a wide range of situations for evaluation. Simulations were run from the  
165 initialization to the end of the leaching measurement period. The leaching estimated by AqYield-N was  
166 compared to that observed for the same measurement period.

## 167 **2.4 Use of the STICS model**

168 The STICS soil-crop model is a dynamic model that simulates, at a daily time step, crop development and  
169 carbon and N uptake as a function of climate, soil characteristics, and crop management (Brisson et al.,  
170 2003, 1998). Like AqYield, STICS does not consider pests or diseases. It has been widely calibrated and  
171 evaluated in the scientific literature, especially for N leaching (Constantin et al., 2012), but also for N  
172 uptake, plant biomass and soil moisture content for more than 15 crops in a wide range of temperate  
173 pedoclimatic conditions (Coucheney et al., 2015).

174 We used STICS simulations in two steps:

- 175 1) During model development, to identify key points or phenological stages for potential N uptake  
176 curves of crops: wheat, sunflower, maize, rapeseed, soybean, fava bean and cover crops. We  
177 used STICS because it was evaluated as “very good” for estimating crop N uptake during the  
178 growing season (Coucheney et al., 2015). We assumed that it correctly estimated N uptake  
179 dynamics.
- 180 2) During model evaluation, in addition to comparing AqYield-N estimates of N leaching to  
181 observed leaching, we compared them to those of STICS. This reinforced the evaluation of the  
182 simpler AqYield-N by comparing its estimates to those of a more complex and calibrated model.  
183 STICS was run for the same situations as those used to evaluate AqYield-N, with the same  
184 initialization, climate, soil and management practices, and during the same periods. The same  
185 statistical criteria were calculated to compare the ability of both models to estimate N leaching.

## 186 2.5 Statistical analysis for model evaluation

187 To evaluate estimates of N leaching, three statistical criteria — mean deviation (MD), relative root mean  
188 square error (rRMSE) and model efficiency (Ef) — were calculated.

$$189 \quad MD = \frac{1}{n} \sum_{i=1}^n (S_i - O_i) \quad (\text{Eq. 1})$$

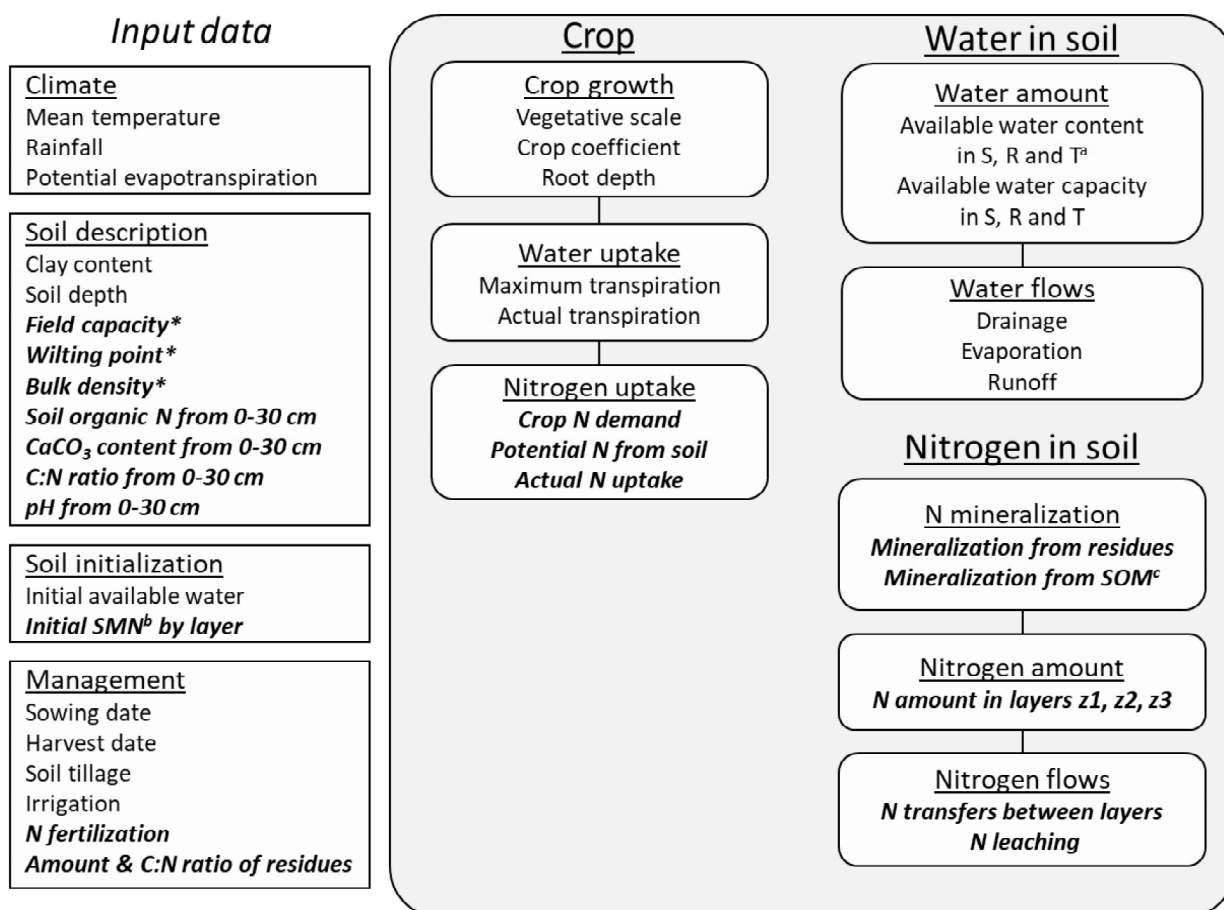
$$190 \quad rRMSE = \frac{\sqrt{\frac{1}{n} \sum_{i=1}^n (S_i - O_i)^2}}{\bar{o}} \quad (\text{Eq. 2})$$

$$191 \quad Ef = 1 - \frac{\sum_{i=1}^n (S_i - O_i)^2}{\sum_{i=1}^n (O_i - \bar{o})^2} \quad (\text{Eq. 3})$$

192 where n is the number of observations,  $O_i$  and  $S_i$  are observed and simulated values, respectively, and  $\bar{o}$   
193 is the mean of observed values. MD provides the deviation of estimates from the line  $x=y$ . rRMSE  
194 provides the relative absolute error and ranges from 0 to infinity, with 0 as the ideal. Ef represents model  
195 accuracy relative to the mean of observed data (range = -∞ to 1). As Ef approaches 1, the similarity  
196 between observed and estimated values increases; it becomes negative when the mean of observed  
197 values lies closer to observed values than to estimated values. The mean difference between observed  
198 and estimated values of leaching was also calculated in absolute value.

## 199 3 Results

### 200 3.1 AqYield-N overview



201 **Figure 1. Description of model inputs (left), modules (in the gray box) and associated variables of AqYield-N.**

202 Original variables and inputs of AqYield are in normal font, new variables and inputs for AqYield-N are in bold  
 203 italics. <sup>a</sup>S, R and T are the shallow, root and total soil compartments, respectively. <sup>b</sup> SMN is soil mineral nitrogen. <sup>c</sup>  
 204 SOM is soil organic matter. \* These three inputs replace the “available water capacity” (AWC) previously used in  
 205 AqYield, since AWC can be calculated from them and soil depth.  
 206

207 The N model was developed like other modules of AqYield, with the goal of adding as few inputs as  
 208 possible (Fig. 1). AqYield-N consists of four new modules: crop N uptake, N mineralization, amount of N  
 209 in the soil and N flows in the soil. Only nine new inputs were necessary, mainly for soil description.

### 210 3.2 Model structure and equations

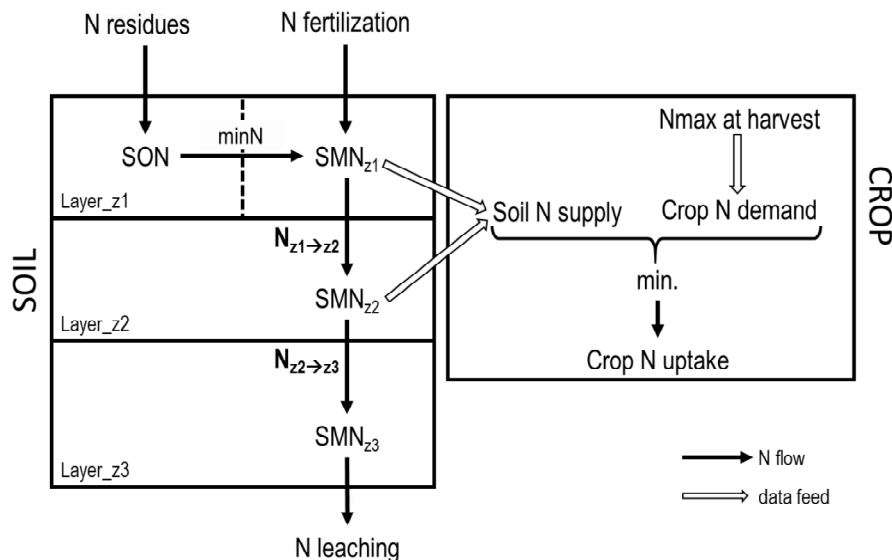
211 The formalisms of AqYield, available in Constantin et al. (2015), were not modified. The N module of  
 212 AqYield-N contains new variables related to N dynamics (Table 2).

213 **Table 2. Name, description, unit and time step of the new variables used in the equations of the N module of**  
 214 **AqYield-N.** All variables are calculated at a daily time step, except for  $N_{max}$ , which is calculated once per cropping  
 215 season.

Variable name	Description	Unit
$AWC_{z_i}$	Available water content (amount of water available in layer $z_i$ )	mm
$maxAWC_{z_i}$	Maximum available water content (in layer $z_i$ )	mm
$Dr$	Amount of water outgoing beyond soil depth	mm
$W_{z_i \rightarrow z_j}$	Amount of water transferred from layers $i$ to $j$	mm
$minN$	Amount of N provided by mineralization from SOM (soil organic matter) and residues	kg N ha <sup>-1</sup>
$N_{demand}$	Amount of N required by the crop	kg N ha <sup>-1</sup>
$N_{ferti}$	Amount of N provided by fertilization and available in layer $z_1$	kg N ha <sup>-1</sup>
$N_{leach}$	Amount of N lost by leaching beyond soil depth	kg N ha <sup>-1</sup>
$N_{max}$	Maximum crop N uptake at harvest	kg N ha <sup>-1</sup>
$N_{uptake}$	Amount of crop N uptake	kg N ha <sup>-1</sup>
$N_{z_i \rightarrow z_j}$	Amount of N transferred from layer $i$ to $j$	kg N ha <sup>-1</sup>
$PotN_{Soil}$	Amount of N in soil that plants can potentially take up	kg N ha <sup>-1</sup>
$SON$	Amount of soil organic N in layer $z_1$	t N ha <sup>-1</sup>
$SMN_{afUp}$	Amount of soil mineral N in layer after N uptake and before N transfer	kg N ha <sup>-1</sup>
$SMN_{z_i}^f$	Amount of soil mineral N in layer $z_i$ after N transfer	kg N ha <sup>-1</sup>
$SMN_{z_i}^i$	Amount of soil mineral N in layer $z_i$ before N uptake and N transfer	kg N ha <sup>-1</sup>

216 **3.2.1 Amount of water in soil layers and water transfers**

217 In AqYield, soil is represented by compartments characterized by a depth and a maximum AWC. To  
 218 adapt the N module to AqYield, we redefined the soil into superimposed layers instead of nested  
 219 compartments (Fig. 2).



220  
 221 **Figure 2. Description of the new process represented by AqYield-N.** SON is Soil Organic N, SMN is soil mineral N, and minN is  
 222 net N mineralization.  $N_{z_i \rightarrow z_j}$  is the N transfer from layer  $z_i$  to layer  $z_j$ .

223 We thus recalculated the amount of water in each layer based on AqYield simulations. Layer\_z1  
 224 extends from 0-30 cm deep. Layer\_z2 extends from 30 cm deep to the rooting depth. Layer\_z3  
 225 extends from the rooting depth to the bottom of the soil (soil depth). Layer\_z2 and Layer\_z3 thus  
 226 differ in thickness, available water capacity and amount of SMN as a function of rooting depth.

227 The amount of water in the first layer z1 ( $AWC_{z1}$ ) was already available in the model since it is the  
 228 AWC from 0-30 cm. For the two other layers, it was calculated (in mm) as follows:

229 - layer z2:  $AWC_{z2} = RootAWC - AWC_{z1}$  (Eq. 4)

230 - layer z3 :  $AWC_{z3} = TotAWC - RootAWC$  (Eq. 5)

231 with  $RootAWC$  and  $TotAWC$  the AWC in the root and total compartments, respectively, described by  
 232 Constantin et al. (2015). The root compartment corresponds to that explored by the roots (i.e. down to  
 233 rooting depth). The total compartment corresponds to the total soil profile (i.e. soil depth). Each layer's  
 234 maximum AWC was calculated in the same way as its AWC.

235 When a layer's AWC reaches the layer's maximum AWC, the additional water transfers to the layer  
 236 below, as follows:

237  $W_{z1 \rightarrow z2} = AWC_{z1(d-1)} + R + Irr - EVA - TR_{z1} - maxAWC_{z1}$  (Eq. 6)

238 with  $R$  the rainfall,  $Irr$  the irrigation,  $EVA$  the evaporation and  $TR_{z1}$  the transpiration from the layer z1.

239  $W_{z2 \rightarrow z3} = AWC_{z2(d-1)} + W_{z1 \rightarrow z2} - (TR - TR_{z1}) - maxAWC_{z2}$  (Eq. 7)

240  $Dr = AWC_{z3(d-1)} + W_{z2 \rightarrow z3} - maxAWC_{z2}$  (Eq. 8)

241 with  $TR$  the daily actual transpiration from the crop described in Constantin et al. (2015). Using these  
 242 equations, drainage ( $Dr$ ) is calculated from separate layers and water transfers, but is identical to *drain*,  
 243 which is the drainage calculated by the original AqYield model. We verified that AqYield-N's method  
 244 estimated the same drainage as AqYield's method.

### 245 3.2.2 Amount of nitrogen in soil layers

246 The initial amount of SMN in each layer is provided as input data. N from fertilization and mineralization  
247 from residues and soil organic N is pooled in SMN of layer z1 (Fig. 2). N taken up by crops is removed  
248 from layers z1 and z2 (see section 3.2.4.3). N is transferred with water transfers between layers (z1 to z2  
249 and z2 to z3), and N is leached with drainage from layer z3 when water in the AWC of the layer is at its  
250 maximum ( $AWC_{zi} = \max AWC_{zi}$ ) and there is water input. The amount of SMN in each layer (in  $\text{kg N ha}^{-1}$ ) is  
251 the result of these different processes and is calculated for a given day (d) from the final amount of SMN  
252 on the previous day ( $SMNf_{(d-1)}$ ):

253 1) Incoming N from fertilization and mineralization (z1) or from root growth (z2 and z3) on this day,  
254 to determine initial SMN of the day ( $SMNi$ ), using the following equations:

255 - layer z1:  $SMNi_{z1} = SMNf_{z1(d-1)} + Nferti + minN$  (Eq. 9)

256 - layer z2:  $SMNi_{z2} = SMNf_{z2(d-1)} + RootAlloc$  (Eq. 10)

257 - layer z3:  $SMNi_{z3} = SMNf_{z3(d-1)} - RootAlloc$  (Eq. 11)

258 with  $Nferti$  the amount of incoming N from fertilizer on this day (in  $\text{kg N ha}^{-1}$ ) that is set to 0 if  
259 there is no fertilization on the given day (see section 3.2.3.1) and  $minN$  the daily N mineralization  
260 of soil organic matter and residues (in  $\text{kg ha}^{-1}$ ) (see sections 3.2.3.2 and 3.2.3.3).  $RootAlloc$  is the  
261 amount of N (in  $\text{kg N ha}^{-1}$ ) that passes from one layer to the next due to daily root growth, which  
262 changes the thickness of layers z2 and z3, existing only when roots are deeper than 30 cm:

263  $RootAlloc = (RootAWC_{\max(d-1)} - RootAWC_{\max}) \times \frac{SMNf_{z3(d-1)}}{AWC_{z3}}$  (Eq. 12)

264 with  $RootAWC_{\max}$  the maximum AWC of the “root” compartment (mm) described by  
265 Constantin et al. (2015).

266 2) Crop N uptake, to determine the SMN after crop N uptake ( $SMNafUp$ ), which occurs only in  
267 layers z1 and z2, using the following equation:

268  $SMNafUp_{zi} = SMNi_{zi} - Nuptake_{zi}$  (Eq. 13)

269 with  $i = 1$  or  $2$  depending on the layer considered.

270 3) Incoming N from the layer above and outgoing N to the layer below, to determine the final SMN

271 amount for the day ( $SMN_f$ ), using the following equations:

272 - layer z1:  $SMN_{f_{z1}} = SMN_{afUp_{z1}} - N_{z1 \rightarrow z2}$  (Eq. 14)

273 - layer z2:  $SMN_{f_{z2}} = SMN_{afUp_{z2}} + N_{z1 \rightarrow z2} - N_{z2 \rightarrow z3}$  (Eq. 15)

274 - layer z3:  $SMN_{f_{z3}} = SMN_{i_{z3}} + N_{z2 \rightarrow z3} - N_{leach}$  (Eq. 16)

275 with  $N_{z1 \rightarrow z2}$  and  $N_{z2 \rightarrow z3}$  the amount of N transferred by water flows between layers and  $N_{leach}$

276 the amount of N lost by leaching due to drainage (outgoing N and water from layer z3) (see

277 section 3.2.5).

### 278 3.2.3 Nitrogen inputs in the soil

#### 279 3.2.3.1 Nitrogen fertilization

280  $N_{ferti}$  refers to the addition of mineral N in the soil after gaseous N losses have occurred. The N provided

281 by fertilization is homogeneously available in z1 (0-30 cm) only after a cumulative water input of 5 mm

282 (rain and irrigation), as in the SUNFLO model (Casadebaig et al., 2011). The model does not distinguish

283 among different fertilizers.

#### 284 3.2.3.2 Nitrogen mineralization of soil organic matter

285 For N mineralization of soil organic matter, we used the formalism of Clivot et al. (2017), based on

286 measurements on 65 contrasting bare soils in France. We chose the soil model Vp5 (A1), which estimates

287 mineralization of soil organic matter well, with no bias and an efficiency of 0.61. Time was expressed as

288 “normalized days” (nday) under standard conditions of temperature and soil water, calculated using the

289 equation of Mary et al. (1999). Prediction error ( $RMSE_p$ ) of soil organic matter mineralization was 0.22 kg

290  $N \text{ ha}^{-1} \text{ nday}^{-1}$  for the entire database. This equation requires five basic soil inputs: organic N content (SON

291 in  $t \text{ ha}^{-1}$ ), C:N ratio, pH,  $CaCO_3$  content (in  $g \text{ kg}^{-1}$ ) and clay content (Clay in  $g \text{ kg}^{-1}$ ). It estimates the daily

292 potential net N mineralization rate ( $Vp$  in  $kg \text{ ha}^{-1} \text{ nday}^{-1}$ ) as follows:

293 
$$Vp = 0.346 \times SON \times e^{-2.519 \times \frac{Clay}{1000}} \times e^{-0.112 \times (pH-8.5)^2} \times (0.8 \times e^{-0.06 \times (C:N-11)^2} + 0.2) \times \frac{1}{1+1.114 \times CaCO_3/1000} \quad (\text{Eq. 17})$$

294 The calculation requires adding three additional inputs to AqYield-N: wilting point (% of dry soil), field  
 295 capacity (% of dry soil) and bulk density (kg m<sup>-2</sup>). The N provided by mineralization is assumed to be  
 296 homogeneously available in z1 (Fig. 2). For fields with a long history of cropping systems with  
 297 conventional tillage, we suggest using default values for soil parameters if they are not available: 9.5 for  
 298 the C:N ratio and 1.45 kg m<sup>-2</sup> for bulk density.

299 **3.2.3.3 Nitrogen mineralization of crop residues**

300 For N mineralization of crop residues, we used equations of Nicolardot et al. (2001) with the updated set  
 301 of parameters of Justes et al. (2009), which accurately estimate the amount of mineral N produced by  
 302 decomposition of multiple types of both mature and non-mature (e.g. cover crop) residues. These  
 303 equations and parameters are now also used in STICS to estimate N mineralization of crop residues  
 304 (Brisson et al., 2008). It is based on modeling three distinct pools of organic matter:

- 305 - Fresh crop residues, not yet degraded
- 306 - Microbial biomass, which includes decomposing biomass and the microbial community that  
 307 decomposes it
- 308 - “Humus”, corresponding to the humified organic matter that is ultimately pooled with soil  
 309 organic matter

310 Modeling the N fluxes determined daily net mineralization and the amount of mineral N in AqYield-N  
 311 that is homogeneously available in z1 (Fig. 2). The input data required for these equations – the amount  
 312 of N per kg of residue and the C:N ratio – are used to calculate the “fresh crop residues” pool. The N pool  
 313 in microbial biomass is set at 0 at the beginning of the simulation and increases as fresh crop residues  
 314 decompose. The humified organic matter is initialized using the new input of soil organic N in the upper  
 315 30 cm of soil.



### 316 **3.2.4 Crop nitrogen uptake**

317 In AqYield-N, crop N uptake is determined by comparing plant N demand to soil N supply, as in most  
318 dynamic crop models (Casadebaig et al., 2011). Thus, AqYield-N estimates daily crop N demand as a  
319 function of phenological stage, cumulative degree days and maximum total N uptake at harvest. It also  
320 estimates daily potential N supply from the soil as a function of transpiration and N concentration in the  
321 root zone.

#### 322 **3.2.4.1 Crop nitrogen demand**

323 Crop N demand ( $N_{demand}$ , in  $\text{kg N ha}^{-1} \text{ day}^{-1}$ ) is the amount of N that the crop needs to grow when not  
324 stressed (N, water, pests and disease). Most crop models estimate it from the daily increase in biomass.  
325 Since AqYield does not represent biomass, we represented dynamics of the maximum daily N  
326 requirement of the crop using linear regressions between key phenological stages (in cumulative degree  
327 days). First, we estimated the maximum total N uptake at harvest ( $N_{max}$ , in  $\text{kg N ha}^{-1}$ ) from the potential  
328 yield ( $Yield_{max}$ , in  $\text{t ha}^{-1}$ ) and the amount of N required to produce 1 t of yield ( $YieldNeed$ , in  $\text{kg N t}^{-1}$ , Table  
329 3), as follows:

$$330 \quad N_{max} = Yield_{max} * YieldNeed \quad (\text{Eq. 18})$$

331  $Yield_{max}$  is the potential yield of the crop, which is an input value of the model determined by expert  
332 knowledge.  $YieldNeed$  values came from a lookup table of COMIFER (2017), Mchet et al. (2017) and  
333 other experimental data (data not shown). These sources determined the N (per unit of grain  
334 production), for a variety of crops, required to produce a target grain yield.

335 **Table 3. Parameters and equations of N demand (*Ndemand*) for crops and cover crops in AqYield-N**

Species	YieldNeed (kg N t <sup>-1</sup> )	$\Sigma T_{em}$ (DD)	$\Sigma T_{flo}$ (DD)	$\Sigma T_{mat}$ (DD)	StartNeeds (DD)	Cropping period	Crop N demand per DD
Maize Soybean (type I)	22 (13 for silage maize) 80	80 120	875-1072* 700	1745-2070* 1760	190 190	StartNeeds → Maturity:	$N_{max} / (\Sigma T_{mat} - StartNeeds - \Sigma T_{em})$
Sunflower Rapeseed	45 70	80 80	1050-1120* 1200	1630-1720* 1900	190 390	StartNeeds → Flowering: Flowering → Maturity:	$0.8 \times N_{max} / (\Sigma T_{mat} - StartNeeds - \Sigma T_{em})$ $0.2 \times N_{max} / (\Sigma T_{mat} - \Sigma T_{flo})$
Wheat	30-37**	80	1300	2015	0	StartNeeds → End of photoperiod effect: End of photoperiod effect → Flowering: Flowering → Maturity:	$0.0227$ $(0.8 \times N_{max} - N_{upEndPhot}) / (\Sigma T_{flo} - \Sigma T_{EndPhot})$ $0.2 \times N_{max} / (\Sigma T_{mat} - \Sigma T_{flo})$
Fava bean	48	110	880	2100	0	Emergence → Emergence + 500DD Emergence + 500DD → Maturity	$0.0044$ $(N_{max} - N_{up500DD}) / (\Sigma T_{mat} - (\Sigma T_{em} + 500DD))$
Brassicaceae cover crop	-	125	1200	-	90	StartNeeds → Cover destruction	$(-0.0008 \times \text{sowing date} + 0.3317)$
Graminae cover crop	-	110	1500	-	190	StartNeeds → Cover destruction	$(-0.0011 \times \text{sowing date} + 0.3589)$

336 'YieldNeed' is the amount of N required to produce 1 t of yield.

337  $\Sigma T_{em}$ ,  $\Sigma T_{EndPhot}$ ,  $\Sigma T_{flo}$  and  $\Sigma T_{mat}$  are the sum of degree days needed to reach emergence, the end of the photoperiod effect, flowering and physiological maturity, respectively.

339 'StartNeeds' is the number of degree days after emergence before crop N demand begins.

340 'Nmax' is maximum N demand.

341 'NupEndPhot' is the amount of N uptake at the date of the end of photoperiod effect.

342 'Nup500DD' is cumulative N uptake after 500 degree days.

343 'DD' is degree-day.

344 \*Values depend on cultivar precocity.

345 \*\* Values depend on cultivar and area.

346 'Sowing date' is expressed as a day of year.

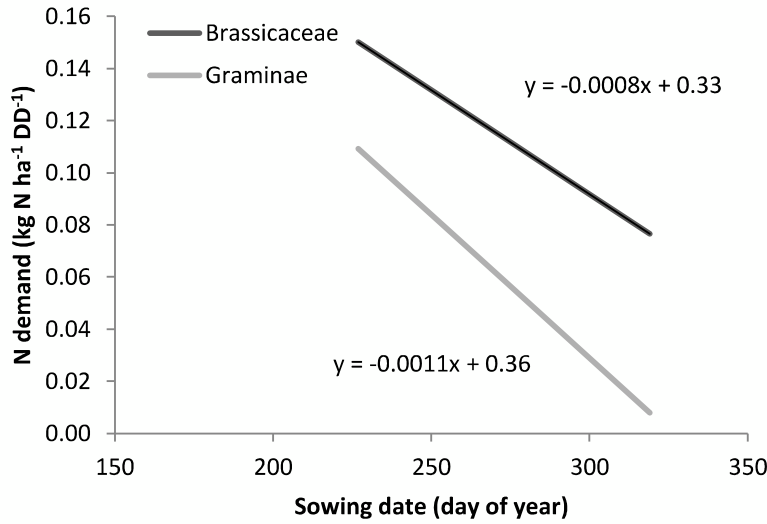
347  
 348 Using the STICS estimates of N accumulation in unstressed plants over time, we determined a generic  
 349 curve of cumulative N uptake demand for each crop, as a function of crop development (Table 3). We  
 350 ran STICS for five sites across France with contrasting soils and climates with typical sowing dates and  
 351 nitrogen fertilization and irrigation that avoided N and water stresses. From each crop's simulated curves  
 352 of N uptake without stress, we determined the crop's generic cumulative curve of N demand as a  
 353 function of cumulative degree days. The N demand curves included several key points, depending on the  
 354 crop, according to STICS estimates:

- 355 • The beginning of high N requirements, set as the number of degree days from emergence until  
 356 N uptake of 3 kg N ha<sup>-1</sup> was reached in STICS simulations, assuming that N uptake was negligible  
 357 before.
- 358 • The end of the photoperiodic effect for wheat, before which N demand is low and assumed to  
 359 be constant.

- 360 • Flowering, which is an inflection point for several crops, after which daily N demand is lower. For  
361 this stage, we also determined the percentage of N<sub>max</sub> the crop had already acquired (e.g. 80%  
362 for sunflower, wheat and rapeseed).
- 363 • Maturity, after which N demand is null.

364 For simplicity, we assumed a constant N demand between two key points equal to the slope of a linear  
365 interpolation. The maximum number of equations for representing N demand was three, with two  
366 inflection points. As a result, AqYield-N required only two additional crop parameters (*YieldNeed* and  
367 *StartNeeds*, Table 3) in addition to the 11 existing ones.

368 For cover crops sown in late summer or autumn under French conditions (August-November), we  
369 determined a constant daily N demand as a function of sowing date (Table 3) because no inflection  
370 points were identified in the STICS simulations and to consider the decrease in N demand with late  
371 sowings. Daily N demand remains constant throughout cover crop development but decreases as sowing  
372 occurs later in the year because of slower crop growth due to lower temperature and global radiation  
373 (Fig. 3). It also varies among crops; for example, mustard has a higher daily N demand than oat for the  
374 same sowing date.



375  
 376 **Figure 3. Relationship between N demand and sowing date for two cover crops (Brassicaceae and Graminae). DD is degree**  
 377 **day.**

378 **3.2.4.2 Potential nitrogen supply from the soil**

379 N supply from the soil (*PotNsoil*, in kg N ha<sup>-1</sup>) in the layers explored by roots (*z1* and *z2*) is estimated at a  
 380 daily time step in a simple manner: actual transpiration × N concentration in the soil, as in other models,  
 381 such as SUNFLO (Casadebaig et al., 2011). This approach was too limiting during winter, however, when  
 382 transpiration was extremely low. As a result, the crop did not take up N even though N was available in  
 383 the soil and the crop had not met its daily requirements. To address this underestimation of N uptake by  
 384 the crop, we calibrated a value of 1.5 kg N ha<sup>-1</sup> day<sup>-1</sup> that can be taken up if it is available in the soil and  
 385 meets the crop N requirements. The equation for daily N supply from the soil is as follows:

386 if  $(SMNi_{z1} + SMNi_{z2}) > 1.5 \text{ kg N ha}^{-1}$ ,

387 
$$PotNsoil = 1.5 + TR \times \frac{SMNi_{z1} + SMNi_{z2}}{AWC_{z1} + AWC_{z2}} \quad (\text{Eq. 19})$$

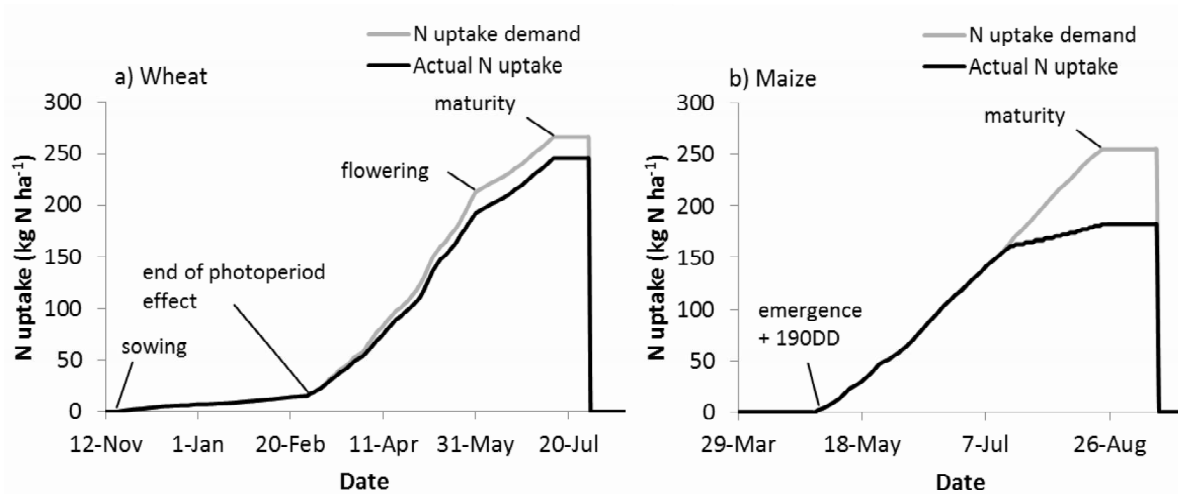
388 else,

389 
$$PotNsoil = TR \times \frac{SMNi_{z1} + SMNi_{z2}}{AWC_{z1} + AWC_{z2}} \quad (\text{Eq. 20})$$

390 with  $TR$  the actual transpiration in mm (described by Constantin et al., 2015),  $SMNi_{z1}$  and  $SMNi_{z2}$  the  
391 amount of N (in  $\text{kg N ha}^{-1}$ ) in layers  $z1$  and  $z2$ , respectively, and  $AWC_{z1}$  and  $AWC_{z2}$  the amount of available  
392 water (in mm) in layers  $z1$  and  $z2$ , respectively (see section 3.2.1).

### 393 3.2.4.3 Actual nitrogen uptake

394 Daily actual N uptake ( $N_{\text{uptake}}$ , in  $\text{kg N ha}^{-1} \text{ day}^{-1}$ ) equals the minimum of  $N_{\text{demand}}$  and  $PotN_{\text{soil}}$   
395 described previously (sections 3.2.4.1 and 3.2.4.2). Thus, N uptake decreases if crop N demand exceeds  
396 N supply from the soil.



397  
398 **Figure 4. Illustration of N demand and actual N uptake curves for wheat and maize simulated in**  
399 **AqYield-N. \*DD means degree-days.**

400  
401 In an example simulation, wheat had low N uptake during winter until the end of the photoperiod effect,  
402 after which daily demand increased until flowering and then decreased until maturity (Fig. 4a). In this  
403 example, almost all N demand was met due to low N stress and high N supply in the soil. In an example  
404 simulation of maize, N demand and uptake began at  $StartNeeds$ , with a relative constant daily N demand  
405 until maturity (Fig. 4b). In this example, N availability in the soil was limiting, which caused significant N  
406 stress (N demand higher than N supply from the soil), resulting in lower actual N uptake.

407 Once daily actual N uptake is calculated, it is divided between the two layers explored by roots ( $z_1$  and  
 408  $z_2$ ) in proportion to their relative thickness and up to the limit of N available in each layer ( $SMNi_z$ ), as  
 409 follows:

$$410 \quad N_{uptake_{zi}} = \frac{N_{uptake} * thickness_{zi}}{RootDepth} \quad (Eq. 21)$$

411 with  $thickness_z$  the thickness (in cm) of layer  $z$ :  $thickness_{z1}$  always equals 30 cm and  $thickness_{z2} =$   
 412  $RootDepth - thickness_{z1}$ ;  $RootDepth$  is the daily root depth (cm) calculated as a function of cumulative  
 413 degree days and the phenological stages of the crop (see details in Constantin et al., 2015).

414 If N is lacking in one layer but available in the other, the proportion is adapted to reach the total crop N  
 415 uptake if possible. For legume species, the amount of N acquired by symbiotic fixation can be calculated  
 416 as the  $N_{demand}$  minus  $N_{uptake}$ .

### 417 3.2.5 Nitrogen transfers and leaching

418 N transfers and leaching are calculated for each layer by adapting the Burns (1975) equation, which  
 419 estimates the proportion of N leached from a uniform soil profile during drainage. This equation has  
 420 been tested in the literature and determined to be satisfactory for estimating soil leaching (Addiscott  
 421 and Wagenet, 1985). Although the equation was initially developed for a larger soil profile and time step,  
 422 we adapted it to represent movement of N at a daily time step and for each soil layer. Thus, AqYield-N  
 423 represents the amount of N in each layer and its daily dynamics. The equation was applied only when  
 424 water transfers or drainage occurred. The equations for the amounts of N transferred between layers or  
 425 leached ( $\text{kg N ha}^{-1}$ ) are as follows:

426 From an upper layer  $z_i$  to a lower layer  $z_j$ :

$$427 \quad N_{zi \rightarrow zj} = \frac{SMNafUp_{zi}}{AWC_{zi}} \times W_{zi \rightarrow zj} \times \left( \frac{W_{zi \rightarrow zj}}{W_{zi \rightarrow zj} + \left( \frac{FC \times BD}{100} \right)} \right)^{25} \quad (Eq. 22)$$

428 with, between parentheses, the proportion of N leached or transferred, adapted from Burns (1975),  $FC$   
 429 the soil field capacity and  $BD$  the bulk density, which is assumed to be the same for the entire soil profile

430 in AqYield, for simplification. N leaching ( $N_{leach}$ ) corresponds to the N transferred from  $z_3$  beyond the  
 431 soil profile:

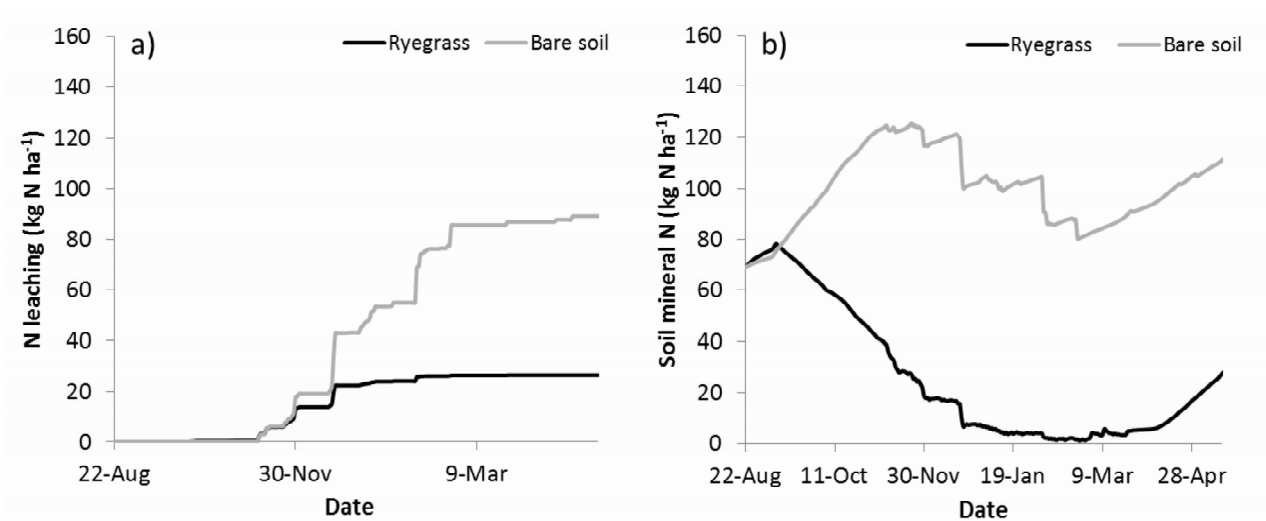
$$432 \quad N_{leach} = \frac{SMNi_{z_3}}{AWC_{z_3}} \times Dr \times \left( \frac{Dr}{Dr + \left( \frac{FC \times BD}{100} \right)} \right)^{25} \quad (\text{Eq. 23})$$

433 The parameter value set equal to 25 (cm) corresponds to the  $h$  parameter of Burns' equation, which  
 434 represents the mean displacement of N as a soil parameter. This value is based on those of Burns (1975)  
 435 for medium to heavy (clay) soils, which correspond to most French soils. This value can be adapted for  
 436 sandier soils.

### 437 3.3 Model assessment

#### 438 3.3.1 Examples of simulations

439



440

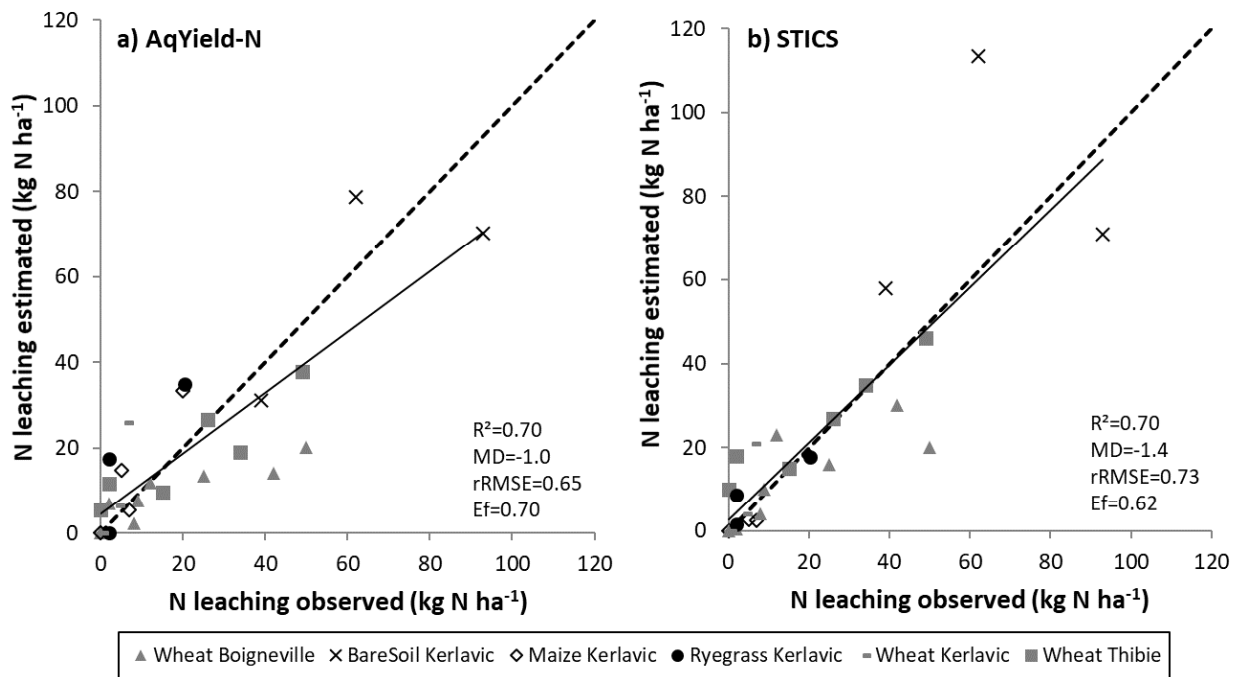
441 **Figure 5. Examples of AqYield-N simulations of N leaching and soil mineral N for a fallow period with bare soil or**  
 442 **an Italian ryegrass cover crop.**

443

444 Example AqYield-N estimates of N leaching and SMN during a fallow period with bare soil or Italian  
 445 ryegrass (sown in late August) show much less leaching from ryegrass during winter, which is a drainage

446 period (Fig. 5). Overall, sowing ryegrass reduced leaching by 97 kg N ha<sup>-1</sup> (a 54% decrease), due to  
 447 ryegrass taking up SMN (susceptible to leaching) during autumn. By the date that the drainage period  
 448 began (24 October), ryegrass had already reduced SMN by 66 kg N ha<sup>-1</sup> (i.e. 49 kg N ha<sup>-1</sup>, vs. 115 kg N ha<sup>-1</sup>  
 449 for bare soil).

450 **3.3.2 Evaluation of AqYield-N estimates of nitrogen leaching and comparison to those of**  
 451 **STICS**



452  
 453 **Figure 6 Cumulative N leaching observed over 4-8 months (leaching period in Table 1) vs. that estimated by a) AqYield-N and**  
 454 **b) STICS for three sites (Boigneville, Kerlavic and Thibie) under bare soil, wheat, maize or ryegrass. MD is mean deviation,**  
 455 **rRMSE is relative root mean squared error and Ef is efficiency.**

456 Observed N leaching ranged from 0-93 kg N ha<sup>-1</sup> (Fig. 6). AqYield-N accurately estimated a range of  
 457 situations with low to high N leaching: estimated values ranged from 0-79 kg N ha<sup>-1</sup>. AqYield-N obtained  
 458 a good model efficiency (0.70) and a low mean deviation (-1.0 kg N ha<sup>-1</sup>), even though the variability in  
 459 estimated leaching (rRMSE) was relatively high (0.65). In absolute value, the mean difference between  
 460 estimated and observed values was 9.1 kg N ha<sup>-1</sup>. All sites and situations were estimated relatively well.



461 The ability of AqYield-N to estimate leaching was generally similar to that of STICS. Even though STICS  
462 had a slightly lower  $E_f$ , higher MD and higher rRMSE, the mean difference in absolute value (8.1 kg N  
463  $\text{ha}^{-1}$ ) was better than that of AqYield-N. The statistical criteria of STICS were influenced mainly by a  
464 particularly large overestimation of N leaching under bare soil in Kerlavic. STICS also greatly  
465 underestimated one of the two observed leaching situations that AqYield-N underestimated for  
466 Boigneville.

## 467 **4 Discussion**

### 468 **4.1 Ability of AqYield-N to estimate nitrogen leaching**

469 AqYield-N is a simple soil-crop model that estimates N leaching at the field scale, based partly on  
470 previously published equations and new simple equations. Although most crop models consider a few  
471 sets of crops (Di Paola et al., 2016), few models that simulate the N cycle include the main crop species  
472 grown on temperate arable farms (Cannavo et al., 2008). The genericity of AqYield-N for simulating a  
473 variety of crops (e.g. spring crops, winter crops, legumes, cover crops) enables estimating N leaching for  
474 a variety of crop rotations at a large scale. The small number of inputs and parameters required makes it  
475 easy apply the model, and the simplicity of the formalisms makes it easy to calibrate them for new  
476 species or soils. Compared to the more complex STICS, which had 40 inputs, AqYield increased its  
477 number of inputs from 15 (Constantin et al., 2015) to 24. Most new model inputs were related to N  
478 mineralization, which is already simulated by STICS, and came from the formalism of Clivot et al. (2017),  
479 which the latter considered the most parsimonious model for estimating net N mineralization well.  
480 These authors performed a sensitivity analysis and found that the most influent factor was soil organic N,  
481 followed by clay, pH and C:N ratio. The number of new parameters for crop N remained much lower,  
482 however: two in AqYield-N vs. more than 10 in STICS. This new module added 23 equations, which seems  
483 reasonable for modeling the entire N cycle.

484 AqYield was previously evaluated as satisfactory for estimating water variables, especially drainage  
485 (Constantin et al., 2015; Tribouillois et al., 2018). In the present study, AqYield-N estimated observed N  
486 leaching sufficiently well, with the ability to reproduce contrasting leaching situations, from no leaching  
487 to high leaching. AqYield-N obtained an  $R^2$  of 0.70, which is considered “good” according to Cannavo et  
488 al. (2008), while an  $R^2$  greater than 0.5 is “acceptable” according to Moriasi et al. (2007). These authors  
489 also consider models “good” if  $E_f$  is greater than 0.50, which was the case for AqYield. AqYield-N’s MD  
490 (5.5%) is also considered “good” according to Cannavo et al. (2008). The only criterion considered “poor”  
491 according to Cannavo et al. (2008) is the high rRMSE of 0.65. However, when normalized by the standard  
492 deviation of observed data, as Coucheney et al. (2015) did, the resulting value of 0.54 falls into the  
493 “good” category defined by Cannavo et al. (2008).

494 Like the evaluation of AqYield for estimating water variables (Constantin et al., 2015), AqYield-N  
495 generally estimated leaching as well as much more complex models such as STICS. Although the two  
496 models showed some differences in their leaching estimates, they sometimes overestimated or  
497 underestimated a given leaching situation in the same way. This suggests that some observed data may  
498 have been measured with some uncertainty, due to the difficulty of measuring N leaching from  
499 experimental fields; for this reason, estimates of N leaching are rarely evaluated. Similar overestimates  
500 or underestimates could also have been due to both models failing to represent certain processes.  
501 AqYield-N estimated leaching dynamics (Fig. 6) consistent with results found in the literature on the  
502 ability of cover crops to reduce N leaching compared to that from bare soil (e.g. Thorup-Kristensen et al.,  
503 2003). This is a relevant point, since cover crops are an important management tool for designing more  
504 agroecological cropping systems. Tribouillois et al. (2016) and Plaza-Bonilla et al. (2015) identified these  
505 leaching dynamics using STICS. AqYield-N can thus represent well the expected dynamics and amount of  
506 N leaching for multiple field crop situations, which was the study’s main objective. We did not evaluate  
507 intermediate variables because i) total N leaching was the main objective; ii) estimated drainage, which

508 strongly influences estimated leaching, was previously evaluated as sufficient (Tribouillois et al., 2018);  
509 iii) mineralization and leaching equations were based on previously published and evaluated equations  
510 (Burns, 1975; Clivot et al., 2017; Justes et al., 2009; Nicolardot et al., 2001) and iv) the N uptake demand  
511 of crops was based on STICS simulations, which were also previously evaluated as satisfactory (Brisson et  
512 al., 2008; Coucheney et al., 2015).

## 513 **4.2 Validity range and limits**

514 Leaching was evaluated for three French soils and climate sites with contrasting conditions, especially for  
515 rainfall and climate years, to evaluate the model for a wide range of leaching amounts. The validity range  
516 for N leaching estimates is thus temperate climates typical of Europe. The equations for mineralization  
517 added to AqYield-N are valid only for crop residues; however, parameters for mineralization of organic  
518 residues, such as manure, are available in the literature (Brisson et al., 2008) and can be used easily in  
519 AqYield-N since the equations remain the same.

520 AqYield-N was able to estimate the range of leaching amounts observed in contrasting situations and  
521 amounts of initial soil mineral N. To keep AqYield-N simple, we represented N uptake directly without  
522 simulating biomass dynamics and thus without representing photosynthesis. The variation in global  
523 radiation according to location, which can influence crop growth and thus N and water uptake, was not  
524 included. As in several other crop models that simulate the N cycle, AqYield-N ignores  $N_2O$  and  $N_2$   
525 emissions (Cannavo et al., 2008). AqYield-N does not directly simulate volatilization after N fertilizer  
526 application. Consequently, volatilization should be estimated and subtracted from *Nfert<sub>i</sub>*, for example  
527 using IPCC emission coefficients or more process-based models such as Volt'air (Génermont and Cellier,  
528 1997). AqYield-N also ignores N inputs from irrigation water and atmospheric deposition; however, they  
529 are assumed to have little impact on the N balance. Because the AqYield-N's objective was to predict  
530 leaching, and N gases were not represented, AqYield-N cannot predict greenhouse gas emissions,  
531 especially  $N_2O$ , of cropping systems or agroecological practices. However, annual N losses from leaching

532 are considered to be ten times as high as those from N<sub>2</sub>O emissions in arable systems (Stenberg et al.,  
533 2012; Webb et al., 2000).

534 Using a simple model to simulate complex mitigation scenarios has disadvantages since complexity and  
535 data requirements generally increase with the number of processes that a model can represent  
536 (Bouraoui and Grizzetti, 2014). This means that certain scenarios, such as intercropping or agroforestry,  
537 cannot be tested with this version of AqYield; they would require additional development of AqYield-N  
538 or a more complex model. Nonetheless, since AqYield-N is a process-based model that operates at a  
539 daily time step, it is adapted to simulate the fate of N and the processes involved. Despite its limitations  
540 and simple equations, AqYield-N is reliable for predicting N leaching in a variety of situations.

## 541 **5 Conclusion**

542 The present study presented the development and formalisms of AqYield-N. The model's estimates of N  
543 leaching were evaluated as satisfactory based on experimental data measured in three contrasting  
544 pedoclimatic situations and under various crops and bare soil, with contrasting levels of soil mineral N  
545 before drainage. Although the model is simple and requires only a few input data, it was as accurate as  
546 more complicated crop models widely used and evaluated in the agronomic literature, such as STICS. The  
547 study demonstrated the model's potential to evaluate the influence of cover crops on N leaching, which  
548 is an important management option for mitigating environmental N losses. AqYield-N, whether alone or  
549 in integrated modeling approaches, could be used to predict leaching during crop rotations at field and  
550 larger scales to assess the influence of various agroecological practices on N losses in groundwater and  
551 thus on water quality.

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