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

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

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Abstract

Evaluating and improving cropping systems is essential to reduce nitrate leaching, improve drinking water quality and prevent eutrophication. Since the intensity of nitrogen (N) leaching varies greatly spatially and is difficult to measure, crop models are useful tools to quantify the influence of climate, soil and agricultural practices on N leaching. Our objective was to develop a simple model with low input data and calibration requirements to predict nitrate leaching from a variety of crop fields over large areas, such as watersheds, for which data are often limited. The AqYield model is a simple model with few inputs that has estimated sufficiently well drainage and water flows for several crops and rotations. Based on this model, we developed AqYield-N, which considers the major N flows in the soil–plant system, including mineralization, plant uptake and leaching at a daily time step. The present study presents the development and formalisms of AqYield-N. We developed AqYield-N based on simple and robust formalisms and low requirements for input data and parameters. As much as possible, we used equations already published and validated in the scientific literature. We then evaluated AqYield-N using observed experimental N leaching data. Its estimates were satisfactory for three contrasting pedoclimatic situations and for various crops and bare soil. Although the model is simple and requires only a few inputs, it was as accurate as more complex crop models widely used and evaluated in the agronomic literature, such as STICS. The study demonstrated the potential of AqYield-N to estimate the influence of management practices on N leaching. AqYield-N, whether alone or integrated in larger-scale modeling approaches, can be used to predict leaching during crop rotations at field and large scale to evaluate the influence of various agroecological practices on N leaching.

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

1 Introduction

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

Soil-crop models are useful tools to quantify the influence of climate, soil and agricultural practices on nitrate leaching (Hoffmann and Johnsson, 1999). These models can be distributed over a large area to quantify the influence of agricultural practices on nitrate leaching at a large scale (Wagenet and Hutson, 1996). They can be applied on a small region or watershed of few km², on large watershed of hundreds of km² or a whole country. Linking a soil-crop model to current climates, agricultural soils, cropping practices and a given agricultural region allows prediction of N leaching at the large scale for current and alternative scenarios of improved agricultural practices, its impact on water quality (Hall et al., 2001) and the potential of these improved practices to decrease water pollution. Model assessment depends on the realism of its formalisms, the quality of calibration and the reliability of input data (Loague and Corwin, 1996). However, the availability of data for calibration or model input is often an obstacle to applying soil-crop models at a high resolution over large areas (Therond et al., 2009). For regional assessments, the model must consider large areas that have contrasting soils, climates and management practices. Estimating the influence of multiple cropping systems and pedoclimatic conditions in a region requires a robust and generic model that can simulate a variety of crops (e.g. spring and winter cash crops, cover crops) and crop management practices (e.g. sowing dates, crop rotations). Many crop models require considerable calibration and many inputs, which can result in a lack of adequate and sufficient data to run the model at a large scale, such as a region or watershed (Faivre et al., 2004). In this context, using a simple model with simple formalisms, low input data requirements and as few parameters as possible, is necessary to accurately estimate leaching at this scale under current conditions. Since N dispersal in the soil depends strongly on soil water fluxes, one key issue for modeling N leaching is to estimate these water flows accurately (Addiscott and Wagenet, 1985).

The soil-crop model AqYield is a simple and generic model that demonstrated its ability to simulate dynamic water balance components (soil water content and evapotranspiration) as accurately as a more complex model for a variety of crop species, crop rotations and management practices (Constantin et al., 2015; Tribouillois et al., 2018). These two studies demonstrated the model's ability to simulate water flows with good accuracy, particularly evapotranspiration and water drainage, highlighting the potential to develop an additional module that estimates nitrate leaching. AqYield has already been applied at the watershed scale in MAELIA, the integrated simulation platform that can also simulate hydrology (Therond et al., 2014), since it requires only a few inputs. Crop models can be combined with hydrological models to study interactions between agricultural practices and the physical characteristics of watersheds (Ferrant et al., 2011; Martin et al., 2016). This combination with hydrological models enables analysis of impacts of agricultural management on water flows in rivers, levels of pollution and interactions between water resources in the watershed and irrigation requirements (Cannavo et al., 2008). Due to its strong parsimony of equations and parameters, it has the advantage of easier calibration and shorter calculation times and requires only basic input data that are easily collected at a large scale. These properties also allow to avoid the “black box” effect that results from a lack of transparent internal structure and a complicated model behavior (Constantin et al., 2015).

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

2 Materials and methods

2.1 AqYield overview

The AqYield model is a simple dynamic soil-crop model that estimates water fluxes at the field scale at a daily time step. It was previously calibrated and evaluated for spring crops with and without irrigation under various pedoclimatic conditions in southern France (Constantin et al., 2015) and for winter crops, both separately and in rotations (Tribouillois et al., 2018). Its ability to estimate soil water content dynamics, water drainage and evapotranspiration under crops or bare soil has been assessed as satisfactory. The model simulates daily water balance components, phenological stages and annual crop yield. It requires a few inputs: three soil properties (clay content, soil available water capacity and soil depth), three daily climate features (daily mean temperature, rainfall and reference evapotranspiration) and the dates of sowing, harvest, irrigation and tillage as well as the amount of irrigation and soil tillage depth for crop management. Its simplicity comes mainly from not simulating biomass; instead, the influence of crop development on water fluxes is considered using only a crop coefficient (Kc). The Kc varies according to crop (i.e. phenology, maximum Kc) and pedoclimate (i.e. day length, daily mean temperature and water stress). It influences evaporation and maximum transpiration, which determine the soil water available for the crop. Soil is represented using a classic tipping-bucket approach and the concept of available water capacity. Detailed description of equations used in AqYield is provided in Constantin et al. (2015) and Tribouillois et al. (2018).

2.2 Modeling approach used to develop AqYield-N

AqYield-N was based on the functioning of AqYield to estimate N leaching at the field scale at a daily time step, like for water fluxes. We developed AqYield-N by keeping the same objectives as those of AqYield: simple formalisms and low requirements for input data and parameters. To obtain an efficient simple model, we used, as much as possible, equations already published and validated in the scientific literature. We identified the key processes and most important N inputs, outputs and stocks of the soil-plant system needed to estimate N leaching: mineral N fertilization and associated N gas losses, N mineralization from organic residues and soil organic matter, soil mineral N content (SMN) and its transfer in the soil, crop N uptake and N leaching. Like other models that simulate N leaching, N_2O and N_2 gas emissions from the soil were not represented, since they represent a negligible loss of N compared to that lost by leaching (Stenberg et al., 2012; Webb et al., 2000). For example, total N_2 and N_2O losses have been estimated at less than 10 kg N ha^{-1} yr^{-1} for unfertilized crops in a wheat-maize cropping system (Chen et al., 2019). For N volatilization losses, according to the review of Bussink and Oenema (1998), losses from ammonium nitrate-based fertilizers are generally less than 5% of total N. These authors also observed that soils and crops are not a major source of NH_3, with a net loss from crops less than 2 kg NH_3 ha^{-1} yr^{-1} in fertilized fields, and even less in unfertilized fields. As a result, these processes were not included in the AqYield-N module to estimate nitrate leaching.

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

The general approach included four steps:

1) We investigated whether the scientific literature contained formalisms that were already evaluated and published for each key process. The chosen formalisms must be simple, require few inputs and be generic enough to apply to the wide range of pedoclimatic conditions and cropping systems.
2) When no corresponding formalism was found, we developed simple equations from a more complex model already evaluated and published in the scientific literature. Since AqYield does not represent biomass, and we found no formalism linking Kc and N uptake, we developed equations for the daily N demand by crops without requiring data on biomass.
3) We evaluated AqYield-N's estimates of N leaching under crop fields by comparing them to observed data on N leaching in a variety of experimental field situations.
4) We compared our model to a more complex model already evaluated as accurate for estimating leaching.

2.3 Experimental data for evaluating leaching

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

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

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

Site	Crop	Years	Clay content (%)	AW* capacity (mm)	SOM content (%)	C:N	Bulk density	Rainfall (mm yr^{-1})	Initial SMN (kg N ha^{-1})	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]
Kerlavic	Silage maize	4	16	213	4.8	10.7	1.2	1138	[32;54]	[77;100]	[Mar-Oct]
	Wheat	3							[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]

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

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

Each simulation used to evaluate leaching was initialized between the harvest of the preceding crop and sowing of the next one, using the mean SMN and available water content (AWC) measured for a given crop (mean of the 3 replicates). The initialization date was always before the start of the leaching measurement period. Depending on the year and crop, initialization conditions and leaching values differed among years, providing a wide range of situations for evaluation. Simulations were run from the initialization to the end of the leaching measurement period. The leaching estimated by AqYield-N was compared to that observed for the same measurement period.

2.4 Use of the STICS model

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

We used STICS simulations in two steps:

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

2.5 Statistical analysis for model evaluation

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

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

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

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

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

3 Results

3.1 AqYield-N overview

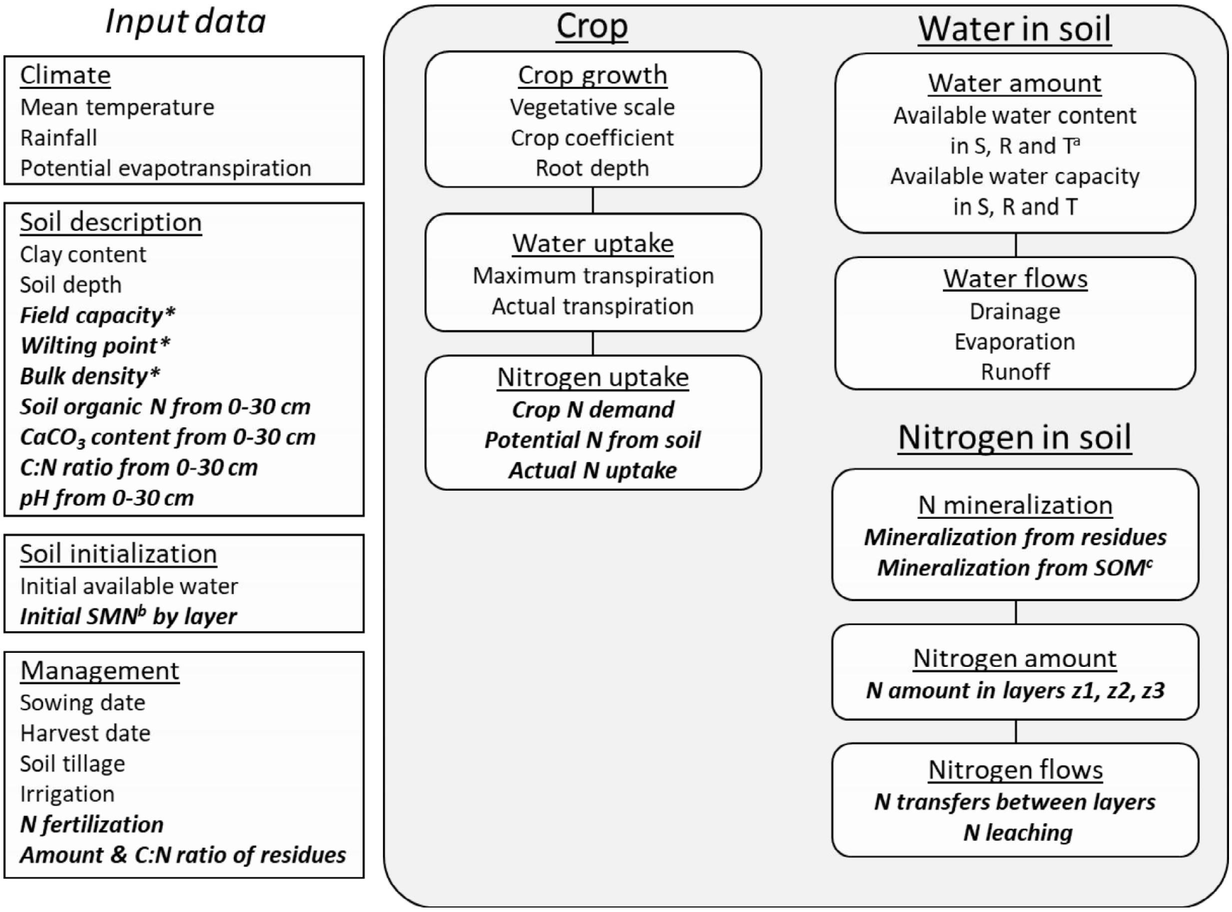

Figure 1. Description of model inputs (left), modules (in the gray box) and associated variables of AqYield-N. Original variables and inputs of AqYield are in normal font, new variables and inputs for AqYield-N are in bold italics. ^{a} S, R and T are the shallow, root and total soil compartments, respectively. ^{b} SMN is soil mineral nitrogen. ^{c} SOM is soil organic matter. * These three inputs replace the “available water capacity” (AWC) previously used in AqYield, since AWC can be calculated from them and soil depth.

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

3.2 Model structure and equations

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

Table 2. Name, description, unit and time step of the new variables used in the equations of the N module of AqYield-N. All variables are calculated at a daily time step, except for Nmax, which is calculated once per cropping season.

Variable name	Description	Unit
AWC_{zi}	Available water content (amount of water available in layer z_i)	mm
$maxAWC_{zi}$	Maximum available water content (in layer z_i)	mm
Dr	Amount of water outgoing beyond soil depth	mm
$W_{zi \to zj}$	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^{-1}
Ndemand	Amount of N required by the crop	kg N ha^{-1}
Nferti	Amount of N provided by fertilization and available in layer z_1	kg N ha^{-1}
Nleach	Amount of N lost by leaching beyond soil depth	kg N ha^{-1}
Nmax	Maximum crop N uptake at harvest	kg N ha^{-1}
Nuptake	Amount of crop N uptake	kg N ha^{-1}
$N_{zi \to zj}$	Amount of N transferred from layer i to j	kg N ha^{-1}
PotNSoil	Amount of N in soil that plants can potentially take up	kg N ha^{-1}
SON	Amount of soil organic N in layer z_1	t N ha^{-1}
SMNafUp	Amount of soil mineral N in layer after N uptake and before N transfer	kg N ha^{-1}
$SMNf_{zi}$	Amount of soil mineral N in layer z_i after N transfer	kg N ha^{-1}
$SMNi_{zi}$	Amount of soil mineral N in layer z_i before N uptake and N transfer	kg N ha^{-1}

3.2.1 Amount of water in soil layers and water transfers

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

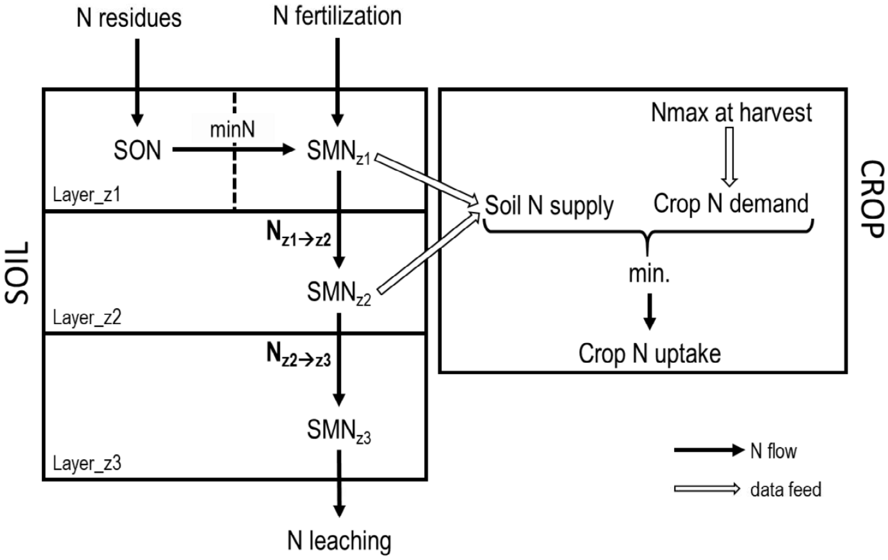

Figure 2. Description of the new process represented by AqYield-N. SON is Soil Organic N, SMN is soil mineral N, and minN is net N mineralization. $N_{zi \to zj}$ is the N transfer from layer z_i to layer z_j.

We thus recalculated the amount of water in each layer based on AqYield simulations. Layer_z1 extends from 0-30 cm deep. Layer_z2 extends from 30 cm deep to the rooting depth. Layer_z3 extends from the rooting depth to the bottom of the soil (soil depth). Layer_z2 and Layer_z3 thus differ in thickness, available water capacity and amount of SMN as a function of rooting depth.

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

- layer z2: $AWC_{z2} = RootAWC - AWC_{z1}$ (Eq. 4)
- layer z3 : $AWC_{z3} = TotAWC - RootAWC$ (Eq. 5)

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

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

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

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

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

$$\mathrm{D}r = AWC_{z3(d-1)} + W_{z2\rightarrow z3} - maxAWC_{z2} \quad \text{(Eq. 8)}$$

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

3.2.2 Amount of nitrogen in soil layers

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

1) Incoming N from fertilization and mineralization (z1) or from root growth (z2 and z3) on this day, to determine initial SMN of the day (*SMNi*), using the following equations:
    - layer z1: $SMNi_{z1} = SMNf_{z1(d-1)} + Nferti + minN$ (Eq. 9)
    - layer z2: $SMNi_{z2} = SMNf_{z2(d-1)} + RootAlloc$ (Eq. 10)
    - layer z3: $SMNi_{z3} = SMNf_{z3(d-1)} - RootAlloc$ (Eq. 11)

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

    $$RootAlloc = \left(RootAWC_{\max\,(d-1)} - RootAWC_{\max}\right) \times \frac{SMNf_{z3(d-1)}}{AWC_{z3}} \quad \text{(Eq. 12)}$$

    with $RootAWC_{max}$ the maximum AWC of the "root" compartment (mm) described by Constantin et al. (2015).

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

    $$SMNafUp_{zi} = SMNi_{zi} - Nuptake_{zi} \quad \text{(Eq. 13)}$$

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

3) Incoming N from the layer above and outgoing N to the layer below, to determine the final SMN amount for the day (*SMNf*), using the following equations:

   - layer z1: $SMNf_{z1} = SMNafUp_{z1} - N_{z1\rightarrow z2}$ (Eq. 14)
   - layer z2: $SMNf_{z2} = SMNafUp_{z2} + N_{z1\rightarrow z2} - N_{z2\rightarrow z3}$ (Eq. 15)
   - layer z3: $SMNf_{z3} = SMNi_{z3} + N_{z2\rightarrow z3} - Nleach$ (Eq. 16)

   with $N_{z1\rightarrow z2}$and $N_{z2\rightarrow z3}$ the amount of N transferred by water flows between layers and $Nleach$ the amount of N lost by leaching due to drainage (outgoing N and water from layer z3) (see section 3.2.5).

3.2.3 Nitrogen inputs in the soil

3.2.3.1 Nitrogen fertilization

Nferti refers to the addition of mineral N in the soil after gaseous N losses have occurred. The N provided by fertilization is homogeneously available in z1 (0-30 cm) only after a cumulative water input of 5 mm (rain and irrigation), as in the SUNFLO model (Casadebaig et al., 2011). The model does not distinguish among different fertilizers.

3.2.3.2 Nitrogen mineralization of soil organic matter

For N mineralization of soil organic matter, we used the formalism of Clivot et al. (2017), based on measurements on 65 contrasting bare soils in France. We chose the soil model Vp5 (A1), which estimates mineralization of soil organic matter well, with no bias and an efficiency of 0.61. Time was expressed as “normalized days” (nday) under standard conditions of temperature and soil water, calculated using the equation of Mary et al. (1999). Prediction error ($RMSE_P$) of soil organic matter mineralization was 0.22 kg N ha^{-1} $nday^{-1}$ for the entire database. This equation requires five basic soil inputs: organic N content (SON in t ha^{-1}), C:N ratio, pH, $CaCO_3$ content (in g kg^{-1}) and clay content (Clay in g kg^{-1}). It estimates the daily potential net N mineralization rate (*Vp* in kg ha^{-1} $nday^{-1}$) as follows:

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

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

3.2.3.3 Nitrogen mineralization of crop residues

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

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

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

3.2.4 Crop nitrogen uptake

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

3.2.4.1 Crop nitrogen demand

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

$$Nmax = Yield_{max} * YieldNeed \qquad \text{(Eq. 18)}$$

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

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

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

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

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

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

'Nmax' is maximum N demand.

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

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

'DD' is degree-day.

*Values depend on cultivar precocity.

** Values depend on cultivar and area.

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

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

- The beginning of high N requirements, set as the number of degree days from emergence until N uptake of 3 kg N ha^{-1} was reached in STICS simulations, assuming that N uptake was negligible before.
- The end of the photoperiodic effect for wheat, before which N demand is low and assumed to be constant.

- Flowering, which is an inflection point for several crops, after which daily N demand is lower. For this stage, we also determined the percentage of Nmax the crop had already acquired (e.g. 80% for sunflower, wheat and rapeseed).
- Maturity, after which N demand is null.

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

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

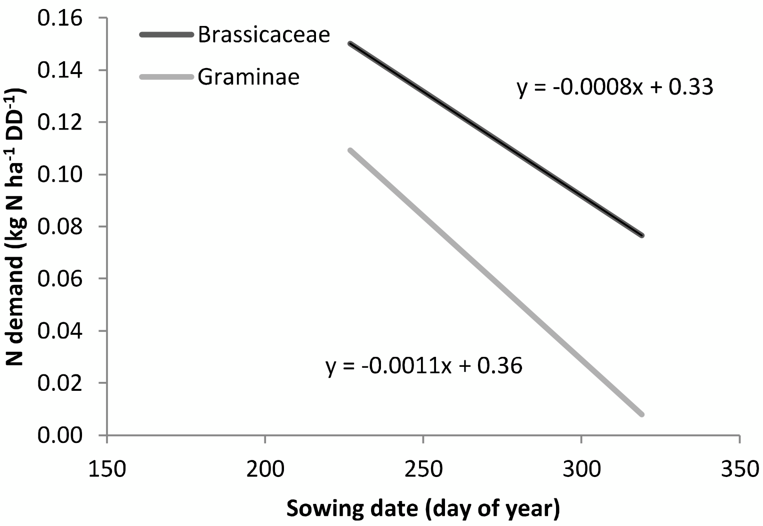

Figure 3. Relationship between N demand and sowing date for two cover crops (Brassicaceae and Graminae). DD is degree day.

3.2.4.2 Potential nitrogen supply from the soil

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

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

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

else,

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

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

3.2.4.3 Actual nitrogen uptake

Daily actual N uptake (*Nuptake*, in kg N ha^{-1} day^{-1}) equals the minimum of *Ndemand* and *PotNsoil* described previously (sections 3.2.4.1 and 3.2.4.2). Thus, N uptake decreases if crop N demand exceeds N supply from the soil.

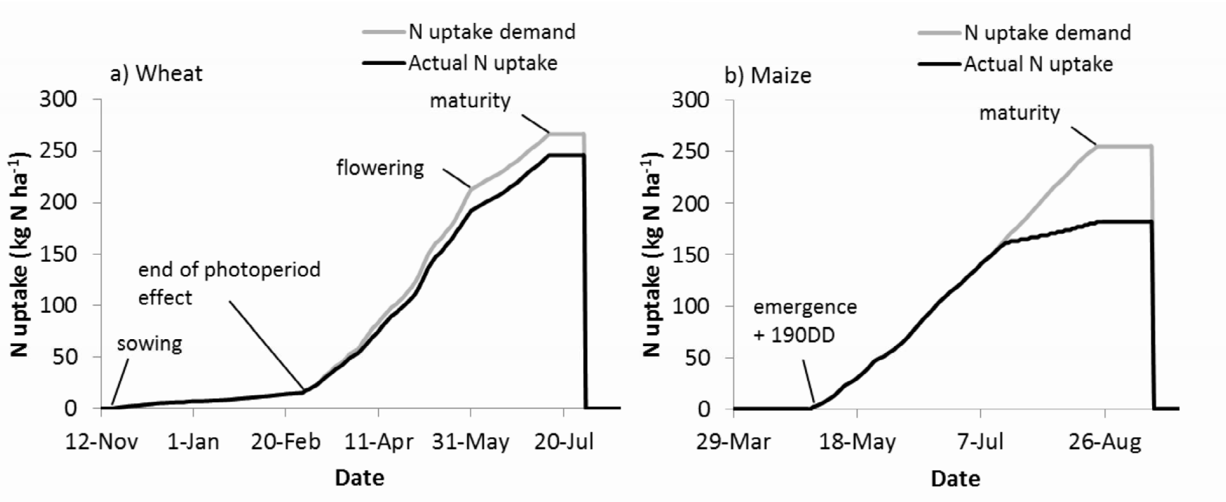

Figure 4. Illustration of N demand and actual N uptake curves for wheat and maize simulated in AqYield-N. *DD means degree-days.

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

Once daily actual N uptake is calculated, it is divided between the two layers explored by roots (z1 and z2) in proportion to their relative thickness and up to the limit of N available in each layer ($SMNi_z$), as follows:

$$Nuptake_{zi} = \frac{Nuptake * thickness_{zi}}{RootDepth} \qquad \text{(Eq. 21)}$$

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

If N is lacking in one layer but available in the other, the proportion is adapted to reach the total crop N uptake if possible. For legume species, the amount of N acquired by symbiotic fixation can be calculated as the *Ndemand* minus *Nuptake*.

3.2.5 Nitrogen transfers and leaching

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

From an upper layer zi to a lower layer zj:

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

with, between parentheses, the proportion of N leached or transferred, adapted from Burns (1975), FC the soil field capacity and BD the bulk density, which is assumed to be the same for the entire soil profile in AqYield, for simplification. N leaching (*Nleach*) corresponds to the N transferred from z3 beyond the soil profile:

$$Nleach = \frac{SMNi_{z3}}{AWC_{z3}} \times Dr \times \left(\frac{Dr}{Dr+\left(\frac{FC \times BD}{100}\right)}\right)^{25} \quad \text{(Eq. 23)}$$

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

3.3 Model assessment

3.3.1 Examples of simulations

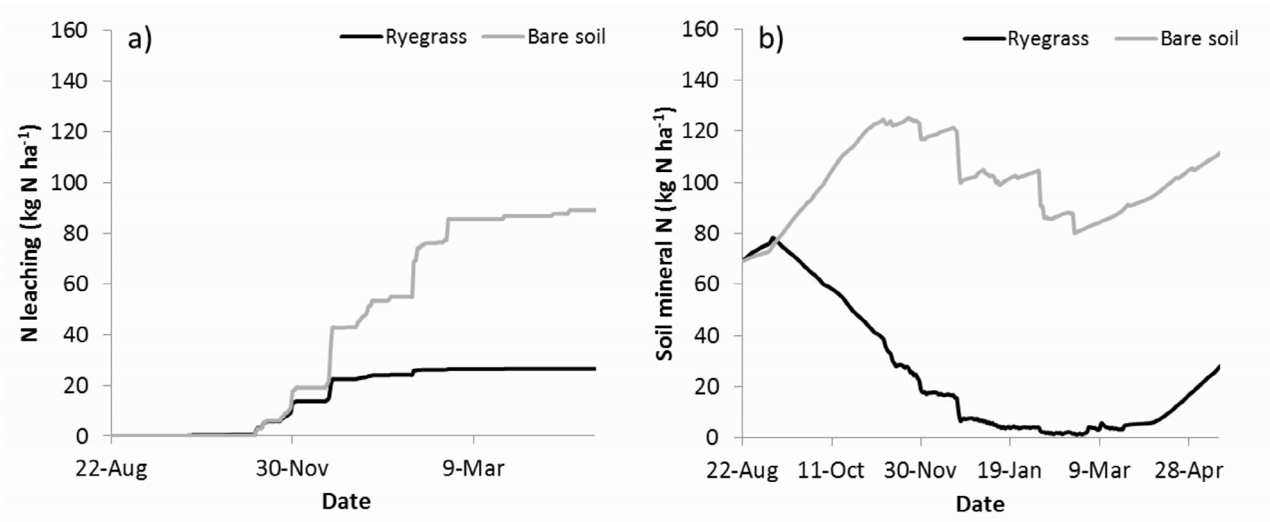

Figure 5. Examples of AqYield-N simulations of N leaching and soil mineral N for a fallow period with bare soil or an Italian ryegrass cover crop.

Example AqYield-N estimates of N leaching and SMN during a fallow period with bare soil or Italian ryegrass (sown in late August) show much less leaching from ryegrass during winter, which is a drainage period (Fig. 5). Overall, sowing ryegrass reduced leaching by 97 kg N ha^{-1} (a 54% decrease), due to ryegrass taking up SMN (susceptible to leaching) during autumn. By the date that the drainage period began (24 October), ryegrass had already reduced SMN by 66 kg N ha^{-1} (i.e. 49 kg N ha^{-1}, vs. 115 kg N ha^{-1} for bare soil).

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

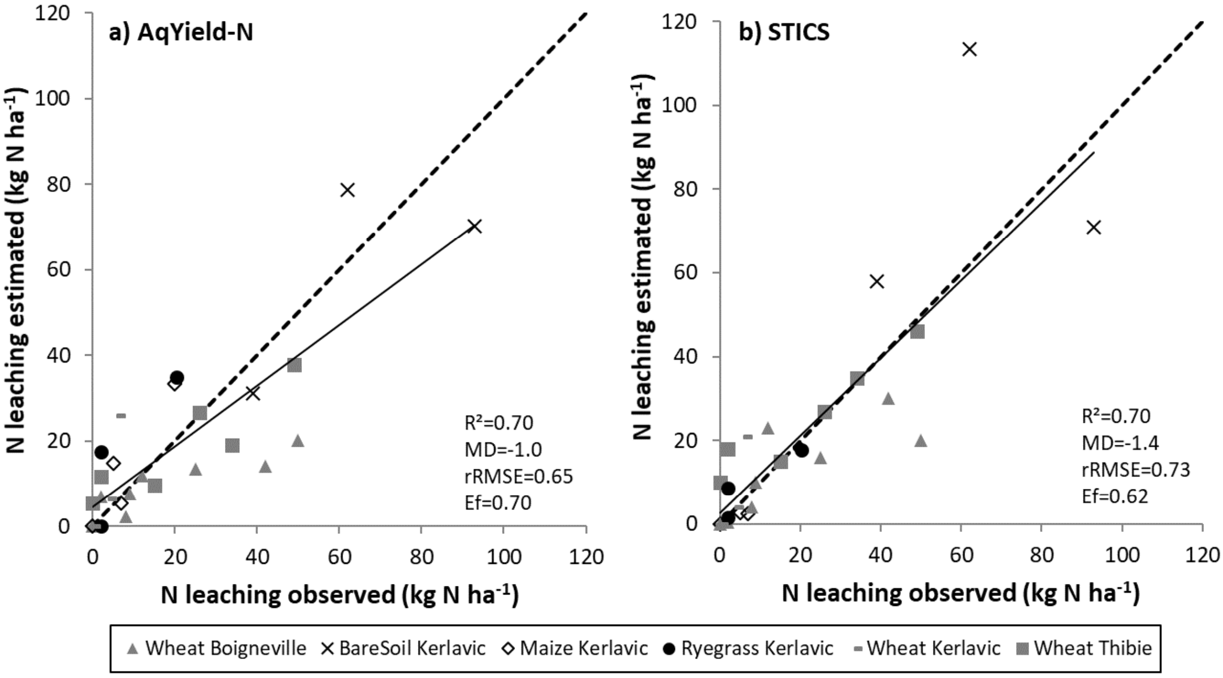

Figure 6 Cumulative N leaching observed over 4-8 months (leaching period in Table 1) vs. that estimated by a) AqYield-N and b) STICS for three sites (Boigneville, Kerlavic and Thibie) under bare soil, wheat, maize or ryegrass. MD is mean deviation, rRMSE is relative root mean squared error and Ef is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

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

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

4 Discussion

4.1 Ability of AqYield-N to estimate nitrogen leaching

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

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

Like the evaluation of AqYield for estimating water variables (Constantin et al., 2015), AqYield-N generally estimated leaching as well as much more complex models such as STICS. Although the two models showed some differences in their leaching estimates, they sometimes overestimated or underestimated a given leaching situation in the same way. This suggests that some observed data may have been measured with some uncertainty, due to the difficulty of measuring N leaching from experimental fields; for this reason, estimates of N leaching are rarely evaluated. Similar overestimates or underestimates could also have been due to both models failing to represent certain processes. AqYield-N estimated leaching dynamics (Fig. 6) consistent with results found in the literature on the ability of cover crops to reduce N leaching compared to that from bare soil (e.g. Thorup-Kristensen et al., 2003). This is a relevant point, since cover crops are an important management tool for designing more agroecological cropping systems. Tribouillois et al. (2016) and Plaza-Bonilla et al. (2015) identified these leaching dynamics using STICS. AqYield-N can thus represent well the expected dynamics and amount of N leaching for multiple field crop situations, which was the study’s main objective. We did not evaluate intermediate variables because i) total N leaching was the main objective; ii) estimated drainage, which strongly influences estimated leaching, was previously evaluated as sufficient (Tribouillois et al., 2018); iii) mineralization and leaching equations were based on previously published and evaluated equations (Burns, 1975; Clivot et al., 2017; Justes et al., 2009; Nicolardot et al., 2001) and iv) the N uptake demand of crops was based on STICS simulations, which were also previously evaluated as satisfactory (Brisson et al., 2008; Coucheney et al., 2015).

4.2 Validity range and limits

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

AqYield-N was able to estimate the range of leaching amounts observed in contrasting situations and amounts of initial soil mineral N. To keep AqYield-N simple, we represented N uptake directly without simulating biomass dynamics and thus without representing photosynthesis. The variation in global radiation according to location, which can influence crop growth and thus N and water uptake, was not included. As in several other crop models that simulate the N cycle, AqYield-N ignores N_2O and N_2 emissions (Cannavo et al., 2008). AqYield-N does not directly simulate volatilization after N fertilizer application. Consequently, volatilization should be estimated and subtracted from *Nferti*, for example using IPCC emission coefficients or more process-based models such as Volt'air (Génermont and Cellier, 1997). AqYield-N also ignores N inputs from irrigation water and atmospheric deposition; however, they are assumed to have little impact on the N balance. Because the AqYield-N's objective was to predict leaching, and N gases were not represented, AqYield-N cannot predict greenhouse gas emissions, especially N_2O, of cropping systems or agroecological practices. However, annual N losses from leaching are considered to be ten times as high as those from N_2O emissions in arable systems (Stenberg et al., 2012; Webb et al., 2000).

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

5 Conclusion

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

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7 References

Addiscott, T., Wagenet, R.J., 1985. Concept of solute leaching in soil: a review of modelling approaches. J. Soil Sci. 36, 411–424.

Bouraoui, F., Grizzetti, B., 2014. Modelling mitigation options to reduce diffuse nitrogen water pollution from agriculture. Sci. Total Environ. 468–469, 1267–1277. https://doi.org/10.1016/j.scitotenv.2013.07.066

Brisson, N., Gary, C., Justes, E., Roche, R., Mary, B., Ripoche, D., Zimmer, D., Sierra, J., Bertuzzi, P., Burger, P., Bussiere, F., Cabidoche, Y.M., Cellier, P., Debaeke, P., Gaudillère, J.P., Hénault, C., Maraux, F., Seguin, B., Sinoquet, H., 2003. An overview of the crop model STICS. Eur. J. Agron. 18, 309–332. https://doi.org/10.1016/S1161-0301(02)00110-7

Brisson, N., Launay, M., Mary, B., Beaudoin, N., 2008. Conceptual basis, formalisations and parameterisation of the STICS crop model, Editions Q. ed.

Brisson, N., Mary, B., Ripoche, D., Jeuffroy, M.-H., Ruget, F., Nicoullaud, B., Gate, P., Devienne-barret, F., Recous, S., Tayot, X., Plenet, D., Cellier, P., Machet, J., Marc, J., Delécolle, R., 1998. STICS : a generic model for the simulation of crops and their water and nitrogen balances . 1 . Theory and parameterization applied to wheat and corn. Agronomie 18, 311–346.

Burns, I.G., 1975. An equation to predict the leaching of surface-applied nitrate. J. agric. Sci., Camb 85, 443–454. https://doi.org/10.1017/S0021859600062328

Bussink, D.W., Oenema, O., 1998. Ammonia volatilization from dairy farming systems in temperate areas: A review. Nutr. Cycl. Agroecosystems 51, 19–33. https://doi.org/10.1023/A:1009747109538

Cannavo, P., Recous, S., Parnaudeau, V., Reau, R., 2008. Modeling N Dynamics to Assess Environmental Impacts of Cropped Soils. Adv. Agron. 97, 131–174. https://doi.org/10.1016/S0065-2113(07)00004-1

Carr, G.M., Neary, J.P., 2008. Water quality for ecosystem and human health. UNEP/Earthprint.

Casadebaig, P., Guilioni, L., Lecoeur, J., Christophe, A., Champolivier, L., Debaeke, P., 2011. SUNFLO, a model to simulate genotype-specific performance of the sunflower crop in contrasting environments. Agric. For. Meteorol. 151, 163–178. https://doi.org/10.1016/j.agrformet.2010.09.012

Chen, T., Oenema, O., Li, J., Misselbrook, T., Dong, W., Qin, S., Yuan, H., Li, X., Hu, C., 2019. Seasonal variations in N2 and N2O emissions from a wheat–maize cropping system. Biol. Fertil. Soils 55, 539–551. https://doi.org/10.5846/stxb201412292597

Clivot, H., Mary, B., Valé, M., Cohan, J.P., Champolivier, L., Piraux, F., Laurent, F., Justes, E., 2017. Quantifying in situ and modeling net nitrogen mineralization from soil organic matter in arable cropping systems. Soil Biol. Biochem. 111, 44–59. https://doi.org/10.1016/j.soilbio.2017.03.010

COMIFER, 2017. Guide de la fertilisation raisonnée. https://comifer.asso.fr/en/publications-en/the-comifer-brochure.html.

Constantin, J., Beaudoin, N., Launay, M., Duval, J., Mary, B., 2012. Long-term nitrogen dynamics in various catch crop scenarios : Test and simulations with STICS model in a temperate climate. Agric. Ecosyst. Environ. 147, 36–46. https://doi.org/10.1016/j.agee.2011.06.006

Constantin, J., Mary, B., Laurent, F., Aubrion, G., Fontaine, A., Kerveillant, P., Beaudoin, N., 2010. Effects of catch crops, no till and reduced nitrogen fertilization on nitrogen leaching and balance in three long-term experiments. Agric. Ecosyst. Environ. 135, 268–278. https://doi.org/10.1016/j.agee.2009.10.005

Constantin, J., Willaume, M., Murgue, C., Lacroix, B., Therond, O., 2015. The soil-crop models STICS and AqYield predict yield and soil water content for irrigated crops equally well with limited data. Agric. For. Meteorol. Meteorol. 206, 55–68. https://doi.org/10.1016/j.agrformet.2015.02.011

Coucheney, E., Buis, S., Launay, M., Constantin, J., Mary, B., García de Cortázar-Atauri, I., Ripoche, D., Beaudoin, N., Ruget, F.F., Andrianarisoa, K.S., Le Bas, C., Justes, E., Leonard, J., 2015. Accuracy, robustness and behavior of the STICS v-8 soil-crop model for plant, water and nitrogen outputs: evaluation over a wide range of agro-environmental conditions. Environ. Model. Softw. 64, 177–190. https://doi.org/10.1016/j.envsoft.2014.11.024

Di, H.J., Cameron, K.C., 2002. Nitrate leaching in temperate agroecosystems : sources , factors and mitigating strategies 237–256.

Di Paola, A., Valentini, R., Santini, M., 2016. An overview of available crop growth and yield models for studies and assessments in agriculture. J. Sci. Food Agric. 96, 709–714. https://doi.org/10.1002/jsfa.7359

Faivre, R., Leenhardt, D., Voltz, M., Benoît, M., Papy, F., Dedieu, G., Wallach, D., 2004. Spatialising crop models. Agronomie 24, 205–217. https://doi.org/10.1051/agro

Ferrant, S., Oehler, F., Durand, P., Ruiz, L., Salmon-Monviola, J., Justes, E., Dugast, P., Probst, A., Probst, J.-L., Sanchez-Perez, J.-M., 2011. Understanding nitrogen transfer dynamics in a small agricultural catchment: Comparison of a distributed (TNT2) and a semi distributed (SWAT) modeling approaches. J. Hydrol. 406, 1–15. https://doi.org/10.1016/j.jhydrol.2011.05.026

Génermont, S., Cellier, P., 1997. A mechanistic model for estimating ammonia volatilization from slurry applied to bare soil. Agric. For. Meteorol. 88, 145–167. https://doi.org/10.1016/S0168-1923(97)00044-0

Hall, M.D., Shaffer, M.J., Waskom, R.M., Delgado, J.A., 2001. Regional nitrate leaching variability: what makes a difference in northeastern Colorado. J. Am. Stat. Assoc. 37, 139–150.

Hoffmann, M., Johnsson, H., 1999. A method for assessing generalised nitrogen leaching estimates for agricultural land 4, 35–44.

Justes, E., Mary, B., Nicolardot, B., 2009. Quantifying and modelling C and N mineralization kinetics of catch crop residues in soil: parameterization of the residue decomposition module of STICS model for mature and non mature residues. Plant Soil 325, 171–185. https://doi.org/10.1007/s11104-009-9966-4

Köhler, K., Duynisveld, W.H.M., Böttcher, J., 2006. Nitrogen fertilization and nitrate leaching into groundwater on arable sandy soils. J. Plant Nutr. Soil Sci. 169, 185–195. https://doi.org/10.1002/jpln.200521765

Loague, K., Corwin, D.L., 1996. Uncertainty in Regional-Scale Assessments of Non-Point Source Pollutants. Soil Sci. Soc. Am. J. 677.

Lord, E.I., Sheperd, M.A., 1993. Developments in the use of porous ceramic for measuring nitrate leaching. J. Soil Sci. 44, 435–449.

Machet, J.-M., Dubrulle, P., Damay, N., Duval, R., Julien, J.-L., Recous, S., 2017. A Dynamic Decision-Making Tool for Calculating the Optimal Rates of N Application for 40 Annual Crops While Minimising the Residual Level of Mineral N at Harvest. Agronomy 7, 73. https://doi.org/10.3390/agronomy7040073

Martin, E., Gascoin, S., Grusson, Y., Murgue, C., Bardeau, M., Anctil, F., Ferrant, S., Lardy, R., Le Moigne, P., Leenhardt, D., Rivalland, V., Sánchez Pérez, J.M., Sauvage, S., Therond, O., 2016. On the Use of Hydrological Models and Satellite Data to Study the Water Budget of River Basins Affected by Human Activities: Examples from the Garonne Basin of France. Surv. Geophys. 37, 223–247. https://doi.org/10.1007/s10712-016-9366-2

Mary, B., Beaudoin, N., Justes, E., Machet, J., 1999. Calculation of nitrogen mineralization and leaching in fallow soil using a simple dynamic model. Eur. J. Soil Sci. 50, 549–566.

Moriasi, D.N., Arnold, J.G., Van Liew, M.W., Bingner, R.L., Harmel, R.D., Veith, T.L., 2007. Model Evaluation Guidelines for Systematic Quantification of Accuracy in Watershed Simulations. Trans. ASABE 50, 885–900. https://doi.org/10.13031/2013.23153

Nicolardot, B., Recous, S., Mary, B., 2001. Simulation of C and N mineralisation during crop residue decomposition : A simple dynamic model based on the C : N ratio of the residues. Plant Soil 83–103.

Plaza-Bonilla, D., Nolot, J.M., Raffaillac, D., Justes, E., 2015. Cover crops mitigate nitrate leaching in cropping systems including grain legumes: Field evidence and model simulations. Agric. Ecosyst. Environ. 212, 1–12. https://doi.org/10.1016/j.agee.2015.06.014

Silgram, M., Anthony, S.G., Fawcett, L., Stromqvist, J., 2008. Evaluating catchment-scale models for diffuse pollution policy support: some results from the EUROHARP project. Environ. Sci. Policy 11, 153–162. https://doi.org/10.1016/j.envsci.2007.12.002

Singh, B., Sekhon, G.S., 1977. Some measures of reducing leaching loss of nitrates beyond potential rooting zone III. Proper crop rotation. Plant Soil 47, 585–591. https://doi.org/10.1007/BF00011028

Stenberg, M., Ulén, B., Söderström, M., Roland, B., Delin, K., Helander, C.A., 2012. Tile drain losses of nitrogen and phosphorus from fields under integrated and organic crop rotations. A four-year study on a clay soil in southwest Sweden. Sci. Total Environ. 434, 79–89. https://doi.org/10.1016/j.scitotenv.2011.12.039

Taylor, S.D., He, Y., Hiscock, K.M., 2016. Modelling the impacts of agricultural management practices on river water quality in Eastern England. J. Environ. Manage. 180, 147–163. https://doi.org/10.1016/j.jenvman.2016.05.002

Therond, O., Belhouchette, H., Janssen, S., Louhichi, K., Ewert, F., Bergez, J., Wery, J., Heckelei, T., Alkan, J., Leenhardt, D., Ittersum, M. Van, 2009. Methodology to translate policy assessment problems into scenarios : the example of the SEAMLESS integrated framework 12, 619–630. https://doi.org/10.1016/j.envsci.2009.01.013

Therond, O., Sibertin-blanc, C., Lardy, R., Gaudou, B., Sauvage, S., Taillandier, P., Vavasseur, M., Mazzega, P., Balestrat, M., Ong, Y., Louail, T., Mayor, E., Bai, V., 2014. Integrated modelling of social-ecological systems : The MAELIA high-resolution multi-agent platform to deal with water scarcity problems, in: 7th Intl. Congress on Env. Modelling and Software, San Diego, CA, USA. June, p. 8.

Thorup-Kristensen, K., Magrid, J., Jensen, L.S., Magid, J., Jensen, L.S., Magrid, J., Jensen, L.S., Magid, J., Jensen, L.S., 2003. Catch crops and green manures as biological tools in nitrogen management in temperate zones. Adv. Agron., Advances in Agronomy 79, 227–302. https://doi.org/10.1016/S0065-2113(02)79005-6

Tribouillois, H., Cohan, J.-P., Justes, E., 2015. Cover crop mixtures including legume produce ecosystem services of nitrate capture and green manuring: assessment combining experimentation and modelling. Plant Soil 401, 347–364. https://doi.org/10.1007/s11104-015-2734-8

Tribouillois, H., Constantin, J., Willaume, M., Brut, A., Ceschia, E., Tallec, T., Beaudoin, N., Therond, O., 2018. Predicting water balance of wheat and crop rotations with a simple model: AqYield. Agric. For. Meteorol. 262, 412–422. https://doi.org/10.1016/j.agrformet.2018.07.026

Wagenet, R.J., Hutson, J.L., 1996. Scale-Dependency of Solute Transport Modeling/GIS Applications. J. Environ. Qual. 25, 499–510.

Webb, J., Harrison, R., Ellis, S., 2000. Nitrogen fluxes in three arable soils in the UK. Eur. J. Agron. 13, 207–223. https://doi.org/10.1016/S1161-0301(00)00075-7