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# Modelling direct field nitrogen emissions using a semi-mechanistic leaching model newly implemented in Indigo-N v3

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## Abstract

Nitrogen plays a major role in agroecosystems as the key nutrient in agricultural production as well as a source of different emissions, which exceed currently planetary boundaries. N losses, are conditioned by both pedoclimatic conditions and agricultural strategies (e.g. rotations, fertilisation), predominantly take the form of ammonia (NH<sub>3</sub>) volatilisation, nitrate (NO<sub>3</sub>) leaching, nitrification-driven nitric oxide (NO<sub>x</sub>) emission to air, and denitrification-driven nitrous oxide (NO<sub>x</sub> and N<sub>2</sub>O) emissions to air. The multiplication of initiatives and studies on nitrogen modelling resulted in a broad offer of complex simulation models (Tier 3) on one extreme of the gradient between feasibility and integration of processes. On the other side, a multiplication of initiatives has led to a broad offer of causal indicators in the form of proxies and considering one or a few input variables (Tier 1). A relevant compromise between those extremes lies in the development of operational models using a restricted number of parameters and input variables (Tier 2). Here, we propose a new semi-mechanistic operational model for the estimation of direct field N emissions (NH<sub>3</sub>, NO<sub>3</sub>, NO<sub>x</sub> and N<sub>2</sub>O) from contrasting agricultural situations: the Indigo-N v3 (I-N3) model. The gaseous emissions are based on Tier 1 (NO<sub>x</sub>) and Tier 2 (NH<sub>3</sub>, N<sub>2</sub>O) methods taken from the literature, with some enhancements, while we developed a totally new semi-mechanistic approach for nitrate leaching. A comparison of I-N3 outputs was performed with measurements of nitrate leaching in three countries (15 arable fields in France, 3 sugar cane fields at Reunion Inland, and 5 cropped fields in Kenya) and showed a reasonable predictive quality for temperate arable fields, and for some of the tropical fields (1 in Reunion and 3 in Kenya). It also performed better than the previous version of Indigo-N (IN-2) and the SALCA/SQCB models. In comparison with previous Tier 2 models, the newly developed Indigo-N v3 presents an original position on the gradient between integration of processes and feasibility of the simulation of processes. Another novelty of I-N3 lies in its broad scope, designed to be valid for temperate and non-temperate crops, including annual field crops, short-cycle vegetables, temporary grasslands and perennial grasses (such as sugarcane, miscanthus or switchgrass). Parameterisation and validation should be continued for further crops, such as associations and short cycle vegetables.

**Keywords:** ammonia volatilisation; contrasting agricultural situations; life cycle inventories, nitrate leaching; nitrous oxide emissions; organic fertilisation

## 1 Introduction

The relevance of nitrogen (N) as a limiting factor for primary productivity has been well established, as well as the important impacts associated with N emissions from agricultural systems linked to biogeochemical flows (Stevens, 2019; Sutton, 2011). Those are considered having exceed planet boundaries (Campbell et al., 2017), besides erosion of biodiversity and phosphorus biogeochemical flows. N losses, conditioned by both pedoclimatic conditions and agricultural strategies (e.g. rotations, fertilisation), predominantly take the form of

ammonia (NH<sub>3</sub>) volatilisation, nitrate (NO<sub>3</sub>) leaching, nitrification-driven nitric oxide (NO<sub>x</sub>) emission to air and denitrification-driven nitrous oxide (NO<sub>x</sub> and N<sub>2</sub>O) emissions to air (EMEP/EEA, 2019). Those are sources of losses to the different environmental compartments, causing a series of impacts, the so called “nitrogen cascade” (Fowler et al., 2013).

Agricultural systems differ in terms of the type of produced crops (e.g. field crops, vegetable gardening, perennials), underlying pedoclimatic conditions (e.g. temperate, tropical and sub-tropical conditions; predominantly sandy, silty or clayey soils), and agricultural practices adopted (e.g. crop rotations/sequences, fertilisation strategies and irrigation). This variety of management and pedoclimatic circumstances can be labelled as **contrasting agricultural situations**, which have been addressed by modellers via major nitrogen modelling efforts over the last decades (Bhar et al., 2021; Cannavo et al., 2008).

Despite these efforts, the lack of a universally valid and operational model to estimate direct field emissions in the context of applications such as life cycle assessment (LCA) has been repeatedly indicated in the literature (Avadí et al., 2022; Nitschelm et al., 2018; Pereira Andrade et al., 2021; van Lent et al., 2015). Indeed, in the context of LCA, practitioners require simpler models rather than complex ones to estimate direct field emissions to be included in life cycle inventories (Avadí et al., 2022). Complex models, such as crop-soil models (e.g. Brisson et al., 2003; Parnaudeau et al., 2012; Tribouillois et al., 2020), have been indeed used in LCA, but their correct calibration and interpretation of outputs require advanced agronomical expertise. The multiplication of initiatives and studies on nitrogen modelling resulted in a broad offer of complex simulation models on one extreme of the gradient between feasibility and integration of processes (Bhar et al., 2021; Bhattacharyya et al., 2021; Bockstaller et al., 2015; Cannavo et al., 2008). On the other side, a multiplication of initiatives has led to a broad offer of causal indicators in the form of proxies and taking into account one or a few input variables, with nitrogen balances being among the most popular (Bockstaller et al., 2015; Rasmussen et al., 2017; Weckesser et al., 2021; Zhang et al., 2019). A relevant compromise between those extremes lies in the development of operational models using a restricted number of parameters and input variables, as reviewed by Buczko and Kuchenbuch (2010). In this review, models behind the reviewed indicators belong to the Tier 1 (simplified approaches based, on scoring methods or on emission coefficients) or Tier 2 levels (e.g. semi-mechanistic, with relatively modest data needs). More recently Nitrogen Footprint is another example of Tier 1 model (Li et al., 2022; Mohanty et al., 2020). However, most of the models present a very large degree of simplification; characteristic of Tier 1 approaches, and/or are limited regarding their scope, emissions covered by the model or in the range of agricultural situations they cover.

Therefore, models assessing direct nitrogen emissions and adapted to cover a broad range of agricultural situations beyond those featuring conventionally fertilised temperate field crops are needed to *inform* (i.e. to provide key data elements to) agricultural life cycle inventories or the data needs of other multi-criteria assessments in agricultural contexts. Such model development remains a challenge. Here, we propose a new **Tier 2 semi-mechanistic operational model** for the estimation of direct field N emissions from contrasting agricultural situations: the **Indigo-N v3 (I-N3)** model. I-N3 is built upon previous iterations of the INDIGO model (Bockstaller et al., 2008; Bockstaller and Girardin, 2010), as well as on more recent models and approaches which attempt to semi-mechanistically represent the drivers and mechanisms for N losses from agricultural systems. The novelty of I-N3 lies in the better integration of mechanisms for the nitrate leaching component than in Tier 1 models reviewed by Buczko and Kuchenbuch (2010) or in Tier 2 models, such as the previous version of **Indigo-N** (Avadí et al., 2022) or the SALCA model (Nemecek et al., 2020), while maintaining the need of input data at reasonable level —i.e. considerably lower level compared to Tier-3 ones (Avadí et al., 2022;

Pereira Andrade et al., 2021). The broad scope of the model is another progress in comparison with previous models. I-N3 was designed to be valid for temperate and non-temperate crops, including annual field crops, short-cycle vegetables, temporary grasslands and perennial grasses (such as sugarcane, miscanthus or switchgrass). The model is not (yet) valid for rice production, associated crops or perennials (e.g., fruit trees, oil palm, grapevines). Future development of the model will increase its scope and functionality to include these crops.

## **2 Methods**

In a previous study (Avadí et al., 2022), we compared the feasibility and accuracy of commonly used Tier 1-2 models to predict agricultural N emissions. Based on the recommendations from that study, we performed a literature review to identify equations, formulas, approaches and models dealing with the aspects identified as deficient in the revised models. The retained solutions were those identified as capturing the main determinants of emissions, and whose parameters could be successfully determined to represent contrasting agricultural situations. The retained sub-models are listed in Table 1.

**Table 1. Elements of the Indigo-N v3 model**

<b>Emission and/or mechanism</b>	<b>Model for mineral fertilisation</b>	<b>Model for organic fertilisation</b>	<b>Suitability for tropical and sub-tropical agriculture</b>	<b>Suitability for horticulture and perennials</b>	<b>Notes</b>
Ammonia (NH <sub>3</sub> ) volatilisation	EMEP/EEA (2016 or 2019) Tier 2 → a product of N applied, annual average temperature, soil pH, and emission rate per type of mineral fertiliser; modified by correction factors for soil incorporation	For manure and slurry: EMEP/EEA (2016 or 2019) Tier 2; for compost, digestate and sludge: Brockmann et al. (2018) → a product of TAN, an emission rate per type of organic fertiliser; modified by correction factor for spreading technology and soil incorporation	Only a partial adaptation for mineral fertilisers (i.e. correction for pH and average annual temperature), but not for organic ones, as limited by the emission factors, which are valid for temperate conditions.	Yes	Emission factors from EMEP/EEA (Amon et al., 2019, 2016; Hutchings et al., 2019, 2016) and Brockmann et al. (2018) for mineral and organic fertilisers are corrected using factors for agricultural management proposed in Brockmann et al. (2018) and AGRAMMON <sup>a</sup> technical parameters documentation v2018 (Kupper, 2018).
Nitrogen oxides (NO <sub>x</sub> ) emission to air	EMEP/EEA (2019) Tier 1 model (Hutchings et al., 2019) → emission factors derived from Stehfest and Bouwman (2006)		In principle yes, as the EMEP/EEA observations dataset <sup>b</sup> includes global agricultural systems	In principle yes, as the EMEP/EEA observations dataset <sup>b</sup> includes global agricultural systems	No Tier 2 is available.
Nitrous oxide (N <sub>2</sub> O) emissions to air	IPCC (2006) Tier 1 → Direct N <sub>2</sub> O emissions: a product of N from fertiliser and crop residues with a fixed emission factor; modified by correction factors from Bockstaller and Girardin (2010), according to soil type, soil management and irrigation. Indirect N <sub>2</sub> O emissions: linked to NH <sub>3</sub> volatilisation, NO <sub>x</sub> emissions and NO <sub>3</sub> leaching/run-off		In principle yes, as the IPCC observations dataset includes global agricultural systems	In principle yes	
Nitrate (NO <sub>3</sub> ) leaching	Leaching factors computed from a new formalism combining the Burns model (Burns, 1976; Scotter et al., 1993) with the N balances before and during each drainage period		Yes, variable draining regimes and mineralisation dynamics are considered	Yes (for market vegetables and perennial grasses only)	The formalism allows a great flexibility for representing different draining regimes (e.g. winter rains in temperate climates, rainy seasons in tropical climates) and agricultural systems featuring different cycle lengths (e.g. vegetable cycles of <2 months vs. long crop rotations).

Mineralisation of exogenous organic matter (crop residues and organic fertilisers)	N/A	Mineralisation curves from literature (Bouthier et al., 2009; Lashermes et al., 2010; Machet et al., 2017), based on normalised days (Mary et al., 1999)	In principle yes, as based on temperature and humidity normalised days. The curves are mainly parametrised on French data	Yes	The formalism allows a great flexibility for representing various crop rotations and fertilisation strategies.
Main and intermediate crop N needs and absorption dynamics	N needs computed per unit of yield and/or per ha (standard/generalised practice) and absorption dynamics expressed as temperature sums between seeding and harvest dates	Yes	Yes	Yes	Absorption dynamic, approached as sigmoid or linear depending on the crop, allows a great flexibility to estimate the absorption for any crop on any climate
Mineralisation of soil organic matter	Clivot et al. (2017) → empirical model based on 65 field experiments in France, where mineralisation is predicted from 5 soil parameters (soil N <sub>org</sub> , clay, pH, C/N and CaCO <sub>3</sub> )	Yes: normalised days are used	Yes: a period of analysis from harvest to the end of draining is considered	Yes	Mechanism relevant for computing NO <sub>3</sub> lixiviation.

<sup>a</sup> AGRAMMON model (<https://www.agrammon.ch/>) as used in ecoinvent 3 (Nemecek and Schnetzer, 2012); <sup>b</sup> Data associated with Stehfest and Bouwman (2006)

## 2.1 Model definition: general principles

Indigo-N v3 is based on the following principles, objectives and functionalities:

- Calculate all N emissions at the field scale for a crop, a crop sequence or rotation, with a focus on nitrate leaching, identified as the main N agricultural emission (in quantity) and the most complex one to assess (Avadí et al., 2022). The model combines different existing approaches to estimate  $\text{NH}_3$ ,  $\text{NO}_x$  and  $\text{N}_2\text{O}$  emissions and proposes a new formalism to estimate  $\text{NO}_3$  losses.
- Represent a wide variety of field crops, vegetables and grasslands/meadows, under various pedoclimatic conditions worldwide.
- Provide worldwide default values for pedoclimatic and agricultural parameters, to keep the user data demand as low as possible.
- The time period of a crop is considered from the previous main crop destruction to the crop destruction. The catch crops are thus included into the time period of the following main crop.

In many agricultural situations —not least for arable crops in temperate conditions, which represent a great cropped area— nitrate leaching occurs during the drainage between two crops, thus it does not depend on only one crop but at least on the characteristics of the preceding and the studied crop (Beaudoin et al., 2005).

In Indigo-N v3, it is possible to model either a crop rotation or a crop sequence. In a crop rotation, the last crop described connects with the first crop. In a crop sequence, which is linear, the last crop does not influence the first crop. The latter approach enables studying single crops, by considering a short sequence featuring a crop of interest and certain elements of the previous crop (at least residue management, as it impacts on the crop of interest).

By default, we will refer to rotations in this work, unless otherwise indicated. All the emissions are calculated at the rotation scale. We propose an emissions allocation method among crops in the rotation in section 2.4.

The overall architecture of I-N3 is depicted in Fig. 1.

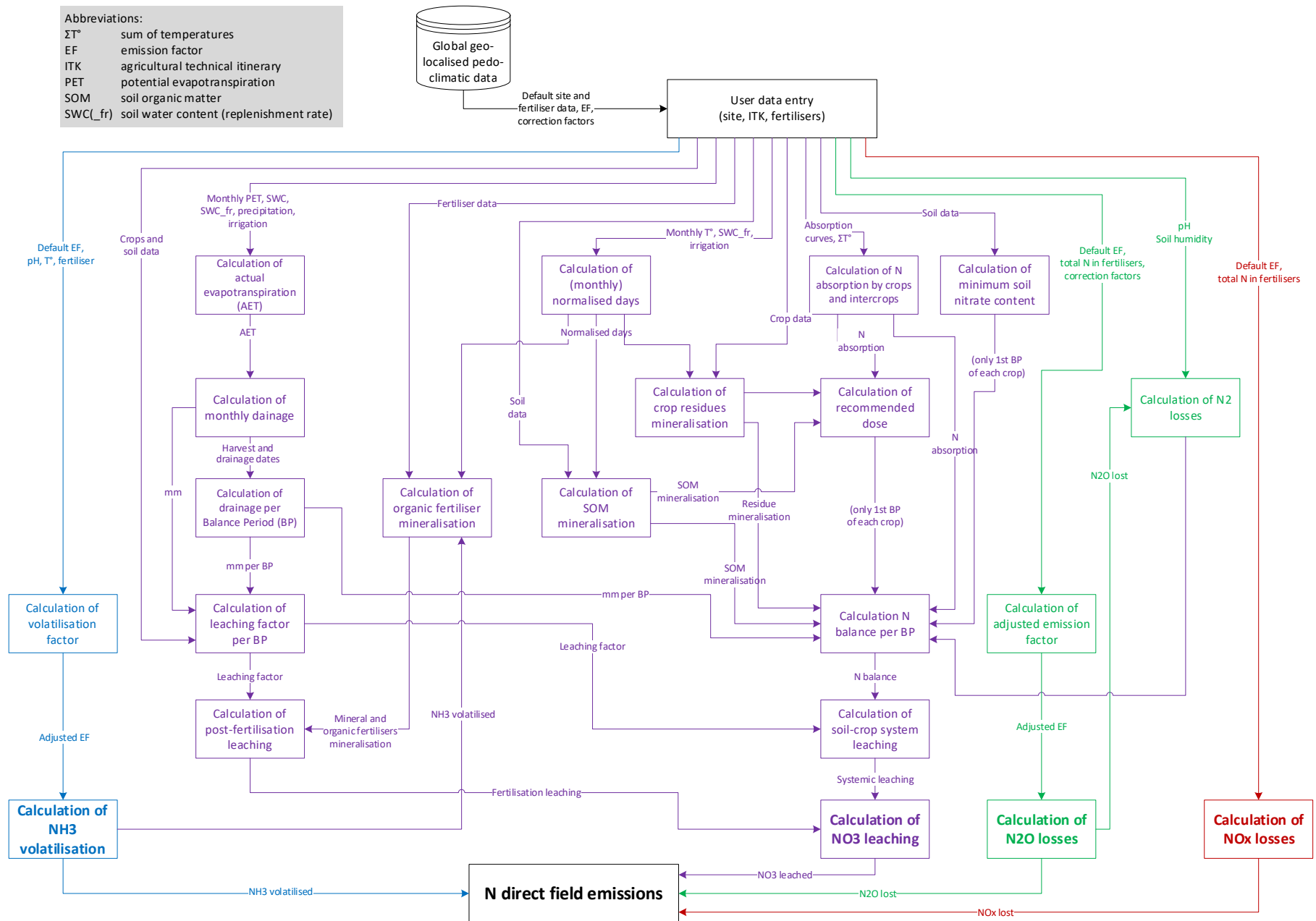


Fig. 1. Architecture of the Indigo-N v3 model



## 2.2 Model definition: gaseous losses

Gaseous N emissions are fairly well computed with Tier 1 and 2 models (Avadí et al., 2022).

Ammonia volatilisation, which takes place before all other emissions (Sommer et al., 2004), is computed per fertiliser. The calculation is based on EMEP/EEA (versions 2016 or 2019, to be chosen by the user), Chapter 3.D Crop production and agricultural soils (Hutchings et al., 2019, 2016) Tiers 1 or 2 for mineral fertilisers and Tier 1 for organic fertilisers, Chapter 3.B Manure management (Amon et al., 2019, 2016) Tiers 1 or 2 for animal effluents (i.e. excretions); complemented with emission factors from Brockmann et al. (2018) and correction factors from AGRAMMON (Kupper, 2018). Ammonia emissions from each fertiliser are then allocated among the crops according to rules described in section 2.4.

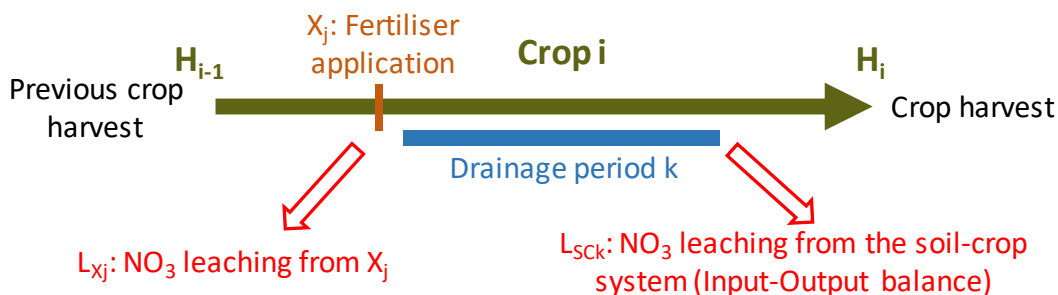
Nitrogen oxide emissions are computed directly per fertiliser. The calculation is based on EMEP/EEA (2019), Chapter 3.D Crop production and agricultural soils (Hutchings et al., 2019) Tier 1.

Nitrous oxide emissions include both direct and indirect (i.e.  $N_2O$  emissions taking place through indirect pathways, namely volatilisation, leaching and runoff (De Klein et al., 2006)) pathways.  $N_2O$  emissions are computed directly for each crop. The calculation is based on IPCC (2006), Volume 4: Agriculture, Forestry and Other Land Use, Chapter 11:  $N_2O$  Emissions from Managed Soils, and  $CO_2$  Emissions from Lime and Urea Application (De Klein et al., 2006) Tier 1, complemented with correction factors from Bockstaller and Girardin (2010).

## 2.3 Model definition: nitrate ( $NO_3$ ) leaching

$NO_3$  leaching is a vertical transfer of N dissolved in drainage water that can impact groundwater if an underground water body is present or surface water in case of in depth hydrogeological transfer or by artificial drainage (Van Drecht et al., 2003). The computation of leaching for the harvest-to-harvest period associated with crop  $i$  includes two distinctive mechanisms, as depicted in Fig. 2: i) a leaching from t

he soil surface of N input  $X_j$  ( $L_{X_j}$ ), function of the amount of mineral input and a leaching coefficient, and ii) a leaching across the soil profile associated with the soil-crop system ( $L_{SCK}$ ), calculated from a soil-crop input-output balance for each draining event  $k$  and a leaching coefficient.



**Fig. 2. Generic representation of surface leaching from N inputs ( $L_{X_j}$ ) and profile leaching from the soil-crop system ( $L_{SCK}$ ) for the draining period  $k$ , for crop  $i$ , between the harvest of the previous crop ( $H_{i-1}$ ) and the crop harvest**

Leaching coefficients are computed with the adapted Burns model (Burns, 1976; Scotter et al., 1993). The overall surface leaching from all N inputs ( $L_{X_i}$ ) is the sum of all  $L_{X_j}$ , and the overall leaching from the soil-crop system ( $L_{SCK}$ ) is the sum of all  $L_{SCK}$ .

Surface leaching following N input ( $L_{X_j}$ ) is calculated for each fertiliser application on the crop  $i$ , and the overall surface leaching from all N inputs is the sum of all  $L_{X_j}$  (Eq. 1).

$$L_{X_i} = \sum L_{X_j} \quad \text{Eq. 1}$$

The soil-crop system leaching is calculated for each drainage period  $k$  occurring during crop  $i$ , from a crop N balance on this period of time. The overall leaching on the soil profile is the sum of all  $L_{Sck}$  (Eq. 2).

$$L_{SC_i} = \sum L_{Sck} \quad \text{Eq. 2}$$

The total leaching of crop  $i$  ( $L_{N-NO_3i}$ ) [kg N-NO<sub>3</sub>] is the sum of total surface and soil-crop leaching (Eq. 3).

$$L_{N-NO_3i} = L_{X_i} + L_{SC_i} \quad \text{Eq. 3}$$

### 2.3.1 Surface leaching following N input

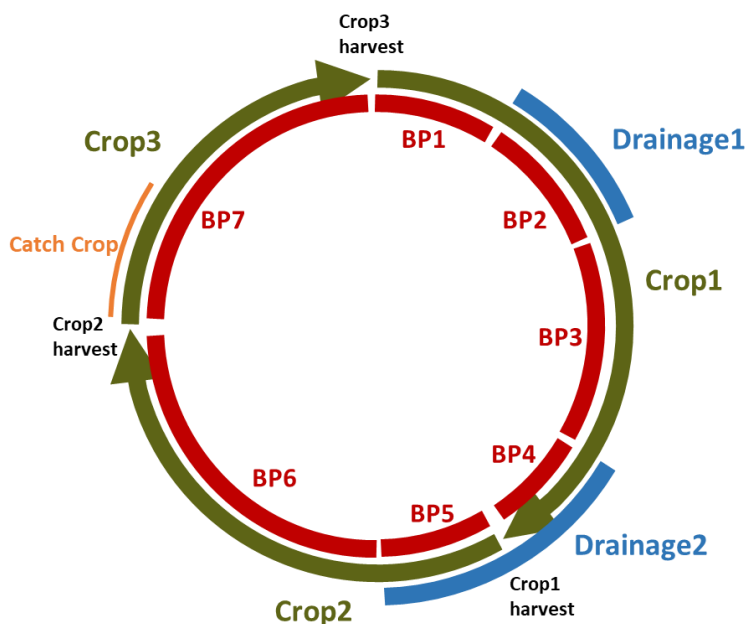
A leaching coefficient is calculated for each fertiliser application following the adapted Burns model (Burns, 1976; Scotter et al., 1993). Parameters for this coefficient are estimated based on user data (see section 3.5 in the Supplementary Material). The leachable N from the fertiliser is determined by deducting ammonia volatilisation, and then it is multiplied by the leaching coefficient to determine surface leaching.

### 2.3.2 Leaching across the soil profile associated with the soil-crop system ( $L_{Sck}$ ), for all crops except grasslands

To calculate the leaching associated with the soil-crop system, the rotation is cut into specific time periods called Balance Periods (BP). A BP is the time period during which a N balance, associated with a leaching coefficient (computed with the adapted Burns model), will be calculated. The time period of a crop is considered from the previous crop harvest to the current crop harvest, without taking into account intermediate catch crops.

The BP are defined as follows, a new BP starts with i) a crop harvest + 1 day (the crop time period always begins with a new BP), ii) the start of a drainage period, or iii) the end of a drainage period + 1 day. Temporary grasslands are an exception, see 2.3.3.

This method is generic enough to calculate the BP on any combination of crop/rotation/drainage time period. An example is presented in Fig. 3.



**Fig. 3.** An example of the cutting of a random rotation into balance periods (BP). Here, we have 3 crops (with their respective time period represented in green) and 2 drainage periods (with their respective time period represented in blue). This two information (crops time periods and drainages time periods) allow us to cut the rotation into specific balance period with the rules presented above (here we have 7 BP)

### 2.3.3 Leaching across the soil profile associated with the soil-crop system ( $L_{sck}$ ), temporary grassland specificities

Grasslands are not considered to have a high nitrate leaching potential (Padilla et al., 2018), except on high N inputs conditions (Jarvis, 2000). The exception are leguminous plants considered as grasslands, such as alfalfa, which contribute non-negligible amounts of N to the soil, being continuously mineralised (Justes et al., 2001; CIVAM, 2010). Under low to moderate nitrogen rate, grass cover uptakes N during the whole vegetative cycle except in dry conditions, without any period of bare soil fostering leaching exists. Furthermore, some specificities do not allow a modelling similar to that for annual crops, such as multiple harvest, grazing, etc. For those reasons, the N leaching across the soil profile is considerably simplified for temporary grassland.

The grassland time period (between the previous crop harvest +1 day and the grassland destruction) is split in two: part 1 and part 2.

Part 1: at the beginning of this time period, grasslands are supposed to have the same behaviour as other annual crops for the nitrate leaching dynamic, thus the nitrate leaching calculation is the same as described in 2.3.2. Part 1 lasts from the previous crop harvest +1 day to grassland seeding + x sum of temperatures (base 0). This amount of sum of temperature is fixed at 1170°C (the sum of temperatures between 1 October and 1 March in Ille-et-Vilaine, typical region of grassland in temperate medium conditions). This parameter may be adapted to other regions.

Part 2: from grassland seeding + x sum of temperatures to grassland destruction. This part is considered as one single balance period and the leaching on this period is calculated as follows. Fig. 4 shows an example of a crop rotation featuring a grassland. A single N balance is calculated for the part 2 time period.

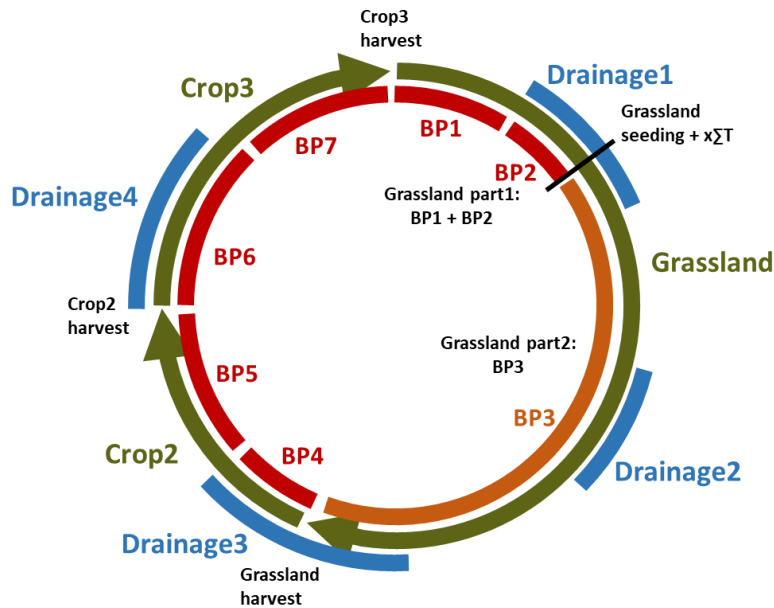


Fig. 4. Example of a rotation with one grassland and 2 other crops. The leaching on BP 1-2-4-5-6-7 will be calculated as described in 2.3.2. The leaching in BP3 will be calculated as described in 2.3.3

### 2.3.4 Preliminary calculations

#### *Normalised days*

Normalised days are computed based on a temperature function and a soil humidity function, per calendar day  $d$  (Mary et al., 1999). Usually the humidity normalisation function depends on the soil water content at field capacity, at wilting point and at day  $d$ , this for each layer of soil. Here, we propose to simplify the approach by reducing the soil to one single layer and using for water content, the available water content (AWC). As the data are available at a monthly scale, we assumed homogenous days per month to calculate it at a daily scale.

#### *Drainage*

Drainage is one of the most important parameters of drainage leaching (Padilla et al., 2018). The challenge is to know not only the amount of drained water, but also the period of the year when it occurs. We propose a method (and all the data associated, at monthly scale) to estimate the amount of drained water, based on precipitation, irrigation, actual evapotran

spiration and soil available water content data. As the data were available at a monthly scale (Galland et al., submitted), we assumed homogenous days per month to calculate it at a daily scale.

For more consistency in the calculation of the Balance Period, we assumed that the total drainage occurring during a specific month should be superior to 10 mm, e.g. the drainage calculated for January (or every other month) should be superior to 10 mm. If not, every day of this month is supposed to be 0 mm of drainage.

Irrigation data, not being globally available at the required level of detail (e.g. Pfister and Bayer 2014), is requested as user data in implementations of the model.

#### *Recommended N dose ( $X_R$ )*

The recommended dose is calculated for each crop (except grasslands) in order to estimate a possible over fertilisation. An N balance is calculated to estimate the crop needs of N from fertilisers. This balance will be

done for a specific time period, from balance opening to crop harvest. By default, the balance opening is the previous crop harvest +1 day (e.g. the N balance for the recommended dose is done for the whole crop time period). But the balance opening date can be personalised by the user.

### **2.3.5 N balance items**

Mineralisation and absorption are computed per specific period required, namely per balance period for nitrate leaching and per crop cycle to determine the recommended N dose. A day-by-day computation, which in itself is meaningless, is carried out in order to easily extract mineralisation or absorption amounts associated with specific periods.

#### ***Minimal mineral nitrogen in soil ( $N_{mnh}$ and $Nof$ )***

Minimal mineral nitrogen in soil at harvest ( $N_{mnh}$ ) is estimated from soil texture and depth class, following COMIFER (2013), and adjusted for high drainage conditions. The increase of the residual amount of mineral N in soil due to over-fertilisation ( $Nof$ ) is calculated following Bockstaller and Girardin (2010). This parameter is not calculated for grasslands.

#### ***Mineralisation of soil organic matter ( $N_{som}$ )***

The potential soil net N mineralisation rate  $V_p$  [kg N/ha/nday] is calculated for the used soil following model A1.5 in Clivot et al. (2017), adapted for a better fit for calcareous soils (e.g., the parameter  $p_{calc}$  is modified from the original 1.114 to 1.5, H. Clivot, pers. comm.).

#### ***Mineralisation of crop and catch crops residues ( $N_{res}$ )***

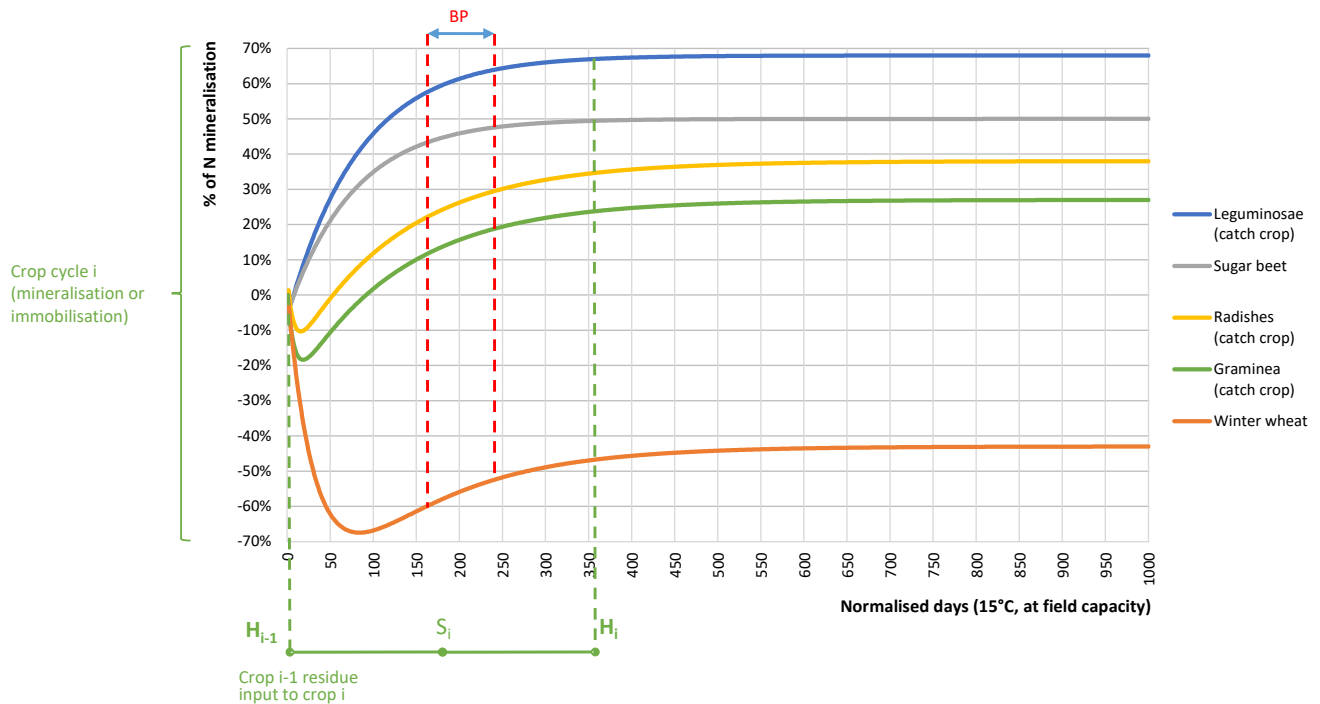
The mineralisation of crop residues ( $N_{res}$ ) is based on mineralisation (asymptotic) curves per class of inputs, following Machet et al. (2017), Lashermes et al. (2010) and discussions with experts (V. Parnaudeau, L. Thuriès and T. Morvan, 2019-2020 pers. comm.). The parameterisation and shape of these curves are discussed in Galland et al. (submitted).

Lashermes et al. (2010) proposed a typology of exogenous organic matter (organic fertilisers and crop residues), based on a number of chemical characteristics not readily available for all crop residues and their fractions (above- and belowground), including cellulose, hemicellulose, lignin, and organic C and N content. Some mineralisation kinetics presented in Machet et al. (2017) are not calibrated in the first part of the cycle in autumn, winter (e.g. maize), because they were created with a different goal, which privileges accuracy during the intensive nitrogen uptake phase of the crop in spring. Alternative approaches, such as the model suggested in Nicolardot et al. (2001), are too data demanding. Given the large uncertainty involved in these kinetics, we retained a subset of five Machet et al. (2017) curves, representing various typical behaviours (Fig. 5). Based on our expertise and the typology of Lashermes et al. (2010), we assigned these five curves to all crop residues parameterised in our model:

- Winter wheat: represents crop residues featuring low water and high lignocellulosic content with high C/N ratio, such as those from most cereals, fibre and oil seeds.
- Leguminosae (catch crop): represents crop residues and whole plants with high N content and mineralisation speed.
- Graminea (catch crop): represents crop residues and whole plants with the lowest mineralisation (among all classes other than Winter wheat).

- Sugar beet and Radishes (catch crop): represent crop residues with relatively high N content, such as leafy residues from vegetables, and a mineralisation behaviour intermediate between Leguminosae and Graminea.

Mineralisation curves are generally asymptotic, from approximately 500 normalised days on. The amount of N mineralised following a crop residue input ( $N_{orgi}$ ), in kg N/ha, is allocated to a crop  $i$  between the date of the previous harvest ( $H_{i-1}$ ) and the harvest ( $H_i$ ) (Fig. 5).



**Fig. 5. Allocation of a crop residue input to a crop and a balance period, based on N mineralisation curves per type of crop residue**

### ***Mineralisation of organic fertilisers ( $N_{org}$ )***

The mineralisation of organic fertilisers ( $N_{org}$ ) is modelled, for each applied organic fertiliser, based on mineralisation (asymptotic) curves per class of inputs, following Bouthier et al. (2009) and Lashermes et al. (2010). Each fertiliser is associated to a class based on Bouthier et al. (2009), but adapted by expert opinion. Each class is associated with specific mineralisation parameters and a typical behaviour. Mineralisation curves are asymptotic, from approximately 500 normalised days on (Fig. 6). The parameterisation and shape of these curves are discussed in Galland et al. (submitted).

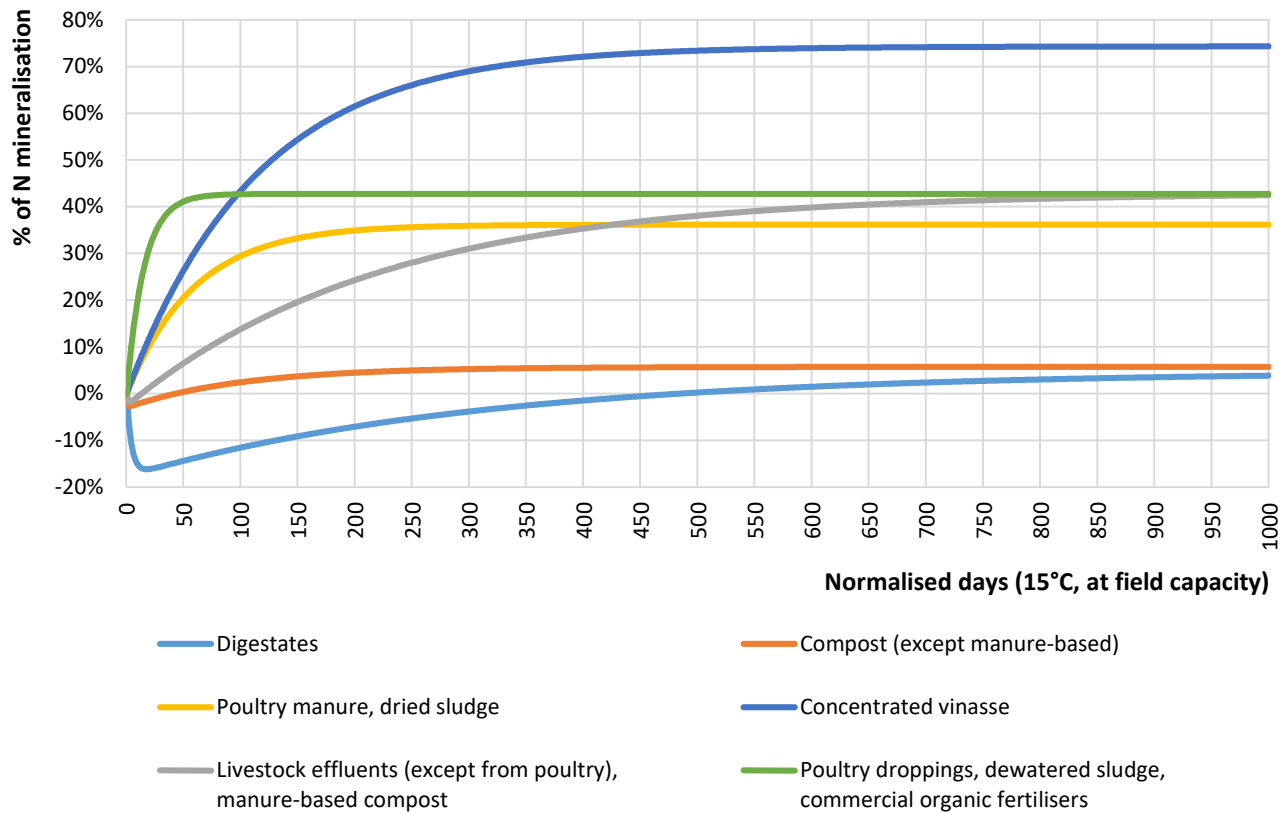
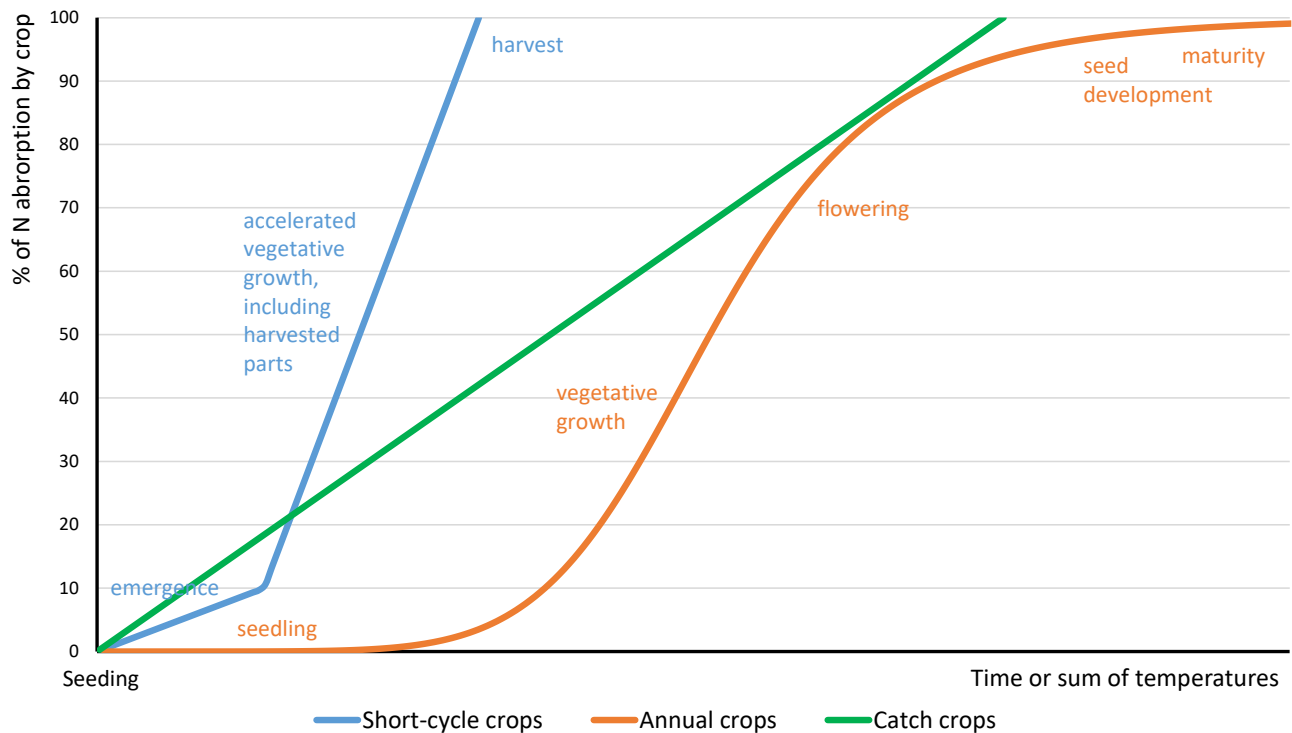


Fig. 6. N mineralisation curves per type of fertiliser

### Absorption by crops and catch-crops ( $N_{abs}$ )

First, the total amount of N absorbed by the crop is estimated. It is typically calculated as the sum of N in above ground residues, N in below ground residue and N in harvested part. This amount of N will be absorbed by the plant according to a simplified absorption curve to estimate the N absorption dynamic.

The absorption dynamic of N by catch crops and main crops ( $N_{abs}$ ) is computed based on the assumptions that the main variable explaining N uptake is the sum of temperatures since the date of seeding (Tribouillois et al., 2020), and that the crop N needs as a function of its yield are known. Moreover, as the main absorption periods of different crop types usually differ (COMIFER, 2013), different absorption curves were retained, namely, sigmoid for cereals, oily seeds and other annual crops, and linear for catch crops, market vegetables and grasslands. Such decision is founded on the common shapes of absorption curves for different crops, as depicted in the literature (e.g. see review in Geisseler and Horwath (2019)). These typical shapes are valid for most crops both in terms of time (i.e. days from seeding) and sum of temperatures (Fig. 7). For a few cases of crops featuring special absorption kinetics (e.g. rapeseed), these generic curves were also retained.



**Fig. 7. Typical shapes and of absorption curves for annual and short-cycle crops**

For catch crops as the crop doesn't reach its full maturity before harvest or destruction, a simplification is made. The absorption is considered linear (in sum of temperature) between seeding and destruction.

### ***N<sub>2</sub> from denitrification to calculate N-balances***

N<sub>2</sub> emissions are a product of denitrification, together with N<sub>2</sub>O, but denitrification models usually compute N<sub>2</sub>O only, or both gasses aggregated. The mole ratio (in g N-N<sub>2</sub>O per g N-N<sub>2</sub>O+N<sub>2</sub>) is extremely variable, between <0.05 and 1 so that the N<sub>2</sub> fraction may represent a non-negligible amount of nitrogen (Mathieu et al., 2006; Saggari et al., 2013). In IN-3, N<sub>2</sub> emissions are estimated with an empirical equation from Le Gall et al. (2014). Then, they are allocated to each BP proportionally of the length of each BP in normalised days.

## **2.4 Allocation of N losses among crops in the rotation**

For each fertiliser, an allocation coefficient is calculated to allocate the emissions of this fertiliser between the crops of the rotation. For mineral fertilisers, all N applied is available for the crop receiving it, thus the allocation factor will be 1 for the crop receiving the fertiliser and 0 for the others. Organic fertilisers can be partially used by the following crops (through fertiliser organic N mineralisation) thus the weight of the emission should be shared on the whole rotation. The allocation factor is proportional to the quantity of mineral N from the fertiliser available for each crop of the rotation.

Every fertiliser dependent emission (i.e. NH<sub>3</sub>, NO, NO<sub>3</sub> leaching following N input and direct N<sub>2</sub>O from fertiliser) will be allocated between the crops with this allocation factor. Direct N<sub>2</sub>O from crop residues and from over-fertilisation is allocated to the crop producing the residues or the potential over-fertilisation. Indirect N<sub>2</sub>O is calculated using the allocated NH<sub>3</sub>, NO and NO<sub>3</sub> emissions and is considered as already allocated.

NO<sub>3</sub> leaching due to the soil-crop system is the result of complex interactions among crops, mineralisation, the fertilisation plan of the rotation and pedoclimatic data. We recommend the following approach: "NO<sub>3</sub> losses



from the soil-crop system are allocated equally between the crop time period receiving the losses and all the previous crop time periods until the one with a drainage period". If there is a drainage on every crop time period (the common case for temperate crop for example), it means that the losses are equally shared between the crop and the previous crop only.

## 2.5 Data

### 2.5.1 Background data

As the goal of the model is to support the construction of agricultural life cycle inventories representing contrasting agricultural situations, its implementation was supported with the inclusion of a database containing global data pertaining to pedoclimatic conditions and crop characteristics. The database provides the soil data and monthly climatic data, as well as crops and fertilisers data, necessary to run the model. Pedoclimatic data are available for each combination of country and Global Ecological Zone (FAO, 2012) worldwide, as well as for each French department. All background data are presented in the accompanying data paper (Galland et al., submitted), and are directly available as a downloadable dataset.

The model's list of crops aims at representing the most important global agricultural products. The list was constructed based on data availability on crop characteristics (e.g. harvest ratios, N content of plant parts, N absorption kinetics, etc.). All crops were assigned a crop category (Table 2), and reference values were included per category in such a way that crops not explicitly listed could be modelled if their crop category is known.

**Table 2. Crop categories in I-N3**

Crop category	Examples
Cereals (fodder)	Maize, oats
Cereals (grain)	Maize, oats, barley, rye, wheat
Green manure	Crucifers, cereal + vegetable mixes
Market vegetables	Cucurbitaceae, tomato, leafy vegetables
Oily seeds	Rapeseed, flaxseed
Annual grasses	Ray grasses
Perennial grasses	Sugarcane, miscanthus, switchgrass
Pulses	Beans, peas
Tubers	Potatoes, cassava, yams

Source: Galland et al. (submitted)

### 2.5.2 Data for model testing and validation

The model was implemented as a spreadsheet tool, and was tested with several datasets of agricultural itineraries, depicting contrasting agricultural situations. The agricultural datasets, described in Table 3, were used to test the model. Observed values of leached nitrate were plotted against predicted values, and a set of non-correlated statistics were computed according to Yang et al. (2000), since a single criterion is insufficient for assessing model performance (Bellocchi et al., 2010). We thus computed the following statistics to assess the predictive quality of the model: i) the mean deviation (MD) assessing whether the model over- or underestimates the observation (Eq. 4), ii) the mean square error (RMSE) assessing the mean deviation around the prediction (Eq. 5), and iii) the model efficiency assessing the lack of model bias, if efficiency is equal to 1 (Eq. 6).

$$MD = 1/n \cdot \sum_{i=1}^n (O_i - P_i) \quad \text{Eq. 4}$$

$$RMSE = \left( 1/n \cdot \sum_{i=1}^n (O_i - P_i)^2 \right)^{1/2} \quad \text{Eq. 5}$$

$$EF = 1 - \sum_{i=1}^n (O_i - P_i)^2 / \sum_{i=1}^n (O_i - \hat{o})^2 \quad \text{Eq. 6}$$

where  $n$  is the number of observations,  $O_i$  and  $P_i$  are observed and predicted values, respectively, and  $\hat{o}$  is the mean of observed values.

Moreover, I-N3 estimations were compared with those of I-N2 (Bockstaller et al., 2008; Bockstaller and Girardin, 2010), SALCA-NO3 V4.81a (Nemecek et al., 2020; Richner et al., 2014; Agroscope, pers. comm) and SQCB (de Willigen, 2000; Faist Emmenegger et al., 2009), all of which were either implemented or available as a spreadsheet tool.

**Table 3. Agricultural datasets used to illustrate/validate the model**

Variable	Site 1: France - Seine Basin	Site 2: Reunion - SOERE PRO	Site 3: Kenya - Central Province
Sources	UPCM, M. Benoit, pers. comm. and Benoit et al. (2015, 2016)	CIRAD, A. Versini, pers. comm., SOERE PRO Network ( <a href="https://si-pro.fr/">https://si-pro.fr/</a> ) and Versini et al. (2020)	FIBL, N. Adamtey, pers. comm. and ICIPE, M. Musyoka, pers. comm., from the SysCom project ( <a href="https://systems-comparison.fibl.org/">https://systems-comparison.fibl.org/</a> ), and Musyoka et al. (2019b, a)
Description	(1) Fava beans/cereals/alfalfa, (2) various crops, with and without CC, (3) various crops, with and without CC	Sugarcane	(1) Potato, (2) Maize, (3) Cabbage
Locations	Seine-et-Marne, France	Reunion island (France), Indian Ocean	Chuka and Thika, Kenya
Global Ecological Zones (FAO, 2012)	Temperate oceanic forest	Tropical mountain system	Tropical mountain system
Periods of seeding and harvest	(1) Unknown – late summer (2) CC: late summer – early fall, crops: fall – early summer (3) CC: summer - late fall, crops: late fall – early summer	Early October – early October	(1) Mid October – early February (2) Late March – early September (3) Early November – late February
Years represented	2013-2014	2017-2018	2012-2014
Tillage	Conventional, a few no-tillage cases	Conventional	Conventional
Irrigation	No	No	Yes
Average yields (t/ha) (DM: dry matter, FM: fresh matter)	(1) 4.6 (wheat) - 10.8 (CC + beans) (DM) (2) 2.5 (CC + faba beans) - 18.4 (CC + sugar beet) (DM) (3) 0.5 (faba beans) - 18.1 (beans) (DM)	36.0 (DM) 91.0 – 102.0 (FM)	(1) 15.9 – 25.9 (FM) (2) 3.4 – 4.9 (DM) (3) 53.5 – 46.8 (FM)
Catch crops (CC)	Yes: pulses	No	No
Fertilisation	8 conventional mineral treatments, 7 organic treatments (no fertiliser, only CC)	3 treatments: a) Dried sludge + mineral, b) Swine slurry + mineral, c) Mineral	2 sites, 1 treatment: farmyard manure + di-ammonium phosphate + calcium ammonium nitrate
Nitrate measurement methods	Vertical ceramic cups at 90 cm, measurement for the drainage period (winter)	Lysimetric plate at 100 cm, measurement for the whole crop period	Self-integrating accumulators (Bischoff, 2007) at 100 cm, measurement for the drainage period (winter)

## 3 Results

### 3.1 Example of calculation

As shown in Table 4, where a selection of test results is depicted, tropical systems (Reunion and Kenya) yielded higher emissions than temperate ones, as well as systems based on organo-mineral than pure mineral fertilisation strategies. Three exceptions are, respectively, the third French system for high nitrate leaching due to the mineralisation of alfalfa crop residues—which is supported by literature (Justes et al., 2001)—, sugar cane under a mineral fertilisation strategy (Reunion) with ammonia emissions due the high rate of urea, and the cabbage crop in Kenya with low leaching. The systems with sugarcane (Reunion) showed high value for gaseous emissions, especially for ammonia due to fertiliser (i.e. urea and slurry with high emission coefficients), as well as high leached nitrate amount after fertilisation. It should be noticed that for the sugarcane systems, nitrate leaching in the soil crop system was lower than after fertilisation. This is may be due to a high value of drainage (> 1500 mm) regularly spread throughout almost the whole year. In the temperate French system with deep soil, drainage during the fertilisation period is much lower so that leaching is close to zero.

**Table 4. Indigo-N v3 calculation of different emissions (NH<sub>3</sub>, NO<sub>x</sub>, N<sub>2</sub>O, NO<sub>3</sub> due to fertilisation and soil crop system) and their main components (e.g. emission factor (EF))**

Site	Preceding crop/crop	Fertilisation strategy	Fertilisation (kg N/ha) (type)	NH <sub>3</sub> emission		NO <sub>x</sub> emission		N <sub>2</sub> O emission			NO <sub>3</sub> leaching		Soil crop leaching NO <sub>3</sub> (kg NO <sub>3</sub> -N/ha)
				EF NH <sub>3</sub> (kg NH <sub>3</sub> -N/kg N)	Emission NH <sub>3</sub> (kg NH <sub>3</sub> -N/ha)	Emission NO <sub>x</sub> (kg N-NO <sub>x</sub> )/ha	direct EF N <sub>2</sub> O (kg N <sub>2</sub> O-N/kg N)	Correction factor	Direct (indirect) emission N <sub>2</sub> O (kg N <sub>2</sub> O-N/ha)	Leaching after fertilisation (kg NO <sub>3</sub> -N/ha)	N balance (kg N/ha)	Leaching factor (Clix )	
France 1	F/WW	mineral	200 (AN)	0.026	<b>5.3</b>	<b>3.6</b>	0.01	1.25 (soil)	<b>3.7 (0.2)</b>	<b>0.1</b>	<b>20</b>	0.47	<b>9.4</b>
France 2	WW/GM	mineral	160 (AN)	0.012	<b>2.0</b>	<b>2.9</b>	0.01	1.25 (soil)	<b>0.3 (0.2)</b>	<b>0.1</b>	13	0.47	<b>6.3</b>
France 3	Al/WW	no	0	0	<b>0.0</b>	<b>0</b>	0	1.25 (soil)	<b>1.9 (0.2)</b>	<b>0</b>	57	0.47	<b>27.0</b>
France 4	WW/cc/So	no	0	0	<b>0.0</b>	<b>0</b>	0	1	<b>0.9 (0)</b>	<b>0</b>	10	0.24	<b>2.4</b>
Reunion mineral	SC	mineral	142 (Urea)	0.13	<b>18.8</b>	<b>2.3</b>	0.01	0.95 (tillage)	<b>4.2 (0.4)</b>	<b>16.1</b>	12.5	0.92	<b>11.6</b>
Reunion slurry	SC	organo-mineral	190 (Slurry) 88 (Urea)	0.29/ 0.13	<b>66.6</b>	<b>4.4</b>	0.01	0.95 (tillage)	<b>6.3 (1.0)</b>	<b>20.70</b>	12.5	0.92	<b>11.6</b>
Reunion sludge	SC	organo-mineral	0.2 95	0.50 0.13	<b>12.5</b>	<b>2.0</b>	0.01	0.95 (tillage)	<b>4.5 (0.4)</b>	<b>21.4</b>	12.5	0.92	<b>11.6</b>
Kenya Chuka Conv high	BM/Po	organo-mineral	107 (FYM) 54 (CAN)	0.68/ 0.007	<b>10.1</b>	<b>2.2</b>	0.01	2 (soil)	<b>3.8 (0.3)</b>	<b>3.2</b>	30	0.66	<b>19.7</b>
Kenya Chuka Conv high	Po/GM	organo-mineral	50 (FYM) 36 (DAP) 27 (CAN)	0.68/ 0.042/ 0.007	<b>6.3</b>	<b>1.7</b>	0.01	2.4 (irrigation, soil)	<b>4.7 (0.3)</b>	<b>6.2</b>	46.7	0.53	<b>24.8</b>
Kenya Chuka Conv high	GM/Ca	organo-mineral	33 (FYM) 81 (CAN)	0.68/ 0.007	<b>3.5</b>	<b>1.9</b>	0.01	2.4 (irrigation, soil)	<b>4.4 (0.1)</b>	<b>1</b>	30	0.66	<b>19.7</b>

Crop abbreviations: Al: alfalfa, BM: baby maize, Ca: cabbage, cc: cover crop, F: faba beans, GM: grain maize, Po: Potatoes, SC: sugar cane, So: soybean, WW: winter wheat, Conv high: conventional with high input system. Fertiliser abbreviations: AN: ammonium nitrate, CAN: Calcium ammonium nitrate, DAP: di-ammonium phosphate, FYM: farmyard manure.

Notes: The emission factor for NO<sub>x</sub> emission is always the same (= 0.019). For system description see Table 3. The emission factor for NH<sub>3</sub> emission is higher for France 1 than for France 2 because of a soil pH >7 in the former location and a soil pH < 7 for the latter location.

### 3.2 Validation of model results

Fig. 8 shows that a majority of points are scattered around the XY diagonal, except five points corresponding to two sugarcane systems from Reunion (mineral and sludge) and maize (2 plots) and cabbage (1 plot) from Kenya. For the two sugarcane systems, predicted values of the component “soil crop system leaching” of the model, given in Table 4, were close to the measurements. The discrepancy may be explained by the importance of leaching due to fertilisation, which may be uptaken by crop or runoff. For the maize plots in Kenya, low nitrate leaching observed may be due among others to the immobilisation of N during the early stage of maize (Musyoka et al., 2019b, 2019a). This process was not well managed by the model. Therefore, it is not surprising that model efficiency showed a very poor predictive quality (<0) as given in Table 5. For the French dataset, the models showed acceptable results for all the statistical criteria, being close for MD and MEF to the performance of other models (Tribouillois et al., 2020). A value for MEF = 0.70 was considered by these authors as “good”, based on the review by Cannavo et al. (2008). It should be noticed that for the whole dataset and the French dataset, model respectively tended to slightly over- or underestimate the observations.

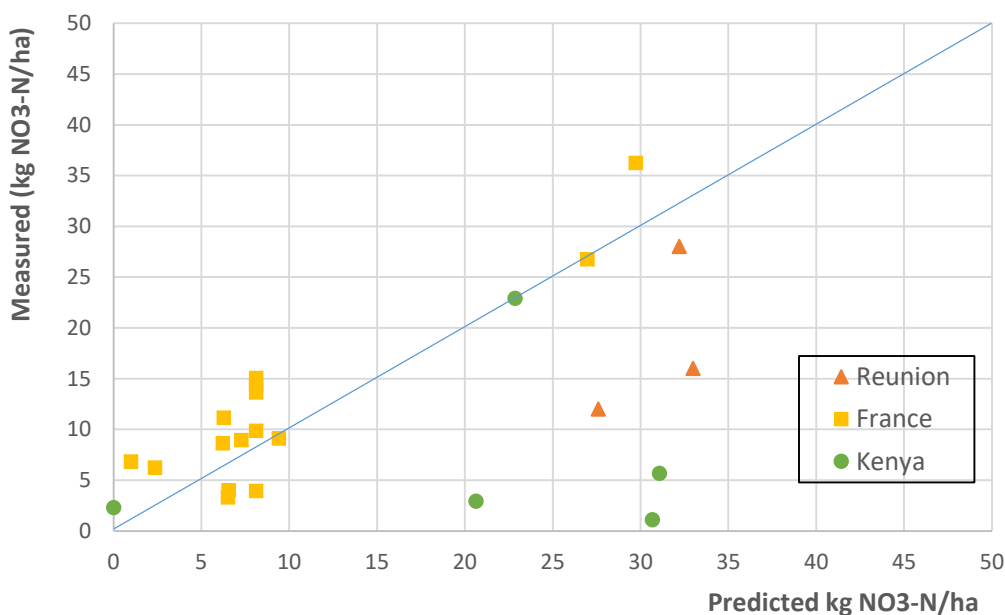


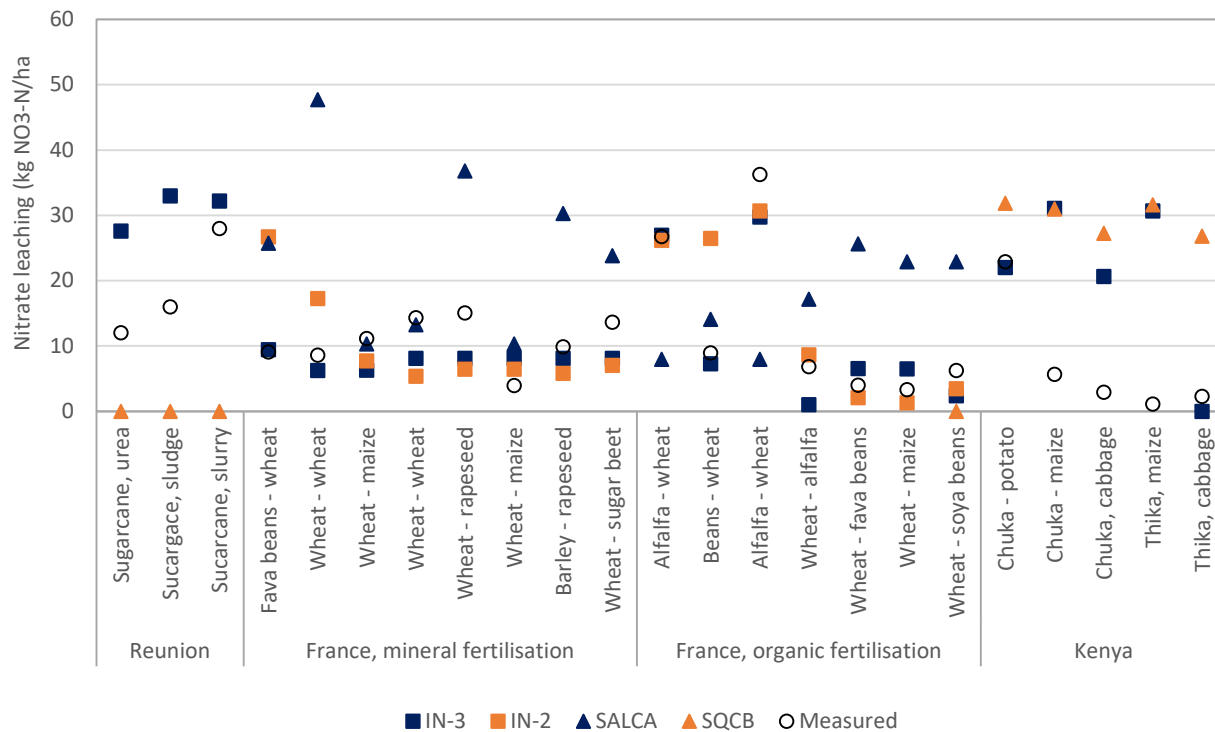
Fig. 8. Cumulative nitrate leaching measured for the cropping period (harvest previous crop harvest of the crop) vs. estimated leaching by Indigo-N v3 for three sites (see Table 3)

Table 5. Main statistical criteria for model validation

	Mean deviation (MD)	Root mean square error (RMSE)	Model efficiency (MEF)
All points	- 3.1	10.8	- 0.43
France	2.3	4.3	0.75

As discussed in Avadí et al., (2022), the nitrate models used by ecoinvent are among the most widely applied models in agricultural LCA. These models are SALCA-NO3 (Richner et al., 2014) for temperate (i.e. Swiss)

conditions and SQCB for all other (i.e. tropical) conditions. A comparison of the predictions by Indigo-N v3 with those of INDIGO-N v2 and SALCA-NO<sub>3</sub>/SQCB, for the three illustrative datasets, is presented in Fig. 9.



**Fig. 9. Comparison of nitrate leaching estimations by Indigo-N v3, INDIGO-N v2 and SALCA/SQCB for three sites (see Table 3)**

For temperate conditions (n=15), IN-3 yielded the estimations closest to the measured values while for tropical (n=8) estimations I-N3 outperformed SQCB. In organic systems, I-N2 estimations were generally closer to measured values). Overall I-N2 presented respectively a lower mean deviation (MD=-0.2), but a higher root mean square error (RMSE=8), and a lower model efficiency (MEF=0.13) than I-N3. SALCA-NO<sub>3</sub> showed a lower predictive quality than the INDIGO models: MD=-12.1, RMSE=22.3, MEF=-5.7). SALCA-NO<sub>3</sub> uses higher default N mineralization rates than calculated by I-N2 or I-N3 and was calibrated for Swiss pedo-climatic conditions and cropping systems, while it was applied here for French conditions. Thus, I-N3 performed better than other models, although it needs further improvement for tropical conditions.

## 4 Discussion

### 4.1 Construction of the model

The design of a new model always involves a compromise between the need to correctly simulate main processes to deliver valid outputs (reality), and a request of feasibility for an utilisation of the model by non-experts. The latter requires parsimony in the number of parameters and input variables, but also availability of input data for users outside the context of the model design. The formalism of Indigo-N v3 is original by its positioning on the gradient between integration of processes and feasibility, when considering the ranking proposed in (Avadí et al., 2022). Furthermore, it follows recommendations of these authors regarding the integration of main processes. In any case, it is much more complex than models relying on emissions coefficients, simple regressions, or nitrogen balances (i.e. the most popular indicator used for nitrogen losses

assessment (Bockstaller et al., 2015)). By modelling nitrate leaching for drainage periods, Indigo-N v3 cannot be compared to more complex dynamic models based on a daily modelling such as Syst’N (Parnaudeau et al., 2012), DAISY (Hansen et al., 1991), STICS (Brisson et al., 2003), APSIM (MacCarthy et al., 2009), etc. DAISY was recently identified as a good candidate model to inform LCIs, despite its large amount of required input data (Pereira Andrade et al., 2021). Indigo-N v3 is close to models like SALCA and the N emissions components of INDIGO-N v2 (which includes indicators other than N-related), going however further in the complexity by considering drainage period and introducing dynamic aspects for mineralisation of crop residues and crop nitrogen absorption.

This complexification was guided first by the aim to extend the validity domain to all climatic and agronomic contexts, while INDIGO-N v2 was restricted to arable crops in a temperate climate, where nitrate leaching occurred mainly in winter (Beaudoin et al., 2005). Furthermore, soil and crop mineralisation, and crop uptake, were simulated in a very simple and rough way. We updated the soil mineralisation equation with the latest versions provided in Clivot et al. (2017) and introduced crop residue and organic fertiliser mineralisation curves (Bouthier et al., 2009; Lashermes et al., 2010; Machet et al., 2017) as well as crop uptake curves (adapted from Geisseler and Horwath 2019). The model was parametrised for 61 crops from all over the world, seven types of cover crops (alfalfa included in this classification) and three types of grasslands (plus four crop “families” for generic modelling: cereals, pulses, roots and tubers, and vegetables). It is not yet valid for crop associations, perennials, rice or cotton, all of which demand important design adaptations. In any case, the quality of parametrisation depends on the amount of knowledge and research effort made for each crop. If for main field crops such as maize, wheat, etc. the knowledge set is large, this is not the case for minor crops, and especially not for short cycle crops like market garden vegetables. For these crops, an effort would be required to improve the parameter dataset before a validation experiment should be performed. In spite of several attempts, it was not possible to find an adequate dataset for this aim. For organic fertilisers, mineralisation curves were taken from studies in temperate areas. Furthermore, curves which are more representative of tropical organic fertilisers have to be added. Some studies, like those of Thuriès et al. (2002) and Rothé et al. (2019), may offer possibilities in the spreadsheet implementation of the model and the associated database. Lastly, a simplified approach inspired partially from the work of Pervanchon et al. (2005) was applied for grasslands, so that grazing excretions are considered as punctual fertilising inputs, instead of as a continuous distributed input over a specific time period. Here again, we proposed a compromise to avoid an over complexification of the model. Actually, nitrate leaching from grasslands is low when they are not over fertilised (Vellinga et al., 2001), which is taken into account in the model, while the ploughing of a grass cover causes a peak of nitrogen mineralisation, source of high nitrate leaching (Kayser et al., 2015; CIVAM, 2010), which is considered by the model.

In spite of the complexification of the model in comparison with the previous version, we made an attempt to improve the feasibility of the model by integrating pedoclimatic data for the whole world. The geographical granularity of pedoclimatic data (combination of country and Global Ecological Zone, or French department) may be a source of high uncertainty. However, it is possible for the user to introduce local data. Concerning the time-step, the choice to work on a basis of monthly weather data and replenishment of the soil’s water content to field capacity may flatten flash events such as very intensive short-lived precipitation. We considered that it is the right compromise between the annual time-step adopted in simple models and the data-intensive daily or hourly one required by simulation models.



## 4.2 Evaluation of the model quality for nitrate leaching

As amply discussed in LCA and modelling literature (e.g. Heijungs and Huijbregts, 2004; Heijungs and Lenzen, 2014; Igos, 2018; Shi et al., 2018), there are several sources and categories of uncertainty in models, including model uncertainty (e.g. due to the formalisms themselves) and data uncertainty. It is our position that for evaluating the robustness of predictions from an emission estimation model, at least data and model uncertainty should be explored. In this article, we explored only model sensitivity, because analysis of data and model uncertainty would have been beyond the scope of this article. Due to lack of time, we did not perform a systematic analysis based on a computational experimental plan, but explored model sensitivity to key parameters by identifying the parameters that produce considerable different responses to a relatively small change. It should be noticed that some publications on nitrate leaching did not present a sensitivity analysis at all (e.g. Tribouillois et al. (2020)).

Formalisms and emission coefficients for gaseous emissions were taken mainly from grey literature based on experts work. Most original work in I-N3 was done for nitrate leaching. However, according to our knowledge of the model and experience with others ones, we consider that the following groups of input data or intermediate variables play a major role in the determination of nitrate leaching:

- i. Potential N net soil mineralisation rate ( $V_p$ ): The soil mineralisation can be a major source of leachable mineral nitrogen and thus is a key parameter to estimate. Because of the complexity of interactions driving this mineralisation, this parameter is also highly uncertain. Soil mineralisation is driven by the "potential N net soil mineralisation rate", a calculated intermediate parameter coming from the soil parameters: %N total in soil, soil pH, %clay in soil, soil bulk density and %CaCO<sub>3</sub> in soil (Clivot et al., 2017). When possible, the user should use personal measured data for those soil parameters.
- ii. Minimal mineral nitrogen in soil at harvest ( $N_{mnh}$ ) and the amount of N absorbed by the crop ( $N_{abs}$ ) are two important entries of the N balances. Thus, this intermediate values should be carefully checked. The main parameters driving this two values are: the crop yield, residues buried or not, residues exported or not (user inputs) and the harvest index and the %N in residues (background data).
- iii. Available water content (AWC): The soil AWC has a high impact on the drainage calculation and thus a high impact on nitrate losses. This parameter is also highly variable between soils and therefore must be customised if possible. The monthly rain and evapotranspiration also have a high impact on the drainage, but are considered as less uncertain.
- iv. Leaching coefficient parameters  $V_m$  (volumetric field capacity) and  $h$  (rooting depth) are two key variables in the Burn's equation used to calculate the leaching factor. Therefore they should be determined accurately.
- v. Drainage calculation vs. user drainage data, as drainage is the most important input variable of the Burn's equation.

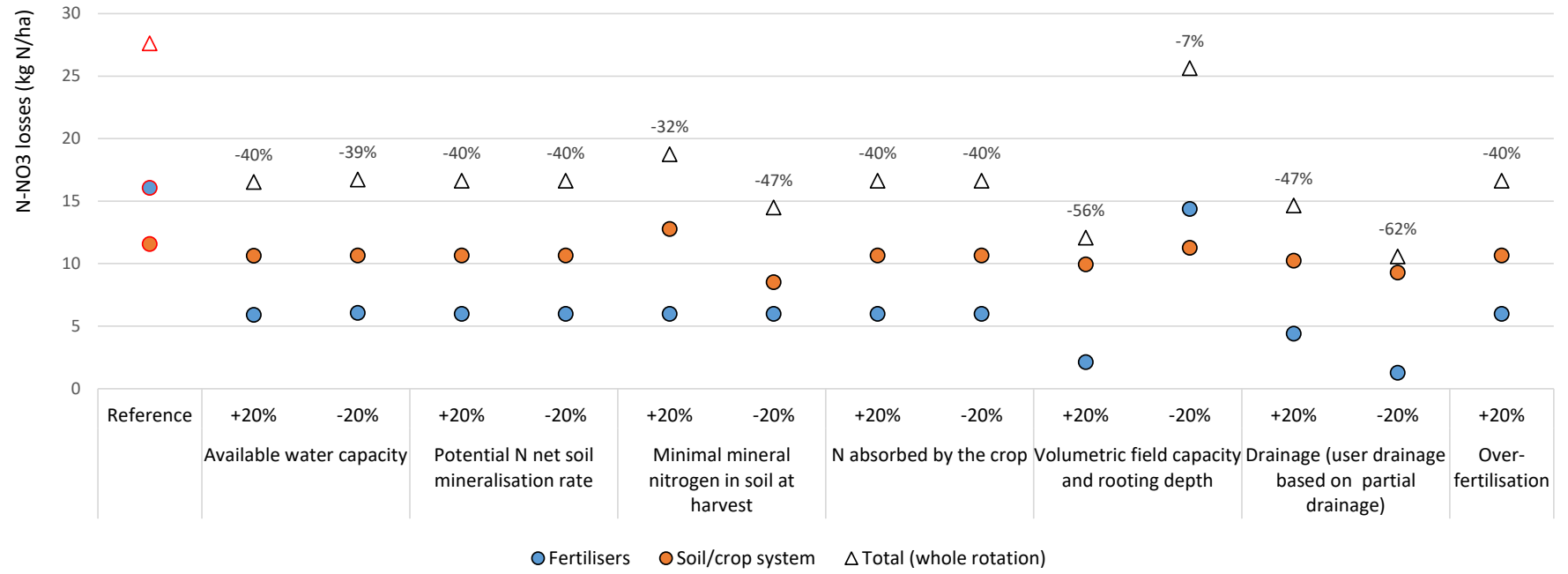
This theoretical analysis shows that the model is highly sensitive to soil and drainage data, thus introducing uncertainty when user data is not used to replace default data. However, when the model is used to compare cropping systems and not deliver absolute results this uncertainty may be mitigated.

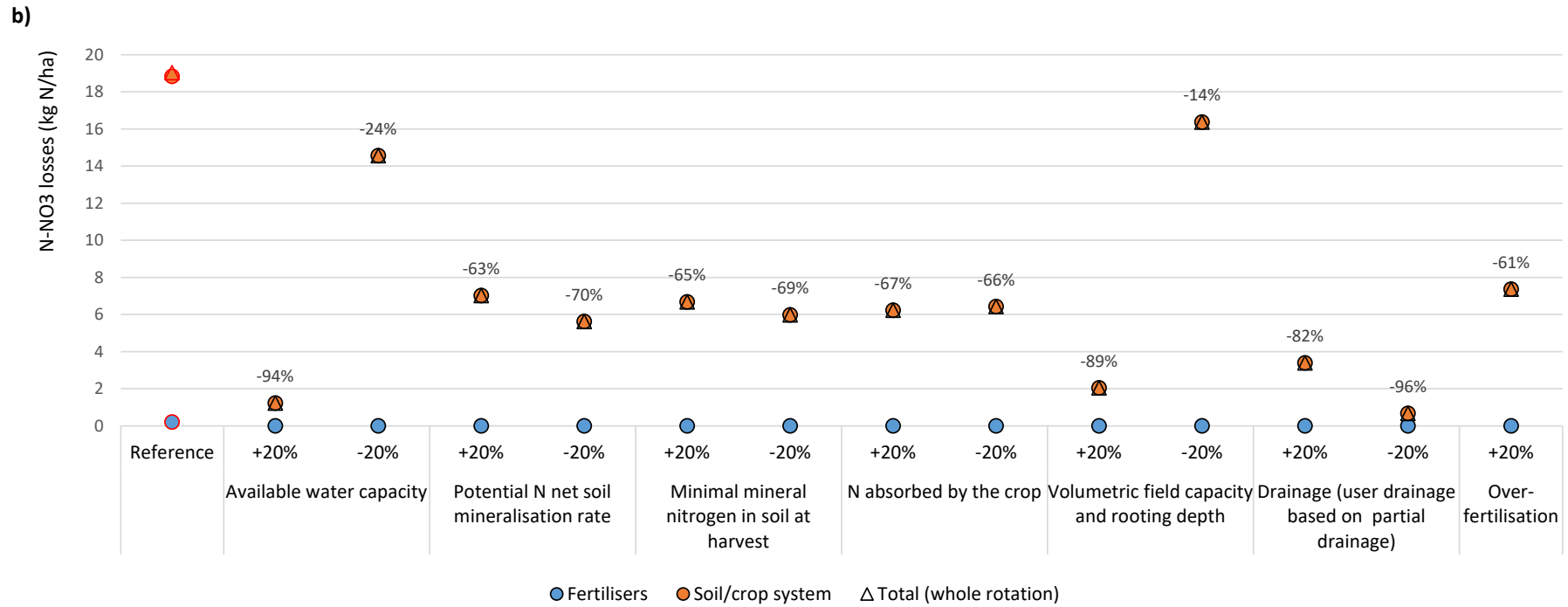
To illustrate, two rotations were calculated for a range of values for some key variables, and the results show the magnitude of the model's sensitivity (Fig. 10). Monte Carlo or other uncertainty propagation methods were not used to test for the model sensitivity to parameters' values, because such bootstrapping-oriented methods, when used alone, are more suitable for understanding data uncertainty, not model uncertainty or model sensitivity (Groen and Heijungs, 2017). For a true global sensitivity analysis, a bootstrapped dataset (e.g.

via Monte Carlo) would have to be further processed to identify the relative contribution of each parameter to the model's outputs (Xiao et al., 2017), via for instance variance decomposition methods (e.g. Puy et al., 2021) or regression-based relative importance analysis methods (e.g. Grömping, 2006; Igos, 2018). Such an exercise was deemed unnecessary, because the parameter sensitivity of Indigo-N v3 is well understood from its theoretical basis.

Sensitivity of variables differed between both sites, one with high drainage during the whole cycle in tropical conditions (Fig. 10a) and the other with low drainage during the winter period (Fig. 10b). For the latter site, leaching after fertilisation was always zero. For tropical conditions with a high level of drainage, the parameters of the leaching equation (volume capacity and rooting depth) are the most sensitive variables, followed by the drainage and mineral nitrogen in soil at harvest. Conversely, potential N net soil mineralisation rate like crop nitrogen uptake and over-fertilisation do not influence nitrate leaching. This is due to the high potential of nitrogen uptake of sugarcane so that the N balance (Eq. 11 and 12 in the Supplementary Material) that will be used to calculate the nitrate leaching remains at the minimum value whatever the value of the terms of the Eq. 14 in the Supplementary Material (crop uptake, soil mineralisation or increase of soil mineral nitrogen due to over-fertilisation). For the French temperate situation with low drainage, again the parameters of leaching equation (volume capacity and rooting depth), but in this case all the variables and parameters linked to the calculation of leaching coefficient, drainage and soil water capacity; have a strong effect on the calculation. The other variables linked to the calculation of the N balance have a lower effect, especially crop intake. These results are in accordance with those of Jabloun et al. (2018) who found that hydraulic parameters, especially during dry seasons, mostly controlled N leaching. This highlights the importance of personalised high quality data for hydraulic variables determining drainage. Even if default data exist, data collection should always be performed as much as possible, especially for soil data.

a)





**Fig. 10. Sensitivity of the Indigo-N v3 model illustrated by modifying certain key parameters of a) the Reunion sugarcane with slurry scenario and b) a France fava beans – wheat – beetroot with mineral fertilisation (percentages represent change relative to the Reference)**

The validation test showed that the model presented acceptable predictive performances for temperate arable conditions and outperformed other models like the previous version of I-N (Bockstaller et al., 2008; Bockstaller and Girardin, 2010), or the models used in ecoinvent (SALCA-NO<sub>3</sub> and SQCB), but remains to be improved for tropical conditions. However, the dataset from Benoit et al. (2016) contained 14 points for three pedoclimatic situations with mainly wheat fields, where pedoclimatic conditions remained quite close since fields were located around Paris. Nonetheless, this dataset was interesting because it contained conventional and organic fields, the latter having been poorly fertilised. A temperate situation with heavy organic fertilisation should be tested with the model. Likely, further efforts have to be made to test the model for more cropping systems and conditions like short cycle crops, like vegetables or grasslands. Thus, the results presented here have to be considered as a first validation attempt. Actually, as pointed out in Keating (2020), validation of model should be a continuous process.

### **4.3 Use of the model**

To support the implementation of the model, a prototype calculator was performed in Excel, and is available with this article. Concurrently, an application programming interface (API) has been implemented into the MEANS platform (<https://pfmeans.inra.fr/means>), which aims at facilitating the computation of sustainability indicators for agricultural systems, including LCA indicators for the environmental dimension. This implementation will enable the use of the model through multiple connected interfaces.

Users from the agri-food sector (e.g. agro-industrial systems) interested in performing LCA should either model their background system (i.e. the agricultural phase of their industrial system) or, if they are willing to model in the foreground the agricultural phase of their product, to collect the required life cycle inventory and emissions modelling data. Such latter approach would be advisable for users with knowledge of the agricultural practices.

Indigo-N v3 offers the possibility to test impacts of the main drivers to reduce emissions, such as the amounts, types, timing and modes of spreading of fertilisers per ha, as well as irrigation and the impact of the crop rotation design. It is suitable for eco-design-oriented LCA projects, as its data requirements are moderate and it is very sensible to the specificities of the modelled technical itinerary. It was designed to handle crop rotations (where the last crop precedes the first) or at least crop sequences (a linear sequence of crops). It is less interesting to be used to study single crops, because the important effect of the crop rotation on individual constituencies is lost.

Regarding data requirements, the model adapts to the amount and quality of available user data. It is possible to run the model with a few user data while relying on the underlying pedoclimatic, crop and fertiliser database. It is also possible to be much more precise by feeding the model detailed user data. The model should be used with system-specific data, and not with aggregated averages or generic data. A list of minimum data requirements is proposed in Table 6. Some of the data are available from the model implementation's database or generated after intermediate calculations, but results would gain in robustness if those would be personalised (highly variable and high impact on final results).

**Table 6. Minimum data requirements of Indigo-N v3 and data which may be updated by the user.**

Data category	Datum
Minimum list	
Pedoclimatic	Country
	Global ecological zone or French department
	Soil type
Technical itinerary, for each crop and catch crop	Crop type
	Seed date
	Harvest date
	Yield
	Residues exported or not
Fertilisation, for each fertiliser application	Residues incorporated or not
	Fertiliser type
	Application date
	Quantity
	Soil incorporation (class)
	Spreading technology (class, for organic fertiliser)
	Monthly irrigation
Data to be updated by user, if needed	
Soil data	Available Water Content
	Topsoil Gravel Content
	Topsoil Sand Fraction
	Topsoil Silt Fraction
	Topsoil Clay Fraction
	Topsoil Bulk Density
	Topsoil Organic Carbon
	Topsoil pH (H <sub>2</sub> O)
	Topsoil Calcium Carbonate
	Topsoil N content
Crop data	N from residues left in soil after harvest
	N absorption by the crop

#### 4.4 Allocation of nitrate

When using the model for LCA, users have to cope with the allocation strategy to attribute emissions to each crop in the rotation. For emissions linked to fertiliser, this is not a problem. Conversely, allocation of NO<sub>3</sub> leaching in the crop soil system among crops in a rotation is a complex problem with a huge potential impact on results and interpretation (Espagnol et al., 2016; Wilfart et al., 2016). NO<sub>3</sub> leaching is the result of intricate interactions between crops rotation soil and climate. Leaching on a specific crop is highly dependent on the previous crops (toward residues mineralisation, fertiliser mineralisation, etc.) as on the crop of the study period. This is the reason why studying nitrate leaching on one crop only is mainly irrelevant.

If two rotations are studied, we recommend to compare the emissions for the whole rotation using kg N leached/year. However, if a product LCA is computed, requiring the identification of crop specific related emissions, allocation is unavoidable. Due to the complexity of the system, no method will be fully exhaustive and accurate. We recommend the following approach "NO<sub>3</sub> losses from the soil-crop system are allocated

equally between the crop time period receiving the losses and all the previous crops time period until the one with a drainage period". For a typical temperate field crop, this method allowed to share the nitrate losses during a crop time period equally between the crop and the previous crop. When several crops in a row (typically short cycle vegetable) are harvested without drainage (thus no nitrate loss during those crop time period), the losses happening during the next drainage period will be shared between all these crops.

## 5 Conclusions

The newly developed model Indigo-N v3 (I-N3) presents an original position on the gradient between integration of processes and feasibility of the simulation of processes. Although more simple than daily step simulation models, it integrated some dynamic aspects with a simple parametrisation for some main processes involved in nitrate leaching. This modelling of nitrate leaching at the level of drainage periods was not covered by previous Tier 2 models. Conversely, I-N3 may be apparently complex, compared with other models or indicators used in environmental assessment like nitrogen balances or Tier 1 models, based on very simple regressions or emission coefficients. To sustain its feasibility, the model was informed by background climatic and soil data from the whole world and a set of parameters for many crop productions, arable and vegetable. This broad scope is undoubtedly another novelty of the model. First results of the model validation yielded acceptable results for arable crops in temperate conditions, but not for all situations in tropical conditions, but discrepancies require additional investigations. In any case, I-N3 outperformed the previous versions, I-N2 and the SALCA and SQCB models. The model provides a global emissions value per crop cycle or year, with allocation factors taking into account knowledge on processes, but also detailed results per fertilizers or contribution of different components (e.g. residue mineralisation, crop uptake, etc.) to the soil crop system leaching. This enables an use for environmental assessment in an LCA based or "conventional" method (Repar et al., 2017) as well as in the design of innovative cropping systems with an eco-design goal. In spite of its broad scope, a consequent effort remains to be made to adapt the model to crop associations, perennials, rice or cotton.

## Software and data availability

An operational implementation (prototype) in Excel of the Indigo-N v3 model, as well as all detailed model equations, are available from the Supplementary Material. All associated data is described in Galland et al. (submitted) and available as a downloadable dataset: Galland, Victor; Avadí, Angel; Bockstaller, Christian; Paillat, Jean-Marie, 2020, "Data to inform the modelling of direct nitrogen field emissions from global agriculture", <https://doi.org/10.15454/RM6TYT>, Portail Data INRAE, V1.

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## Figure captions

Fig. 1. Architecture of the Indigo-N v3 model

Fig. 2. Generic representation of surface leaching from N inputs (L<sub>Xj</sub>) and profile leaching from the soil-crop system (L<sub>Sck</sub>) for the draining period k, for crop i, between the harvest of the previous crop (H<sub>i-1</sub>) and the crop harvest

Fig. 3. An example of the cutting of a random rotation into balance periods (BP). Here, we have 3 crops (with their respective time period represented in green) and 2 drainage periods (with their respective time period represented in blue). This two information (crops time periods and drainages time periods) allow us to cut the rotation into specific balance period with the rules presented above (here we have 7 BP)

Fig. 4. Example of a rotation with one grassland and 2 other crops. The leaching on BP 1-2-4-5-6-7 will be calculated as described in 2.3.2. The leaching in BP3 will be calculated as described in 2.3.3

Fig. 5. Allocation of a crop residue input to a crop and a balance period, based on N mineralisation curves per type of crop residue

Fig. 6. N mineralisation curves per type of fertiliser

Fig. 7. Typical shapes and of absorption curves for annual and short-cycle crops

Fig. 8. Cumulative nitrate leaching measured for the cropping period (harvest previous crop harvest of the crop) vs. estimated leaching by Indigo-N v3 for three sites (see Table 3)

Fig. 10. Sensitivity of the Indigo-N v3 model illustrated by modifying certain key parameters of a) the Reunion sugarcane with slurry scenario and b) a France fava beans – wheat – beetroot with mineral fertilisation (percentages represent change relative to the Reference)