Optimisation of nutrient budget in agriculture

D2.1 Initial report on the design of the Nutrimodel Framework

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Version 1.1	The following changes were made upon the request of the PO and internal reviewers: - “Summary” section on page 4 turned into “Executive Summary” and re-written in a way to present results and conclusions - Section 1.1 now clarifies that the baseline will be published in D2.2, and not in D2.1

	- Section 2.7 clarifies now that the simulation approaches are based on a balance between the level of detail that can be modelled and the available input data at EU and farm level.
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Preface

The NutriBudget project aims to help the agricultural sector in the transition towards sustainable growth by developing and implementing a prototype of an integrated nutrient management platform as a decision support tool (DST). In general, platforms serve a single goal and stakeholder, but this platform aims to serve multiple stakeholders operating at different scale levels (e.g., farmers, advisors, European policymakers, and regional authorities) and evaluate the effect of measures along five goals (e.g., soil quality, water quality, GHG emission, biodiversity, and agricultural production). This helps stakeholders to get a full picture of the opportunities and trade-offs regarding the optimisation of agronomic and environmental nutrient use in the area they operate. This full picture can stimulate the implementation of measures as it helps making well-founded decisions.

The NutriBudget project uses Nutrimodels (i.e., measure-impact models) to assess nutrient (N, P, K, S, Mg, Ca, Zn) budgets that are agronomically and environmentally important. Besides these nutrients, carbon (C) budgets will also be assessed as this is an important soil quality indicator.

The modelling approach is one of its kind, and therefore a framework that explains the operability of the modelling approach and how it fits within the wider scope of the project will be described in this report. This framework helps us in the further development and co-creation of the tool. In the end, this will result in a tool that can help stakeholders in their decisions regarding improved nutrient and carbon management. This report includes an explanation of the NutriModels, the spatial and temporal boundaries of the modelling approach, a description of the nutrient dynamics, and a description of how two additional farm-level models can help to improve the results of the farm-level NutriModel.

Executive Summary

This report describes the NutriModel framework and how this framework is linked to the overall scope of the NutriBudget project. The report is part of Work Package 2 (WP2), Task 2.1, where inclusive measure-impact models for the nutrient management platform are developed and implemented. These so-called NutriModels spatially predict nutrient (N, P, K, S, Mg, Ca, Cu, Zn) and carbon (C) flows of major European farming systems from regional to farm scale. The NutriModels communicate through an application programming interface (API) with a decision support tool (DST). The NutriModels can assess the current nutrient status of farming systems and the effect of nutrient management measures. Therefore, these models are a key element of the NutriBudget project as they provide direct results to the nutrient management platform (NutriPlatform). This report does not contain modelling results. The baseline of the NutriModels will be published in D2.2.

Insight in nutrient budgets is agronomically and environmentally important to feed a growing population in a sustainable way. Different stakeholders aim to meet the growing feed and food demand, and simultaneously reduce nutrient losses by at least 50%. **Chapter 1** provides some more background information on the topic, and describes the motivation and objective of this report.

The design of the NutriModel framework is describe in **Chapter 2**. To serve different stakeholders, results need to be scalable, because a farmer operates at a different level compared to a policy maker. The calculation steps of the NutriModels, including a regional model (i.e., MITERRA-Europe) and a farm-level model (i.e., NutriFarm), are aligned, which makes up- and downscaling of the results possible. The input data of MITERRA-Europe are downscaled and used as default input data of NutriFarm. The boundaries of the NutriModel framework, e.g., on the farming system and the spatial and temporal scale, are also described in Chapter 2, even as the calculation steps on how nutrient and carbon fluxes flow through the soil system and how nutrient and carbon budgets are calculated.

The NutriFarm model makes use of two additional farm-level models to improve the results for specific regions or nutrient flows (CHN and FSF). These complementary models and their role in improving the modelling results are described in **Chapter 3**.

The next steps that are required to make the NutriModels operable within the NutriModel framework are described in **Chapter 4**. These results, and potential updates on the design described in this report, will be presented in Deliverable 2.2.

In this report some essential decisions on the processes within and the connections between the NutriModels were made. For example, decisions on the level of detail that can be modelled at EU level based on available input data, and the connections between the input database of MITERRA-Europe, the data requirements of NutriFarm, and the farm-specific input data required from a user. Therefore, the presented NutriModel framework helps with the ongoing development of the NutriModels, so they can function as Decision Support Tool on the NutriPlatform. Besides, some focus points (Chapter 4) that require further analysis once the NutriModels become operational were identified (e.g., downscaling procedures).

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List of Abbreviations

API	Application Programming Interface
BIO	Microbial biomass
C	Carbon
Ca	Calcium
CH_4	Methane
CO_2	Carbon dioxide
CORINE	Coordination of Information on the Environment
Cu	Copper
DPM	Decomposable plant material
DST	Decision Support Tool
FSF	ForSafe-FarmFlow model
GAINS	Greenhouse Gas - Air Pollution Interactions and Synergies
HUM	Humified organic matter
IMAGE	Integrated Model to Assess the Global Environment
IOM	Inert organic Matter
IPCC	Intergovernmental Panel on Climate Change
K	Potassium
LAI	leaf area index
Mg	Magnesium
N	Nitrogen
N_2O	Nitrous oxide
NH_3	Ammonia
NO_x	Nitrogen oxide
P	Phosphorus
RPM	Resistant plant material
S	Sulphur
Zn	Zink

1. Introduction

1.1.Background and objective

European agricultural systems are under high pressure. On one hand, the demand for food and feed is increasing because of the growing population (Shah and Wu, 2019), and on the other hand nutrient losses, e.g., caused by excessive use of fertilizers, need to be reduced by at least 50% by 2050 according to the goal set in the Farm to Fork Strategy; one of the central pillars of the European Green Deal (European Union, 2020). The Horizon Europe project NutriBudget was launched to help decision makers in their choice selecting sustainable agronomic and environmental nutrient management practices by developing and implementing a prototype of an integrated nutrient management platform as a decision-support tool (DST) for farmers, advisors, European policymakers and regional authorities.

The specific objective of this report is to develop a modelling framework to assess the spatial variation in fate of soil nutrients and C on regional and farm level. This report describes the NutriModel framework for spatial nutrient and carbon flow analysis as part of Work Package 2 (WP2), Task 2.1. This framework helps running the NutriModels for the baseline 2020, which will be published in Deliverable 2.2. Within WP2 an inclusive measure-impact model for the nutrient management platform is developed and implemented. This model can spatially predict soil nutrient (N, P, K, S, Mg, Ca, Cu, Zn) and carbon (C) flows of major European farming systems from regional to farm scale.

1.2 Included nutrient and carbon flow dynamics

Macro- and micronutrients are both essential for the agricultural sector to produce food and feed, but these nutrients can have negative consequences when ending up in the environment (White and Brown, 2010). Therefore, all nutrients important for plant growth (N, P, K, S, Mg, Ca, Cu, Zn) and their interactions, including C flows, should be included when studying the nutrient budgets of agricultural systems from an agronomical and environmental perspective.

In general, dynamic nutrient and carbon models focus on one single nutrient or a limited set of nutrients and therefore the model developed during the NutriBudget project is one-of-its-kind. From an agronomic perspective, the developed models can assess the soil nutrient use efficiency, and from an environmental perspective it assesses emissions to air (NH_3, N_2O, NO_x, CH_4 and CO_2), nutrient flows to surface- and groundwater (N, P, cations, metals), and current and potential C and nutrient budgets.

Key Performance Indicators (KPIs, described in Deliverable 3.1) are being defined in view of current and desired agricultural impact of NH_3 emissions on nature quality, N and P leaching to ground- and surface water on water quality and aquatic biodiversity, soil nutrient status on crop yield, and the emissions of NO_x and greenhouse gasses on climate change and human health. The impact will be graded according to their performance on biodiversity improvements, drinking and surface water quality, human health, and greenhouse gas emissions. The approach to identify these KPIs and their thresholds (either critical limits or target values) has been underpinned by Task 3.1. (see D3.1). The models presented in this report will be used to quantify these KPIs as well as their threshold values on farm and field level, and at regional scale level (Task 2.2).

1.3 Operating at multiple scales

Where a farmer or a farm advisor requires information on nutrient budgets and the effect of nutrient management measures at the farm or field level, a policymaker requires information on the potential nutrient loss reduction at regional, national or European level. Within the NutriBudget project, a model framework will be developed that can provide information on both scale levels. This will help creating consensus between different stakeholders regarding sustainable nutrient management options.

Two dynamic models (i.e., NutriModels), one operating at European level (MITERRA-Europe, described in Section 2.2) and one operating at farm level (NutriFarm, described in Section 2.3), will be developed to make this multi-scale analysis possible. Both models use the same algorithms, although some more detail could be added to the calculations of the farm-level model. Also, the results of the farm-level model can be improved by making use of two additional farm-level models (CHN, described in Section 3.1, and FSF, described in Section 3.2). The input data of the European model will be used as default data for the farm-level model. More detailed data can overwrite the default data when these are available.

2. NutriModel framework

2.1. Design of the NutriModel framework

Figure 1 presents the design of the NutriModel framework and illustrates how WP 2 contributes to the overall objective of the NutriBudget project. The framework consists of the regional model MITERRA-Europe, the farm scale-model NutriFarm and two other farm-scale models that aim to complement NutriFarm; the CHN and ForSafe-FarmFlow (FSF) model. MITERRA-Europe (described in Section 2.2) calculates nutrient budgets at European scale and provides the input and default data for the farm scale model. The default data consist of the downscaled input data and the calculated nutrient budgets of MITERRA-Europe and cover the Europe Union, including Switzerland.

An API (Application Programming Interface) will be used to communicate with the default data inputs to the NutriFarm model and the Decision Support Tool (DST) that will be developed under WP 5. With the DST, a user can assess nutrient budgets and get support on which land-management and fertilization measures will help reach the desired state. A list of potential measures and their effect is compiled in WP 1. The DST can be applied at field or farm level, or at regional level, depending on the user's request. The calculation steps of MITERRA-Europe and NutriFarm are aligned. However, the results of the NutriFarm level model can be improved by two complementary farm-level models (CHN and FSF), that describe soil nutrient and crop nutrient processes in more detail. These models can improve the results in the area they operate and for the nutrients they include. Potential improvements on the results of the NutriFarm model are part of the modelling approach, and therefore included in the results exposed by the API.

Note that this report describes the design of the NutriModel framework. Potential updates on this design, caused by new insights or improved operability of the design, will be described in Deliverable 2.2.

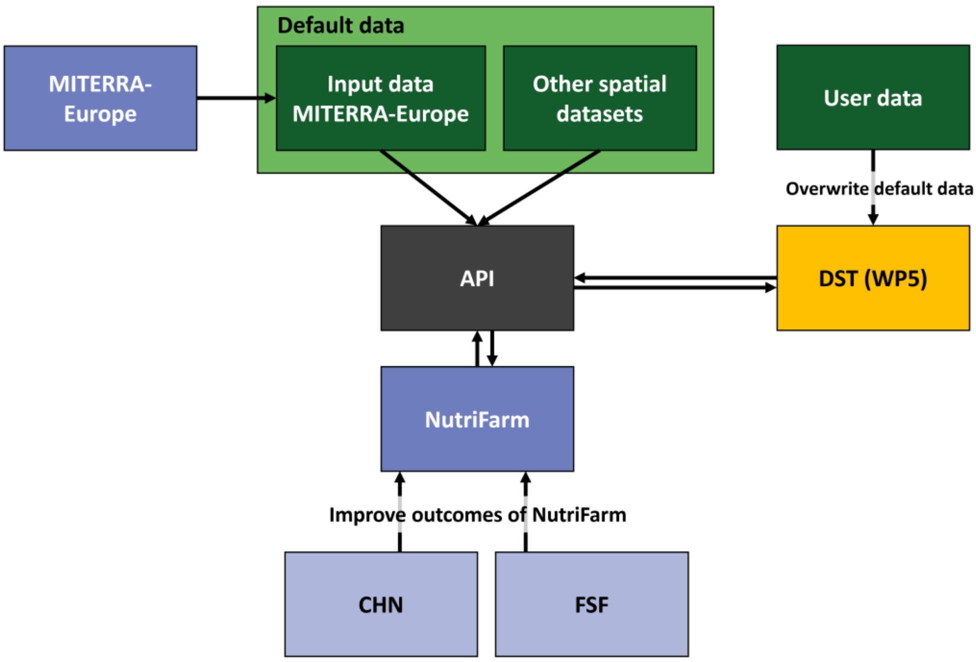

Figure 1. The design of the NutriModel framework.

2.2 Regional NutriModel: MITERRA-Europe

The model framework builds on the existing dynamic nutrient flow models MITERRA-Europe (Velthof et al., 2009) and INTEGRATOR (Reinds et al., 2012; De Vries et al., 2023), which have been successfully applied in European studies (e.g., Duan et al., 2020; Lesschen et al., 2011; Velthof et al., 2014; Kros et al., 2018). The algorithms of INTEGRATOR (for P, K, S, Mg, Ca, Cl, Cu, Zn) based on De Vries et al. (2023) will be integrated into MITERRA-Europe which assesses N and C flows based on Velthof et al. (2009) and Coleman and Jenkinson (2014) . MITERRA-Europe is a deterministic emission and nutrient flow model, which calculates greenhouse gas (CO_2, CH_4 and N_2O) emissions, nitrogen emissions (N_2O, NH_3, NOx and NO_3), N and P flows and soil organic carbon stock changes on annual basis, using emission factors and leaching fractions. The model was developed to assess the effects and interactions of policies and measures in agriculture on N losses on a Nomenclature of Territorial Units for Statistics (NUTS) 2 level in the EU-28 (Velthof et al., 2009; de Vries et al., 2011, Velthof et al., 2014). The MITERRA-Europe model was originally based on the models CAPRI (Common Agricultural Policy Regionalised Impact, http://www.capri-model.org), and GAINS (Greenhouse Gas and Air Pollution Interactions and Synergies, Höglund-Isaksson et al., 2020), and was supplemented with a N leaching module, a soil carbon module and a module for greenhouse gas mitigation measures. The MITERRA-Europe model is described in more detail by Velthof et al. (2009), Lesschen et al. (2011) and Duan et al. (2022).

The input data MITERRA-Europe currently uses are listed in Annex 1A. To make the model operable within the NutriModel framework, adaptations are required (Annex 1B). The input data needs to be downscaled to NUTS 3 level and even further (e.g., based on De Vries et al., 2011) to make the data applicable as default dataset for NutriFarm, and the input data also needs to be updated towards the 2020 baseline. Adaptations to the model include, among others, the incorporation of the calculation rules of the nutrients P, K, Ca, Mg, S, Zn and Cu, an update or incorporation of interactions between nutrients and carbon flows where necessary, and an analysis on critical C and nutrient budgets to set agronomic and environmental targets following, for example, the approaches as being developed for nitrogen by De Vries et al. (2021) and Schulte-Uebbing and De Vries (2021).

2.3 Field scale model: NutriFarm

Within the EU Horizon 2020 project Nutri2Cycle, a farm-level model that can assess C and N flows was established. The calculation steps of this model are aligned with the MITERRA-Europe model and were therefore used as a starting point for the development of the NutriFarm model.

NutriFarm quantifies nutrient budgets and flows at farm scale (including fields) by integrating various key nutrients and trace elements. The NutriFarm model simulates the C cycling, and the soil solution chemistry of all nutrients, including changes in total soil concentrations of C and N (total), adsorbed concentrations of P and S, exchangeable concentrations of Ca, Mg and K and dissolved concentrations of N (NH_4, NO_3), P, S, Ca, Mg, K, Cu and Zn and pH. The cycling of C is based on the RothC model (Coleman and Jenkinson, 2014), for N as included in MITERRA-Europe (Velthof et al., 2009) and for the other elements as described by De Vries et al. (2023). The soil solution chemistry of included nutrients is determined by the element input of mineral and organic fertilizers, biosolids (compost, sludge, manure) and deposition (and fixation in case of N), net uptake by plants, net mineralization/immobilization as well as by soil buffering processes, including adsorption-desorption (P, S, Cu and Zn), cation exchange, and weathering (Ca, Mg and K), while nitrification and denitrification play a role in N transformations. The nutrient concentrations are simulated by a set of: (i) rate limited and linear equations for C and N cycling due to microbial processes and (ii) mass balance equations combined with equilibrium equations or empirical relationships for the other elements.

2.4 NutriModel farming system boundary

Farming systems are diverse and complex. Simplifications in the modelling approach are required to simulate the whole farming system. The farming system can be divided in modules (Figure 2). Each module interacts with another module and can therefore influence the in- and outflow of nutrients and carbon. Because nutrient and carbon flows are assessed spatially within the NutriBudget project, the farming system boundary is set to be land-bound. Nevertheless, modules that fall outside the boundary can still influence the results due to their interaction with other modules.

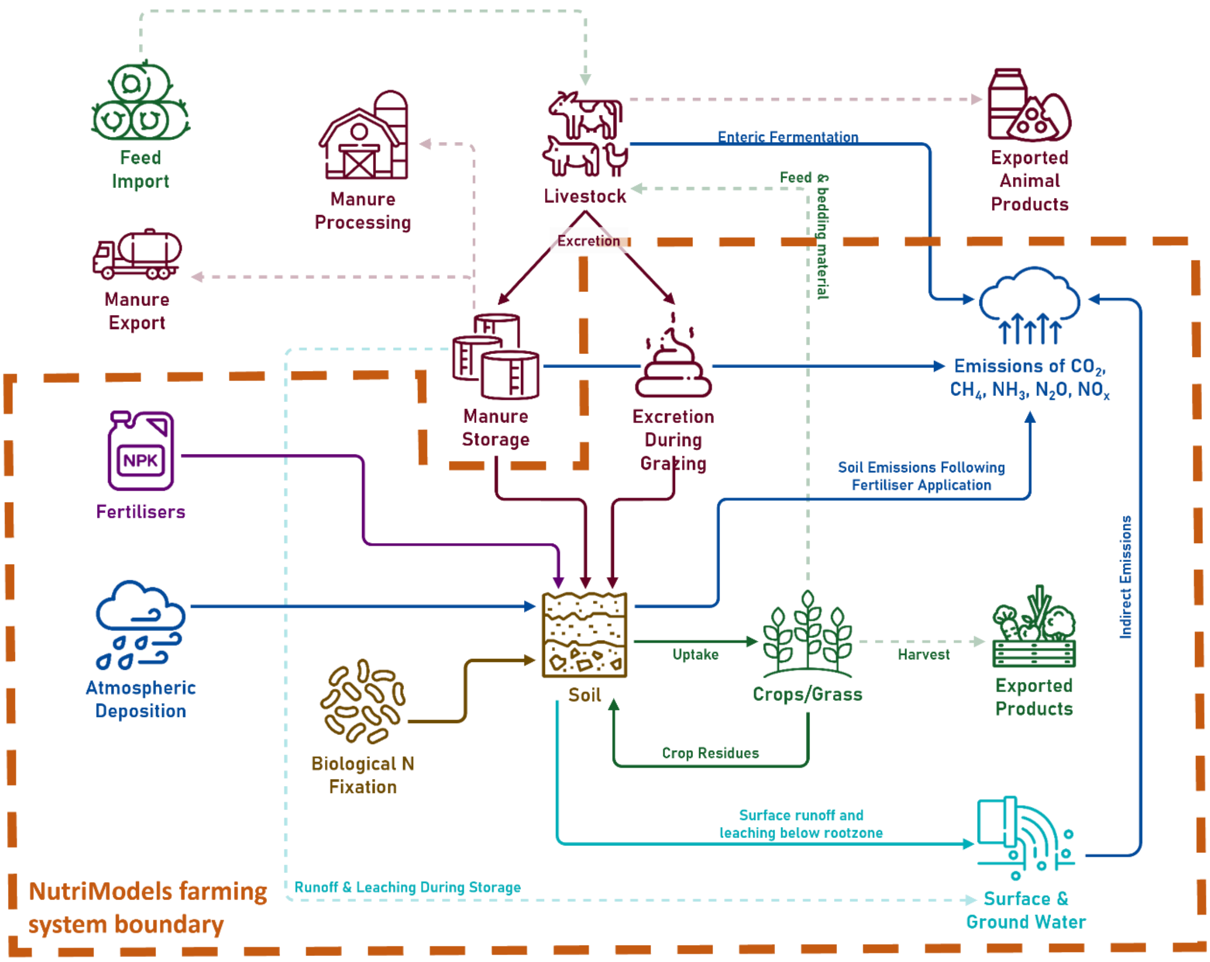

Figure 2 The modules included by the NutriModels. The arrows show the interactions between modules and the dashed arrows show the outflows. The orange dashed box illustrates the farming system boundary of the NutriModels.

2.5. Spatial and temporal boundaries

2.5.1 Spatial boundaries

At European level, MITERRA-Europe currently assesses nutrient and carbon budgets at NUTS2 level for EU27 and United Kingdom. Within the NutriBudget project, the level of detail at which the model calculates will be downscaled to NUTS3 level, and the spatial coverage will be extended with data for Switzerland. This NUTS 3 level will be used to assess nutrient inputs and gaseous emissions related to nitrogen inputs. Soil related processes, such as leaching and adsorption, will be simulated at more detailed level, to account for local differences. Downscaling within a NUTS3 region takes place via unique combinations of, for example, soil type, topography, and land use (based on De Vries et al., 2011). A calculate first average later approach will be applied, as suggested by Heuvelink and Pebesma (1999), for aggregating the simulated results of soil related processes. The resolution of the gridded maps depends on the quality of the underlying spatial data, i.e., we prefer to calculate at a lower resolution when a very detailed map has a high uncertainty. Besides, the optimum between simulation time and resolution of the spatial data still has to be determined to avoid an exponentially increase in the number of model simulations when increasing the spatial resolution to a level that does not add any additional detail or information.

2.5.2 Temporal boundaries

The base year of the NutriModels is 2020. At European level, the effect of mitigation measures will be projected against this baseline. The NutriFarm model is dynamic in time. Time steps of a year are used for all nutrients except P, for which a day is used since rate-limited dissolution equations are included to properly simulate the fate of P. However, in the end, the results of all nutrients will be projected in annual time steps. Mitigation measures run for a 30-year period (2020-2050). The initialisation period might differ per nutrient depending on the time needed for equilibrium and the data availability to calibrate this.

2.6 Nutrient fluxes through the soil system

2.6.1 Water flux

The NutriModels will assess nutrient and C budgets of the topsoil (0-30cm). To assess the surface runoff, subsurface runoff, and leaching within the upper 30 cm, MITERRA-Europe uses a water-flux model based on Keuskamp et al. (2012). Total precipitation surplus is divided over waterflow to ground water and to surface water. Surface runoff fractions were derived as a function of slope, land use and soil texture, and depth to hard rock. Leaching fractions were derived as a function of soil texture, temperature, rooting depth, land use and soil organic carbon content.

The NutriFarm model will assess the water flux in more detail by making use of a two-layered approach (0-30 cm and 30-100 cm). Within NutriFarm, the fraction of the transpiration and of the nutrient uptake in each layer is based on the fine root distribution of the crop. The runoff of nutrients to surface water is calculated as an aggregated value of the surface and the interflow of the two soil layers, while leaching to groundwater is calculated at a depth of 100 cm (see Fig. 3).

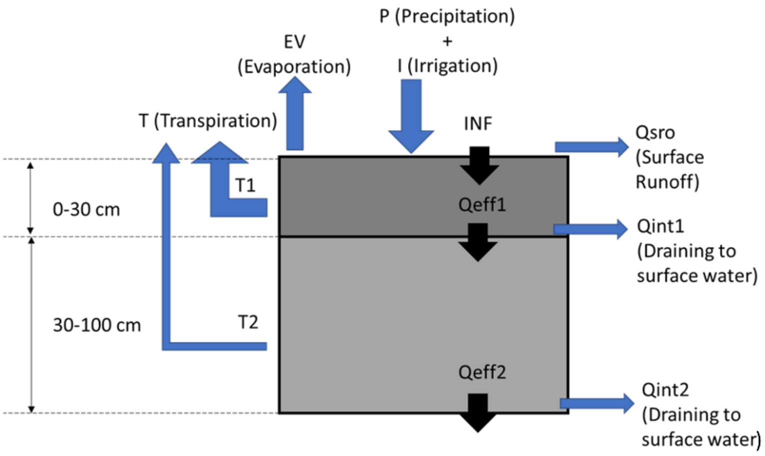

Figure 3 Scheme of the partitioning of the total runoff, being equal to water input by precipitation (P) and irrigation (I) minus the evapotranspiration (sum of EV and T), divided over surface runoff (Qsro), subsurface runoff (Qint), and leaching (Qeff).

The water flow at soil surface (infiltration, INF), at 30 cm depth (Q_{eff1}) and at 100 cm depth (Q_{eff2}), is calculated according to Eq.1-3.

$$INF = P + I - EV - Q_{sro} \quad (1)$$

$$Q_{eff1} = INF - T1 - Q_{int1} \quad (2)$$

$$Q_{eff2} = Q_{eff1} - T2 - Q_{int2} \quad (3)$$

Where P is precipitation, I is irrigation, EV is soil evaporation, T is transpiration, Q_{sro} is surface runoff, Q_{eff} is leaching and Q_{int} is interflow (subsurface runoff) and 1 and 2 refer to layer 1 (0-30cm) and layer 2 (30-100 cm) with all fluxes given in $m^3\ ha^{-1}\ yr^{-1}$ (mm yr^{-1} multiplied by a factor 10). The water flow at 1 meter depth (Q_{eff2}) is taken from Keuskamp et al (2012).

The water flow at 30 cm depth (Q_{eff1}) can be derived as $Q_{eff1} = Q_{eff2} + T2 + Q_{int2}$ (see Eq. 3) where T2 is a fraction of the total transpiration.

2.6.2 Crop nutrient uptake

The crop nutrient uptake in MITERRA-Europe is calculated as crop yield multiplied by the nutrient content of the crop. This is calculated both for the harvested crop part as well as the crop residues. For straw crops, a certain fraction of removal is assumed according to Velthof et al. (2009).

Crop uptake in NutriFarm is partitioned over soil layers equal to the fractions of transpiration. For each nutrient, the concentration in the soil layer is determined by a nutrient mass-balance equation (Eq.4a and 4b) that describes the in- and outputs and the accumulation divided by the water flux.

$$[X]_1 = (X_{in1} - X_{up1} - X_{acc1}) / (Q_{eff1} + Q_{int1}) \quad (4a)$$

$$[X]_2 = (X_{le1} - X_{up2} - X_{acc2}) / (Q_{eff2} + Q_{int2}) \quad (4b)$$

where $[X]_1$ and $[X]_2$ is the concentration in the topsoil and subsoil solution respectively (in $mg.l^{-1}$ or $g\ m^{-3}$), X_{in1} is the total nutrient input to the field entering the topsoil ($g.ha^{-1}.yr^{-1}$) and X_{le1} is the nutrient leaching from the topsoil to the subsoil, X_{up1} and X_{up2} is the crop nutrient uptake, X_{acc1} and X_{acc2} is the nutrient accumulation in the topsoil and subsoil respectively (Section 2.6.3, Eq.5a and 5b). All fluxes of nutrient X are given in either $kg.ha^{-1}.yr^{-1}$ (for N, P, S, K, Ca, Mg) or $g.ha^{-1}.yr^{-1}$ (for Cu and Zn).

Crop nutrient uptake is calculated by multiplying a given crop yield with literature-derived nutrient contents in the harvested parts (e.g. grains, or biomass for forage). Crop yields or plant nutrient concentrations may change with changes in soil nutrient concentrations, due to accumulation or releases. These impacts are not included in the modelling approach except for Zn concentrations in the plant, which is directly dependent on soil Zn concentrations. The uptake of Zn (or concentration of Zn in the plant) are derived based on a non-linear relationship with the soil metal concentrations.

2.6.3 Nutrient accumulation in the soil

Nutrient accumulation in the soil is calculated according to Eq. 5a and 5b.

$$X_{acc1} = X_{in} - X_{up1} - X_{le1} - X_{ro1} \quad (5a)$$

$$X_{acc2} = X_{le1} - X_{up2} - X_{le2} - X_{ro2} \quad (5b)$$

Where X_{le2} is the nutrient leaching from the subsoil. Leaching (X_{le}) and runoff (X_{ro}) are calculated by Eq. 6 and 7 respectively.

$$X_{le} = Q_{eff,i} * [X]t(i)/10 \quad (6)$$

$$X_{ro} = Q_{int,i} * [X]t(i)/10 \quad (7)$$

where 10 is the conversion factor from $g.m^{-2}.yr^{-1}$ to $kg.ha^{-1}.\ yr^{-1}$ and *i* Is the soil layer (topsoil or subsoil). Note that leaching and runoff are calculated from the concentration of *X* in the previous time step multiplied by the relevant water fluxes, i.e. Q_{eff} for leaching and Q_{int} for runoff.

Accumulation and release (negative $X_{acc,i}$) can be caused by: (i) an organic pool linked to the SOC changes, and (ii) a mineral pool due to adsorption or desorption and mineral weathering. Note that nutrient accumulation in the topsoil, and related nutrient concentrations, is directly influenced by the nutrient input, whereas nutrients in the subsoil are calculated as the leaching of the topsoil minus the uptake, leaching and runoff from the subsoil.

The change in the pool of nutrient *X* in soil layer *i* is calculated according to Eq. 8.

$$X_{t+1} = X_t + (X_{acc,t} / z\rho\gamma) * \Delta t \quad (8)$$

where $X_{,t}$ and $X_{,t+1}$ are the sizes of the total X pool at time t and time t+1, respectively ($g\ kg^{-1}$) , X_{acc} is the accumulation of nutrient X in soil ($g.ha^{-1}.yr^{-1}$), z is the thickness of the topsoil (m), ρ is the bulk density of the soil ($kg.m^{-3}$) , Δt is the length of the time step (yr^{-1}) and γ is a conversion factor (1/10.000) for the conversion of $g.ha^{-1}\ yr^{-1}$. For major nutrients $g\ kg^{-1}$ is a proper unit but for minor nutrients $mg.kg^{-1}$.is generally used.

2.7 Calculation of nutrient and carbon budgets

The NutriModels simulate soil C flows and the soil and soil solution chemistry of all nutrients is determined by element input of mineral and organic fertilizers, biosolids and deposition (and fixation in case of N), net uptake by plants, net mineralization/immobilization as well as soil buffering processes, including adsorption-desorption (P, S, Cu and Zn), cation exchange and weathering (Ca, Mg and K), while nitrification and denitrification play a role in N transformations. The nutrient concentrations are simulated by a set of: (i) rate limited and linear equations for C and N cycling due to microbial processes and (ii) mass balance equations combined with equilibrium equations or empirical relationships for the other elements. The simulation approaches are based on a balance between the level of detail that can be modelled and the available input data at EU and farm level.

The approaches will be explained in more detail in the next sub-chapters, but can be summarized as follows:

- Carbon (section 2.7.1): in mineral soils, the turnover of carbon (C) pools is calculated with the RothC model (Coleman and Jenkinson, 2014). This model requires relatively little input data, which is available at European level and often also collected at farm level. Therefore, the model is practically implementable. The model distinguishes 5 carbon pools: decomposable plant material (DPM), resistant plant material (RPM), microbial biomass (BIO), humified organic matter (HUM) and inert organic matter (IOM). The model will be linked to the mineralisation of organic N, P, S, Ca, Mg and K via carbon-nutrient ratios (C/N, C/P, C/S, C/Ca, C/Mg and C/K) (De Vries et al., 2023).
- Nitrogen (section 2.7.2): a steady state linear approach is applied, as used in MITERRA-Europe. Emissions of ammonia and nitrous oxides and N surface runoff are included as a function of N input, and N leaching as a function of N surplus, while accounting for relevant site properties, including soil texture, soil organic matter content, ground water level and precipitation surplus.
- Phosphorus (section 2.7.3): included by using a Langmuir equilibrium, supplemented with rate limited diffusion based on De Vries et al. (2023).
- Sulphur (section 2.7.4): is included by an extended Freundlich equation, where extended refers to the inclusion of pH impacts on the adsorption constant (Gustafsson et al., 2015).
- K, Mg, Ca (Section 2.7.5): the sum of these base cations (BC) is included by a charge balance relationship where BC release is derived by equating BC leaching to anion leaching (where anions include NO_3, SO_4, Cl and HCO_3) and accounting for BC input and BC uptake to get BC release according to De Vries et al (2023). The change in pH is then derived by a simple literature-based pH-Base saturation relationship. Finally, the division in Ca, Mg and K is based on the fractions of Ca, Mg and K on the exchange complex.
- Cu and Zn (Section 2.7.6): a Freundlich equation is used with an adsorption constant that depends on clay, SOM and pH (De Vries et al., 2022; De Vries et al., 2023).

2.7.1 Carbon dynamics and organic matter turnover

The carbon dynamics in mineral soils are based on the well-established RothC-26.3 model (Coleman and Jenkinson, 2014). RothC is a dynamic soil organic carbon turnover model for mineral topsoil. The model divides soil organic carbon in four active so-called carbon pools: decomposable plant material (DPM), resistant plant material (RPM), microbial biomass (BIO), humified organic matter (HUM); and one inactive carbon pool: inert organic matter (IOM). Each pool has its own decomposition rate, and the IOM pool is resistant to decomposition. The decomposition rate depends on soil type, temperature, moisture content and plant cover.

Each organic matter input (i.e., organic manure, compost, green manure, crops, and crop residues) is divided into an easily decomposable and a resistant compartment, depending on their decomposability. In each time step, a fraction of each decomposable compartment decomposes by a first-order process with its own characteristic rate, and converts into BIO, HUM, and CO_2 (Fig.4).

The decomposition of soil organic carbon is closely coupled with the release of other nutrient elements (N, P, S, Ca, Mg, K) from soil organic matter. Nutrient elements are released from organic matter decomposition, and in the meantime assimilated by BIO and HUM pools. The amount released and assimilated can be determined using C:X ratio of each pool, and the balance between release and assimilation determines the net mineralisation or immobilisation of each element in the soil. Based on these principles, the NutriModels include an extension to the RothC model to account for other elements during soil organic matter turnover.

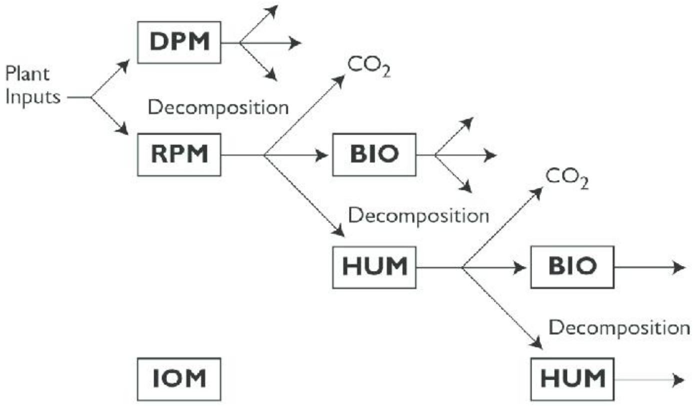

Figure 4 Schematic overview of the soil organic carbon turnover in the RothC model (Coleman and Jenkinson, 2014).

For organic soils a different approach is used, which only calculates CO_2 emissions from drained peat soils. For now, the emissions are calculated using the IPCC 2014 emission factors (IPCC, 2013). For the extent of peatland areas, an overlay is made between the peatland map of Tannenberger et al. (2017) and the area of cropland and grassland as derived from the CORINE land cover map (CLC2018) (EEA, 2020). Climate zones have been derived from the IPCC classification.

2.7.2 Nitrogen dynamics

The NutriModels include nitrogen accumulation or release from the organic carbon pool. This is linked to the SOC change derived by RothC divided by the C/N ratio of the soil. The N flows to and from the soil are given in Figure 5.

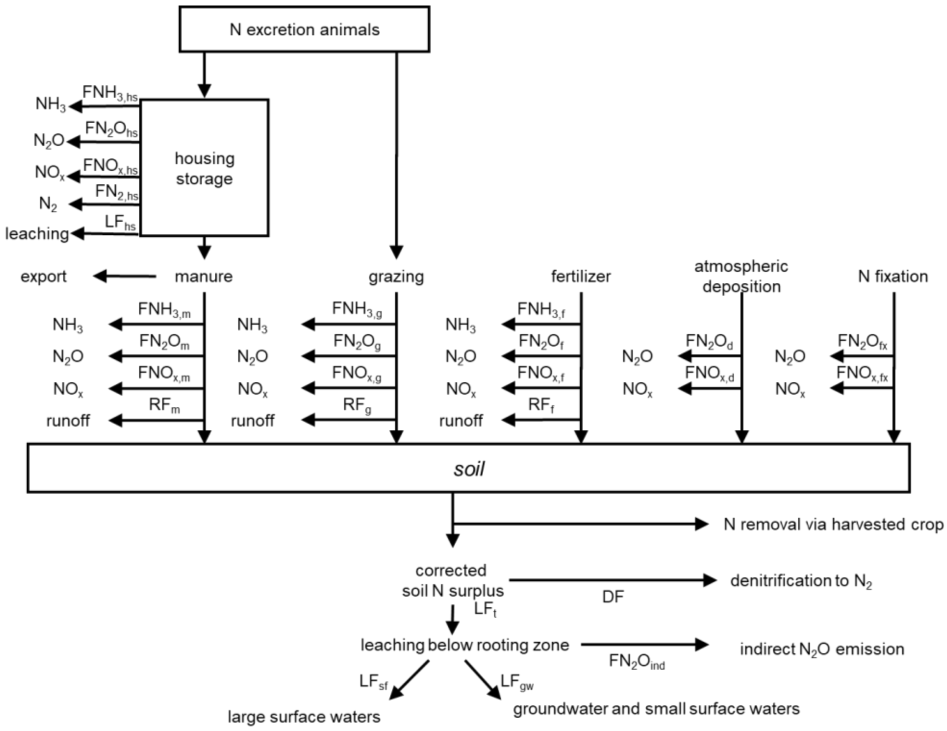

Figure 5 Schematic presentation of the calculated N flows in the NutriModels (based on Velthof et al., 2009).

The models do not included interactions due to adsorption or desorption of N. We assume complete nitrification of NH_4 in clay soil. The NutriModels also include nitrogen accumulation or release from the organic matter pool, which is linked to the SOC change modelled by RothC.

The NutriModels focus on the soil N balance (losses due to emissions of NH_3, N_2O, NO_x and N_2 and runoff of N in housing systems as a fraction of the N excretion; Figure 4). NO_3-N concentrations in the soil are calculated according to Eq.9.

$$[NO3\text{-}N] = (N_{in} – N_{up} – N_{acc} – N_{em})/(Q_{eff} + Q_{int}) \quad (9)$$

where NO_3-N is the NO_3-N concentration, N_{acc} refers to accumulation or release in the organic N pool and N_{em} stands for the emission of NH_3, N_2O, NO_x and N_2.

The emissions of NH_3, N_2O, NO_x are calculated as a fraction of the N inputs. The emission of N_2 is equal to the denitrification flux, which is calculated as a fraction of the N surplus. The emissions of NH_3, N_2O and NO_x and N_2 are assumed to take place in the topsoil only. The N losses to air and water depend on site properties as given in Table 1. The various N loss fractions are all given in De Vries et al (2022).

Table 1 N loss fractions to air (NH_3, N_2O, NO_x and N_2 emissions) and water (N leaching and runoff)

Model inputs	Assessment
NH_3 emission fractions	Grazing: average emission fraction. Housing and manure storage systems: Country-specific N emission fractions distinguished per animal type and manure type (solid and liquid) for different housing systems and manure storage. Soils: Country-specific data from the GAINS model. For manure, emission are distinguished between animal categories and manure type of manure (solid and liquid) and manure application technique. For fertilizer, emission fractions are distinguished between urea-based fertilizers and nitrate-based fertilizers.
N_2O emission fractions	Housing and manure storage systems: country specific fractions based on GAINS model data. Soils: Two options: 1) Tier 1 approach according to IPCC 2019 guidelines (IPCC, 2019) or 2) function of N source (manure type, fertilizer type, crop residue type, grazing, mineralisation, fixation and deposition), application technique, soil type, land use and precipitation and temperature, based on Lesschen et al. (2011).
NO_x emission fractions	Grazing: average emission fraction at country level based on GAINS model. Housing and manure storage systems: 0.3% of N excretion Soils: EF depending on precipitation class (Velthof et al., 2014).
N_2 emission fractions	Housing and manure storage: 9 x NO_x emission, i.e. 2.7% of N excretion (Oenema et al., 2000). Soils: set equal to denitrification rates, being equal to N surplus minus N leaching.
N leaching fractions	Housing and manure storage systems: fraction of N excreted in these systems that depends on the type of manure system and the type of floor (Velthof et al., 2009). Soils: fraction of soil N surplus (includes N input by grazing) depending on soil type, land use, soil organic content, precipitation surplus, temperature and rooting depth (Velthof et al., 2009).
N surface runoff fractions	Fraction of N input to soil by inorganic and organic fertilizers, calculated as a function of slope class, land use, precipitation surplus, soil type and depth to rock (Velthof et al., 2009).
N subsurface runoff fractions	Fraction of N leaching below the root zone, calculated as a function of soil type, moisture class and slope, derived from the IMAGE groundwater model described in Keuskamp et al. (2012).

2.7.3 Phosphorus dynamics

Apart from input and uptake, the P concentration in the topsoil and subsoil is affected by P accumulation. Modelling of P accumulation or release is included by using a Langmuir equilibrium, supplemented with rate limited diffusion, based on the approach used in the INITIATOR model (Van der Salm et al., 2016; De Vries et al, 2023). The P pools are divided in (i) an inert P pool with no change over time, (ii) a stable P pool changing slowly according to rate limited reaction with dissolved P in the soil solution, and (iii) a labile P pool, changing rapidly according to an equilibrium reaction with dissolved P in soil solution. The changes in both, the labile and stable P pools, are included as adsorption or desorption.

The sum of the labile and stable pool is assumed to be approximated by oxalate extractable P (P_{ox}), further denoted as the reactive P pool. The labile pool is at the start assumed as 1/3 of P_{ox}, and the stable pool is assumed as 2/3 of P_{ox}. The change in the reactive P pool is calculated by a mass balance equation. The P accumulation in the topsoil is calculated as the P input minus P uptake minus the change in the organic P pool. P uptake equals the crop P removal times a fraction root uptake. Note that we only include a daily time step for P to properly include rate limited processes but the variation in P inputs and P uptake over the year is not accounted for. Annual inputs and uptake are simply divided by 365 (or 366 in the case of leap years) to get daily values and results are presented again at an annual time step. The change in the labile P pool of the topsoil is calculated by a mass balance, whereas the change in the stable P pool of the topsoil is calculated using a rate-limited Freundlich equation (Van der Zee, 1988).

P leaching and runoff are calculated according to the total (inorganic and organic) P. To calculate leaching of inorganic P, assumptions have to be made with respect to the relationship between inorganic P and total P in the soil solution. We propose to use the approach of Chardon et al. (2007) for P leaching. This approach uses an exponential relationship between total P and inorganic P based on measurements in soil solution, drainage water and surface water, as this seems to be the best approach (according to Chardon et al., 2007). P leaching is currently not included in MITERRA-Europe, as this approach can only be adopted in MITERRA-Europe if EU maps on P_{ox} are available at EU level.

2.7.4 Sulphur dynamics

The SO_4 concentration in the soil is determined by input, uptake and accumulation using a mass balance equation, just like the P concentration. The SO_4 accumulation is calculated as the S input minus the S uptake, the S losses through leaching and runoff, and the change in the organic S pool.

The SO_4 accumulation or release is limited to an adsorption-desorption isotherm that governs the flux of SO_4 between dissolved and sorbed phases. No distinction is made between the stable and labile pool, like it was done for P. The SO_4 adsorption-desorption is included by using an extended Freundlich equation (Van der Zee, 1988). Extended refers to the inclusion of pH impacts on adsorption constant, according to (Martinson et al., 2003; Gustafsson et al., 2015).

2.7.5 Base cation dynamics (K, Mg, and Ca)

Soil acidification due to the release of base cations (i.e., the sum of Ca, Mg, K, and Na) occurs when the sum of leaching and uptake exceeds the sum of external inputs (e.g., organic and chemical fertilizer, and deposition). This is generally the case when the loss of nitrate from the soil is accompanied by base cations. The BC release is similar to a negative accumulation, which is calculated according to Eq. 10.

$$BC_{acc} = \Sigma(Ca + Mg + K + Na)_{in} - \Sigma(Ca + Mg + K + Na)_{up} - \Sigma(Ca + Mg + K + Na)_{loss} \qquad (10)$$

where *in* is total external input, *up* is uptake and *loss* is the leaching plus runoff.

The input of base cations by fertilizer and manure is determined by fertilizer and manure application rates and their composition (Ca, Mg, K and Na concentrations in either fertilizer or manure) while the BC removal by crop harvesting is determined by crop yield and Ca, Mg, K and Na concentrations in crops, respectively.

Base cation loss by leaching and runoff is calculated by multiplying the water flux with Ca, Mg, K and Na concentrations. These concentrations are calculated by assuming charge balance, implying that the sum of cations is equal to the sum of anions. Anions is the sum of SO_4, NO_3, Cl and HCO_3. The calculation of NO_3 and SO_4 concentration in the soil is described in Section 2.7.2 and 2.7.4, respectively.

The Cl concentration in solution is derived by dividing the Cl leaching with the water flux. The HCO_3 concentration in non-calcareous soils is calculated by assuming an equilibrium between the HCO_3 concentration, the CO_2 pressure in the soil and soil pH, according to De Vries and Breeuwsma (1986). In non-calcareous soils, the change in exchangeable base cation pool is equal to the cation exchange capacity (CEC) multiplied by the base saturation. The base saturation is the sum of the BC released and weathering. Information on BC weathering can be derived by Sverdrup and Warfvinge (1993) or approximated by a combination of soil texture class and parent material (De Vries et al., 1994; UBA, 2004).

Changes in pH can be derived by a literature-based pH-base saturation (BS) relationship, such as the Gaines-Thomas and Gapon equations (described by De Vries and Posch, 2003). However, a simpler approach is to use a pH-base saturation relationship based on model results and measurements (based on Xu et al., 2020). Based on these results, a linear relationship between pH 4 and pH 6.5 was derived (Eq.11).

$$pH = 4.0 + 0.025\ BS \quad (11)$$

The results of Xu et al. (2020) are in line with Clark and Hill (1964), Bowman and Lannan (1995) and Ranney et al. (1974). Differences are mainly due to the estimation of the CEC, which is pH dependent. When data on CEC and cation saturation are lacking, it can be derived from Eq. 11 and 12 using available data on SOC, clay and pH.

$$CEC = (0.44 * pH + 3.0) \cdot clay + (5.1 * pH - 5.9) \cdot SOC \quad (12)$$

The change in exchangeable BC is proportioned over Ca, Mg, K and Na. The cation fractions are set at 0.7 for Ca, 0.2 for Mg, 0.1 for K and 0.0 for Na up to pH 4.5, being equal to a base saturation at 20%. Below pH 4.5 (BS of 20%), aluminium (Al) comes increasingly into solution and thus increasingly dominates the exchange complex (see also De Vries, 1994). Then the Ca fraction is set at 0.2.

In calcareous soils, base saturation is set equal to 100% and the change in base saturation is assumed negligible since the acid production rate is fully counteracted by the dissolution of $CaCO_3$. In calcareous soils, the initial pH is assumed to stay constant. To gain insight in the losses of $CaCO_3$, the HCO_3 concentration is calculated by assuming equilibrium with the CO_2 pressure in the soil (De Vries and Breeuwsma, 1986) (Eq. 13).

$$\log[HCO_3]^- = -1.94 + \log(pCO_2)/3 \quad (13)$$

2.7.5 Heavy metal dynamics (Cu and Zn)

The concentration of heavy metals Cu and Zn in the soil is determined by a mass-balance equation that describes the inputs, outputs and accumulation.

The Cu and Zn uptake is calculated by multiplying the crop yield with the metal content in crops. It is assumed that this concentration is soil independent (in the case of Cu) and derived by a non-linear relationship with the soil metal concentration in the topsoil for Zn (Adams et al., 2004; Brus et al., 2002; De Vries et al., 2008).

The leaching and runoff rates are calculated by multiplying either the runoff rate or leaching with a dissolved metal concentration. The dissolved metal concentration is related to the reactive soil metal concentration according to a Freundlich equation. For more detail, we refer to De Vries et al. (2008).

3. Improving modelling results by complementary models

The results of NutriFarm will be improved by two other farm-scale models: CHN and FSF. Where the crop phenology in NutriFarm is described in a relatively generic way, CHN (Clivot et al., 2019) includes these processes in detail and has a specific focus on CN behaviour in arable soil. Therefore, CHN can complement NutriFarm. The model is currently calibrated for the Atlantic climatic zone (in France) and for conventional maize and wheat farming systems. FarmFlow (Modin-Edman et al., 2007) and ForSAFE (Wallman and Svensson, 2005) include more detailed mechanistic soil process descriptions for all nutrient budgets (N, P, K, S, Mg, Ca, Cu, Zn) compared to NutriFarm, and can therefore complement NutriFarm. An overview of the models included in the NutriModel Framework and the nutrients they represent are given in Figure 6.

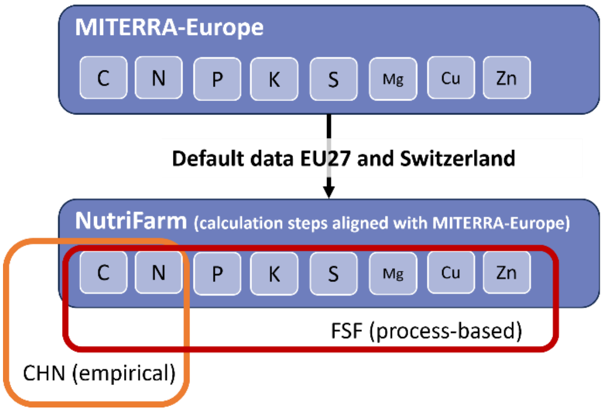

Figure 6 The NutriModels (i.e., Miterra-Europe and NutriFarm) and the complementary models CHN and ForSafe-FarmFlow (FSF).

3.1 The CHN model

The main objective of the CHN model is to be used during the agricultural season as a decision support tool for farmers. It has been designed as a conceptual and mechanistic model. The main processes simulated are plant development and growth, carbon, water and nitrogen fluxes and stocks in the soil, plant and atmosphere compartments (Fig.7). The model is built around 3 main modules:

- The 'carbon' module (C), with, for the soil compartment, the formalisms and parametrizations of the AMG model (Andriulo et al., 1999), and, for the plant compartment, the Monteith's carbon accumulation principle (Monteith and Moss, 1977);
- The 'water' module (H), with the water balance model, based on the work of Lecoeur (2000) and the PILOTE model (Khaledian et al., 2009);
- The ‘nitrogen’ (N) module, based on the principle of the nitrogen nutrition index (Justes et al., 1994) for the plant compartment. Four forms of nitrogen are considered: organic nitrogen, urea, ammonia and nitrate.

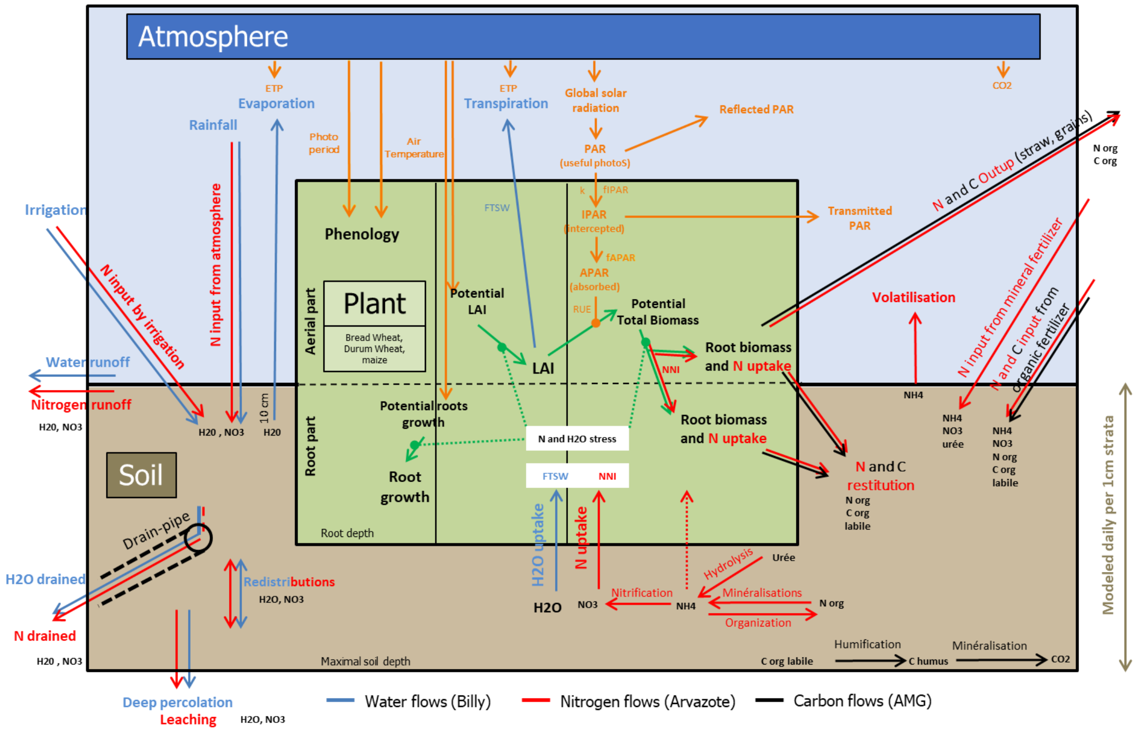

Figure 7 Flowchart of the CHN model.

Soil nitrogen and water fluxes are provided on a daily time-step and at each 1 cm soil layer depth, at field spatial resolution, whereas the soil carbon budget runs over a period of one year.

The soil compartment is linked to a national soil database, which contains nearly 500 soil types with a detailed description of each of the horizons. The soil transfer functions are also used to estimate some agronomic characteristics useful for CHN, such as bulk density or field capacity and permanent wilting point; data measured on the site can also be integrated.

The atmospheric compartment is linked to a meteorological database, which gathers daily information from meteorological station. ARVALIS has access to the daily data from more than 700 weather stations in France. In addition, mapping models for meteorological data have been developed by ARVALIS (Deudon et al., 2017).

The plant compartment is based on the Monteith principle (Monteith and Moss, 1977): leaf growth is modelled using a formalism inspired by Baret (1986), and the leaf area index (LAI) intercepts solar radiation, which is then converted into biomass production. Root growth is also modelled and allows the estimation of the amount of nitrogen and water available to the plant. Leaf growth and biomass accumulation are also affected by stresses related to water and nitrogen availability, according to response functions based on the work of Sinclair (1986). The total biomass produced is then partitioned into aerial and root parts, according to the principles of Savary and Willocquet (2012). Crop development is simulated by phenological models, also mounted to the national cultivar databases containing more than 400 maize, 350 bread wheat and 50 durum wheat varieties. This cultivar database is updated every year.

3.1.1 Carbon module

The carbon flows follow the principles of the AMG model (Andriulo et al., 1999). This module simulates the evolution of the soil organic carbon stock over the long term.

3.1.2 Water module

Concerning water flows, ARVALIS has developed a water balance model represented in Figure 8.

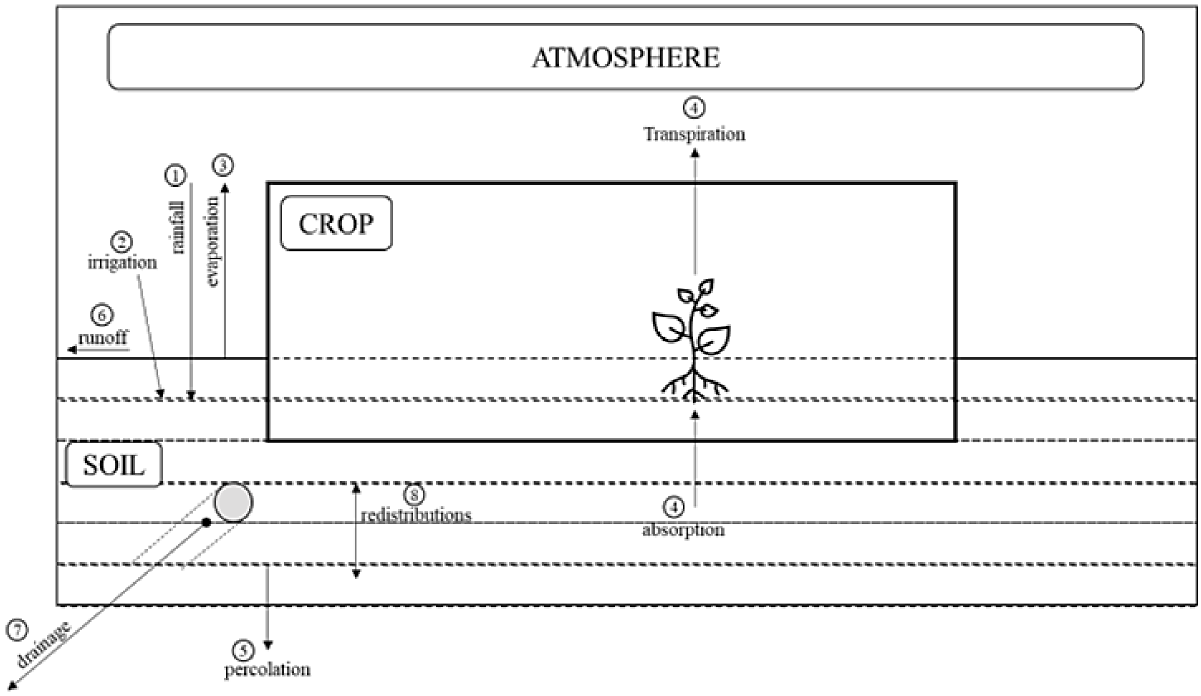

Figure 8 Water balance model developed by ARVALIS. Fluxes are represented with arrows. The numbers indicate the order of execution within the framework of a simulation. Processes displaying the same number are computed at the same time.

The water balance model used in CHN combines the tipping bucket principle (Van Keulen, 1975) with Richard's approach (Richard, 1931). Similar approaches have been used in other crop models (APSIM; Holzworth et al., 2006; 2014; Van Ittersum et al., 2003). As indicated above, each stratum is characterized by an available and usable daily water holding capacity (Assouline et al., 2014). The main fluxes are rainfall and irrigation, soil evaporation, transpiration, percolation, runoff, drainage, and redistribution across strata.

Rainfall and irrigation: All daily water inputs (rainfall and irrigated water) are accounted for in the water balance, assuming a soil infiltration capacity of 100% for the first superficial stratum.

Evaporation: It is assumed that only the first 10 centimetres of soil contribute to evaporation. On bare soil, evaporation depends on ETP (as calculated by Penman-Monteith; Allen et al., 1998; https://www.fao.org/3/x0490e/x0490e00.htm) and a weighted conductivity criterion per stratum, assuming a gradient of water transferability with soil depth. In the presence of a canopy, radiation absorption efficiency (Ead) is used for the calculation of transpiration.

Transpiration: Transpiration flux is governed by the balance between water demand and supply. Daily water demand (Wd_d) is described according to Eq. 14-18.

$$Wd_d = Transpiration_{maxd} * \text{water stress factor} \quad (14)$$

$$Transpiration_{maxd} = K_{cmax} * E_{ad} * ETP_d \quad (15)$$

$$E_{ad} = E_{admax} * (1\text{-}exp(-k * LAI_d)) \quad (16)$$

$$\text{Water stress factor} = 2 / (1+exp(-k_{cmax}*FTSW_d)))-1 / (2 / 1+exp(-k_{cmax}))-1 \quad (17)$$

$$FTSWd = \text{available water}_d / \text{total available water} \quad (18)$$

where $Transpiration_{maxd}$ is dependent on daily radiation absorption efficiency (E_{ad}), the maximal adsorption (E_{admax}), evapotranspiration ETP_d and a species coefficient K_{cmax}. A $water\ stress\ factor$ is computed based on K_{cmax} and the fraction of transpirable soil water ($FTSW_d$), calculated as soil available water content ($available\ water$) divided by soil $total\ available\ water$. K_{cmax} is computed for each process affected by water stress (i.e. leaf area index, aboveground and root dry matter and transpiration) and for each species.

Soil water supply (WS_d) corresponds to Eq. 19 and 20.

$$WS_d = \sum \text{available water per stratum} * \text{cessibility} \quad (19)$$

$$\text{Cessibility} = (\text{water stock}_t - \text{water stock}_{fc}) / (\text{water stock}_t - \text{water stock}_{wp}) \quad (20)$$

where $cessibility$ is the ease with which water (and nitrogen) can be extracted, depending on the moisture of each stratum.

Daily extraction by the roots is defined as Eq. 21.

$$\text{Rootextractiond} = \sum \min(Wd_d, Wd) / WS_d * \text{available water per stratum} \quad (21)$$

Where n corresponds to individual soil layers.

Water transfer across strata: As the layers progressively fill with water, several types of transfer can occur, modulated by the humidity level within each stratum.

Percolation: If the actual moisture content on day d is higher than the moisture content at field capacity within two consecutive periods, then percolation of the excess water is considered to occur. A percolation coefficient is applied to the first 10 strata of soil. Below the part of the profile exploitable by the roots, this percolation is described as deep percolation.

Drainage: When drains are present, a fraction (currently 90%) of the excess water leaves the system at the level of the stratum corresponding to the depth of the collectors. The remaining excess water percolates.

Runoff: Following drainage and percolation, any remaining surplus water may contribute to waterlogging due to soil water saturation. Waterlogging is considered to occur in an upward direction and to produce runoff (calculated from a runoff threshold). The process is applied to the first thirty cm of soil. If the soil is shallower than 30 cm, the process will be applied to the full depth of the soil. Runoff may also occur in case of heavy rainfall, through soil surface infiltration.

Redistributions: Finally, if the moisture content in each set of consecutive 1 cm strata (9 by default) is lower than that at field capacity, the daily difference in average water stock per stratum is calculated to account for redistribution processes resulting in a movement from wetter to drier areas (ascending or descending). If a compartment is saturated with water, runoff and drainage may occur and percolation may also be slowed.

3.1.3 Nitrogen module

On a daily step, the CHN updates the nitrogen stocks in each centimetre of soil, based on the following flows:

- mineral or organic nitrogen fertilizer inputs, which must be entered by the user from the databases on mineral fertilizers and organic waste products
- atmospheric inputs and possible nitrogen inputs from irrigation water, whose nitrate content is an input parameter of the model
- soil supplies, including humus mineralisation, residue mineralisation from the previous crop (Nicolardot et al., 2001) and from the intermediate crop (Justes et al., 2009), organic residue mineralisation (Bouthier et al., 2009), as well as mineralisation due to grassland turning (Laurent et al., 2004), which depend on the calculation of standardized days (Mary et al., 1999)
- symbiotic fixation of legumes
- losses to fertilizer (volatilisation and organisation)
- losses related to soil water functioning (runoff, drainage and leaching), using the Burns model (Burns, 1976)

o fluxes between soil strata (i.e. 1 cm of soil), including diffusion, redistribution and homogenization following tillage
o the nitrogen uptake by the plant, involving the notion of critical nitrogen content (Justes et al., 1994)

The output of the CHN model will be used to improve the output of the NutriFarm model. Currently, CHN can improve the results of NutriFarm in France and for wheat and maize crops only. We will explore the potential of expanding the area in which CHN operates and the number of crops for which the CHN model can run within the NutriBudget project.

3.2 The FSF model

The aim of ForSAFE is to simulate the biogeochemical cycles of C, N, Ca, Mg, K, P, Cl, S, Al within a terrestrial ecosystem (Gaudio et al., 2015; Zanchi et al., 2021). The model is represented by the biota, soil organic matter, solid soil and soil solution. The model simulates both the flows of the elements under organic and inorganic states, as well as the chemical and biological interactions between the cycles of the elements. ForSAFE was never used for agricultural systems, and lacks some of the heavy metals thereof relevant. This is where FarmFlow comes in. We will combine crop parametrization and management information from FarmFlow (e.g, Modin-Edman et al., 2007; Stockwell et al., 2012), together with new elements (such as Cd) into a modified version of ForSAFE. We will preserve the daily time step and high resolution of biogeochemical reactions governing the flows of the ions. The boundaries of the model will also be preserved, including anthropogenic inputs (atmospheric deposition, fertilisation (mineral and organic), and mineral stoichiometry at the source of the weathering fluxes). A schematic overview of FSF is provided in Figure 9.

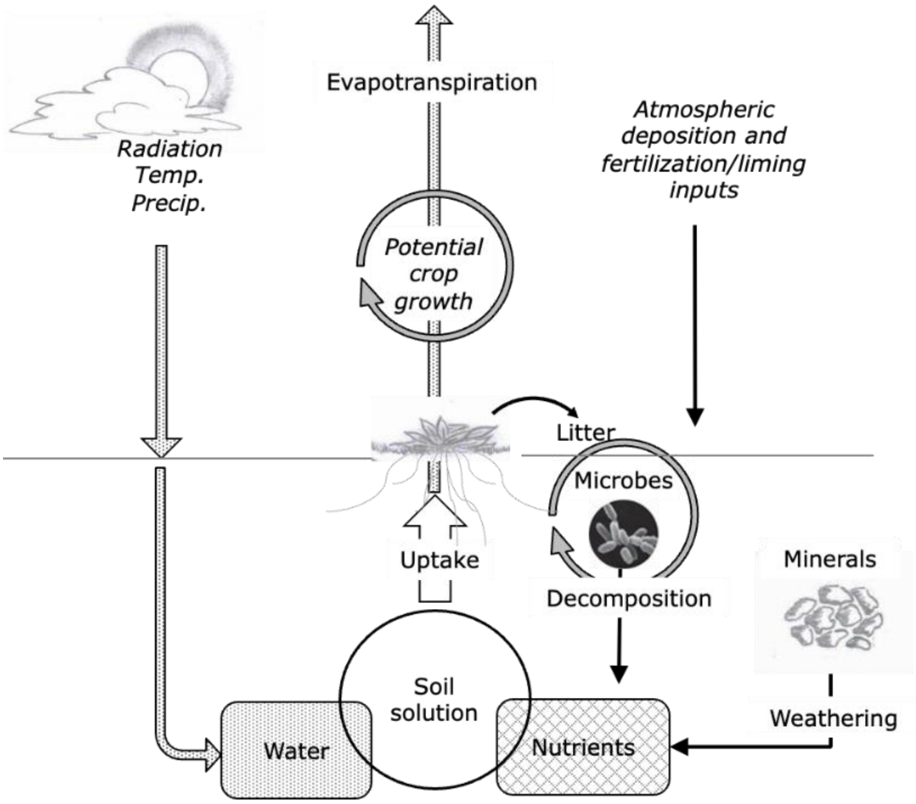

Figure 9 An schematic overview of the scope of FSF. Italics indicate system boundaries that will be provided as input, to keep the focus of the model on soil processes. (Adpated from Zanchi et al, 2014).

We will build on the soil module in ForSAFE, preserving all biogeochemical processes that are internally simulated (ion exchange, mineral weathering, decomposition or organic matter, mineralisation, volatilization and leaching). The soil modules, both organic and inorganic, in their present form simulate the mass balances of C, N, P, Ca, Mg, K, Na, Cl, S and Al in the soil (see Figure 10 below), and the direct and indirect interactions between these. The soil has three phases: aqueous, gaseous, and solid. In the soil and aqueous phases, elements are found in both organic and inorganic compounds. Soil microclimate and chemistry regulate microbial activity and thereby decomposition and mineralisation rates, which are applied to the organic matter substrate fed by litter or other organic input (manure) to estimate the net mineralisation rates of all the elements. Mineralisation is fed into soil solution thereby contributing to its chemical composition, and particularly soil Acid Neutralising Capacity (ANC). All elements dissolved in the soil solution are subject to leaching, but also available to soil exchange, precipitation and plant uptake. Volatile elements, like certain C and N species, are also subject to volatilisation and leave the soil in gaseous phase. The model keeps track of the equilibria between all the phases and uses soil conditions (temperature, moisture, porosity, chemistry, cation exchange capacity and mineralogy) to regulate the fluxes in Figure 10.

Within Nutribudget, we will bring two modifications to the model:

- replace the vegetation with crops, including new management activities (fertilization, ploughing, rotations of crops to start with).
- bring in new elements that are not currently in the model but are relevant for our questions.

Both crops and elements will be first drawn from FarmFlow, and from other sources when needed.

The model is then able to identify: i) the risk for elemental surplus that can leach, and ii) the risk of specific elements that can cause deficiency compared to potential uptake.

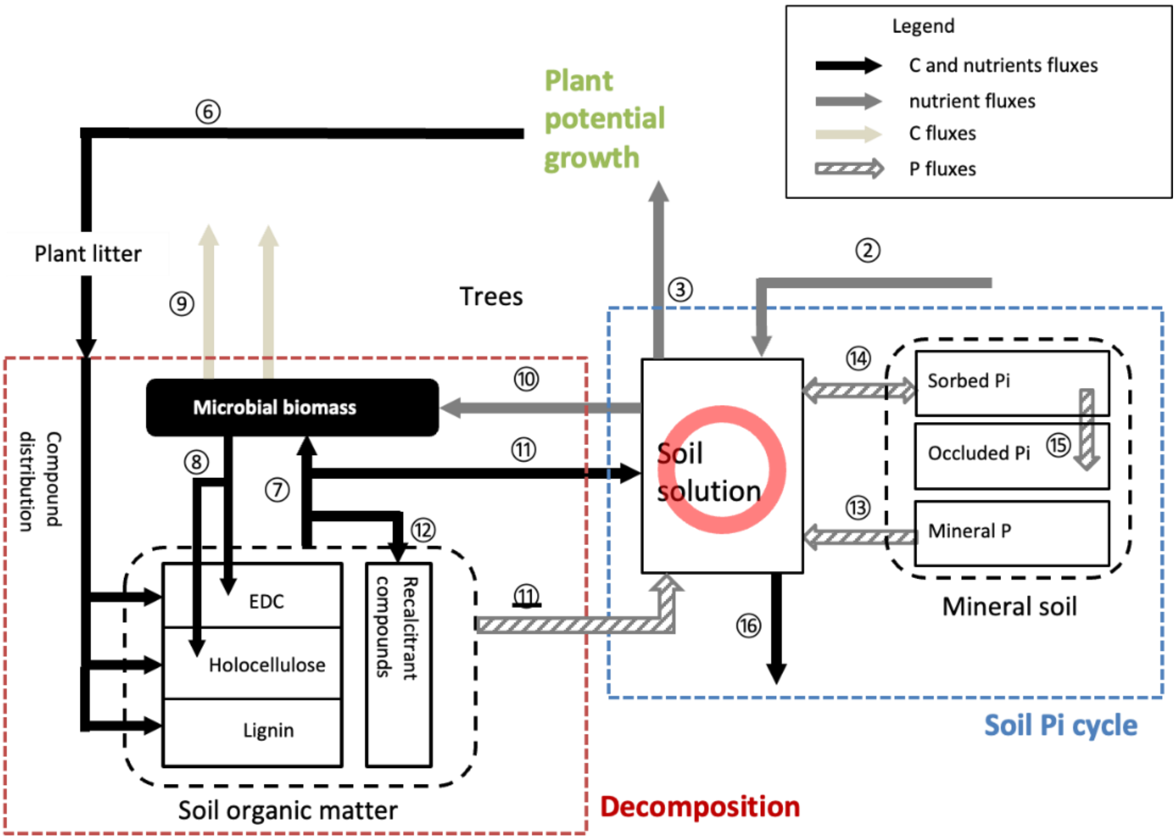

Figure 10 A closer look at the elemental fluxes and pools simulated by FSF, with an illustrative example of P. Other elements follow a similar architecture. The soil is treated as a multidimensional matrix of elemental pools and fluxes that are interact through mutual regulation of flux rates. (Adapted from Yu et al., 2018).

3.3 How CHN and FSF can complement the NutriModels

3.3.1 The role of CHN

The CHN model assumes the pivotal role of augmenting the NutriModels platform by furnishing precise insights into nitrogen and water fluxes throughout the crop's growth season. This is particularly indispensable for nitrogen-intensive crops like wheat, where enhanced precision in daily and sometimes hourly farm management practices proves crucial for optimizing nutrient efficiency. Adhering to the 5R principles of nitrogen fertilization, is essential, encompassing the right source, right rate, right time, right place, and right water supply to achieve nitrogen efficiency. These principles guide farmers toward practices that elevate nutrient efficiency while mitigating environmental losses. Developed primarily for real-time decision support, CHN facilitates the simulation of precision nitrogen and water supply, enabling the estimation of nitrogen and water use efficiency as well as stress indicators impacting overall biomass, on a daily base.

For the accurate simulation of nutrient management practices and their alignment with the 5R principles of precision agriculture (Ahmad and Nabi, 2021), CHN necessitates the validation and updating of model parameters. This process involves leveraging long-term field experimental data from European experiments, ensuring the model's broad applicability across diverse arable farming systems in Europe. Furthermore, CHN allows for the quantification of the impacts of various management activities such as ploughing, irrigation, manuring, crop diversification, cultivar nitrogen use efficiency, etc., on a daily base, offering insights into both short- and long-term effects on carbon and nitrogen dynamics (Laberdesque et al., 2017). The model exhibits heightened sensitivity to key variables, including phenological growth stages, nitrogen input amounts and supply dates, soil water holding capacity, soil organic matter content, and soil mineral nitrogen stocks at the conclusion of the leaching period (post-winter).

3.3.2 The role of FSF

The role of the FSF adaptation in NutriBudget is to complement NutriFarm by providing a stronger focus on how soil chemical reactions can affect the bioavailability and risk for leaching of a set of macro- and micro-nutrients in agricultural soils.

We base the new adaptation on the existing ForSAFE model, which depicts entirely mechanistic soil biogeochemical processes of carbon, nitrogen (including speciation), phosphorous, calcium, magnesium, potassium, sodium, chloride, aluminium and hydrogen. The model simulates the full biogeochemical cycles, but we will only isolate the soil chemical modules. This basis will be complemented with processes from the Farmflow model to depict cadmium and other heavy metals, and be extended to include other micronutrients as detailed in the project proposal.

The model is fully mechanistic in that it depends on singular causal relationships between any two components (one example being the Arrhenius temperature response function regulating the weathering rate of a given mineral). This structure makes the model less dependent on calibration, but heavily dependent on through empirical bases for the causal relationship it is constructed of. It also allows the model to be more responsive to changes in drivers that may have plural impact on the soil (such as moisture and acidity) and, where relevant, able to regulate these drivers in turn through feedback mechanisms. The mechanistic nature of the model also means that it keeps track of interactions between the cycles of different elements, since the rate variables (chemical reaction rates, physical change rates, or biological activity rates) are dependent on the state variables (such as element concentrations and substrate availability), which are regulated by these rates. This implies that a change in the mineralization rate for nitrogen will have an impact on soil solution pH, which will in turn affect the adsorption of potassium, and thereby the bioavailability of the latter.

This last aspect of the FSF model, the integrated mechanistic architecture, is the added value to the project, since it allows to identify critical thresholds and indirect impacts of agricultural measures meant for one element on the other elements.

We are currently working on mapping and isolating the main processes that we want to lift off from ForSAFE, and identifying how to add elements not yet implemented. For this, we are currently creating conceptual causal networks describing the soil biogeochemical processes governing bioavailability and leaching for the elements listed above. In parallel, data for model set up and testing is being processed in cooperation with the Swedish Agricultural University on the same dataset that is being made available to the other models in the ensemble.

The model is focused on mass balances in the soil, keeping track of mass conservation as fluxes and chemical transformations affect how much of any element is available under which form. The forms dealt with are in the solid, aqueous and gaseous phases. The solid phase include mineral, exchangeable and organic form. The aqueous phase refers to the soil solution where chemical reactions can occur, both in speciation (such as oxidation and reduction reactions) and precipitation into secondary minerals. The aqueous phase acts as a conduit to allow gaseous elements, such as CO_2 and N_2O, to volatilise out of the soil. The rates governing the reactions in the aqueous phase, as well those regulating the exchanges with the solid and aqueous phases, are all controlled by microenvironmental conditions and relative concentrations of the different elements.

FSF is meant to track simultaneous changes in the element cycles, and their mutual interactions in response to management and micro-environmental changes. To keep the focus on soil, the model will read crop related fluxes (uptake and litterfall) externally, either as assessed by the other models, or from empirical data.

FSF will identify conditions within which nutrients are bioavailable while the risk for leaching is kept low. These conditions are dictated by how the different elements interact, affecting ultimately the concentrations of nutrients in the soil solution. In this manner, we intend to create a set of dynamic response curves that describe the boundary beyond which a certain nutrient may become deficient, or when the risk for leaching becomes high. These curves will delimit a space of viable sustainability within low leaching risk and will inform the other model to back-calculate agricultural measures that are able to keep the elements concentrations withing the said spaces.

4. Next steps

Now that the framework is designed, a few elements still need to be elaborated further, including:

- Parametrisation and calibration. Especially at farm-level, the parametrisation and calibration need to be revised to analyse whether values used at European level are also valid at farm level.
- Initialisation. To find the initial soil nutrient and carbon status, the current initialisation method will be compared with an initialisation method that involves running the model until equilibrium (the so-called 'spin-up run').
- Validation. In the end, the NutriModels need to be validated. Besides a co-creation workshop that aims to test the validity of the modelling results, independent validation datasets will be collected. At European level, these datasets include regional and European datasets, whereas at farm-level these datasets include long-term experiments or local farm-data. The pilot studies of WP4 also provide data. These data will be used to test how well NutriFarm assesses the effect of measures.
- Downscaling procedure. The input data of MITERA-Europe are used as default data for NutriFarm. Decisions on how to downscale the data to farm or field level have to be decided. The question is to whether these downscaled data are reliable enough or whether users of the platform have to (and want to) provide some basic input data to improve the reliability of the results significantly. This question will also be addressed during the first co-creation workshop that will take place in spring 2024.
- Improving NutriFarm results. Although the roles of CHN and FSF have been described in this report, the modelling results of these models need to be compared to the modelling results of NutriFarm using a test-dataset. Analysing the origin of differences between NutriFarm and the complementary models can help defining which processes or in which regions NutriFarm results can be improved. The test datasets include long-term experiments and a dummy dataset.
- Critical thresholds/target values. Critical thresholds and target values need to be set for all nutrients and carbon to evaluate the desired state regarding the five objectives (soil quality, water quality, GHG emission, biodiversity, and agricultural production). This element is essential in the evaluation of nutrient management measures.

To make the NutriModels operable within the NutriModel framework, some additional model and data developments are required, including:

- Update input data. The current baseline of MITERRA-Europe is 2018. To run the model for baseline 2020, input data have to be updated. While updating the data, potential methodologies for future NutriData collection will be explored as part of sub-task 2.1.1.
- Refine to NUTS3 level. The MITERRA-Europe model is currently designed for NUTS2 calculations. Therefore, the model needs to be refined to NUTS3 level, including the input data.
- Default input dataset. The input data of MITERRA-Europe will be downscaled even further making use of spatial datasets. Different methods will be tested to define the optimum between simulation time and resolution. A next step is to link the default dataset (e.g., gridded data) to the input data required by NutriFarm (field or farm data).
- Elaborate MITERRA-Europe. At the moment, MITERRA-Europe assesses N, P, and C flows. To make the model operable for all nutrients (N, P, K, S, Mg, Ca, Zn) and C, the calculation steps of another European model called INTEGRATOR (Reinds et al., 2011; De Vries et al., 2011; De Vries et al., 2023) will be integrated.
- Elaborate FSF. The FSF model currently focusses on forest soil. To make the model operable for arable soils, elements of the FarmFlow model will be integrated in FSF.

Annexes

Annex 1A Input data the MITERRA-Europe model currently uses.

Dataset	Parameter	Source	Spatial use	Year(s) used
LUCAS – European Soil Data Centre	SOC content, pH, CEC, soil texture, bulk density, depth to bedrock, availability of CaCO3, NPK content, perennial grass cover (used for C balance)	Tóth, G., Jones, A., Montanarella, L. (eds.) 2013. LUCAS Topsoil Survey. Methodology, data and results. JRC Technical Reports. Luxembourg. Publications Office of the European Union, EUR26102 – Scientific and Technical Research series.	Average of LUCAS 2009 point data per NUTS2 region	2009
FAOSTAT	Fertilizer use and type, livestock production	Food and Agriculture Organization of the United Nations, 1997. FAOSTAT statistical database. Rome: FAO.	National data	Average between 2016-2018
EUROSTAT	Milk yield, fat and protein content of milk, percentage and area of natural grassland (not fertilized land)	European Commission, 2019. Eurostat statistical database. Brussels: European Commission.	NUTS2 level	Average between 2016-2018
CAPRI	Animal numbers, crop areas, and crop yields	Britz, W., Witzke, P., 2014. CAPRI model documentation 2014. Bonn, Institute for Food and Resource Economics.	NUTS2 level	2015
National GHG inventory submissions	N excretion of animals, CH_4 emissions from manure management and enteric fermentation	United Nations Framework Convention on Climate Change, 2019. National Inventory Submissions 2019. Bonn: United Nations Climate Change	National data	2017
FSS and SAPM	Arable farm size, farming system, crop rotation, livestock units, areas with organic farming, irrigation, crop cover (arable land)	European Commission, 2019. Farm Structure Survey - Survey Coverage. Brussels, European Commission.	NUTS2 level	2016
GAINS	NH_3 emission factors, NH_3 mitigation measures.	International Institute for Applied Systems Analysis, 2018. The GAINS model. Laxenburg: IIASA.	National data	2005
IPCC	N_2O, CO_2 (peatland) emission factors, global warming potentials,	IPCC, 2006. 2006 IPCC Guidelines for National Greenhouse Gas Inventories, Volume 4, Agriculture, Forestry and Other Land Use. IPCC National Greenhouse Gas Inventories Programme. Institute for Global Environmental Strategies (IGES), Kanagawa, Japan.	Tier 1 approach, based on climate zones	2006

WorldClim	Precipitation, evapotranspiration, temperature	Fick, S.E. and R.J. Hijmans, 2017. WorldClim 2: new 1km spatial resolution climate surfaces for global land areas. International Journal of Climatology 37 (12: 4302-4315.	1x1km resolution aggregated to NUTS2 level	Monthly average 1970-2000
Keuskamp et al. (2012)	Precipitation surplus, surface runoff and groundwater leaching fractions	Keuskamp, J.A., Van Drecht, G., Bouwman, A.F., 2012. European-scale modelling of groundwater denitrification and associated N2O production. Environ. Pollut. 165, 67–76. https://doi.org/10.1016/j.envpol.2012.02.008	Aggregated to NUTS2 level	2012
ESDB v2.0 and soil erosion maps (JRC)	Soil type, soil depth, soil erosion	The European Soil Database distribution version 2.0, European Commission and the European Soil Bureau Network, CD-ROM, EUR 19945 EN, 2004.	Dominant soil type and depth per NUTS2 region	2001

Annex 1B Potential updates and refinements to be made on the input data of MITERRA-Europe.

Dataset	Parameter	Potential changes to be made or explore:
LUCAS – European Soil Data Centre	SOC content, pH, CEC, soil texture, bulk density, depth to bedrock, availability of $CaCO_3$, NPK content, perennial grass cover (used for C balance)	- Include soil property maps (S, Ca, Mg, Cu, and Zn) based on the LUCAS database. - Explore the use of the soil property maps of SoilGrids (1km resolution) and compare these maps with the soil property maps of LUCAS.
FAOSTAT	Fertilizer use and type, livestock production	- Calculate averages over 2019-2021.
EUROSTAT (FSS, Agricultural Production Database, and SAPM)	Fat and protein content of milk, percentage and area of natural grassland (not fertilized land), animal numbers, crop areas, and crop yields, arable farm size, farming system, crop rotation, livestock units, areas with organic farming, irrigation, crop cover (arable land).	- Refine to NUTS3 level. - Update data to 2020.
NIS	N excretion of animals, CH_4 emissions from manure management and enteric fermentation	- Keep using these national data. - Update data to 2020
GAINS	NH_3 emission factors, NH_3 mitigation measures.	- Explore using the EMEP calculation rules including some additional data of EUROSTAT instead of using the GAINS data.
WoldClim	Precipitation, evapotranspiration, temperature	- Switch to ERA5 and update the climate data to the average 1990-2020 data.
Keuskamp et al. (2012)	Precipitation surplus, surface runoff and groundwater leaching fractions	- Explore the potential use of the more detailed Variable Infiltration Capacity (VIC) model (Liang et al., 1994) instead of Keuskamp (2012).
ESDB v2.0 and soil erosion maps (JRC)	Soil type, soil depth, soil erosion	- Refine to NUTS3 level.

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Optimisation of nutrient budget in agriculture

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