



# Optimisation of nutrient budget in agriculture



## D2.4 Publishing the second Nutrimodel



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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 that includes a decision support tool (DST) that operates at field level to serve local stakeholders, and insights in regional nutrient (N, P, K, S, Mg, Ca, Cd, Zn) and carbon (C) budgets to serve regional, national and European stakeholders. The models (i.e., NutriModels) and datasets that are used to assess the nutrient budgets at field and regional scale are aligned, which stimulates the conversation on sustainable nutrient and carbon management options among stakeholders. The NutriModels will, in the end, be able to assess the effect of nutrient and carbon mitigation measures. The effect of measures will be pictured along five goals (e.g., soil quality, water quality, GHG emission, biodiversity, and agricultural production) through a user-friendly interface of the DST. In this way, users will get insight into the opportunities and trade-offs regarding the optimisation of agronomically and environmentally sustainable nutrient use in the area they operate. This full picture can stimulate the implementation of measures as it helps making well-founded decisions at different scales.

The publication of this second NutriModel, NutriFarm, includes (i) a model description on the assessment of soil carbon and nutrient budgets at farm level and specifically where NutriFarm differs from MITERRA-Europe (published in D2.3), (ii) a case study in which the results of two other farm-level models are compared to the results of NutriFarm, and (iii) an approach on how the two additional farm-level models can complement NutriFarm.

NutriFarm can assess soil nutrient and carbon budgets for land-bound farming systems in Europe (EU-27, Switzerland and the United Kingdom), because the input data of MITERRA-Europe are used as default data for NutriFarm (D2.3). Users can access the model through a Decision Support Tool (DST), that is currently developed under WP5.

We greatly acknowledge all partners that contributed to the Nutribudget project and the development to the Nutrimodels, direct or indirectly: Ghent University (Belgium), Luke (Finland), Yara International (Norway), PWC (France), Arvalis (France), Beta Technology Center (Spain), Wageningen University & Research (the Netherlands), the Rural Investment Support for Europe Foundation (RICE), the Università Degli Studi di Milano (Italy), Proman Management (Austria), Sveriges Landbruksuniversitet (Sweden), the Nutrient Management Institute (the Netherlands), Acqua & Sole (Italy), Impact (Belgium), Stockholms Universitet (Sweden) and the Forschungsinstitut für Biologischen Landbouw Stiftung (Switzerland). Lastly, we thank Marcos Lana and Harald Ulrik Sverdrup for reviewing this report.

## Executive Summary

The report is entitled 'Publishing the second Nutrimodel' and implies the publication of NutriFarm including the parameters, input data and algorithms, and a case study that illustrates how two other farm-level models (CHN and FarmSAFE) can complement NutriFarm. 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. The NutriFarm model spatially predicts the nutrient (N, P, K, S, Mg, Ca, Cd, Cu, Zn) and carbon (C) budgets at field or farm level annually for each location in Europe (EU-27, Switzerland, and the United Kingdom).

Insight into nutrient budgets is agronomically and environmentally important to feed a growing population in a sustainable way. **Chapter 1** provides a general introduction on how NutriFarm contribute to the overall project goal.

A description of the farm-level models is provided in **Chapter 2**, including a description of NutriFarm, CHN and FarmSAFE. The algorithms of MITERRA-Europe (see D2.3) and NutriFarm are basically the same, except the water flux. In Nutri-Farm the water flux is calculated using a two-layered approach, whereas MITERRA-Europe uses a one-layered approach. At farm level, a more detailed water flux model was required for proper estimations of the nutrient flows in solution, whereas at regional level this effect is averaging out and it is therefore less relevant.

**Chapter 3** shows the results of a case study. All three farm-level models ran for the same field; a long-term experiment (LTE) in Sweden. Results of different modelling processes are compared among the different models, but also with the measured LTE data.

Based on the case study results, the strengths and weaknesses of the three farm-level models could be defined in **Chapter 4**, and an approach on how the models can complement each other, but especially NutriFarm, was formulated. The ambition is to have most impactful elements of the complementation implemented in NutriFarm by the end of the project.

This brings us to the next steps (**Chapter 5**) where we focus on four main activities: 1) description and implementation of the desired state (as part of WP2, T2.2), 2) connect the NutriFarm model to the DST (in collaboration with WP3 and WP5) on the webserver, 3) assess the effect of measures that were formulated in the mitigation measures catalogue (WP1) and measures that are included in the roadmap (WP2, task 2.3), 4) run the three farm-level models for long-term experiments in the other climatic zones to make the complementary values CHN and FarmSAFE have on Nutri-Farm broader applicable and simultaneously use these LTEs for model validation (WP2, task 2.4).

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## List of Abbreviations

BIO	Microbial biomass
C	Carbon
Ca	Calcium
Cd	Cadmium
CEC	Cation Exchange Capacity
CH <sub>4</sub>	Methane
CO <sub>2</sub>	Carbon dioxide
CORINE	Coordination of Information on the Environment
Cu	Copper
DPM	Decomposable plant material
DST	Decision Support Tool
HUM	Humified organic matter
IOM	Inert organic Matter
IPCC	Intergovernmental Panel on Climate Change
K	Potassium
LAI	Leaf area index
Mg	Magnesium
N	Nitrogen
N <sub>2</sub> O	Nitrous oxide
NH <sub>3</sub>	Ammonia
NO <sub>x</sub>	Nitrogen oxide
P	Phosphorus
RPM	Resistant plant material
S	Sulphur
Zn	Zink

## 1. Introduction

To reach the goals regarding nutrient pollution reduction, climate change mitigation and food security in European agriculture, farmers need to be able to make well-founded decisions on their nutrient management plan. Therefore, a farm-level model called NutriFarm was developed as part of WP2 (Task 2.1) in the NutriBudget project. This process-based empirical model assesses soil nutrient (N, P, K, S, Mg, Ca, Cd, Cu, Zn) and carbon (C) budgets of land-bound farming system in Europe (EU-27, Switzerland and the United Kingdom) and aims to facilitate farmers and farm-advisors to optimise the nutrient management plan. This report focusses on the publication of this NutriFarm model. It is the second NutriModel after the publication of the regional MITERRA-Europe model (D2.3). NutriFarm is based on the algorithms of MITERRA-Europe and uses input and output data of this model as default values to run at each location in Europe.

The NutriFarm model will become operable through a Decision Support Tool (DST) that is currently being developed under WP5. On the webserver where the DST operates, the model will run on-the-fly based on the requests of a user. Linking this user-friendly DST to the well-established NutriFarm model, helps farmers getting insight into their current soil C and nutrient state. Based on these insights, farmers can select effective nutrient mitigation measures that suit their situation or farming system (published in D2.6), and explore how they can bridge the gap between current and desired soil nutrient and C budgets (published in D2.5). The results will be evaluated along five goals (soil quality, water quality, GHG emission, biodiversity, and agricultural production) and measures will be tailored along the scores for each goal. In this way, strategic and operational farm management decisions can be made which can help increase the implementation rate of nutrient mitigation measures necessary to reach EU-wide goals.

This report includes (i) a model description on the assessment of soil C and nutrient budgets at farm level pointing out the elements where NutriFarm differs from the MITERRA-Europe model, (ii) a case study in which the results of two other farm-level models (FarmSAFE and CHN) are compared to the results of NutriFarm, and (iii) an approach on how the two additional farm-level models can complement NutriFarm based on the insights that were gained from the case study.

## 2. Description of farm models

### 2.1 Summary description of NutriFarm

The NutriFarm model is a process-based empirical model that simulates carbon (C) and nutrient fluxes (N, P, K, S, Ca, Mg, Cd, Cu and Zn) in agriculture across Europe (EU-27, Switzerland and the United Kingdom). It quantifies the sequestration of C and nutrient accumulation in the soil, the nutrient uptake by crops, and the fate of nutrients to the environment. The temporal scale of NutriFarm is annually, but some processes were calculated at monthly (e.g., C) or daily time scale (e.g., P), before aggregating it to annual scale.

A full description of the NutriFarm model is provided in [Annex 1](#). In general, the algorithms are similar to those of MITERRA-Europe. Therefore, we also refer to D2.3. The main differences between MITERRA-Europe and NutriFarm are that MITERRA-Europe uses a one-layer approach, focussing on the topsoil (0-30cm), while NutriFarm uses a two-layered approach (0-30 and 30-100cm). This ensures that the root zone of all included crops is covered, which is important for calculations at farm level and the assessment of soil nutrient transfer to and from deeper soil layers.

The fraction of the transpiration and of the element uptake in each layer is based on the fine root distribution of the included crops. The runoff of elements to surface water is calculated as an aggregated value for the surface and the interflow of the two soil layers, while leaching to groundwater is calculated at a depth of 100 cm, comparable to the water flux model used by Keuskamp et al. (2012) with results at a 1 km x 1km resolution at the European scale (see Annex 1 - Figure 1).

NutriFarm quantifies nutrient and C 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 ( $\text{NH}_4$ ,  $\text{NO}_3$ ), 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 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.

The algorithms of NutriFarm are aligned with MITERRA-Europe and therefore quite coarse for a farm-level model. Therefore, NutriFarm will be complemented by elements (i.e., data or processes) of two other farm-level models; FarmSafe (see 2.3) and CHN (see 2.4).

### 2.2 Input data of NutriFarm

The input data required by NutriFarm is equal to the input data of MITERRA-Europe (see D2.3). Additionally, NutriFarm requires subsoil data, because it uses a two-layered approach. The model makes use of default input data being representative for the local agroecological

conditions determining the crop production and environmental losses. These default input data originate from the spatial explicit model input and output of MITERRA-Europe (see D2.3).

All input parameters can roughly be divided into input data that are highly dependent on the local farm management situation (e.g., soil properties, crop yields) and more regional input data that are not that variable over space or directly controlled by the farmer (e.g., nutrient deposition rate, climatic conditions). The necessary model inputs can be divided into eight categories. More detail on the input parameters and data sources is available in Annex 2 – Table 2A.

1. **Soil properties.** This category includes physical and chemical soil properties of the topsoil (0-30 cm) and subsoil (30-100cm) as well as categorical soil characteristics such as textural class or soil type. The physical and chemical soil properties were obtained from the European Land Use/Cover Area frame statistical Survey Soil (LUCAS). Subsoil data were assessed by multiplying the topsoil data by a topsoil:subsoil ratio of SoilGrids, as it is better to use a single data source for soil data (Hendriks et al., 2016). The categorical soil characteristics were obtained from the European Soil Database (ESDB). The base cation weathering rate is derived for six combinations of the textural class and the acidity of the parent material, and is assessed based on Reinds et al. (2001). Data on the slope were derived from the Digital Elevation Model (DEM).
2. **Crop properties.** This category includes data on the crop areas and yields of 34 arable crops and three grass categories (i.e., rough grazings, permanent pastures and meadows) (Annex 1 – Table 1C). Depending on the available data, median (2019-2021) crop yields were provided at NUTS2 or NUTS0 level from Eurostat. For some countries only NUTS0 data were available for specific crops (e.g., fodder other on arable land), whereas other countries had data on NUTS2 level available. For these countries the NUTS0 data were disaggregated to NUTS2 using the CORINE land cover map.
3. **Farm and regional properties.** This category includes information on e.g., derogation areas, soil cover, tillage practice, crop residue and manure management. The data mainly comes from EUROSTAT, the Farm System Survey, and the European Commission. The atmospheric deposition data of nutrients come from EMEP or from previous versions of the MITERRA-Europe model.
4. **Emission factors.** These data are used to assess the emissions from livestock (e.g., enteric fermentation, excretion) and from nutrients applied to soil. The factors were derived from IPCC (2019), EMEP, and the national GHG inventory submissions of 2020.
5. **Climate.** This category includes monthly averaged data on evapotranspiration, temperature, and wind speed, and the monthly summed precipitation. The average over climatic period 1990-2010 was taken from the ERA5 climatic database.
6. **Water flux.** The water flux data, including precipitation surplus, surface runoff and groundwater leaching fractions, were derived from Keuskamp et al. (2012).
7. **Nutrient composition** of crop, manure and fertilizers. Crop, fertilizer, and manure composition data are used to assess the nutrient input and uptake. The composition data are derived from multiple sources and are attached in Appendix 2 – Table 2A, 2B and 2C respectively.
8. **Nutrient deposition.** This category includes deposition data of all nutrients. The data come from EMEP or from previous versions of MITERRA-Europe/INTEGRATOR.

For spatial continuous data, the source data was used as default at the original resolution. However, some of these data did not cover all countries in Europe. These data gaps were filled by regional NUTS2 MITERRA-Europe data or by data from neighbouring countries. Besides, no Eurostat data for the United Kingdom (UK) was collected after 2019, and therefore these data can be slightly outdated.

### 2.3 The FarmSAFE model

A full description of the FarmSafe model is provided in D2.2. The model FarmSAFE (in earlier deliverables referred to as FSF) is a new, fully mechanistic model that 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). It is a combination of two existing models, namely ForSafe (Gaudio et al., 2015; Zanchi et al., 2021) and FarmFlow (e.g. Modin-Edman et al., 2007; Stockwell et al., 2012), and it is further elaborated on Cd and C flows. The singular causal relationship structure makes the model less dependent on calibration, but heavily dependent on 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 in turn regulated by these rates. This implies, for example, that a change in the mineralization rate for N will have an impact on soil solution pH, which will in turn affect the adsorption of potassium, and thereby the bioavailability of the latter.

The modular architecture of the model allows to isolate the soil compartment and focus on the cycles of elements in the soil, as impacted by agronomic choices involving crops, residue and fertilisation, as well as climatic factors and site conditions. The model can recreate changes in the bioavailability of N, P, S and base cations. The model further focusses 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 or adsorption onto the ion exchange receptors on clay, silt and organic particles. The aqueous phase acts as a conduit to allow gaseous elements, such as CO<sub>2</sub>, methane and N<sub>2</sub>O, 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.

### 2.4 The CHN model

A full description of the CHN model is available in D2.2. The main objective of the CHN model is to be used during the agricultural season as a decision support tool for farmers to advise them on sustainable C and nutrient management options.

The CHN model was designed as a conceptual and mechanistic model. The main processes simulated are plant development and growth, C, water and N fluxes and stocks in the soil, plant and atmosphere compartments. The model is built around 3 main modules: 1) the 'carbon' module (C), with, for the soil compartment, the formalisation and parameterisation of the AMG model (Andriulo et al., 1999), and, for the plant compartment, the Monteith's C

accumulation principle (Monteith and Moss, 1977); 2) the 'water' module (H), with the water balance model, based on the work of Wery and Lecoœur (2000) and the PILOTE model (Khaledian et al., 2009); and 3) the 'nitrogen' (N) module, based on the principle of the N nutrition index (Justes et al., 1994) for the plant compartment. Four forms of N are considered: organic N, urea, ammonia and nitrate.

### 3. Comparison of farm level models; a case study

#### 3.1 Case study description

All three farm-level models run for a specific case study; a long-term experiment (LTE) in Sweden located in Säby (17.42 longitude; 59.49 latitude). The model run for eight years (2013-2020) and the crop rotation consists of oats, spring barley, two years of grass ley, two years of winter wheat, oats and spring barley. All crops except grass ley receive 450 kg/ha chemical fertilizer YaraBela AXAN (27% N, 0.6% Mg, 3.7% S) and no other (organic) fertilizers. Crop properties were measured annually, and soil properties were measured in 2013 and 2020. The difference between year 2020 and 2013 was used to fill soil data gaps linearly over intermediate years when no data were collected.

Input data requirements that were not measured were filled by either MITERRA-Europe default data or estimated by modelling experts (as more detailed input data were required by CHN and FarmSAFE).

#### 3.2 Elemental budget indicators for comparison

We present two indicators of elemental budgets: 1) element balances, and 2) element surpluses.

1- Balances are given as the difference between elements inputs to, and outputs from the soil at its external boundary. For inputs this includes, for example, deposition, (organic) fertilisation and mineralization, and outputs include, for example, crop harvest, leaching to groundwater (gw), and gaseous emissions.

2- Surpluses are concerned with the accumulation or depletion of elements in the soil, and the risk of exporting them to the environment beyond the agricultural soil, either in gaseous or aqueous form. The surplus implies the elements inputs to the soil and outputs related to crop uptake.

**Table 3.1.** Elemental input and output indicators considered by the model NutriFarm.

Model	Indicator	Flux	Nutrient
NutriFarm	Crop residue	INPUT	C
NutriFarm	Mineralization	INPUT	C and N
NutriFarm	Fixation	INPUT	N
NutriFarm	Manure	INPUT	C, all nutrients and metals
NutriFarm	Deposition	INPUT	All nutrients and metals
NutriFarm	Fertilizer	INPUT	All nutrients and metals
NutriFarm	CO <sub>2</sub>	OUTPUT	C
NutriFarm	Uptake	OUTPUT	N
NutriFarm	NH <sub>3</sub>	OUTPUT	N
NutriFarm	Denitrification	OUTPUT	N
NutriFarm	N <sub>2</sub> O+NO <sub>x</sub>	OUTPUT	N
NutriFarm	Surface runoff	OUTPUT	N
NutriFarm	Subsurface runoff	OUTPUT	All nutrients and metals
NutriFarm	Leaching to groundwater (gw)	OUTPUT	All nutrients and metals

**Table 3.2.** Elemental input and output indicators considered by the model CHN.

Model	Indicator	Flux	Nutrient
CHN	Mineralization	INPUT	N
CHN	Fertilizer	INPUT	N
CHN	Volatilization	OUTPUT	N
CHN	Nitrogen Lixiviation	OUTPUT	N
CHN	Runoff	OUTPUT	N
CHN	Above ground biomass	INPUT	C
CHN	Rhizosphere biomass	INPUT	C

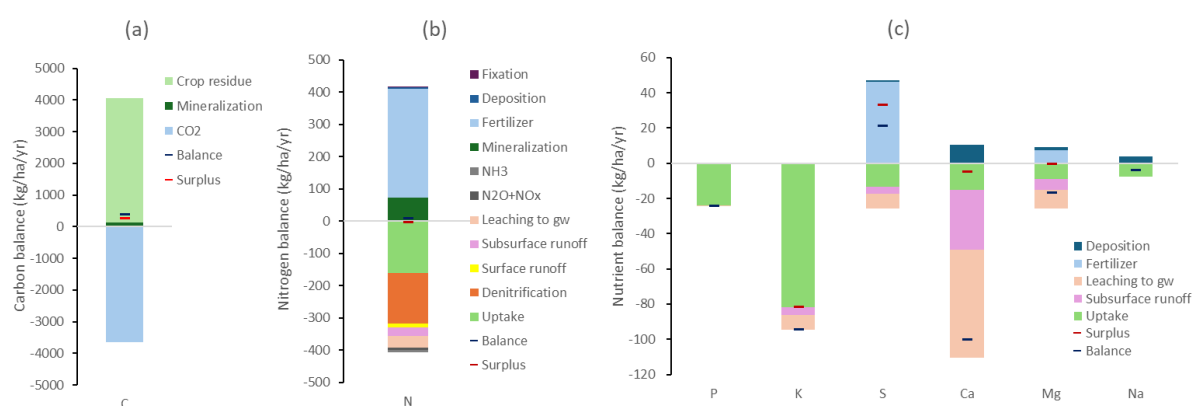
**Table 3.3.** Elemental input and output indicators considered at the moment by the model FarmSafe (more will come in the next iteration of the model development).

Model	Indicator	Flux	Nutrient
FarmSAFE	Fertilizer	INPUT	All nutrients and metals
FarmSAFE	Organic residue & manure	INPUT	C, nutrients & metals
FarmSAFE	Potential uptake	INPUT	All nutrients and metals
FarmSAFE	Deposition	INPUT	All nutrients and metals
FarmSAFE	Actual uptake	OUTPUT	All nutrients & metals
FarmSAFE	Soil C & nutrient partitioning	OUTPUT	C and nutrients
FarmSAFE	Surface runoff	OUTPUT	DOC and nutrients
FarmSAFE	Leaching losses	OUTPUT	DOC, nutrients and Cd

### 3.3 Plausibility of NutriFarm

Results presented here include the average budgets (inputs and outputs), balances and surplus of C, N, P, K, S, Ca, Mg, Na, Cd, Cu and Zn of the LTE case study over the years 2013-2020 (Fig. 3.1 and 3.2).

For C, most input came from crop residue (3925 kg/ha), followed by soil mineralization (128 kg/ha) (Figure 3.1a). CO<sub>2</sub> emission (3646 kg/ha) was the only C output from the soil. The average C surplus was 279 kg/ha/yr and average C balance was 406 kg/ha/yr.



**Figure 3.1.** Soil carbon (a), nitrogen (b) and other nutrient (c) budgets (kg/ha/yr) for a case study in Sweden.

For N, fertilizer was the main input source (on average 338 kg/ha/yr), followed by N mineralization (73 kg/ha/yr), while inputs by deposition and fixation were low, i.e. 3.4 and 2.8

kg/ha/yr, respectively (Figure 3.1b). The crop removal by harvest (grain) was the major output (162 kg/ha/yr), with a N use efficiency (NUE) of 48%, as all crop residues had been incorporated. Denitrification was the main pathway of N losses (156 kg/ha/yr), followed by surface and subsurface runoff (in total 37 kg/ha/yr), leaching to groundwater (36 kg/ha/yr), NH<sub>3</sub> emission (7.8 kg N/ha) and N<sub>2</sub>O and NO<sub>x</sub> emissions (7.5 kg N/ha).

For P, deposition was the only input source (0.20 kg/ha). Crop removal was the major P output (24 kg/ha), followed by leaching to groundwater (0.15 kg/ha) and subsurface runoff (0.06 kg/ha) (Figure 3.1c). Average P surplus and P balance was both -24 kg/ha/yr.

Similar as P, deposition was also the only K input source (0.46 kg/ha/yr) (Figure 3.1c). Crop removal was the major K output (82 kg/ha/yr), followed by leaching to groundwater (8.4 kg/ha/yr) and subsurface runoff (4.6 kg/ha/yr) (Fig 5.4). Average K surplus and K balance was -81 and -94 kg/ha/yr, respectively.

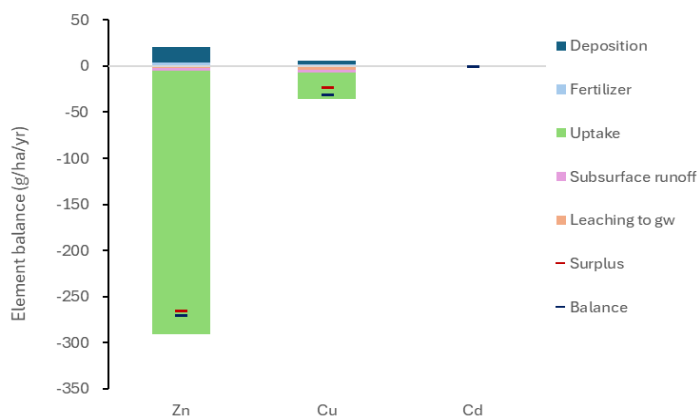
For S, fertilizer was the major input source (46 kg/ha/yr), followed by deposition (0.72 kg/ha/yr) (Figure 3.1c). Crop removal was the major S output (14 kg/ha/yr), followed by leaching to groundwater (8.2 kg/ha/yr) and subsurface runoff (3.8 kg/ha/yr). Average S surplus and S balance was 33 and 21 kg/ha/yr, respectively.

For Mg, similarly, fertilizer was the major input source (7.5 kg/ha/yr), followed by deposition (1.7 kg/ha/yr) (Figure 3.1c). Crop removal was the major Mg output (9.2 kg/ha/yr), followed by leaching to groundwater (11 kg/ha/yr) and subsurface runoff (5.8 kg/ha/yr). Average Mg surplus and Mg balance was 0 and -16 kg/ha/yr, respectively.

For Ca, deposition was the only Ca input source (10 kg/ha/yr) (Figure 3.1c). For output, leaching to groundwater was the major pathway (62 kg/ha/yr), followed by subsurface runoff (34 kg/ha/yr). The least output was crop removal (15 kg/ha). Average Ca surplus and Ca balance was -5 and -100 kg/ha/yr, respectively.

For Na, deposition was also the only input source (4.0 kg/ha/yr), while uptake was the only output pathway (7.5 kg/ha/yr) (Figure 3.1c). Average Na surplus and balance was both -4 kg/ha/yr.

For Zn, deposition was the major Zn input source (18 g/ha/yr), followed by fertilizer (3.4 g/ha/yr) (Figure 3.2). Crop removal was the major output (286 g/ha/yr), while subsurface runoff and leaching to groundwater was both minor (2.7 and 2.0 g/ha/yr, respectively). Average Zn surplus and Zn balance was -265 and -270 g/ha/yr, respectively.



**Figure 3.2.** Soil zinc, copper and cadmium budgets (g/ha/yr) for a case study in Sweden.

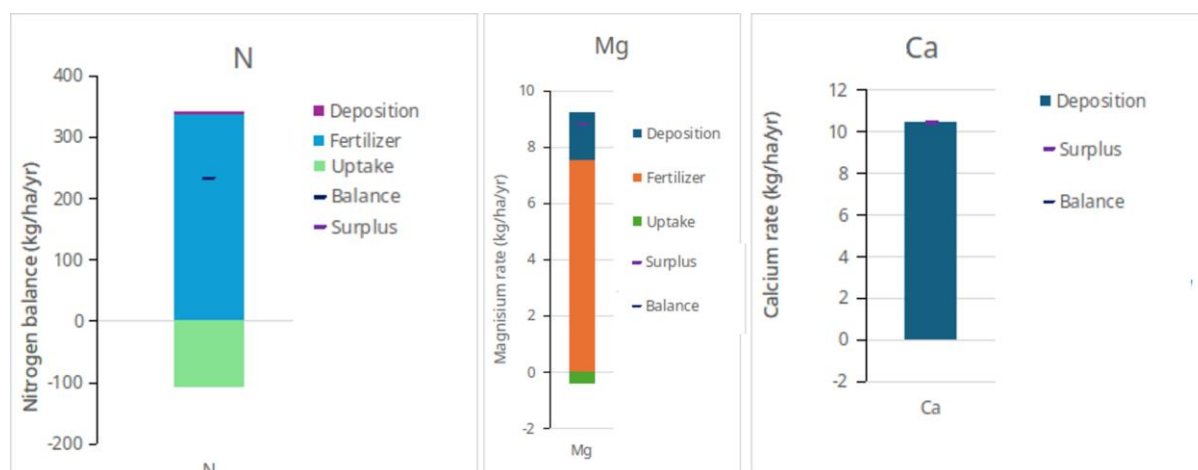
Similar to Zn, deposition was the major Cu input source (3.7 g/ha/yr), followed by fertilizer (1.9 g/ha/yr) (Figure 3.2). Crop removal was the major output (29 g/ha/yr), followed by leaching to groundwater (4.5 g/ha/yr) and subsurface runoff (2.7 g/ha/yr). Average Cu surplus and Cu balance was -23 and -30 g/ha/yr, respectively.

For Cd, deposition was the only input source (0.19 g/ha/yr) (Figure 3.2). Crop removal was the major output (0.68 g/ha/yr), while subsurface runoff and leaching to groundwater was both minor (0.03 and 0.02 g/ha/yr, respectively). Average Cd surplus and Cd balance was -0.49 and -0.54 g/ha/yr, respectively.

### 3.4 Results of FarmSAFE

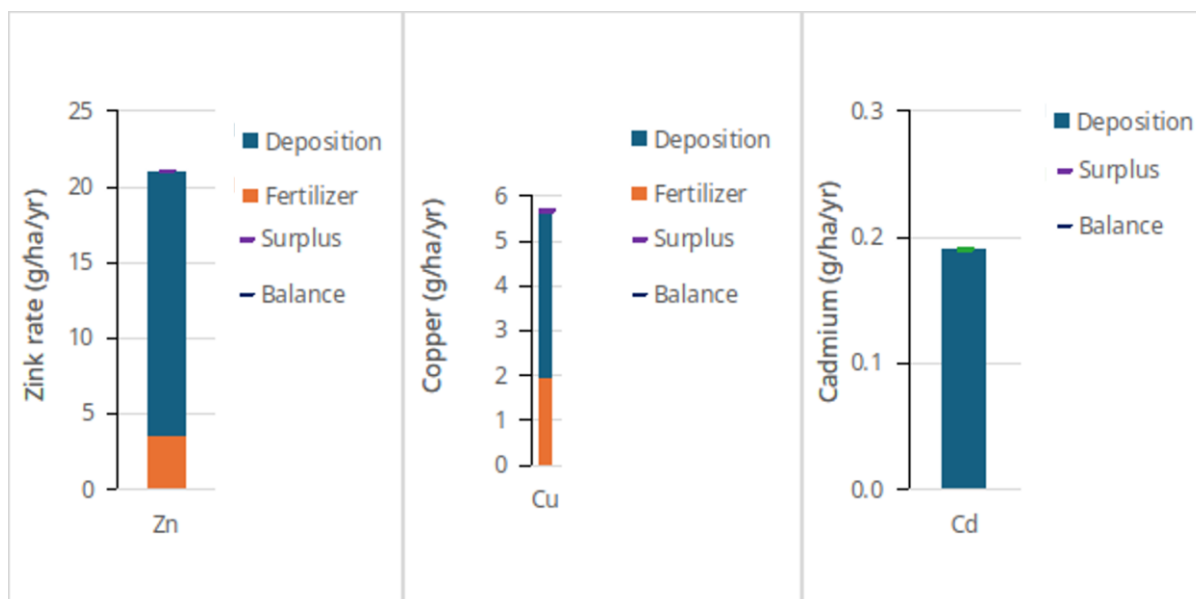
Due to the current implementation of the N cycle in the FarmSAFE model, it does not yet account for gaseous emission from N and C cycles. Therefore, in the calculation of budget calculates fertilisation input and subtracts only crop uptake, whereas balance accounts only for fertilisation, uptake and leaching. While gaseous emissions of C were significant, averaging an annual flux of 527 kg/ha,yr, gaseous emissions of N remained minimal at an annual average of 1.1kg/ha,yr. N fluxes out of the soil were overwhelmingly dominated by leaching and uptake, while there was no significant accumulation not depletion in soil organic N. The low rate of N retention in the soil is due to the short residence time of the latter, explained by the elevated runoff and associated leaching of dissolved inorganic N matching the annual rate of uptake. The result implies a relatively low N use efficiency, probably due to the fertilization type and timing assumed in the simulations.

For the test site, average budgets, balances and surpluses of the nutrients N, Mg, Ca, Zn, Cu and Cd are given in Figure 3.3 for the years 2013-2020 and for the processes FarmSAFE currently can model (more processes will be added in the next iteration of the model development). For N, the highest contributor was fertilisation at 337.5 kg/ha,yr. Only around one third of the added N was taken up by the crop. Mg inputs were fertilisation at 7.6 kg/ha and deposition at 1.7 kg/ha, with the uptake adding up to 0.42 kg/ha. Ca input was deposition at 10.47 kg/ha with uptake of 0.022 kg/ha. (fig. 3.3)



**Figure 3.3.** Soil nitrogen (N), magnesium (Mg) and calcium (Ca) budgets for a case study in Sweden.

Inputs for heavy metals consisted of mostly deposition at 17.6 kg/ha for Zn, 3.73 for Cu and 0.19 kg/ha for Cd. Zn and Cu were added through fertiliser as trace elements at 3.34 kg/ha and 1.94 kg/ha respectively (Fig. 3.4).

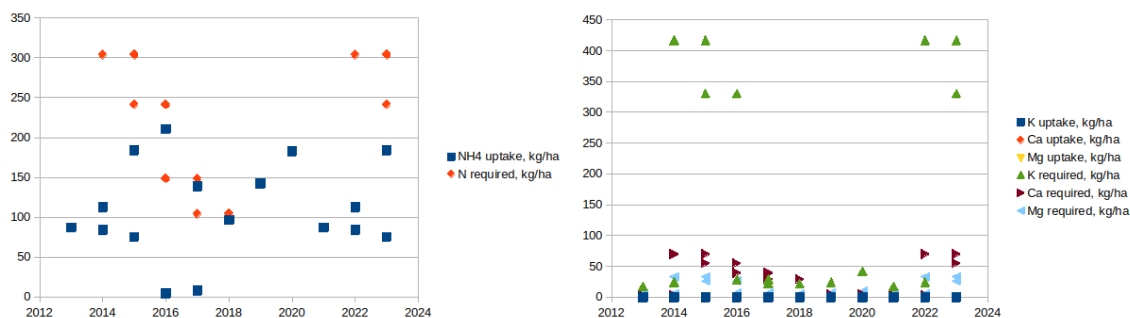


**Figure 3.4.** Zinc (Zn), copper (Cu), and cadmium (Cd) budgets (g/ha/yr) for a case study in Sweden.

The model simulated low P availability, as inputs from weathering rates and ambient atmospheric deposition remained low. We hypothesise that the expected crop yields would not be sustainable with the simulation assumption that there was no P fertilization. At the time of writing, this data remains unavailable, as does data on the pool of exchangeable P.

Due to the daily resolution of the FarmSAFE model, it can provide more insights to the functioning of the system. Actual uptake is one of the potential contributions, because NutriFarm determines the uptake based on a fixed crop nutrient demand. FarmSAFE can provide more information of the susceptibility of nutrient loss (in this case N), as a combined results of application time, leaching due to precipitation events, and soil retention in mineral and organic forms.

Another process that FarmSAFE can provide is the potential uptake, i.e. the nutrient amount requested by the crop. This potential uptake can be compared to the actual uptake to determine the nutrient deficit or surplus. The base cation deficit graph (Fig.3.5) shows that the plant regularly is stressed with unfulfilled uptake requirements, and that deficit adds up to total yearly deficit for N and base cations. The simulation at Säby also shows that the model is unable to achieve the observed regulated soil pH reported at the site. Without prescribed liming, the background soil pH predicted by the model lies around 4. This low pH reflects the relatively low availability of base cations, and confirms the need for liming. Liming, or the addition of other base cation rich material, would not only fill the uptake deficit gap, but also bring the pH to a higher neutral or alkaline level. However, increasing soil alkalinity might also affect the bioavailability of P, which could further exacerbate the risk of P losses. The simulation indicates that adding base cations should go hand in hand with P addition.



**Figure 3.5.** Yearly deficit for nitrogen (N) and base cations (K, Ca, Mg) for the case study in Sweden.

Finally, the model shows a very high variability in daily water balances. The soil being well drain and with a relatively high saturated conductivity makes for short residence times for soil water. Obviously, it is not possible to predict daily precipitation from the perspective of agronomic measures planning (like fertilisation events), but the model can be used to test alternatives altering the hydrological properties of the soil, such as the mentioned saturated conductivity. It would be interesting to explore novel methods such as biochar additions, but also more traditional methods like elevated solid organic inputs. FarmSAFE could be run for several such scenarios to inform NutriFarm on more desirable measures to better even out the high temporal variation in water availability and associated nutrient loss through leaching.

### 3.5 Results of CHN

Results presented here include averaged inputs and outputs of CHN for the LTE over the years 2013-2020 (Fig.3.6).

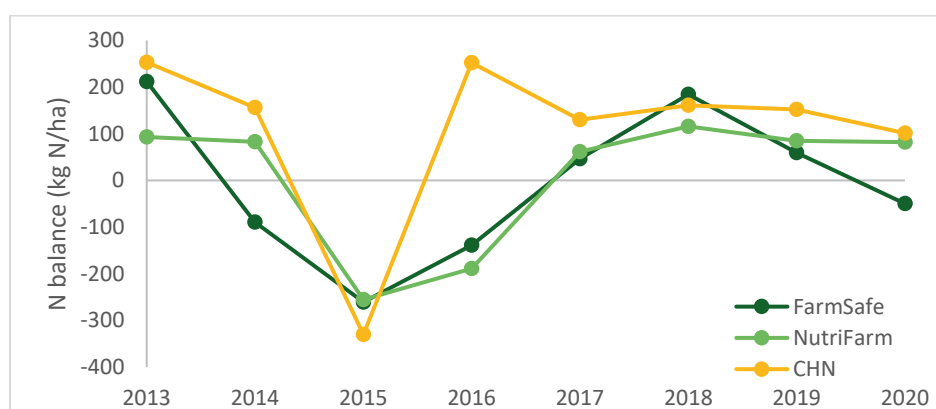


**Figure 3.6.** Annual inputs and outputs of nitrogen (N) (kg/ha/yr) in the LTE test site of Sweden.

For N, fertilizer was the main input source (on 450 kg/ha/yr except for grass lay), followed by N mineralization (72.47 kg/ha/yr), while inputs by mineralisation of harvest residues are quite low, i.e. 1 to 8 kg/ha/yr, respectively (Figure 3.4). The crop removal by harvest (grain) was the major output (average 319 kg/ha/yr aboveground and average 27 for below ground biomass), with a N use efficiency (NUE) of 48%, as all crop residues had been incorporated. NH<sub>3</sub> emission (7.8 kg N/ha) was the major way of N losses (-30 kg/ha/yr).

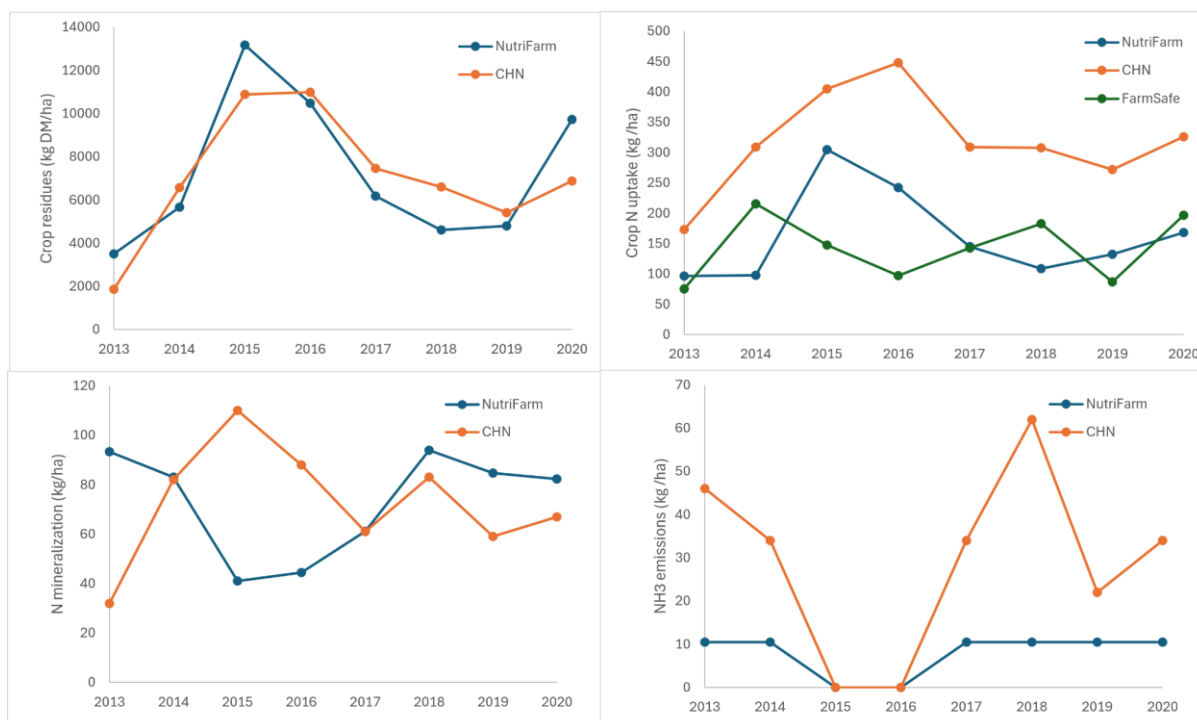
### 3.5 Comparison of modelling results

Comparing the balance (i.e., the difference between elements inputs to, and outputs from the soil; see 3.2), we noticed that every model assesses different inputs and outputs. Although a certain degree as disagreement between models is expected, potentially generating contradictory results, the N balance the difference found between the models used by NUTRIBUDGET are quite comparable (Fig. 3.7), indicating that our approaches are coherent. These elemental differences are also where the models can complement each other.



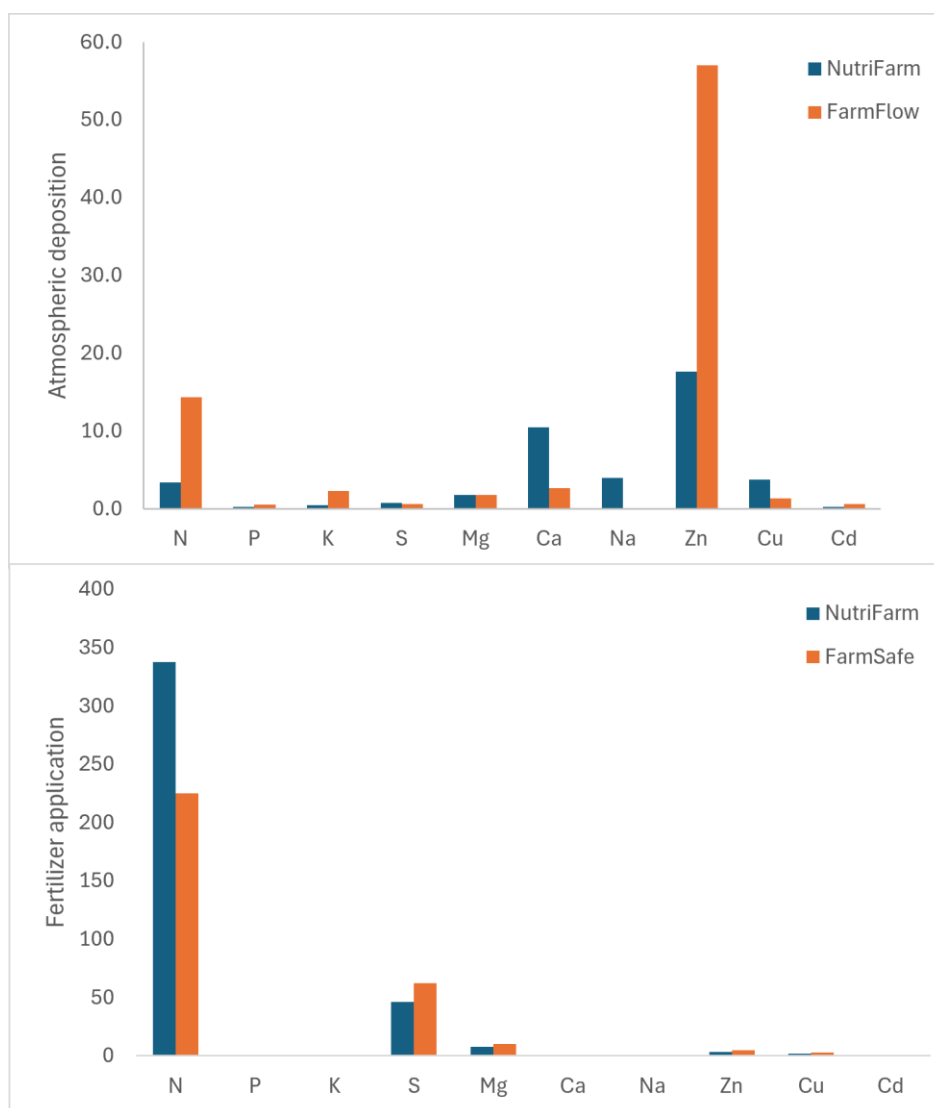
**Figure 3.7.** N balance estimated by three different farm-level models; NutriFarm, FarmSafe, and CHN.

Crop biomass production (in kg DM/ha) is very comparable between NutriFarm and CHN, whereas the N uptake calculated by CHN deviates from NutriFarm and FarmSafe (Fig.3.8). The N mineralization rates are very similar for some years (e.g., 2014 and 2017), but for 2013 and 2015 the estimations deviation quite a lot. Also, NH<sub>3</sub> emissions were significantly higher estimated by CHN compared to NutriFarm. The more detailed dynamics of certain processes in CHN and FarmFlow can help improving NutriFarm (Chapter 4).



**Figure 3.8.** Comparing crop residue production (in kg DM/ha), crop N uptake (in kg/ha), N mineralization (in kg/ha) and NH<sub>3</sub> emissions estimated by the NutriFarm, CHN, and/or FarmSafe model.

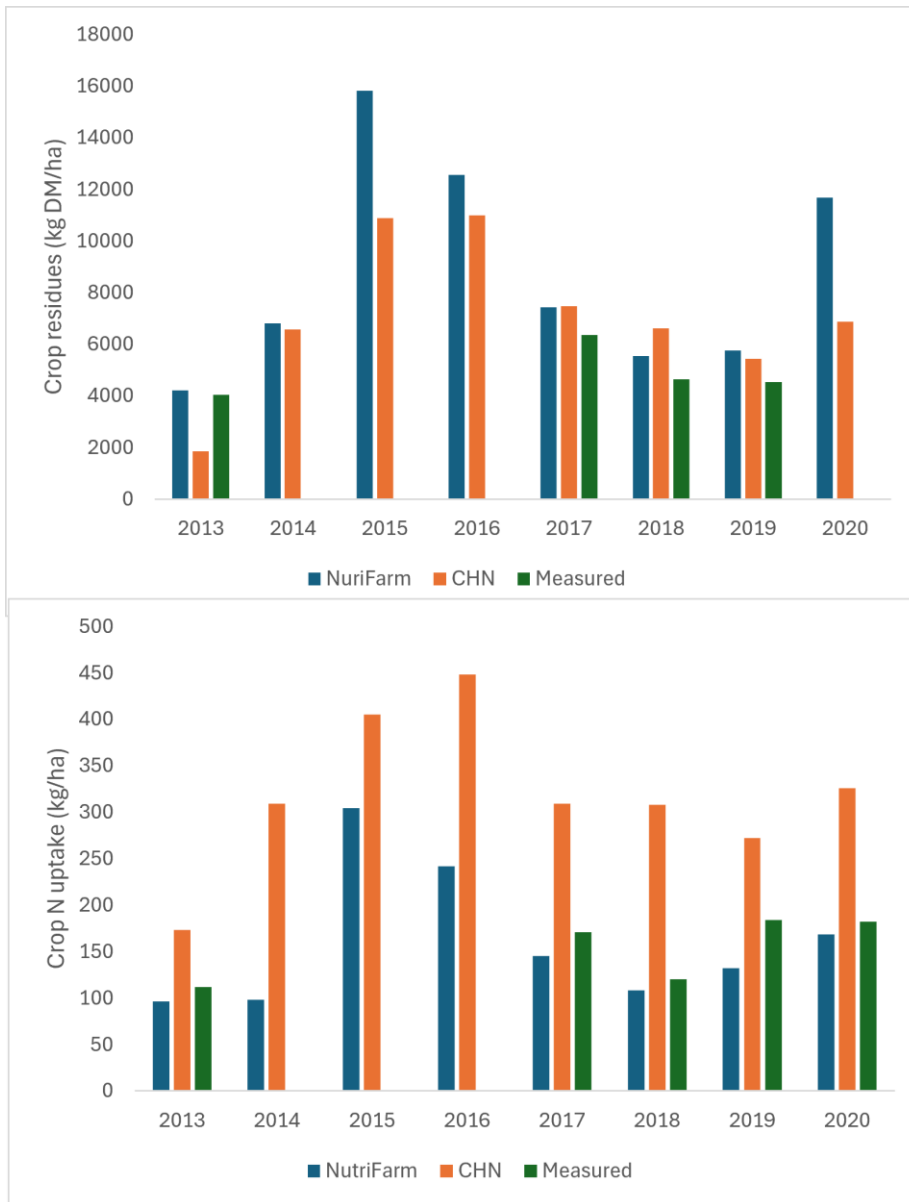
The strength of FarmSafe is that it is a farm-level model that describes soil processes in much detail and integrated the same nutrients as NutriFarm. Comparing two input parameters of the Saby case, atmospheric deposition and fertilizer application, we see that some nutrients show quite similar results (P, S, Mg, Cd), while other nutrient values still deviate from each other (N, K, Ca, Zn, Cu) (Fig. 3.9). Causes for the deviation in results for some nutrients and heavy metals needs to be investigated further to understand if and where FarmSafe can complement NutriFarm.



**Figure 3.9.** Comparing nutrient deposition and fertilizer application between NutriFarm and FarmSafe.

### 3.6 Comparison of model simulations with observations

Crop residue production was measured in the LTE, but also calculated by NutriFarm and CHN, while provided as input data to FarmSAFE, and therefore this parameter could be compared with real measurements (Fig. 3.10). This comparison shows that the models are quite in line with the measured values, although slightly overestimating residue production in three years. NutriFarm uses fixed C inputs or a non-linear relationship between yield and crop residues to estimate crop residue production. The yield is, however, also a fixed number, whereas CHN uses a crop-growth model to estimate yields more realistically. We foresee that this is an element where CHN can complement NutriFarm. The crop N uptake is more in line with NutriFarm compared to CHN, which confirms that NutriFarm estimates N uptake quite well.



**Figure 3.10.** Modelled (NutriFarm and CHN) and measured crop residue inputs (in kg DM/ha) and crop N uptake (in kg/ha).

## 4. Approach on model complementarity

### 4.1 Modelling philosophy of NutriFarm

The main strengths of farm level models include: (i) to simulate fundamental changes in major properties such as field and farm production, soil quality and environmental effects, (ii) to identify the major drivers or causes in view of e.g., agricultural management and climate change, and (iii) to assess the impacts of a wide range of technological innovation and farm-specific policies.

The NutriFarm model is a process-based empirical model, allowing broad applicability across Europe. It is imperative that the model approach is appropriate in view of the model objectives and the spatial and temporal scales addressed. The aim of the NutriFarm model is to assess annual element fluxes over a longer time period at high spatial resolution and evaluate the impacts of multiple feed, housing, nutrient, soil and crop management practices on those fluxes. With the purpose to apply this model on all potential farming systems across Europe, known by its high spatial variability in agroecological conditions, there is a trade-off between model complexity and data availability. When the model complexity increases, the descriptive (model) error decreases but the parameter error increases. The model approach of the NutriFarm model is therefore chosen to minimise the total prediction error in large scale environmental applications.

There are multiple detailed mechanistic models to simulate element fluxes in the field, such as C and N fluxes and GHG emissions, but these models require multiple input data (e.g. initial conditions and parameters) which are often limited or even unknown at the relevant scale. Especially at high spatial resolution, many model parameters cannot be derived in such models and most mechanistic models make use of generic parameter estimates from literature. Mechanistic models are thus very useful to gain insights in processes, in particular for experimental sites that are intensively monitored, but they are mostly not very suitable for large scale applications. This holds even stronger for the implementation of measures, which is generally very hard to parameterize. Considering the aim to predict annual element fluxes, our modelling philosophy was to develop a process-based model at intermediate complexity, including all key processes, well accounting for spatial variability by making use of readily available empirical data based on field measurements. Earlier studies (De Vries et al., 1998; 2023) showed that model simplification, in terms of less detailed formulations of processes (process aggregation) at low temporal resolution (temporal aggregation) is an adequate step in the upscaling of modelling results from a local to a regional scale when interested in annual average element fluxes. The spatial variability was included by using empirical relationships between model parameters and factors driving the variation, including animal category, land use/crop type, soil type/soil properties (such as pH, clay and organic matter content) and groundwater level to maintain transparency and to increase model applicability across the Netherlands.

To strengthen the applicability of the NutriFarm model approach, we tested the plausibility of the observed trends in view of scenarios varying element inputs and removals, and aim to bring relevant insights from process-based models (in this case FarmSAFE) or highly data-demanding models (in this case the CHN model) into the model framework of the NutriFarm model. Potential opportunities for model complementarity and improvements are described in the next section.

## 4.2 Opportunities for complementarity

The three models (farm, crop and soil numerical) included in NutriBudget were selected based on their mutual spatial, temporal and process resolution complementarity. Given its readiness for wide geographical and contextual application, NutriFarm will be the recipient platform where inputs and improvement from both CHN and FarmSAFE will be incorporated. In this section of the report, we document how NutriFarm is informed by the other two models, and the implications of the individual amendments.

We foresee six potential processes where insights from the CHN and FarmSAFE model can complement the current NutriFarm approach, being summarized in table 4.1. First of all, the current simplification of the hydrological fluxes can be improved when the transport of nutrients accounts for the actual runoff and leaching risks that might vary throughout the season whereas these dynamics are ignored in the current annual scale nutrient modelling in NutriFarm. This would require site specific algorithms quantifying how the annual runoff and leaching fraction depends on the rate of change in the precipitation surplus throughout the year. In theory this correction might depend on the water retention capabilities of the soil layer.

Second, whereas the NutriFarm simplifies the cation exchange from major cations to the exchange complex, it would be valuable to add analytical solutions for the exchange of the major cations Ca, Mg, K and Na in response to variation in their inputs. This might have strong implications for the agronomic soil fertility and associated required nutrient inputs as well the soil structure, thereby affecting the nutrient use efficiency and nutrient uptake.

Third, the carbon model in Nutrifarm follows the five-pool C decomposition approach as done with RothC whereas the mineralisation of organic nutrients is simply calculated by their respective C-nutrient ratios. Where this approach is generally valid on annual level, it might be valuable to expand the NutriFarm model with the nutrient supply occurring during the growing season and thereby giving scientific underpinning for the derivation of fertilizer use recommendations.

**Table 4.1.** Processes that can be complemented by CHN and FarmSafe.

Process	Model source	Implication in NutriFarm
Evapotranspiration	CHN & FarmSAFE	More dynamic precipitation surplus and losses in the form of surface runoff and leaching, controlled by daily hydrological balance between precipitation, evaporation and plant processes and scaled to annual water budgets. This will have implications on the annual water surpluses and associated leachates.
Cation exchange	FarmSAFE	Incorporate annual change in base saturation in base cation budgets, which will be reflected more realistically in surpluses
Organic mineralisation	CHN & FarmSAFE	Temporally dynamic estimates of soil organic C decomposition and associated mineralisation of nutrient elements, which will be reflected in elemental budgets and thereby surpluses.
Phosphorus retention	FarmSAFE	Include the net transfer of P between soil precipitates and bioavailable form in response to soil conditions, particularly liming, to better represent the surpluses and deficits in P budgets

Nutrient and water limitations	CHN & FarmSAFE	Corrections of crop growth prognosis in the event of nutrient or water limitation on a rotational scale. This will have implications on surpluses of all nutrient elements.
Organic accumulation/depletion	CHN/ForSAFE	Long-term trends in soil organic matter content in response to practices and climate, which will impact the C budgets, organic nutrient retention, and soil hydrological and physical properties.

Fourth, the NutriFarm assesses the fate of P via a combined Langmuir and Freundlich approach, thereby accounting for the interaction between clay minerals and the levels of available P in soil solution. This approach ignores the potential impact of Ca, leading to the precipitation of Ca-P complexes. In addition, it assumes instant equilibrium whereas this might be affected by the moisture content during the growing season. Insights from the FarmSAFE model can probably be used to correct for common representative situations during the growing season across Europe. Note that then also crop dependent variations in rooting patterns might play a role.

Fifth, the NutriFarm model did not include a crop module, and crop nutrient uptake is basically a model input being used as system boundary. In reality, the nutrient uptake is highly dependent on the actual supply from soil and inputs, and insights of the crop response to nutrient availability can be deduced from both the CHN (for N) and the FarmSAFE model and be implemented as crop-nutrient response relationships in the NutriFarm model.

Lastly, the long-term impacts of organic matter inputs on soil fertility and associated soil processes are explicitly modelled for organic nutrients and their influence on the metal availability is also considered. Whether the RothC approach is applicable for all climate regions across Europe needs still to be evaluated, and the model approaches from CHN or ForSAFE might be useful to validate the simulated fate of SOC and associated impacts on nutrient availability.

Though all these six complementarity issues are beneficial for the accuracy and applicability of the NutriFarm model, pragmatic reasons force us to set priorities in the actual model development. Given the final goals of the project, we need to balance the detail resolution of the NutriFarm with the constraints on implementation as well as usability and transportability of the associated application of the tool. Within the Nutribudget project we would focus on the correction for seasonal weather conditions, the cation exchange, and the crop nutrient response to nutrient availability in soil.

## 5. Next steps

Now, as NutriFarm is published, the current state of soil nutrient and C budgets can be estimated at every land-bound farm in Europe. Next steps are to:

- 1) Describe and implement the desired nutrient and C state and link these to the five goals (soil quality, water quality, GHG emission, biodiversity, and agricultural production) as part of WP2, T2.2.
- 2) Connect the NutriFarm model and default data to the DST (in collaboration with WP3 and WP5) on the webserver. This includes a translation of the NutriFarm results to user-friendly output that farmers or farm-advisers can understand and can implement in their strategic and operational farm management plan (using the results of the co-creation workshops described in M4)
- 3) The effect of nutrient mitigation measures will have an effect on certain model parameters. We need to define, which model parameters will be affected by the measures defined in the mitigation measures catalogue (WP1) (and measures that are included in the roadmap (WP2, task 2.3)), and to which extent these measures will affect the nutrient or C flow.
- 4) Run the three farm-level models for other long-term experiments in different climatic zones to make the complementary value of CHN and FarmSAFE have on Nutri-Farm broader applicable and simultaneously use these LTEs for model validation (WP2, task 2.4)
- 5) Calibrate the relative magnitudes of soil fluxes for all elements among the models. The fluxes include organic accumulation or depletion, as well as losses through leaching, runoff and gaseous emissions.

## Annexes

### Annex 1. Description of NutriFarm

#### 1 Introduction

As agreed in NutriBudget, the considered elements in the project, and thus also in the Nutri-Farm model, are Carbon (C), Nitrogen (N), Phosphorous (P), Sulphur (S), Calcium (Ca), Magnesium (Mg), Potassium (K), Copper (Cu), Cadmium (Cd) and Zinc (Zn). However, in order to predict fluxes of Ca, Mg, K, it is also important to include Sodium (Na), Chloride (Cl) and Bicarbonate ( $\text{HCO}_3$ ) as explained in the Section 2.4 on base cations. Below we describe the modelling approach, divided over (i) Carbon, (ii) Nitrogen, (iii) Phosphorous, (iv) Sulphur, (v) Calcium plus Magnesium plus Potassium and (vi) Copper plus Zinc (Section 2) and model application, including model schematization, initialization and data derivation (Section 3)

#### 2 Model calculations

##### 2.1 Overall approach

The Nutri-Farm model simulates C cycling, the soil and soil solution chemistry of all included 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 ( $\text{NH}_4$ ,  $\text{NO}_3$ ), P, S, Ca, Mg, K, Cu, Cd and Zn and pH. The cycling of C is included as described by RothC (Coleman and Jenkinson, 2014), for N as included in MITERRA Europe (Velthof et al., 2009) and for the other elements as described in INITIATOR (De Vries et al., 2023). Soil and soil solution chemistry of all nutrients is determined by element input of mineral and organic fertilizers, biosolids (compost, sludge) 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.

In more detail, the approaches can be summarized as follows:

- Carbon (Section 2.2): in mineral soils, the turnover of soil organic C (SOC) is calculated with the RothC 26.3 model (Coleman and Jenkinson, 2014). Carbon is already being part of MITERRA-Europe, where it is linked to soil N interactions. RothC distinguishes 4 active (decomposable plant material (DPM), resistant plant material (RPM), microbial biomass (BIO), humified organic matter (HUM)), and one inactive pool (inert organic matter (IOM)). This is linked to organic mineralisation of organic N via C-N ratios as done in INITIATOR (De Vries et al., 2023). In peat soils, the net loss of C pools (and related  $\text{CO}_2$  emissions) is included by an empirical relationship with groundwater (ditchwater) level.
- Nitrogen (Section 2.3): A steady state linear approach, as used in INTEGRATOR/MITERRA. 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 2.4): included by using a Langmuir equilibrium, supplemented

with rate limited diffusion, as given in INITIATOR (De Vries et al., 2023).

- Sulphur (Section 2.5): included by an extended Freundlich equation, where extended refers to the inclusion of pH impacts on adsorption constant (Gustafsson et al., 2015)
- K, Mg, Ca (Section 2.6): 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  $\text{NO}_3$ ,  $\text{SO}_4$ , Cl and  $\text{HCO}_3$ ) 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 (can be update by using exchange equations (as in VSD+).
- Cd, Cu and Zn (Section 2.7); Freundlich equation with adsorption constant that depends on clay, SOM and pH as included in INTEGRATOR (De Vries et al., 2022) and in INITIATOR (De Vries et al., 2023).

### Modeling of water fluxes

The model includes two layers, i.e. a top layer of 0-30 cm and a bottom layer of 30-100 cm to ensure that the root zone of all included crops is covered. The fraction of the transpiration and of the element uptake in each layer is based on the fine root distribution of the included crops. The runoff of elements to surface water is calculated as an aggregated value for the surface and the interflow of the two soil layers, while leaching to groundwater is calculated a depth of 100 cm, comparable to a water flux model used by Keuskamp et al. (2012) with results at a 1 km x 1km resolution at the European scale (see Fig. 1).

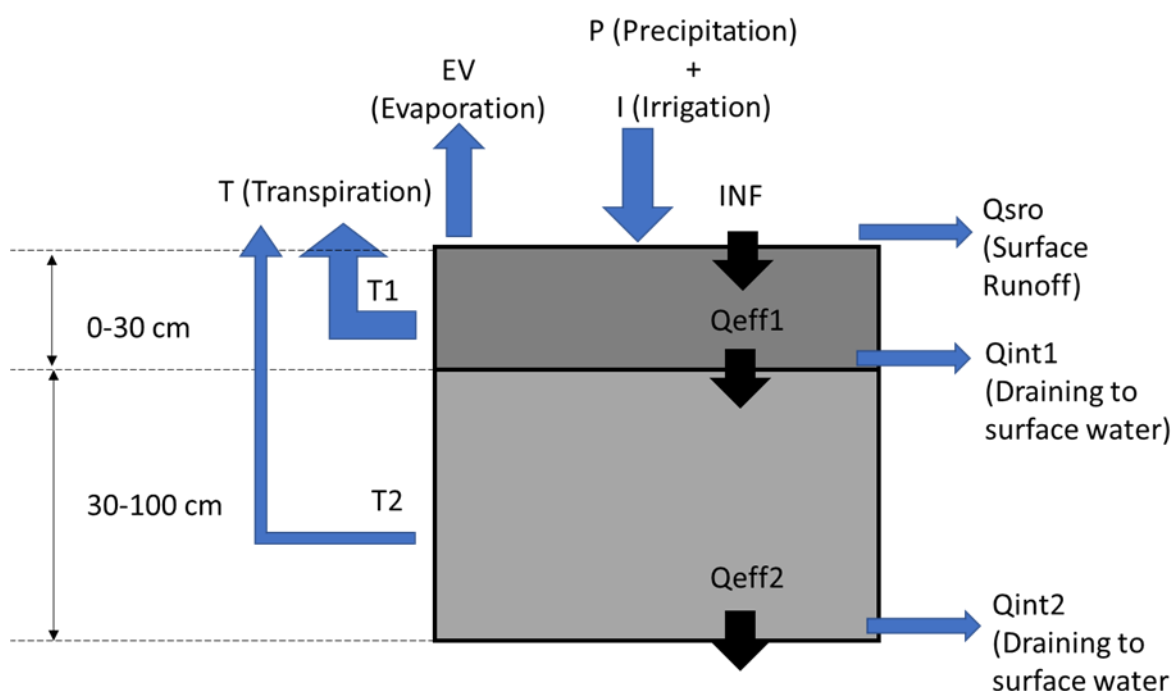


Figure 1. Scheme of the partitioning of the total runoff ( $Q_{tot}$ ), being equal to water input by precipitation and irrigation minus the evapotranspiration, divided over surface runoff ( $Q_{sro}$ ), and leaching recharging shallow groundwater ( $Q_{eff}$ ) in layer 1 (0-30 cm) and layer 2 (30-100 cm).

The water flow at soil surface (infiltration, INF), at 30 cm depth ( $Q_{eff1}$ ) and at 100 cm depth ( $Q_{eff2}$ ) are calculated as (see Figure 1):

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

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

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

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. Idea is to use data on total transpiration from the VIC model and to use data of Fan et al (2016) on the root distributions by 11 crops, assuming that this is directly related to the transpiration, to get the fraction transpiration in layer 1 and layer 2. As a first step we assume that the transpiration is 300 mm of which a fraction is taken up in layer 1 and the remaining fraction in layer 2 (e.g. 80% in layer 1, i.e. 240 mm and 20% in layer 2, i.e. 60 mm. This means that the water flux in layer 1 (runoff and leaching) is 60 mm higher less than in layer 2). Note that for some crops all transpiration occur in layer 1 and the water fluxes in layer 1 and 2 are the same.

### **Modeling of nutrient fluxes**

The concentration of nutrient X (N, P, S, K, Ca, Mg, Cu and Zn), and of Cd which is also included in view of its potential toxic impact, is calculated for the distinguished two layers, a topsoil of 0-30 cm and a subsoil of 30-100 cm in which crop uptake is partitioned equal to the fractions for transpiration. For each nutrient, the concentration in each layer is determined by a nutrient mass-balance equation, that describes the inputs and outputs and accumulation, divided by the water flux according to:

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

$$[X]_2 = (X_{le1} - X_{up2} - X_{acc2}) / (Q_{eff2} + Q_{int2}) \quad (5)$$

where is  $[X]$  is X concentration in the soil solution ( $g m^{-3}$  or  $mg.l^{-1}$ ),  $X_{in}$  is the total nutrient input to the field entering the topsoil,  $X_{up,1}$  and  $X_{up,2}$  is the crop nutrient uptake, and  $X_{acc,1}$  and  $X_{acc,2}$  is the nutrient accumulation from the topsoil (-30cm) and the subsoil (30-100 cm), respectively ( $kg ha^{-1} yr^{-1}$  for the major nutrients N,P, S, Ca, Mg, K and  $g ha^{-1} yr^{-1}$  for the minor nutrients Cu and Zn and for Cd) and where  $Q_{eff1}$  and  $Q_{eff2}$  are the water fluxes at 30 cm and 100 cm depth, respectively ( $m^3 ha^{-1} yr^{-1}$ ). For the micronutrients, of which the unit is  $g ha^{-1} yr^{-1}$  fluxes are multiplied by 1000 to convert kg to g.

Crop nutrient uptake is calculated by multiplying a given crop yield (Eurostat data) with literature derived nutrient contents in the harvested parts. Even though crop yields or plant nutrient concentrations may change with changes in soil nutrient concentrations, due to accumulation or releases, those impacts are not included in the modelling approach except for Cd and Zn concentrations in the plant, which are dependent on soil Cd and Zn concentrations.

Nutrient accumulation is calculated as

$$X_{acc1} = X_{in} - X_{up1} - X_{le1} - X_{ro1} \quad (6)$$

$$X_{acc2} = X_{le1} - X_{up2} - X_{le2} - X_{ro2} \quad (7)$$

Where  $X_{le1}$  and  $X_{le2}$  is the nutrient leaching from the topsoil and subsoil and  $X_{ro1}$  and  $X_{ro2}$  is the nutrient runoff (interflow) from the topsoil and subsoil, where all fluxes of nutrient X are given

in  $\text{g}\cdot\text{ha}^{-1}\cdot\text{yr}^{-1}$  but divided later by 1000 for N, P, S, K, Ca, Mg to present results in  $\text{kg}\cdot\text{ha}^{-1}\cdot\text{yr}^{-1}$ . The leaching ( $X_{le}$ ) and runoff ( $X_{ro}$ ) in each layer  $j$  (topsoil or subsoils), is calculated as:

$$X_{le} = Q_{eff}(j) * [X]_t(j) \quad (8)$$

$$X_{ro} = Q_{int}(j) * [X]_t(j) \quad (9)$$

Also here, a division by 1000 is needed to convert  $\text{g}\cdot\text{ha}^{-1}\cdot\text{yr}^{-1}$  to  $\text{kg}\cdot\text{ha}^{-1}\cdot\text{yr}^{-1}$ . 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 can also be negative (release) and includes both accumulation or release from: (i) an organic pool, linked to the SOC change derived by RothC (this pool change is neglected for metals) 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 content of nutrient  $X$  in a given layer (1 or 2) is calculated as:

$$X_{t+1} = X_t + \left(\frac{X_{acc,t}}{z\rho\gamma}\right) * \Delta t \quad (10)$$

where  $X_t$  and  $X_{t+1}$  are the sizes of the total  $X$  contents at time  $t$  and time  $t+1$ , respectively ( $\text{g}\cdot\text{kg}^{-1}$ ),  $X_{acc}$  is the accumulation of nutrient  $X$  in soil ( $\text{g}\cdot\text{ha}^{-1}\cdot\text{yr}^{-1}$ ),  $z$  is the thickness of the topsoil (m),  $\rho$  is the bulk density of the soil ( $\text{kg}\cdot\text{m}^{-3}$ ),  $\Delta t$  is the length of the time step ( $\text{yr}^{-1}$ ) and  $\gamma$  is a conversion factor ( $1/10.000$ ) for the conversion of  $\text{g}\cdot\text{ha}^{-1}\cdot\text{yr}^{-1}$  to  $\text{g}\cdot\text{m}^{-2}\cdot\text{yr}^{-1}$ . For major nutrients  $\text{g}\cdot\text{kg}^{-1}$  is a proper unit but for minor nutrients  $\text{mg}\cdot\text{kg}^{-1}$  is generally used. Then a multiplication by 1000 is needed.

Note that timesteps of a year are used for all nutrients is a year except P where a daily timestep is used, since rate-limited dissolution equations are included to simulate the fate of P properly (Eq. 18).

## 2.2 Modelling of carbon dynamics

For C dynamics NutriFarm focuses on the first layer. In brief, the turnover of C pools is simulated based on the RothC model (Coleman and Jenkinson, 2014) dividing the soil organic C into five C pools, including decomposable plant material (DPM), resistant plant material (RPM), microbial biomass (BIO), humified organic matter (HUM) and inert organic matter (IOM). Turnover of the first four pools follows first-order processes, modified by temperature, soil moisture and soil cover, as well as clay content in the case of BIO and HUM. The IOM pool does not decompose (see model description of Miterra-Europe in D2.3).

## 2.3 Modelling nitrogen 'dynamics'

With respect to N, the word dynamics is not really correct, since we do not include interactions due to adsorption or desorption of N (only relevant for  $\text{NH}_4$  in clay soil but we assume complete nitrification) but only accumulation or release from an organic pool, 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 2.

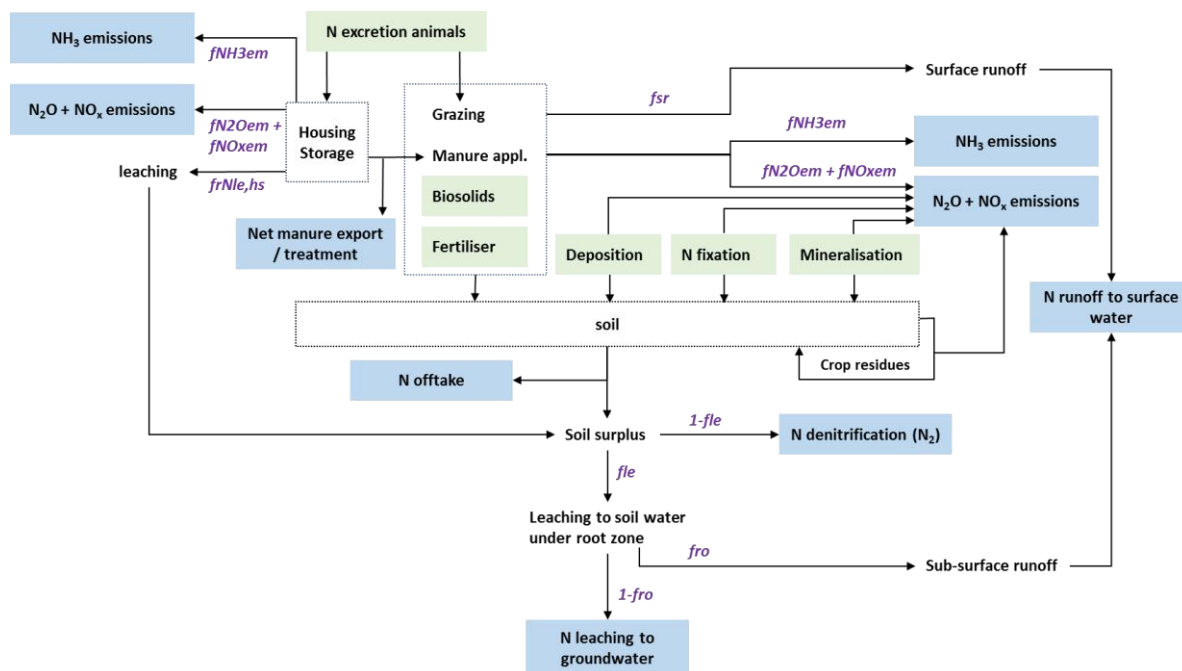


Figure 2 Schematic presentation of the calculated N flows in Nutri-Farm (according to the MITERRA-EUROPE model (Velthof et al., 2009) slightly adapted in INTEGRATOR in terms of calculations of the various fractions (De Vries et al., 2021, 2022)

The method to simulate N dynamics used in NutriFarm is same as Miterra-Europe (see D2.3), except for the calculation of the leaching and subsurface runoff in different soil layers. The NutriFarm model focuses on the soil N balance (losses due to emissions of  $\text{NH}_3$ ,  $\text{N}_2\text{O}$ ,  $\text{NO}_x$  and  $\text{N}_2$  and runoff of N in housing systems are precalculated as a fraction of the N excretion as shown in Figure 2) and  $\text{NO}_3\text{-N}$  concentrations in the soil are calculated according to:

$$[\text{NO}_3 - \text{N}]_1 = (N_{in} - N_{up1} - N_{acc1} - N_{em1}) / (Q_{eff1} + Q_{int1}) \quad (13)$$

$$[\text{NO}_3 - \text{N}]_2 = (N_{le1} - N_{up2} - N_{acc2} - N_{em2}) / (Q_{eff2} + Q_{int2}) \quad (14)$$

Where  $\text{NO}_3\text{-N}$  is the  $\text{NO}_3\text{-N}$  concentration,  $N_{acc}$  refers to accumulation or release in the organic N pool and  $N_{em}$  stands for the emission of  $\text{NH}_3$ ,  $\text{N}_2\text{O}$ ,  $\text{NO}_x$  and  $\text{N}_2$  (being equal to the C pool sequestration derived by Roth C times the N/C ratio in organic matter).

The emissions of  $\text{NH}_3$ ,  $\text{N}_2\text{O}$ ,  $\text{NO}_x$  are all calculated as a fraction of the N input (distinguishing between manure (type), fertilizer (type), biosolids, deposition and fixation) while the emission of  $\text{N}_2$ , is set equal to the denitrification flux, which is calculated as a fraction of the N surplus (see the model description of Miterra-Europe). The emissions of  $\text{NH}_3$ ,  $\text{N}_2\text{O}$  and  $\text{NO}_x$  and  $\text{N}_2$  are all assumed to occur in the first layer and put at zero for the second layer. The denitrification flux ( $\text{N}_2$  emission), assuming to occur in the first layer is calculated as a fraction of the N input minus the total N uptake and total N accumulation in the first and second layer, minus the emission of  $\text{NH}_3$ ,  $\text{N}_2\text{O}$  and  $\text{NO}_x$ , which is all assumed to occur in the first layer, according to:

$$[\text{NO}_3 - \text{N}]_1 = (N_{in} - N_{up1} - N_{acc1} - (\text{NH}_3 + \text{N}_2\text{O} + \text{NO}_x)_{em1} - frNde (N_{in} - N_{up1} - N_{acc1} - N_{acc2}) / (Q_{eff1} + Q_{int1}) \quad (15)$$

$$[\text{NO}_3 - \text{N}]_2 = (N_{le1} - N_{up2} - N_{acc2}) / (Q_{eff2} + Q_{int2}) \quad (16)$$

The fractions used, both in housing systems in the pre-calculation, and in soils, to calculate N losses to air and water depend on site properties as given in Table 1. The various fractions are all given in the model description of Miterra-Europe.

**Table 1** N loss fractions to air ( $NH_3$ ,  $N_2O$ ,  $NO_x$  and  $N_2$  emissions) and water (N leaching and runoff) with the default approach used to calculate them as a function of N inputs.

Model inputs	Assessment
NH <sub>3</sub> emission fractions	<p><u>Grazing</u>: average emission fraction</p> <p><u>Housing and manure storage systems</u>: Country-specific N emission fractions distinguished per animal type and manure type (solid and liquid) for different housing systems and manure storage</p> <p><u>Soils</u>: For solid manure applied to the field or deposited during grazing, NH<sub>3</sub>-N volatilization is calculated as a fraction of the total ammonium N (TAN) applied. For liquid slurry, NH<sub>3</sub>-N emissions are estimated using the ALFAM2 model, which adopts a more dynamic approach taking into account slurry composition, climate, and application method. For fertilizer, NH<sub>3</sub>-N emission factor depends on the type of the fertiliser, and the soil pH.</p>
N <sub>2</sub> O emission fractions	<p><u>Housing and manure storage systems</u>: country specific fractions based on GAINS model data</p> <p><u>Soils</u>: the emission factor depends on climate zones and N sources following the 2019 IPCC Guidelines.</p>
NO <sub>x</sub> emission fractions	<p><u>Grazing</u>: average emission fraction at country level based on GAINS model</p> <p><u>Housing and manure storage systems</u>: 0.3% of N excretion.</p> <p><u>Soils</u>: Emission factor for NO<sub>x</sub> is linked to annual precipitation amount.</p>
N <sub>2</sub> emission fractions	<p><u>Housing and manure storage</u>: 9 x NO<sub>x</sub> emission, i.e. 2.7% of N excretion (Oenema et al., 2000).</p> <p><u>Soils</u>: set equal to denitrification rates, being equal to N surplus-N leaching.</p>
N leaching fractions	<p><u>Housing and manure storage systems</u>: fraction of N excreted in these systems that depends on the type of manure system and the type of floor (Velthof et al., 2009).</p> <p><u>Soils</u>: 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).</p>
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, as described in De Vries et al. (2021, 2022)

## 2.4 Modelling 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 in NutriFarm 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 change in the labile P pool is due to adsorption (denoted as ads) or desorption (denoted as des) depending on where the pools increase (adsorption) or decreases. The change in the stable pool is due to diffusion and dissolution-precipitation.

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, L, is at the start assumed equal 1/3 of  $P_{ox}$ , with the stable pool, S, thus being equal to 2/3 of  $P_{ox}$ . The maximum pool of  $P_{ox}$  is assumed to equal  $0.5 \cdot (Al + Fe)_{ox}$  with  $(Al + Fe)_{ox}$  being the oxalate extractable Al and Fe contents ( $mmol \cdot kg^{-1}$ ). The maximum labile pool  $L_m$  is in principle thus 1/6 (or 0.167) and the maximum stable pool  $S_m$  is thus 1/3 (or 0.333)  $\cdot (Al + Fe)_{ox}$ . The change in the reactive P pool, being equal to the change in total inorganic P (since the inert P pool is assumed to stay constant) is calculated by a mass balance equation:

$$P_{ox,t+1} = P_{ox,t} + P_{acc,t} \cdot \Delta t \quad (17)$$

where  $P_{ox,t}$  and  $P_{ox,t+1}$  are the size of the reactive P pool at time t ( $mmol \cdot kg^{-1}$ ) and time t+1 respectively,  $P_{acc}$  is the P accumulation in soil ( $mmol \cdot kg^{-1} \cdot d^{-1}$ ) and  $\Delta t$  is the length of the time step ( $d^{-1}$ ).

The P accumulation in the topsoil is calculated as the P input minus P uptake minus the change in the organic P pool (being equal to the C pool sequestration derived by Roth C times the P/C ratio in organic matter):

$$P_{acc,t} = \frac{(P_{in,t} - P_{up,t} - \Delta P_{org,t}) \gamma_1}{z \rho M} - \frac{P_{loss,t} \gamma_2}{z \rho M} \quad (18)$$

in which  $P_{acc}$  is the P accumulation in the topsoil per unit soil mass ( $mmol \cdot P \cdot kg^{-1} \cdot d^{-1}$ ),  $P_{in}$  is the input of P ( $kg \cdot ha^{-1} \cdot yr^{-1}$ ),  $P_{up}$  is the uptake of P ( $kg \cdot ha^{-1} \cdot yr^{-1}$ ),  $P_{loss}$  is the loss of P by leaching and runoff ( $kg \cdot ha^{-1} \cdot d^{-1}$ ),  $\Delta P_{org}$  is the change in the pool of organic P ( $kg \cdot ha^{-1} \cdot yr^{-1}$ ) being calculated by the change in C pool derived by Roth C for mineral soils or the C mineralization of peat soils as given in Eq. (12) times the P/C ratio in organic matter, z is the thickness of the topsoil (m),  $\rho$  is the bulk density of the soil ( $kg \cdot m^{-3}$ ), M the molar weight of P (31  $mg \cdot mmol^{-1}$ ) and  $\gamma_1$  is a conversion factor (100/365) from  $kg \cdot ha^{-1} \cdot yr^{-1}$  to  $mg \cdot m^{-2} \cdot d^{-1}$ ,  $\gamma_2$  is a conversion factor (100) from  $kg \cdot ha^{-1} \cdot d^{-1}$  to  $mg \cdot m^{-2} \cdot d^{-1}$ . P input equals the P input by fertilizer, manure, biosolids and deposition in the top layer (0-30cm depth) and the leaching from that layer in the second layer (30-100 cm depth). P uptake equals the crop P removal times a fraction root uptake in each of the two layers, with the sum of both fractions being equal to 1. Note that we only include a daily time step for P to properly include rate limited processes (see below) 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 to get daily values and results are presented again at an annual time step.

The loss of P by leaching and runoff ( $P_{loss}$  in  $kg \cdot ha^{-1} \cdot day^{-1}$ ) is calculated according to Eq. (8) and (9) where [P] refers to the total (inorganic and organic) P, in each layer j (topsoil or

subsoils). To calculate the leaching of inorganic P, assumptions have to be made with respect to the relationship between inorganic P and total P in the soil solution. In NutriFarm, we use an exponential relationship between total P and inorganic P based on measurements in soil solution, drainage water and surface water, by Chardon et al. (2007):

$$cP_t = 1.1 * cP_i + 0.1 * e^{-cP_i} \quad (19)$$

where  $cP_i$  is inorganic (ortho-) P concentration and  $cP_t$  is the total (inorganic and organic P concentration (both in  $\text{mg.l}^{-1}$  equal to  $\text{g.m}^{-3}$ ).

The concentration of inorganic P in soil solution,  $cP_i$ , is calculated from the size of the labile P pool ( $L$ ) according to a Langmuir equation:

$$L = \frac{K_L * cP_i / 1000 * L_m}{K_L * cP_i / 1000 + 1} \quad \text{or} \quad cP_i = \frac{L}{K_L (L_m - L)} * 1000 \quad (20)$$

where  $L$  is the amount of adsorbed (labile) P ( $\text{mmol.kg}^{-1}$ ),  $L_m$  is the adsorption maximum ( $\text{mmol.kg}^{-1}$ ),  $K_L$  is a Langmuir adsorption constant ( $\text{m}^3.\text{kg}^{-1}$ ).  $L_m$  is calculated as a fraction  $\beta$  (-) times the oxalate extractable Al and Fe contents  $(\text{Al} + \text{Fe})_{\text{ox}}$  ( $\text{mmol.kg}^{-1}$ ) where  $\beta$  is set at 0.167. The value of 1000 in both formulas is used to express  $cP_i$  from  $\text{mg P/l}$  to  $\text{kg P/m}^3$ . The Langmuir adsorption constant ( $K_L$  in ( $\text{m}^3.\text{kg}^{-1}$ ) is set at 500 for peat, 1000 for sand (texture class 1), 1500 for loam (texture class 2) and 2000 for clay (texture class 3) after Van der Salm et al (2016).

Eq. (20) implies that the inorganic P in soil solution,  $cP_i$ , can become infinitely high when  $L$  approaches  $L_m$ . We used a maximum value  $cP_i$ , of 90  $\text{mgP/l}$  (after Schoumans, 2013). Following Eq. (20), this results in  $L_{\text{max}} = \frac{K_L * 90 / 1000 * L_m}{K_L * 90 / 1000 + 1}$ . We also used a minimum value  $cP_i$ , of 0.001  $\text{mgP/l}$ . Following Eq. (20), this results in  $L_{\text{min}} = \frac{K_L * 0.001 / 1000 * L_m}{K_L * 0.001 / 1000 + 1}$ . Note that  $0.5 * (\text{Al} + \text{Fe})_{\text{ox}}$  is  $L_{\text{max}} + S_{\text{max}}$  (see text above Eq. (17)) implying  $S_{\text{max}} = (0.5 * (\text{Al} + \text{Fe})_{\text{ox}} - L_{\text{max}})$ . Once the sum of labile and stable P pool reaches its maximal value (at a given time step  $t+1$ ), this pool will not increase despite the ongoing P surplus, being equal to  $P_{\text{in},t} - P_{\text{up},t} - \Delta P_{\text{org},t} - P_{\text{loss},t}$  implying an imbalanced P cycle. In this case, we assume that P is precipitated in “precipitation P pool” ( $I_p$ ), which is calculated as described in the equations below. Note that the amount that is precipitated, which happens when the labile P pool equals the maximal pool size, is generally only part of the P surplus near that point. Inversely, the amount mined from the “precipitation P pool” can be less than the negative P surplus. Therefore, we “corrected” the P pool changes driven by a given P surplus, by the P pool size at that time step and the maximal pool size. The change in the labile P pool of the topsoil is calculated by a mass balance:

$$L_{t+1} = \begin{cases} L_t + P_{\text{disL,corrected},t} * \Delta t & \text{when } L_t + P_{\text{disL,corrected},t} * \Delta t < L_{\text{max}} \text{ and } L_t + P_{\text{disL,corrected},t} * \Delta t \geq L_{\text{min}} \\ L_{\text{max}} & \text{when } L_t + P_{\text{disL,corrected},t} * \Delta t \geq L_{\text{max}} \\ L_{\text{min}} & \text{when } L_t + P_{\text{disL,corrected},t} * \Delta t \leq L_{\text{min}} \end{cases} \quad (21)$$

where  $L_t$  and  $L_{t+1}$  are the size of the labile P pool at time  $t$  ( $\text{mmol.kg}^{-1}$ ) and time  $t+1$ , respectively, and  $\Delta t$  is the length of the time step ( $\text{d}^{-1}$ ).  $P_{\text{disL,corrected},t}$  is the P transfer between P in the soil solution ( $C_{\text{pi}}$ ) and the labile pool ( $L$ ), corrected for the changes in the precipitation P pool ( $I_p$ ).

The theoretical P transfer between P in the soil solution ( $C_{\text{pi}}$ ) and the labile pool ( $L$ ),  $P_{\text{disL},t}$  is defined as:

$$P_{disL,t} = P_{in,t} - P_{up,t} - \Delta P_{org,t} - P_{disS,corrected,t} - P_{loss,t} \quad (22)$$

Where,  $P_{disS,corrected}$  is the corrected P flux from the soil solution to the stable pool of adsorbed P ( $\text{mmol.kg}^{-1}.\text{d}^{-1}$ ) and  $P_{loss,t}$  is the loss of P by leaching and runoff ( $\text{mmol.kg}^{-1}.\text{d}^{-1}$ ).

The corrected P transfer between P in the soil solution ( $C_{pi}$ ) and the labile pool (L) ( $P_{disL,corrected,t}$ ) is calculated as:

$$P_{disL,corrected,t} = \begin{cases} P_{disL,t} & \text{when } P_{disL,t} \geq 0 \\ P_{disL,t} + I_{p,t} + I_{p,change,S,t} & \text{when } P_{disL,t} < 0 \text{ and } I_{p,t} + I_{p,change,S,t} < \text{abs}(P_{disL,t}) \\ P_{disL,t} & \text{when } P_{disL,t} < 0 \text{ and } I_{p,t} + I_{p,change,S,t} \geq \text{abs}(P_{disL,t}) \end{cases} \quad (23)$$

Where  $I_{p,t}$  is the size of the precipitation P pool at timestep t and  $I_{p,change,S,t}$  is the change in the precipitation pool due to changes in the stable pool (S).

The change in the precipitation pool from the labile P pool ( $I_{p,change,L}$ ) is calculated as:

$$I_{p,change,L,t} = \begin{cases} 0 & \text{when } P_{disL,t} \geq 0 \text{ and } L_t + P_{disL,t} * \Delta t < L_{max} \text{ and } L_t + P_{disL,t} * \Delta t > L_{min} \\ L_t + P_{disL,t} - L_{max} & \text{when } P_{disL,t} \geq 0 \text{ and } L_t + P_{disL,t} * \Delta t > L_{max} \\ -(I_{p,t} + I_{p,change,S,t}) & \text{when } P_{disL,t} \geq 0 \text{ and } L_t + P_{disL,t} * \Delta t < L_{min} \text{ and } \text{abs}((L_t + P_{disL,t} * \Delta t) - L_{min}) > \\ I_{p,t} + I_{p,change,S,t} - L_{min} & \text{when } P_{disL,t} \geq 0 \text{ and } L_t + P_{disL,t} * \Delta t < L_{min} \text{ and } \text{abs}((L_t + P_{disL,t} * \Delta t) - L_{min}) > \\ -(I_{p,t} + I_{p,change,S,t}) & \text{when } P_{disL,t} < 0 \text{ and } I_{p,t} + I_{p,change,S,t} < \text{abs}(P_{disL,t} * \Delta t) \\ P_{disL,t} & \text{when } P_{disL,t} < 0 \text{ and } I_{p,t} + I_{p,change,S,t} > \text{abs}(P_{disL,t} * \Delta t) \end{cases} \quad (24)$$

Where  $P_{disL}$  is the theoretical P transfer between P in the soil solution ( $C_{pi}$ ) and the labile pool (L).  $I_{p,t}$  is the size of the precipitation P pool at the timestep t.  $I_{p,change,S,t}$  is the changes in the precipitation pool due to changes in the stable pool (S).

The final precipitation pool size after accounting for changes in both stable and labile P pools is calculated as:

$$I_{p,t+1} = I_{p,t} + I_{p,change,S,t} + I_{p,change,L,t} \quad (25)$$

The change in the stable P pool of the topsoil, S, is calculated as (see footnote in Table 2 for the maximum of S,  $S_{max}$ , related to maximum inorganic P concentration of 90 mg P l<sup>-1</sup> as described in the text below Eq.(20)):

$$S_{t+1} = \begin{cases} S_t + P_{disS,corrected,t} * \Delta t & \text{when } S_t + P_{disS,corrected,t} * \Delta t < S_{max} \\ S_{max} & \text{when } S_t + P_{disS,corrected,t} * \Delta t \geq S_{max} \end{cases} \quad (26)$$

Where  $P_{disS,corrected,t}$  is the corrected P transfer between P in the soil solution ( $C_{pi}$ ) and the stable pool (S). The theoretical P transfer between P in the soil solution ( $C_{pi}$ ) and the stable pool (S),  $P_{disS}$ , is described by a rate-limited Freundlich equation, according to:

$$P_{disS,t} = \begin{cases} \mu_{DisS} * (KF * c_{pi}^n - S) & \text{when } KF * c_{pi}^n \geq S \\ \mu_{SDis} * (KF * c_{pi}^n - S) & \text{when } KF * c_{pi}^n < S \end{cases} \quad (27)$$

where  $\mu_{DisS}$  is the rate constant (d<sup>-1</sup>) for the transfer from soil solution to a stable pool S (mmol kg<sup>-1</sup>),  $\mu_{SDis}$  is the rate constant (d<sup>-1</sup>) for the transfer from a stable pool to soil solution,  $K_F$  is a Freundlich constant of the stable pool (mmol. kg(soil)<sup>-1</sup> (mg.l (water)<sup>-1</sup>)<sup>-n</sup>), n is the exponent of stable pool (-), and  $C_{pi}$  the dissolved P concentration (mg l<sup>-1</sup>). The generic values used in Eq. (27) are given in Table 2.

**Table 2** Generic parameter values for the rate-limited Freundlich equation used in NutriFarm (based on Van der Salm et al., 2016).

$K_{F,i}$ (mmol kg <sup>-1</sup> (mg l <sup>-1</sup> ) <sup>1-n</sup> )	$N_i$ (-)	$\mu_{DisS,i}$ (d <sup>-1</sup> )	$\mu_{SDis,i}$ *(d <sup>-1</sup> )
$(0.5 * (Al+Fe)ox - L_{max}) / 90^{n-1}$	0.26	0.0014	2 10 <sup>-6</sup> for sand and 44 10 <sup>-6</sup> for clay and peat

<sup>1</sup> Note that  $0.5 * (Al+Fe)ox$  is  $L_{max}+S_{max}$  (see text above Eq. (17)) implying  $(0.5 * (Al+Fe)ox - L_{max}) = S_{max}$

This formula is linked to a maximum inorganic P concentration of 90 mg P l<sup>-1</sup>.

The corrected change in the stable P pool ( $P_{disS,corrected,t}$ ) is calculated as:

$$P_{disS,corrected,t} = \begin{cases} P_{disS,t} * \Delta t & \text{when } P_{disS,t} \geq 0 \\ P_{disS,t} * \Delta t + I_{p,t} & \text{when } P_{disS,t} < 0 \text{ and } I_{p,t} < abs(P_{disS,t} * \Delta t) \\ 0 & \text{when } P_{disS,t} < 0 \text{ and } I_{p,t} \geq abs(P_{disS,t} * \Delta t) \end{cases} \quad (28)$$

Where  $P_{disS,t}$  is theoretical P transfer between P in the soil solution ( $C_{pi}$ ) and the stable pool (S).  $I_{p,t}$  is the size of the precipitation pool at timestep t (beginning of the timestep).

The change in the precipitation pool due to changes in the stable P pool is calculated as:

$$I_{p,change,S,t} = \begin{cases} 0 & \text{when } P_{disS,t} \geq 0 \text{ and } S_t + P_{disS,t} * \Delta t < S_{max} \\ S_t + P_{disS,t} * \Delta t - S_{max} & \text{when } P_{disS,t} \geq 0 \text{ and } S_t + P_{disS,t} * \Delta t > S_{max} \\ -I_{p,t} & \text{when } P_{disS,t} < 0 \text{ and } I_{p,t} < abs(P_{disS,t} * \Delta t) \\ P_{disS,t} * \Delta t & \text{when } P_{disS,t} < 0 \text{ and } I_{p,t} \geq abs(P_{disS,t} * \Delta t) \end{cases} \quad (29)$$

Where  $P_{disS,t}$  is the theoretical P transfer between P in the soil solution ( $C_{pi}$ ) and the stable pool (S).  $I_{p,t}$  is the size of the precipitation pool at timestep t (beginning of the timestep).

## 2.5 Modelling sulphur dynamics

S with P, the  $SO_4$  concentration in the topsoil and subsoil determined by input, uptake and accumulation using a mass-balance equation that describes the inputs and outputs and accumulation in each layer. The change in adsorbed  $SO_4$  pools is described by a mass-balance equation:

$$SO4_{ad,t+1} = SO4_{ad,t} + SO4_{acc,t} * \Delta t \quad (30)$$

where  $SO4_{ad,t}$  and  $SO4_{ad,t+1}$  are the size of the adsorbed S pool at time t ( $\text{mol kg}^{-1}$ ) and time t+1 respectively,  $SO4_{acc}$  is the  $SO_4$  accumulation in soil ( $\text{mol kg}^{-1} \text{ yr}^{-1}$ ), which is assumed to be only adsorbed  $SO_4$  and  $\Delta t$  is the length of the time step ( $\text{yr}^{-1}$ ).

As with P, the  $SO_4$  accumulation is calculated as the S input minus S uptake minus S losses through leaching and runoff minus the change in the organic S pool (being equal to the C pool sequestration derived by Roth C times the S/C ratio in organic matter):

$$SO4_{acc,t} = \frac{SO4_{in,t} - SO4_{up,t} - SO4_{loss,t} - \Delta SO4_{org,t}}{z\rho M} \quad (31)$$

in which the various  $SO_4$  flux terms ( $\text{g} \cdot \text{ha}^{-1} \cdot \text{yr}^{-1}$ ) are comparable to those given above for P. However, unlike P, the calculations occur at an annual level. The S losses through leaching and runoff are calculated using equation 8 and 9, with  $SO_4$  concentration calculated in Eq. (33).

$SO_4$  accumulation or release is limited to an adsorption-desorption isotherm that governs the flux of  $SO_4$  between dissolved and sorbed phases. Unlike P, no distinction is made in stable and labile pools, thus not including a rate limited flux from a stable to a labile pool.  $SO_4$  adsorption-desorption is included by using an extended Freundlich equation, where extended refers to the inclusion of pH impacts on adsorption constant, according to (Martinson et al., 2003; Gustafsson et al. (2015):

$$SO4_{ad} = K_F ([SO_4] [H]^n)^m \quad (32)$$

where  $SO4_{ad}$  is the amount of adsorbed  $SO_4$  ( $\text{mol kg}^{-1}$ ),  $[SO_4]$  is the total dissolved concentration of  $SO_4$  ( $\text{mol l}^{-1}$ ),  $[H]$  is the total dissolved proton ( $\text{mol l}^{-1}$ ),  $K_F$  is the Freundlich  $SO_4$  adsorption coefficient, whereas m and n are parameters. After taking the logarithm of both sides, and substituting  $\log\{H^+\}$  for pH-MgCl<sub>2</sub> (assume as pH-CaCl<sub>2</sub> here:  $\text{pH-CaCl}_2 = \text{pH-KCl} * 0.9288 + 0.5262$ ), we obtain:

$$\text{Log}(SO4_{ad}) = \text{Log } K_F + m * (\text{Log}[SO_4] - n * \text{pH}) \quad (33)$$

$$\text{Or } \text{Log}[\text{SO}_4] = (\text{Log}(\text{SO}_{4\text{ad}}) - \text{Log } K_F)/m + n \cdot \text{pH}$$

Based on results given by Gustafsson et al. (2015),  $n$  can be set at 1.7, thus only requiring the derivation of  $K_F$  and  $m$ . Based on model calibration on 5 sites in Sweden, the value of  $K_F$  varied from ca 0.05-5.0 and  $m$  from ca 0.10-0.25.

The initial  $\text{SO}_4$  concentration is calculated by assuming equilibrium with the historic S input and S uptake in soils in the past (e.g. 2020) according to:

$$[\text{SO}_4]_{0,1} = (\text{SO}_{4\text{in},0,1} - \text{SO}_{4\text{up},0,1}) / (Q_{\text{eff}1} + Q_{\text{int}1}) \quad (34)$$

$$[\text{SO}_4]_{0,2} = (\text{SO}_{4\text{le},0,1} - \text{SO}_{4\text{up},0,2}) / (Q_{\text{eff}2} + Q_{\text{int}2}) \quad (35)$$

Where  $[\text{SO}_4]_0$  is the initial concentration of  $\text{SO}_4$  in soil solution ( $\text{mol l}^{-1}$  or  $\text{kmol m}^{-3}$ ),  $\text{SO}_{4,\text{in},0,1}$  is the S input in 2020 by fertilizer, manure and atmospheric deposition and  $\text{SO}_{4\text{up},0,1}$  is the S uptake in 2020 ( $\text{kg ha}^{-1} \text{yr}^{-1}$ ) and water fluxes are in  $\text{m}^3 \text{ha}^{-1} \text{yr}^{-1}$ . To convert units from kg to kmol, the input and uptake fluxes concentrations have to be divided by 32 (molar weight of S) as this leads to a concentration of  $\text{kmol m}^{-3}$  or  $\text{mol l}^{-1}$ . The calculated  $[\text{SO}_4]_0$  is used to calculate the initial  $\text{SO}_{4\text{ad},0}$  in Eq. (33), which is then used in Eq. (30) to determine the  $\text{SO}_{4\text{ad}}$  for the next timestep, based on the  $\text{SO}_4$  accumulation in Eq. (31) in which the  $\text{SO}_4$  loss is based on the initial  $\text{SO}_4$  concentration. The  $\text{SO}_{4\text{ad}}$  for the next timestep is then used in Eq. (33) to quantify the  $\text{SO}_4$  concentration in the next timestep.

## 2.6 Modelling base cation (K, Mg, Ca) dynamics

Soil acidification due to the release of base cations (BC is sum of Ca, Mg, K and Na) occurs when the sum of leaching and uptake exceeds the external input by fertilizer, manure and deposition. This is generally the case since the loss of nitrate from the soil is accompanied by base cations. The BC release is similar to a negative accumulation which is calculated as:

$$\text{BC}_{\text{acc}} = \sum(\text{Ca} + \text{Mg} + \text{K} + \text{Na})_{\text{in}} - \sum(\text{Ca} + \text{Mg} + \text{K} + \text{Na})_{\text{up}} - \sum(\text{Ca} + \text{Mg} + \text{K} + \text{Na})_{\text{loss}} \quad (36)$$

Where  $\text{in}$  is total external input by fertilizer, manure and deposition (base cation weathering is not part of it),  $\text{up}$  is uptake and  $\text{loss}$  is leaching plus runoff in a given layer and where all fluxes are given in  $\text{mol}_c \text{ha}^{-1} \text{yr}^{-1}$ . To come from  $\text{mol}_c \text{ha}^{-1} \text{yr}^{-1}$  to  $\text{kg ha}^{-1} \text{yr}^{-1}$ , results are converted by multiplying with the equivalent weights, being 20 for Ca (40/2), 12 for Mg (24/2), 39 for K and 23 for Na, and then divide by 1000.

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 in a given layer (see above) 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, where cations stands for the sum of Ca, Mg, K, Na (assuming that concentrations of other cations such as ammonium (full nitrification), aluminium or iron are negligible) and anions stands for the sum of  $\text{SO}_4$ ,  $\text{NO}_3$ , Cl and  $\text{HCO}_3$  (assuming that concentrations of other anions, such as phosphate and organic anions are negligible):

$$\sum(\text{Ca} + \text{Mg} + \text{K} + \text{Na}) = \sum(\text{SO}_4 + \text{NO}_3 + \text{Cl} + \text{HCO}_3) \quad (37)$$

The calculation of  $\text{NO}_3$  and  $\text{SO}_4$  concentrations is given above. The Cl concentration is derived by dividing the Cl leaching with the water flux in a given layer (see above) with Cl leaching being calculated by assuming no interaction with the soil (tracer behaviour), implying that the output is equal to the input minus crop removal in the two layers (see Eq. (6) and (7) with accumulation being set at 0. The  $\text{HCO}_3$  concentration  $[\text{HCO}_3]$  in non-calcareous soils and is calculated by assuming equilibrium with the  $\text{CO}_2$  pressure in the soil and soil pH, according to (De Vries and Breeuwsma, 1986):

$$[\text{HCO}_3] = \frac{p\text{CO}_2 \cdot 10^{-7.8}}{[\text{H}]} \quad (38)$$

Where  $[\text{HCO}_3]$  is  $\text{HCO}_3$  concentration ( $\text{mol}_c \cdot \text{l}^{-1}$ ),  $[\text{H}]$  is H concentration ( $\text{mol}_c \cdot \text{l}^{-1}$ ) derived as  $10^{-\text{pH,ss}}$  and  $p\text{CO}_2$  is soil  $\text{CO}_2$  pressure (bar), which is set equal to 0.02 bar (20 mbar). A unit conversion of (61/ 1000) is used to convert from mol/l to mg/l.

In non-calcareous soils, the change in exchangeable base cation pool (meg/kg), being equal to the CEC (meq/kg) multiplied with the base saturation (being the fraction of base cations on the exchange complex) is calculated as

$$\Delta \text{BC}_{\text{exchangeable}} = \text{BC}_{\text{acc}} + \text{BC}_{\text{weathering}} \quad (39)$$

The rationale behind Eq. (39) is that soil acidification due to BC release (negative accumulation) is buffered by weathering and the release of base cations from the exchange complex. The information on BC weathering can be derived by the Profile model when total concentrations of base cations are known (Sverdrup and Warfvinge, 1988). When this is not the case, a first approximation of weathering rates (classes) can be determined by a combination of soil texture class (determined by clay and sand content) and parent material with parent material being classified into acidic, intermediate, basic or organic based on soil type, as given in Table 3 (De Vries et al., 1994a; UNECE Mapping Manual 2004).

The weathering rates thus assigned can be corrected for the effect of temperature according to (Sverdrup, 1990, De Vries et al., 1994a):

$$\text{BC}_{\text{we}}(T) = \text{BC}_{\text{we}}(T_o) \cdot e^{(A/T_o - A/T)} \quad (40)$$

where  $\text{BC}_{\text{we}}(T)$  is the weathering rate at the local mean annual temperature  $T$  (K),  $\text{BC}_{\text{we}}(T_o)$  is the average weathering rate defined in Table 3 for each combination of soil type and texture class at a reference temperature  $T_o$  (K) and  $A$  is a pre-exponential temperature factor (K). For  $A$  a value of 3600 K has been taken (Sverdrup, 1990). Reference temperatures (in  $^\circ\text{C}$ ) in the weathering rate classes were set at 4.3, 2.6, 6.5, 8.3, 8.5 and 8.8 for the classes 1, 1/2, 1/3, 2, 2/3 and 3 respectively (De Vries et al. 1994a).

**Table 3** Relationships between base cation weathering rates and various combinations of parent material class and texture class (indicated by 1, 1/2 etc.). Texture classes have been defined as: 1 (coarse): clay content less than 18%, 2 (medium): clay content between 18 and 35% and 3 (fine): clay content above 35% When two texture classes occur within one mapping unit, this is indicated as 1/2, 2/3 or 1/3.

Parent material class	Weathering rate ( $\text{mol}_c \text{ ha}^{-1} \text{ yr}^{-1} \text{ m}^{-1}$ )					
	1	1/2	1/3	2	2/3	3
Acidic <sup>1)</sup>	250	750		1250	1750	
Intermediate <sup>2)</sup>	750	1250	1750	1750	2250	2750

Basic <sup>3)</sup>	750	1250	2250	2750
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<sup>1)</sup> Acidic: Sand (stone), gravel, granite, quartzite, gneiss (schist, shale, greywacke, glacial till). Schist, shale, greywacke and glacial till are put in brackets since soil types containing these parent materials can be converted to acidic or intermediate parent material class, depending on the other parent materials available.

<sup>2)</sup> Intermediate : Granodiorite, loess, fluvial and marine sediment (schist, shale, greywacke, glacial till)

<sup>3)</sup> Basic : Gabbro, basalt, dolomite, volcanic deposits.

Low temperatures were associated with low weathering rate classes, which mainly occur in northern Europe. The temperature correction procedure given above implies that the weathering rates given in Table 3 are average values which decrease and increase with a lower and higher temperature respectively.

The change in base saturation ( $\Delta BS$ ) is derived as

$$\Delta BS = \Delta BC_{\text{exchangeable}} / (\text{CEC} \times \rho \times T \times 10) \quad (41)$$

Where CEC is cation exchange capacity ( $\text{mmol}_c \cdot \text{kg}^{-1}$ ),  $\rho$  is bulk density of the soil ( $\text{kg} \cdot \text{m}^{-3}$ ) and T is soil thickness (m), for two soil layers and 10 is the conversion factor from  $\text{mmol}_c \cdot \text{m}^{-2} \cdot \text{yr}^{-1}$  to  $\text{mol}_c \cdot \text{ha}^{-1} \cdot \text{yr}^{-1}$ . The change in pH is derived by a simple literature-based pH-Base saturation relationship. The relationship between pH and base saturation can be modelled with exchange equations, such as Gaines-Thomas and Gapon equations with constants for the exchange between protons ( $\text{H}^+$  concentration) and base cations (Ca, Mg, K and Na) as given in de Vries and Posch (2003). However, a simpler approach is to use relationship between pH and base saturation obtained from both model results and measurements on this relationship. We used this approach, based on Xu et al (2020), who gave relationships derived from observations and model results in fertilization and liming experiments at Rothamsted experimental station at a permanent grassland (Park grass) and crop land (Sawyers field). Results all show a linear relationship between pH and base saturation in a pH range between ca 4-7 according to  $\text{pH} = a_0 + a_1 \text{BS}$  with values of  $a_1$  and  $a_2$  given in Table 4, where BS is base saturation in %.

Based on those results we assumed a linear relationship between pH in soil solution from 4.0 to 7.0 with a base saturation varying from 0-100%, according to:

$$\text{pH}_{\text{ss}} = 4.0 + 0.03 \text{BS} \quad (42)$$

where  $\text{pH}_{\text{ss}}$  is the pH in soil solution, which is approximated from pH-KCl according to:  $\text{pH}_{\text{ss}} = \text{pH-KCl} \cdot 0.82 + 1.79$  (De Vries et al., 2008). This result is reasonably in line with the shape presented by Clark and Hill (1964), Bowman and Lannan (1995) and Ranney et al. (1974), who also suggest a slightly non-linear pH-base saturation relationship, with pH mainly changing from 4.5-6.5 in a base saturation range from 10-90% and with results presented by Beery and Wilding (1971), who show linear relationships between 4 and 7 with BS ranging from about 10-90%.

**Table 4** Intercepts and regression coefficients in the relationships between pH in soil solution ( $\text{pH}_{\text{ss}}$ ) and base saturation.

Experiment	Type of results	$a_0$	$a_1$	$R^2$
Park grass	Modelled	3.85	0.03	0.87
	Observed	3.50	0.03	0.88

Sawyers field	Modelled	4.34	0.02	0.83
	Observed	4.35	0.02	0.83

Note that the differences are mainly due to the estimation of the CEC, which is pH dependent, with Xu et al (2020) making use of a CEC buffered at 6.5 while Beery and Wilding (1971) uses a CEC buffered at 8.2.

The reason for using for using a buffered CEC is because the actual CEC in the field situation is not only determined by the clay and organic matter content, but is also pH dependent, with an overall relationship given by Helling et al. (1964):

$$\text{CEC} = (0.44 \cdot \text{pH-H}_2\text{O} + 3.0) \cdot \text{clay} + (5.1 \cdot \text{pH} - 5.9) \cdot \text{SOC} \quad (43)$$

where clay and SOC are the clay and soil organic C content, respectively (%) and the pH in this equation equals pH-H<sub>2</sub>O (pH-H<sub>2</sub>O = pH-KCl \* 0.777 + 2.23). In NutriFarm, we make use of a CEC buffered at pH 6.5 (NH<sub>4</sub> acetate buffered CEC), being generally the upper range of a non-calcareous soil with a base saturation at 100%. This is done to avoid pH dependency on the CEC when the soil acidifies. In the model, acidification implies that the exchangeable proton fraction increases, whereas the exchangeable amount of base cations decreases at a constant buffered CEC. The CEC at pH 6.5 is then only a function of the clay and organic C content. Using a pH value of 6.5 gives a regression coefficient of 5.9 for clay and 27.3 for organic C, which is reasonably consistent with Breeuwsma et al. (1986), who found a relationship between the buffered CEC at pH 6.5 and the clay and organic matter content, with regression coefficients of 5.0 for clay and 30 for organic C. In NutriFarm we use the regression coefficient of 5.9 for clay and 27.3 for organic C as derived by Helling with a pH of 6.5. Note that the data on PH, CEC and BS need to be derived for two spoil layers, i.e. 0-30 cm and 30-100 cm. When data on CEC and cation saturation are lacking, it is derived from Eq. (42) and Eq. (43) using available data on SOC, clay and pH.

The fraction of Ca, Mg, K and Na in the release from or accumulation of BC on the adsorption complex is set equal to the fraction of these elements (Ca/BC, Mg/BC, K/BC and Na/BC) on the adsorption complex. The change in BC<sub>exchangeable</sub> is thus proportioned over Ca, Mg, K and Na<sub>exchangeable</sub> with the initial fractions on the adsorption complex being derived from data and assumed to stay equal over time. 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, near a base saturation at 20% (Eq. 42). Below pH 4.5 (BS of 20%), 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 (Al fraction is 0.5).

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<sub>3</sub>. In calcareous soils, the initial pH is assumed to stay constant (always >6.5). To gain insight into the losses of CaCO<sub>3</sub>, [HCO<sub>3</sub><sup>-</sup>] (unit: eq/l or molc/l) is calculated by assuming equilibrium with the CO<sub>2</sub> pressure (unit: bar) in the soil only, according to (De Vries and Breeuwsma, 1986):

$$\log [HCO_3^-] = -1.94 + \log(pCO_2) / 3 \quad (44)$$

## 2.7 Modelling Cd, Cu and Zn dynamics

As with P and SO<sub>4</sub>, the concentration of the metals Cd, Cu and Zn in the topsoil and subsoil is determined by a mass-balance equation that describes the inputs and outputs and

accumulation in each layer. Note that apart from the micronutrients Cu and Zn, included in the NutriBudget project, we also include Cd in NutriFarm since cd can be an important pollutant in P fertilizers and its long-term behaviour in response to various management strategies is relevant to include in the model calculations.

As with all other nutrients, Cd, Cu and Zn uptake is calculated by multiplying the crop yield with the metal content in crops, which is either assumed to be soil independent (for Cu) or derived by a non-linear relationship with the soil metal concentration in the topsoils (layer 0-30 cm), accounting for the impact of soil properties that control the (bio)availability of metals in soils for Cd and Zn (Adams et al., 2004; Brus et al., 2002), according to (see also De Vries et al., 2008a):

$$Me_{\text{plant}} = K_F Me_{\text{soil}}^n \text{ or } \text{Log } Me_{\text{plant}} = \text{log } K_F + n \text{ log } Me_{\text{soil}} \quad (45)$$

where  $K_F$  is a function of pH and the content of soil organic matter and clay according to:

$$\text{Log } K_F = a_0 + a_1 \cdot \text{pH}_{\text{KCL}} + a_2 \cdot \text{log SOM} + a_3 \cdot \text{log clay} \quad (46)$$

Combining Eq (38) and Eq. (39) gives:

$$\text{log } Me_{\text{plant}} = a_0 + a_1 \cdot \text{pH}_{\text{KCL}} + a_2 \cdot \text{log SOM} + a_3 \cdot \text{log clay} + n \cdot \text{log } Me_{\text{soil,tot}} \quad (47)$$

where  $Me_{\text{plant}}$  is the metal concentration in plant, where Me stand for either Cd or Zn ( $\text{mg.kg}^{-1}$ );  $Me_{\text{soil,tot}}$  is the total metal (Cd or Zn) concentration in soil ( $\text{mg.kg}^{-1}$ ); SOM is the soil organic matter content in the soil (%); clay is the clay content in the soil (%) and n is a coefficient describing the non-linear relationship between the metal concentration in plant and in soil (-). Values for the regression coefficients in Eq. (46) were derived for Cd and Zn in grass, maize, wheat, potatoes and sugar beet while the relation for other crops, mainly including other cereals, was assumed to be equal to wheat. The used values for Cd and Zn are given in Table 5 and Table 6, respectively.

The leaching and runoff rate from the topsoil (0-30cm) and subsoil (30-100 cm) is calculated by multiplying either the runoff rate or leaching with a dissolved metal concentration (see also the scheme in Figure 1 while lumping the layers 1 and 2). The dissolved metal concentration is related to the reactive soil metal concentration according to a Freundlich equation (De Vries et al., 2008b) according to:

$$Me_{\text{soil, re}} = K_F Me_{\text{ss}}^n \quad (48)$$

Rewriting gives:

$$Me_{\text{ss}} = \left( \frac{Me_{\text{soil, re}}}{K_F} \right)^{1/n} \quad (49)$$

where  $Me_{\text{ss}}$  is the concentration of Me in the soil solution ( $\text{mmol.l}^{-1}$ ),  $Me_{\text{soil, re}}$  is the reactive concentration of Me in the soil ( $\text{mol.kg}^{-1}$ ) and  $K_F$  is a Freundlich coefficient ( $\text{mol.l}^{-1n}.\text{kg}^{-1}$ ).

**Table 5** Values for the coefficients  $a_0 - a_3$  and n in the soil– plant relations for Cd according to Eq. (47) in grass, maize, potatoes wheat and sugar beet, based on De Vries et al. (2008a).

Crop	a <sub>0</sub>	a <sub>1</sub>	a <sub>2</sub>	a <sub>3</sub>	n	R <sup>2</sup>	se-y <sub>est</sub> <sup>1)</sup>
Grass	1.45	-0.38		-	1.22	0.63	0.23
Maize	0.90	-0.21		-0.32	1.08	0.62	0.26
Potatoes	0.97	-0.21	-0.41	-0.2	0.81	0.78	0.26
Wheat1	0.22	-0.12	-0.33	-0.04	0.62	0.64	0.20
Sugar beet	1.33	-0.22		-0.13	0.62	0.83	0.15

<sup>1)</sup> The standard error of the y-estimate on a logarithmic basis

**Table 6** Values for the coefficients a<sub>0</sub> – a<sub>3</sub> and n in the soil– plant relations for Zn according to Eq. (47) in grass, maize, potatoes wheat and sugar beet, based on De Vries et al. (2008b).

Crop	a <sub>0</sub>	a <sub>1</sub>	a <sub>2</sub>	a <sub>3</sub>	n	R <sup>2</sup>	se-y <sub>est</sub> <sup>1)</sup>
Grass	2.06	-0.09	1.09	-1.05	0.41	0.49	0.11
Maize	3.05	-0.31		-0.61	0.64	0.67	0.12
Potatoes	0.0	-0.09	-0.64	0.41	0.68	0.74	0.04
Wheat	1.32	-0.06		-0.24	0.45	0.56	0.09
Sugar beet	2.69	-0.41	-0.71	-0.37	1.13	0.67	0.14

<sup>1)</sup> The standard error of the y-estimate on a logarithmic basis

Since input data on the reactive metal concentration are given in mg. kg<sup>-1</sup>, the concentrations are divided by 1000 and by the molar weight of Cd (112.5), Cu (63.5) and Zn (65.5) to get concentration values in mol. kg<sup>-1</sup>. Furthermore, since the metal concentrations in soil solution are used in mg l<sup>-1</sup> the concentrations are multiplied with the molar weights given above to transfer mmol.l<sup>-1</sup> to mg l<sup>-1</sup>.

The value of K<sub>F</sub> is also calculated as a function of the content of organic matter (in %), clay (in %) and pH-H<sub>2</sub>O (-) according to:

$$\log K_F = b_0 + b_1 * \log (\text{SOM}) + b_2 * \log (\text{clay}) + b_3 * \text{pH-H}_2\text{O} \quad (50)$$

where b<sub>0</sub> ... b<sub>3</sub> are the model coefficients, SOM is the soil organic matter content (%), clay is the clay (< 2µm or lutum) content (%) and pH-H<sub>2</sub>O is the pH determined in water (or soil solution). Values for the various regression coefficients were derived from laboratory experiments with approximately 1400 soil samples from Dutch locations (Römken et al., 2004). Values for the coefficients used are given in Table 7 (see also De Vries et al., 2008b).

**Table 7.** Values for the coefficients  $b_0$ - $b_3$  and  $n$  in the relationships relating dissolved total concentrations and reactive soil concentrations of Cu and Zn, according to Eq. 50 (after Römken et al., 2004, Table 3.2).

Metal	$b_0$	$b_1$	$b_2$	$b_3$	$n$	$R^2$	se- $y_{est}$
Cd	-4.85	0.58	0.28	0.27	0.54	0.79	0.33
Cu	-3.55	0.48	0.18	0.16	0.47	0.62	0.35
Zn	-4.51	0.39	0.35	0.45	0.74	0.82	0.40

The reactive metal concentrations in Eq. (48) were derived from available data on total metal concentrations (Cd, Cu or Zn) by accounting for the variation in organic matter and clay content, according to (Römken et al. (2004):

$$\log Me_{soil,re} = c_0 + c_1 * \log (\text{SOM}) + c_2 * \log (\text{clay}) + c_3 * \log Me_{soil,tot} \quad (51)$$

Where both  $Me_{soil,re}$ ,  $Me_{soil,tot}$ , being the reactive and total metal (Cd, Cu or Zn) concentrations in soil, are given in  $\text{mg.kg}^{-1}$  Values for the coefficients used are given in Table 8 (see also De Vries et al., 2008b).

**Table 8.** Values for the coefficients  $c_0$ - $c_3$  in the relationships between reactive and total concentrations of Cd, Cu and Zn, according to Eq. 51 (after Römken et al., 2004, Table A1.1).

Metal	$c_0$	$c_1$	$c_2$	$c_3$	$R^2$	se- $y_{est}$
Cd	-0.089	0.022	-0.062	1.08	0.96	0.11
Cu	-0.331	0.023	-0.171	1.15	0.93	0.13
Zn	-0.703	0.183	-0.298	1.24	0.96	0.16

### 3 Model application

**Base line and scenarios:** The model starts with simulations for the base year (2020) and then evaluates mitigation measures using a standard time period of 30 years (2020-2050), which can be extended to >100 years for exploratory reasons, e.g. for C, P and metal dynamics.

**Model initialization:** The model is initialized for the year 2010, thus using a 10 year simulation period up to 2020 using:

- (i) available data on P-Olsen and P total from LUCAS and relating it to P oxalate,
- (ii) available metal data (Metot) in GEMAS
- (iii) available CEC and pH data from LUCAS/Soil Grids and deriving Base saturation from pH and
- (iv) initializing  $[\text{SO}_4]$  by assuming an equilibrium in 2000 based on input and precipitation surplus followed by 20 years runs. The value of KF and m to be used can be checked by requiring that the calculated initial adsorbed amount of  $\text{SO}_4$  does not exceed the  $\text{SO}_4$  sorption capacity (SSC), which can be approximated as  $0.05 \times (\text{AL} + \text{Fe})_{ox}$  (De Vries et al., 1994b).

**Input data:** Default input data at initial resolution for the Nutri-Farm model will be derived from the raster data on climate, slope, deposition, (crop residue usage) and soil properties. Decisions on which input data to use and whether data can be overwritten when data are available at farm level (e.g., soil data) will be considered.

## Annex 2. Default input parameters used to run NutriFarm

Table 1A. Default input parameters and its sources.

Category	Parameter	Datasets	Source
Soil properties *	Soil pH, CEC, availability of CaCO <sub>3</sub> , NPK content	Soil Chemical properties at European scale based on LUCAS 2009/2012 topsoil data	<a href="#">Ballabio, C., Lugato, E., Fernández-Ugalde, O., Orgiazzi, A., Jones, A., Borrelli, P., Montanarella, L. and Panagos, P., 2019. Mapping LUCAS topsoil chemical properties at European scale using Gaussian process regression. Geoderma, 355: 113912.</a>
Soil properties *	Soil organic carbon (SOC) content	LUCAS 2018 TOPSOIL data	Fernandez-Ugalde, O; Scarpa, S; Orgiazzi, A.; Panagos, P.; Van Liedekerke, M; Marechal A. & Jones, A. LUCAS 2018 Soil Module. Presentation of dataset and results, EUR 31144 EN, Publications Office of the European Union, Luxembourg. 2022, ISBN 978-92-76-54832-4, doi:10.2760/215013, JRC129926. Orgiazzi, A., Ballabio, C., Panagos, P., Jones, A., Fernández-Ugalde, O. 2018. LUCAS Soil, the largest expandable soil dataset for Europe: A review. European Journal of Soil Science, 69(1): 140-153. <a href="https://doi.org/10.1111/ejss.12499">https://doi.org/10.1111/ejss.12499</a> .
Soil properties *	Soil texture, coarse fractions, bulk density, rooting depth	Topsoil physical properties for Europe (based on LUCAS topsoil data)	<a href="#">Ballabio C., Panagos P., Montanarella L. Mapping topsoil physical properties at European scale using the LUCAS database (2016) Geoderma, 261, pp. 110-123.</a>
Soil properties	Soil type ('WRB-LEV1'), soil texture class ('TEXT-SRF-DOM'), soil depth to rock ('DR'), rooting depth ('ROO'), soil	ESDB v2.0 and soil erosion maps (JRC)	The European Soil Database distribution version 2.0, European Commission and the European Soil Bureau Network, CD-ROM, EUR 19945 EN, 2004. Panagos Panos. The European soil database (2006) GEO: connexion, 5 (7), pp. 32-33. De Vries, W.: 1991, Methodologies for the assessment and mapping of critical loads and of the impact of abatement strategies on forest soils, DLO Winand Staring Centre, Wageningen, the Netherlands, Report 46, 109 pp.

	erosion, organic carbon class ('OC_TO P'), parent material ('PAR-MAT-DOM'). Base cation weathering		
Soil properties	Slope	EU-DEM	European Environmental Agency, 2024. European Digital Elevation Model (EU-DEM). DOI: <a href="https://ec.europa.eu/eurostat/web/gisco/geodata/digital-elevation-model/eu-dem#Slope">https://ec.europa.eu/eurostat/web/gisco/geodata/digital-elevation-model/eu-dem#Slope</a> (Accessed on 01-08-2024).
Soil properties	C-factor, erosion	USLE model	Panagos, P., Borrelli, P., Meusburger, C., Alewell, C., Lugato, E., Montanarella, L., 2015. <a href="#">Estimating the soil erosion cover-management factor at European scale</a> . Land Use policy journal. 48C, 38-50.
Crop properties	Crop yields	Eurostat and Agrarstrukturhebung for Germany	Crop production in EU standard humidity by NUTS 2 region. <a href="https://ec.europa.eu/eurostat/databrowser/view/apro_cpshr/default/table?lang=en&amp;category=agr.apro.apro_crop.apro_cp.apro_cpsh">https://ec.europa.eu/eurostat/databrowser/view/apro_cpshr/default/table?lang=en&amp;category=agr.apro.apro_crop.apro_cp.apro_cpsh</a>  Agrarstrukturhebung 2020. <a href="https://www.regionalstatistik.de/genesis/online?language=de&amp;sequenz=statistikTabellen&amp;selectionname=41141">https://www.regionalstatistik.de/genesis/online?language=de&amp;sequenz=statistikTabellen&amp;selectionname=41141</a>
Farm and regional properties	Soil cover and tillage practice	FSS	<a href="#">European Commission, download September 2009</a> URL: <a href="https://ec.europa.eu/eurostat/web/microdata/farm-structure-survey">https://ec.europa.eu/eurostat/web/microdata/farm-structure-survey</a>
Farm and regional properties	Areas under derogation	EC	European Commission, downloaded May 2019. URL: <a href="https://ec.europa.eu/environment/water/water-nitrates/index_en.html">https://ec.europa.eu/environment/water/water-nitrates/index_en.html</a>
Farm and regional	Crop residue removal index	Smerald et al. (2023)	<a href="#">Dataset: Global crop residue management dataset (1997 - 2021)</a>

prop erties			
Emis sion factor s	N excre tio n of animals, CH <sub>4</sub> emis sion s from manure manage ment system and enteric fermenta tion	National GHG inventory submissio ns	United Nations Framework Convention on Climate Change, 2020. National Inventory Submissions 2020. Bonn: United Nations Climate Change.
Emis sion factor s	N <sub>2</sub> O, CO <sub>2</sub> (peatlan d) emis sion factors, global warming potential s,	IPCC	IPCC, 2019. 2006 IPCC Guidelines for National Greenhouse Gas Inventories, Volume 4, Agriculture, Forestry and Other Land Use. IPCC National Greenhouse Gas Inventories Programme. Institute for Globa
Emis sion factor s	NH <sub>3</sub> emis sion factors	EMEP	<a href="https://www.eea.europa.eu/en/analysis/publications/emep-eea-guidebook-2023">https://www.eea.europa.eu/en/analysis/publications/emep-eea-guidebook-2023</a> , Table 3-9, Chapter 3.B for manure; Table 3-2, Chapter 3.D for mineral fertilisers.
Clim ate prop erties	Precipita tion, evapotra nspiratio n, temperat ure, wind speed	ERA5	<a href="https://climate.copernicus.eu/era5-hourly">Hersbach, H., Bell, B., Berrisford, P., Biavati, G., Horányi, A., Muñoz Sabater, J., Nicolas, J., Peubey, C., Radu, R., Rozum, I., Schepers, D., Simmons, A., Soci, C., Dee, D., Thépaut, J.-N. (2023): ERA5 hourly data on single levels from 1940 to present. Copernicus Climate Change Service (C3S) Climate Data Store (CDS), DOI: 10.24381/cds.adbb2d47 (Accessed on 10-09-2024).</a>
Wate r flux	Precipita tion surplus, surface runoff and groundw ater	Keuskam p et al. (2012)	<a href="https://doi.org/10.1016/j.envpol.2012.02.008">J. A. Keuskamp, G. Van Drecht, A. F. Bouwman (2012). European-scale modelling of groundwater denitrification and associated N<sub>2</sub>O production. Environmental Pollution, 165, pp. 67-76, doi: http://dx.doi.org/10.1016/j.envpol.2012.02.008.</a>

	leaching fractions		
Nutrient composition	Composition of organic fertilizers		Multiple sources based on literature and database study
Nutrient composition	Composition of crop (residues)		Multiple sources based on literature and database study
Nutrient composition	Composition of chemical fertilizers		Multiple sources based on literature and database study, including expert judgement of Römken (2024)
Nutrient deposition	Ca, Cd, Cu, K, Mg, Na, NH <sub>3</sub> , NO <sub>x</sub> , SO <sub>x</sub> , Zn deposition	EMEP	Van Loon, M., Tarrasón, L., Posch, M., 2005. Modelling Base Cations in Europe. EMEP/MSW-W&CCE Note2/2005. ISSN 0804-2446. EMEP MSC-W, <a href="https://emep.int/mscw/mscw_moddata.html">https://emep.int/mscw/mscw_moddata.html</a> .

\* Subsoil data were retrieved by taking the LUCAS topsoil data and multiply these data by the ratio topsoil:subsoil of SoilGrids. When parameters are not available from SoilGrids, the topsoil data equal the subsoil data

Table 1B. Livestock and manure categories copied from MITERRA-Europe.

Livestock type	Manure code	Description	Eurostat category
DAIRYCOWS	DAICOW_L	Dairy cows liquid manure	A2300F
OCOW	OCOW_L	Dairy cows solid manure	A2000 - A2300F
PIGS	PIGS_L	Other cows liquid manure	A3100
DAIRYCOWS	DAICOW_S	Other cows solid manure	A2300F
OCOW	OCOW_S	Pigs liquid manure	A2000 - A2300F
PIGS	PIGS_S	Pigs solid manure	A3100
LAYHENS	LAYHENS	Laying hens	A51100
OPOUL	OPOUL	Other poultry	A5000
SHEGOA	SHEGOA	Sheep and goat	A4100 + A4200

HORSES	HORSES	Horses	A1000
FURANI	FURANI	Fur animals	

Table 1C. Crop categories copied from MITERRA-Europe.

<b>Crop code</b>	<b>Description</b>
APPL	Apples pears and peaches
BARS	Spring barley
BARW	Winter barley
CITR	Citrus fruits
DWHE	Durum wheat
FLOW	Flowers
GRAP	Permanent pastures and meadows
GRAR	Rough grazings
MAIF	Fodder maize
MAIZ	Grain maize
NURS	Nurseries
OATS	Oats and summer cereal without triticale
OCER	Other cereals including triticale
OFAR	Fodder other on arable land
OFRU	Other fruits
OIND	Other industrial crops
OLIV	Olives for oil
OOIL	Other oils
OVEG	Other vegetables
PARI	Paddy rice
POTA	Potatoes
PULS	Pulses
RAPE	Rape
ROOF	Fodder root crops
RYEM	Rye and meslin
SOYA	Soya
SUGB	Sugar beet
SUNF	Sunflower
SWHS	Soft spring wheat
SWHW	Soft winter wheat
TABO	Table olives
TAGR	Table grapes
TEXT	Flax and hemp

TOBA	Tobacco
TOMA	Tomatoes
TWIN	Wine

Table 1D. Chemical fertilizer categories copied from MITERRA-Europe.

<b>Fertilizer abbreviation</b>	<b>Description</b>
N_AA	Ammonia, anhydrous
N_AN	Ammonium nitrate (AN)
N_AS	Ammonium sulphate
N_CAN	Calcium ammonium nitrate (CAN) and other mixtures with calcium carbonate
DAP	Diammonium phosphate (DAP)
F_NEC	Fertilizers n.e.c.
MAP	Monoammonium phosphate (MAP)
NPK	NPK fertilizers
N_ONF	Other nitrogenous fertilizers, n.e.c.
Other_NK	Other NK compounds
Other_NP	Other NP compounds
Other_P	Other phosphatic fertilizers, n.e.c.
Other_K	Other potassic fertilizers, n.e.c.
P_rock	Phosphate rock
PK	PK compounds
MOP	Potassium chloride (muriate of potash) (MOP)
KN	Potassium nitrate
N_SN	Sodium nitrate
Super_P	Superphosphates above 35%
Super_P_other	Superphosphates, other
N_Urea	Urea
UAN	Urea and ammonium nitrate solutions (UAN)

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## **INITIATOR and INTEGRATOR Publications relevant to NutriFarm**

### ***Modeling approaches (nitrogen, phosphorus and heavy metals)***

- De Vries, W., J. Kros, J.C. Voogd and G. H. Ros, 2023. Integrated assessment of agricultural practices on the loss of ammonia, greenhouse gases, nutrients and heavy metals to air and water. *Science of the total Environment* 857 (2023) <https://doi.org/10.1016/j.scitotenv.2022.159220>
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### ***Model analysis (focus on nitrogen)***

- Kros, J., G.B.M. Heuvelink, G.J. Reinds, J.P. Lesschen, V. Ioannidi and W. de Vries, 2012. Uncertainties in model predictions of nitrogen fluxes from agro-ecosystems in Europe. *Biogeosciences* 9: 4573-4588.
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### ***Critical losses, surpluses and inputs of nitrogen, phosphorus and heavy metals***

- De Vries, W., J. Kros, J.C.H. Voogd, G. Louwagie and L. F. Schulte-Uebbing, 2021. Spatially explicit boundaries for agricultural nitrogen inputs in the European Union to meet air and water quality targets. *Science of the total Environment* 786 (2021) 147283. <https://doi.org/10.1016/j.scitotenv.2021.147283>
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- De Vries, W., P.F.A.M. Römkens, J. Kros, J.C Voogd and L.F Schulte-Uebbing, 2022. Impacts of nutrients and heavy metals in European agriculture. Current and critical inputs in view of air, soil and water quality. ETC-DI Report 2022/01, 72 pp. [D22 1821 M1 and M2 Nutrients and heavy metals in soils 01032022 ETC-DI 30March.pdf](#)
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