# Modeling Nitrate Leaching in the Gäu Region Using the Farm Model and the DAISY Model

Thesis in partial fulfilment of the requirements for the degree of
Master of Science in the study program Agrosystem Sciences
At the TUM School of Life Sciences of the Technical University Munich.

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**Submitted on** Limburg, 04.05.2021

# Declaration

I hereby declare that the thesis presented here has been written by myself and is a product of my own work, unless otherwise stated by reference of acknowledgement in the text. This thesis, either in whole or in part, has not been submitted for any degree at any university previously.

Limburg, 04.05.2021

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# Abstract

Excessive amounts of nitrogen (N) in the agricultural system can lead to nitrate leaching. Nitrate can reach the groundwater and impair drinking water quality. In 2000, the largest Swiss nitrate project was implemented in the Gäu region, canton Solothurn, to improve drinking water quality. Agricultural measures to mitigate nitrate leaching, comprising adjustments to crop rotations, reduced tillage, and soil cover during the winter, were implemented. In 2017, NitroGäu, a joint research project of several Swiss institutions began, measuring the current nitrate leaching on eleven fields in the Gäu using Self-Integrating Accumulators (SIA), suction cups and $N_{min}$ sampling, and testing additional mitigation strategies. This study was conducted as part of the synthesis of the NitroGäu project and aimed to extrapolate the SIA measurements to a regional scale, as well as modelling nitrate leaching using the Farm Model (FM) and DAISY on five of the eleven fields in the years 2018 and 2019. The FM uses a simple N model, while DAISY is a dynamic soil-plant-atmosphere simulation model. The simulated results were compared to the SIA measurements. Furthermore, farm-gate balances of four farms were calculated for the years 2018 and 2019 and compared to the Suisse Balances of the same farms. Farm-gate budgets showed higher N balances on all farms in both years, by around 18 kg N $ha^{-1}$ on average. The two balancing methods differ in their input data and methodology which can explain the different N balances. Both the FM and DAISY did not simulate nitrate leaching accurately. For the FM, it was difficult to align the results with the SIA measurements, as the model gives an accumulated leaching value of a single crop without an exact time resolution. In DAISY, the crop calibration was suboptimal, as at least one crop of each field's crop rotation was not yet or not well parameterized in the model. Therefore, crop growth and N fluxes were not simulated accurately. The extrapolation of the SIA measurements to the Gäu region showed highest nitrate leaching under winter wheat, as it was widely cultivated (223 ha) and exhibited high relative nitrate leaching rates (133 kg $NO_3$-N $ha^{-1}$). In a typical crop rotation in the Gäu, winter wheat is grown after winter rapeseed or grass clover leys, followed by maize. Both, winter rapeseed and maize leave high amounts of mineral N in the soil after harvest. Only a small part of this is taken up by winter wheat in autumn, while the rest is at high risk of leaching during the winter. A possible additional mitigation strategy is to replace winter wheat with winter barley, as it can take up more N in autumn. Another measure could be field specific fertilization planning, taking $N_{min}$ samples from spring and mineralization from previous crops, especially leguminous leys into account.

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# Introduction

## 1.1. Nitrogen in the Agricultural System

Nitrogen (N) is an important nutrient for crop production and a major yield-defining factor. Global production of mineral N fertilizers increased from 12.7 Tg in 1961 to 120.2 Tg in 2015 (FAOSTAT, 2020). Estimates suggest that without this increase in fertilizer production it would only be possible to sustain roughly 40% of today's population (Smil, 2001). However, the higher N inputs have also led to a multitude of negative environmental effects, as reactive nitrogen is dispersed and accumulated in different sinks on local, regional, and global scale (Galloway et al., 1995). The accumulation of nitrate ($NO_3^-$) in the hydrological system can cause acidification and eutrophication of surface water bodies which can lead to significant loss of biodiversity and habitat degradation (Vitousek et al., 1997, Howarth et al., 2000). Nitrate in drinking water can also be harmful to human health and for example cause Methemoglobinemia which infants are especially susceptible to (Ward et al., 2005). Consequently, the World Health Organization set a guideline value for the nitrate concentration in drinking water of 50 mg $L^{-1}$, which ensures no adverse effects on human health (WHO, 2017). In Switzerland, the Federal Department of Home Affairs set the limit of tolerance to 40 mg $L^{-1}$ within the ordinance of drinking water and water in public swimming pools (TBDV) (EDI, 2016). The Federal Council issued a numerical requirement for groundwater which is intended for drinking water at 25 mg $L^{-1}$ in the Waters Protection Ordinance (WPO) (Der Schweizerische Bundesrat, 1998).

In Europe, agriculture is the main contributor (50-75%) to nitrate concentrations in freshwater (Eurostat, 2018). Sources of nitrate in agriculture are fertilizers containing nitrate, or the process of nitrification in which ammonium ($NH_4^+$) or ammonia ($NH_3$) are converted to nitrate. Nitrate is highly mobile, water-soluble, and not adsorbed to soil particles. Thus, it can be easily transported by seepage when not taken up by vegetation (BAFU, 2019). Nitrate leaching is highly dependent on weather conditions, especially precipitation, soil properties and vegetation cover (Meier et al., 2014). Many projects have devised strategies to reduce nitrate leaching (Osterburg et al., 2007, Dzurella et al., 2012, Hülsbergen et al., 2017). These mitigation strategies often relate to fertilization, crop rotation, soil cultivation, land use, and animal husbandry. Measures in animal husbandry, such as optimal feeding and increased manure storage capacity, do not affect nitrate leaching directly, but target manure composition and timing of application (Hülsbergen et al., 2017). Soil cultivation, often related to incorporation of residues, affects mineralization processes in the soil, which should be aligned with crop uptake of the subsequent crop (Hansen et al., 2019). In crop rotations, cover crops, grown between main crops to retain mineral nitrogen are an efficient measure to reduce nitrate leaching (Constantin et al., 2010, De Notaris et al., 2018). Fertilization can be adjusted according to type, timing, and application technique. Additionally, the amount of fertilizer applied plays a key role for available mineral N and potential leaching. The choice of the measures and their effectiveness strongly depend on regional soil and weather conditions (Hansen et al., 2019).

## 1.2. Nitrogen Budgets

There are several ways to evaluate the risk of nutrient emissions from agriculture, one of the most common being nutrient budgets (Oenema et al., 2003). The principle of these budgets is to sum up all nutrient inputs to and outputs from an agricultural system. The difference between inputs and outputs translates to the nutrient surplus (input > output) or the nutrient deficit (input < output). A nutrient surplus can cause harmful emissions to the ecosystem, while a nutrient deficit over an extensive period, can deplete soil nutrient stocks, decreasing soil fertility. Thus, the goal is an even nutrient balance. Three main approaches are the farm-gate balance (FGB), the soil surface budget and the soil system budget (Figure 1) (Oenema et al., 2003).

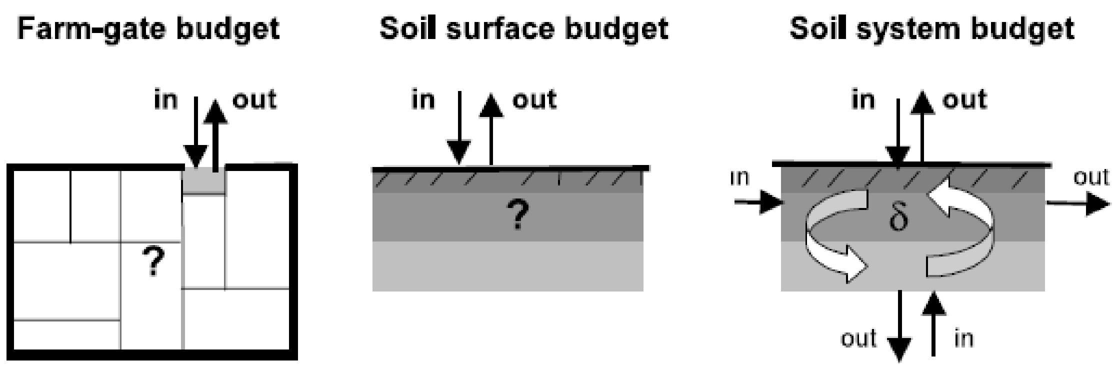


Figure 1. Schematic overview of the differences of the farm-gate budget, soil surface budget and soil system budget. Source: Oenema et al. (2003)

The FGB uses the farm gate as its system boundary, calculating all nutrients entering and leaving the farm operation. The farm itself is treated as a black-box (Oenema et al., 2003). In the soil surface budget, all nutrient inputs entering the soil via the surface and nutrient outputs from harvested crops are considered. Thus, the balance represents possible nutrient losses from the soil. The soil system budget additionally includes nutrient gains and losses within the soil. It allows to distinguish between loss pathways (Oenema et al., 2003). The nutrient balance of FGB and soil surface budget does not generally translate into nutrient losses, as part of these nutrients can also be immobilized in the soil. Generally, budgets should be calculated for several years to see a trend of either nutrient depletion, excessive, or balanced nutrient management (Oenema et al., 2003). There is no standard methodology of nutrient budgets, instead they can be generated at different scales and different levels of detail, depending on their purpose. Possible applications of nutrient budgets are to support farmers in their nutrient management, or to serve policy makers as agri-environmental indicator or as regulatory instrument (Oenema et al., 2003).

In Switzerland, direct payments are only given to farms that comply with the certificate of ecological performance (ÖLN, ökologischer Leistungsnachweis). One requirement is an even farm nutrient balance for nitrogen and phosphorus (P) (KIP, 2008). Nutrient balances are recorded using the Suisse Balance (SB), which serves as a regulatory instrument and as planning aid for farmers (Figure 2). The balance itself resembles a modified soil surface budget where several inputs, such as biological nitrogen fixation (BNF) and atmospheric deposition, are missing, and the output by N removal is replaced by the N demand of the crop production (Bosshard et al., 2012). The derivation of the balance also takes the animal husbandry, and with it, the on-farm nutrient flows into account. The available on-farm organic fertilizer is calculated from the animal husbandry and then compared to the nutrient demand of the crop production. A deficit or surplus of nutrients can be compensated by import or export of fertilizers, which are then taken into account in the final balance (Agridea and BLW, 2015). The implementation of obligatory nutrient budgets in Switzerland in 1992 have helped to decrease the nutrient surplus for nitrogen, phosphorus and potassium (Bosshard et al., 2012).

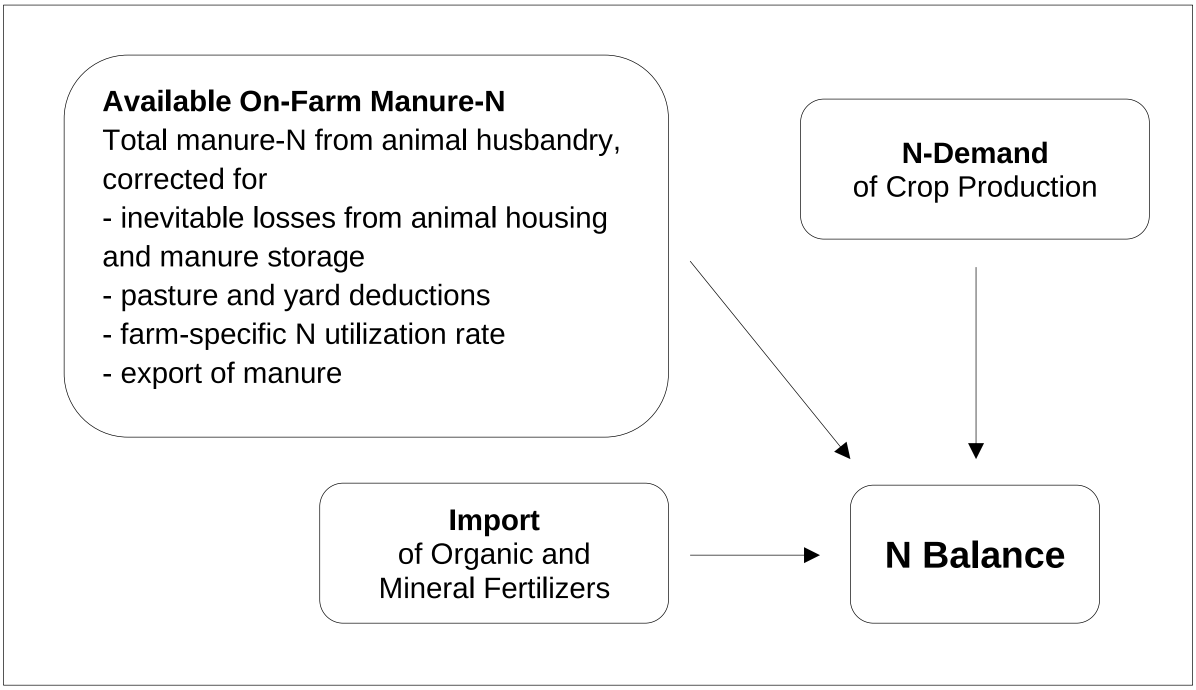


Figure 2. Schematic overview of the N balance of the Suisse Balance. Own representation.

## 1.3. Nitrogen Simulation Models

A more detailed way to evaluate nitrogen emissions to the environment are simulation models. They incorporate the current state of knowledge of the targeted environmental processes in mathematical form. In that, they serve as a review of the current understanding of these processes and can thus complement practical field research. They can also be used to reproduce complex processes that are difficult to observe or quantify, as well as extend them in time and space (Nendel, 2014). Similar to nutrient budgets, the main fields of application are consultations on nutrient management, catchment analyses to protect water resources or habitats, as well as evaluations of environmental and agricultural policies (Nendel, 2014).

There is a multitude of models available that differ in scale, level of detail and complexity. Empirical models combine input and reference data with simplified assumptions and calculations to estimate N content and losses from the soil (Nendel, 2014). An example for this kind of model is the nitrogen model implemented in the Farm Model which was used in this study. The Farm Model is a Life Cycle Assessment (LCA) tool, which is being developed by the Research Institute of Organic Agriculture (FiBL) Switzerland. The principle of LCA is to evaluate a number of environmental indicators for the life of a product or service and the resources used. In agricultural systems it can be used to evaluate crop production, animal husbandry or the entire farm (Payraudeau et al., 2007). The Farm Model can evaluate 13 environmental indicators, such as the contribution to eutrophication of surface water bodies and the greenhouse gas emissions of a farming operation. Emissions and loss pathways from crop production and animal husbandry are quantified in several sub models, regarding e.g. nitrogen and phosphorus. Emission factors and impact assessments are largely based on the ecoinvent 3.5 inventory (Frischknecht et al., 2004, ecovinvent, N.A.), as well as several other standard values, such as emission factors from IPCC (2019). The calculations of the nitrogen model are based on Brock et al. (2012), Meier et al. (2012) and Meier et al. (2014). Loss pathways include nitrate leaching, as well as gaseous losses of nitrogen oxides ($NO_x$), nitrous oxide ($N_2O$) and ammonia ($NH_3$).

Another type of model are the dynamic process-oriented simulation models. These simulate complex ecological processes in time and space (Nendel, 2014). They usually require a large amount of parameters and state variables to describe the surroundings of the simulated system (Jabloun et al., 2018). Two main functions are the simulation of crop growth and the simulation of (C- and) N fluxes, which are realized at different levels of complexity (Nendel, 2014). There are several different models developed and widely used in Europe, for example the Dutch model ANIMO (Renaud et al., 2005), the German models CANDY (Franko et al., 1994) and Expert-N (Engel and Priesack, 1993). In this study, the Danish model DAISY was used to simulate crop growth and nitrate leaching. The model can simulate processes in the plant, soil, and atmosphere. It relies on parameterization of soil and crop characteristics, and the input of daily weather and detailed management data (Hansen et al., 2012). It has been developed by the University of Copenhagen in the late 1980s (Hansen et al., 1990) and has since been widely used and validated in several studies worldwide (Svendsen et al., 1995, Smith et al., 1997, Palosuo et al., 2011).

## 1.4. Nitrate Leaching in the Gäu Region

In Switzerland, 80% of drinking water is derived from groundwater. To ensure the quality and safety of drinking water and to surveil the environmental condition of the aquifer, it is monitored frequently at over 600 monitoring sites within the federal-cantonal program NAQUA National Groundwater Monitoring. Nitrate is the pollutant that most frequently exceeds its numerical requirement in groundwater. Between 2007 and 2014, each year up to 15-20% of all monitoring sites registered nitrate concentrations above the limit value of 25 mg $L^{-1}$. The limit of tolerance of 40 mg $L^{-1}$ was exceeded at 2-4% of monitoring sites (BAFU, 2019). Agriculture was found to be the main emitter of nitrate into the environment (BLW, 2008). In 2014, 40% of monitoring sites under arable land exceeded 25 mg $L^{-1}$ and 12% registered nitrate concentrations above 40 mg $L^{-1}$ (Purtschert and Hunkeler, 2015). Figure 3 shows a correlation between high nitrate concentrations in groundwater and intensive arable farming in the catchment areas.

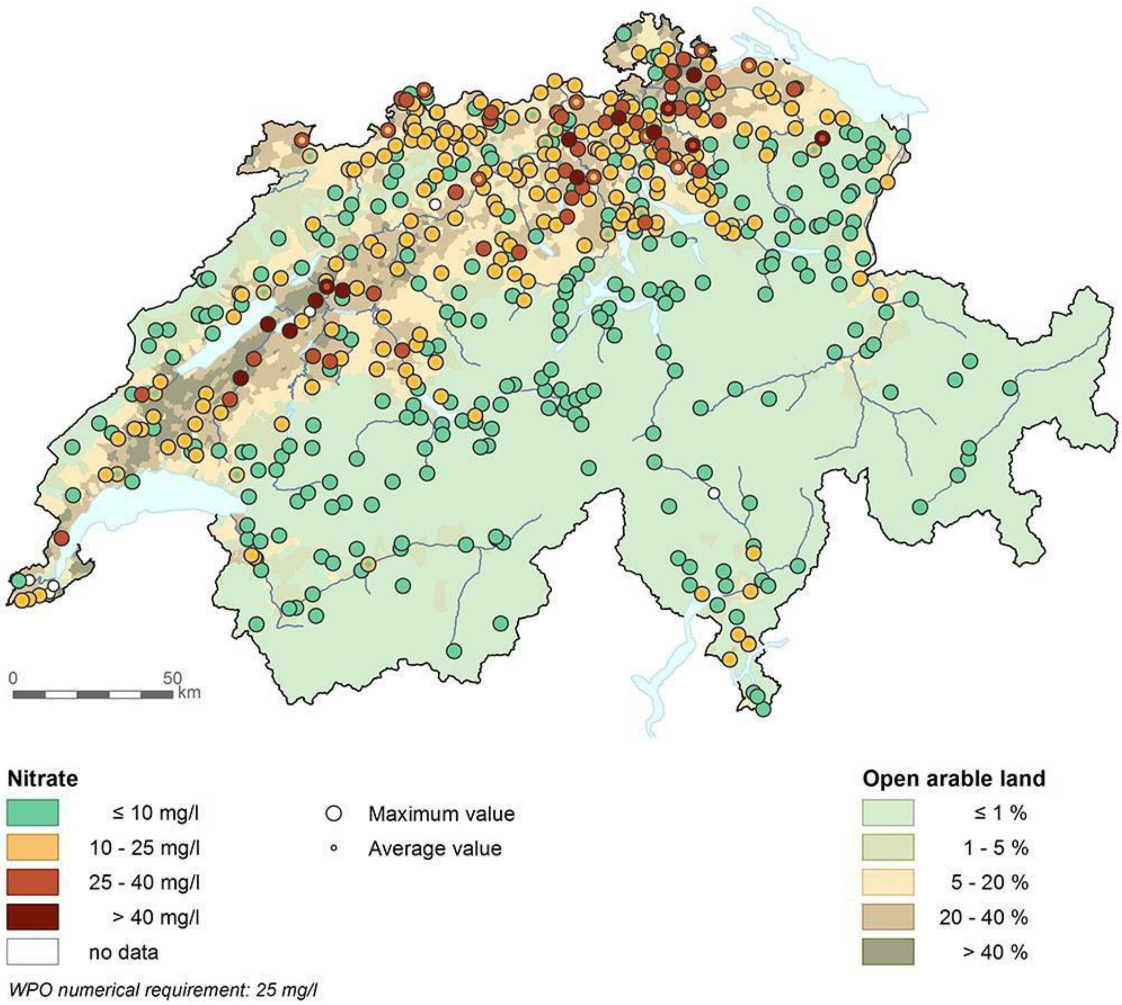


Figure 3. Nitrate in groundwater (2017) and open arable land. Maximum and average concentrations at each NAQUA monitoring site. Source: BAFU. https://www.bafu.admin.ch/bafu/en/home/topics/water/info-specialists/state-of-waterbodies/state-of-groundwater/groundwater-quality/nitrate-in-groundwater.html

In the region Gäu-Olten, the nitrate concentration of the groundwater increased steadily above the quality objective of 25 mg $L^{-1}$ in the 1980s and almost reached the limit of tolerance (40 mg $L^{-1}$) at the pumping station Neufeld in the late 1990s. The aquifer of the Gäu region extends over an area of 41 $km^2$ below the Dünnern valley between Walliswil and Olten. It is fed mainly by infiltration of rainwater from the surface (Hunkeler et al., 2015). There are eight pumping stations extracting drinking water from the aquifer (Purtschert and Hunkeler, 2015). In the year 2000, due to the increased nitrate concentrations, the involved stakeholders, namely the environmental agency of the Canton Solothurn, the pump station operators, and the farmers of the region, began the nitrate project, and a Nitrate Commission was established to accompany the project. It is the largest nitrate project in Switzerland comprising an area of 1000 ha and includes measures for the agricultural practice to avoid nitrate loss in the region. These measures comprise reduced tillage, ground cover during the winter and adjustment of the crop rotation according to the Nitrate Index. It calculates an index for the potential nitrate leaching from agricultural fields according to the specific land management practice. It consists of the basic value (Basispunktzahl) depending on the combination of the previous and the current crop. The basic value is corrected for tillage, time of sowing and type of winter ground cover. The corrected value is calculated for each field and multiplied by the area of the field. All field specific indices are summed up and divided by total farm area to obtain the average nitrate leaching potential for the farm. The smaller the calculated index value, the lower the leaching potential. Within the project, the farmers can decide which measures they implement. They are compensated if they reach a Nitrate Index of either 23 or 25, depending on their contract. By the end of 2013, 136 ha were converted to extensive grassland, 506 ha reached the Nitrate Index of 23 and 364 ha reached the Nitrate Index 25.

Contrary to model simulations at the beginning of the project (Geotechnisches Institut/TK Consult, 1999), the nitrate concentrations did not decrease at a sufficient rate, but rather leveled out at above 25 mg $L^{-1}$, and at the pumping station Neufeld, nitrate concentrations were still close to 40 mg $L^{-1}$ in 2015(Hunkeler et al., 2015). A hydro-chemical investigation of the aquifer by Hunkeler et al. (2015) found that the age of the groundwater was higher than expected. On average, the water needed 5-22 years from the soil surface to the pump stations. This could explain a greater lag in the response of nitrate concentrations in the groundwater to the implemented measures. They also found a lower dilution effect than expected. The aquifer is fed mainly by infiltration of nitrate rich water from the surface (55%). Nitrate poor water from inflowing streams makes up only 45%. Thus, the nitrate rich water is not diluted with nitrate poor water at the rate that was expected (Hunkeler et al., 2015). In 2017, the 4-year project 'NitroGäu' began as a joint research project to evaluate and further develop the Nitrate Index and analyze the processes of nitrate leaching in the region Gäu-Olten. The project had two main objectives:

1. Evaluation of the effectiveness of the Nitrate Index and its control measures
2. Development of additional measures for agricultural practices to improve N efficiency and reduce nitrate leaching.

In the Gäu region, eleven fields on eight different farms were selected according to soil type, planned crop rotation and agricultural practice. The fields had been cultivated according to the measures of the nitrate project with a Nitrate Index of 23. Six fields were compared with regard to differences between organic and conventional cultivation (BIK), and six fields were used to study hydrological processes of the soil and the unsaturated zone (HYD). One field was assessed for both aspects. On all fields nitrate leaching was measured using Self- Integrating Accumulators (SIA). They are cylinders containing an anion exchange resin which adsorbs and immobilizes nitrate from the seepage that passes through them (Bischoff, 2007). In addition, $N_{min}$ samples were taken at the depth of 0-30 cm, 30-60 cm and 60-90 cm in October and February each year. The nitrogen balance for each field and year was calculated using farm specific data on fertilization and N concentrations of organic fertilizers, estimates of atmospheric N deposition, BNF, and N content of the harvested material.

In 2019, additional measures to decrease nitrate leaching were implemented on the HYD fields. These focused on the fertilization of the fields, as this factor was not included in the Nitrate Index. The largest area of the fields was fertilized as usual (control), while one strip received a revised fertilization rate of around 80-100% N compared to the control. On a second strip, fertilization rate was reduced further, or alternative fertilization techniques were tested.

This study was conducted as part of the synthesis of the NitroGäu project. The purpose was to extrapolate the observed nitrate leaching results from field to regional scale. Additionally, the farm-gate balances of the selected farms were calculated and compared to the corresponding Suisse Balances. Another goal were scenario analyses using the Farm Model and the DAISY model to assess the mitigation potential of additional measures. Both models were run on five of the eight fields with the actual management information of 2018 and 2019. Simulated results were compared to the corresponding measured results from the NitroGäu project to assess the models' accuracy. Unfortunately, the results yielded from either model in the simulations did not accurately and reliably match the observed results of nitrate leaching. Therefore, scenario analyses were not attempted.

The following hypotheses were formulated:

(1) The calculated farm-gate budgets will show higher N balances than the Suisse Balances.
(2) The Farm Model will show higher results of nitrate leaching than the SIA measurements, due to the estimation of potential leaching.
(3) Nitrate leaching simulated by DAISY will correlate with the SIA measurements, when the model is calibrated.
(4) Due to the high relative nitrate leaching and the large area under winter wheat, an adjustment of the crop rotation of the Gäu region could decrease nitrate leaching.

# 2. Materials and Methods

## 2.1. NitroGäu project

### 2.1.1. Description of the selected farms

In 2017, the 4-year joint research project ‘NitroGäu’ was initiated to evaluate and further develop the Nitrate Index and analyze the processes of nitrate leaching in the region Gäu-Olten in the canton Solothurn. Eight farms were part of the project of which four were selected for this study, B3, B4, B5 and H2. B3 was an organically managed farm, while the others were under conventional management. B3, B4 and B5 were located near Niederbuchsiten, while H2 was situated near Kappel.

B3 was a dairy farm with around 65 dairy cows with an average milk yield of 6,000 liters per cow per year (Table 1). The farm cultivated 27ha of land with the main purpose of fodder production, mainly growing silage maize and winter wheat in rotation with grass clover leys. The farm B4 changed its production type from dairy to cattle fattening between 2018 and 2019. In 2018, it had 16 dairy cows with a milk yield of 5,500 liters per cow per year. In 2019, dairy production was replaced with calf fattening. There were three production cycles per year, each with around 55 calves being bought in at about 80kg liveweight and fattened for roughly 110 days up to 200kg liveweight. Additionally, the farm cultivated around 16ha of land with crop rotations including cereals, silage maize, a small share of potatoes and grass clover leys. The farm B5 did not have animal husbandry and cultivated 21ha of land. Its crop rotation included cereals, silage maize and temporary grassland. H2 kept around 18 dairy cows with a milk yield of 7,800 liters per cow per year. On the arable land winter barley, spelt, winter rapeseed, silage maize, potatoes, and grass clover leys were grown.

Table 1. Overview of the selected farms B3, B4, B5 and H2 with corresponding animal numbers and area of arable land and grassland.

| **Farms** | **Animals** | **Arable land [ha]** | **Grassland [ha]** |
|---|---|---|---|
| B3 | 65 dairy cows | 11 | 16 |
| B4 | 16 dairy cows (2018), 165 fattening calves | 14 | 2 |
| B5 | No animal husbandry | 18 | 3 |
| H2 | 18 dairy cows | 34 | 19 |

### 2.1.2. Description of the selected fields

For the NitroGäu project, eleven fields of the eight farms were selected according to soil type, crop rotation and agricultural practice. Six fields were compared with regard to differences between organic and conventional cultivation (BIK), and six fields were used to study hydrological processes of the soil and the unsaturated zone (HYD). One field was assessed for both aspects (HYD1). Out of these eleven fields, six were selected for this study, on the basis of availability of further information (Figure 4). HYD2 is a synthesis of fields HYD2 and HYD3, as these fields were initially one field with the same crop rotation and management.

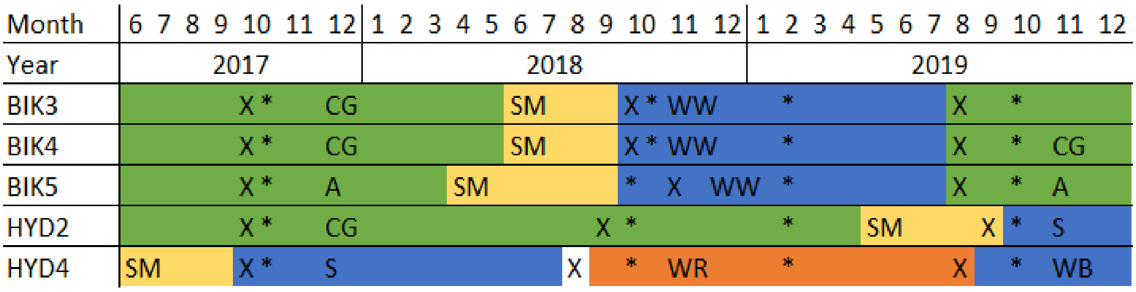


Figure 4. Crop rotation, SIA-changes, and Nmin sampling of the selected fields BIK 3, 4, 5, HYD 2, 4. X represents change of Self-Integrating Accumulators (SIA). * represents Nmin sampling. The crops are Alfalfa (A), Grass Clover Leys (CG), Spelt (S), Silage Maize (SM), Winter Barley (WB), Winter Rapeseed (WR), and Winter Wheat (WW).

HYD2 and 4 belong to the farm H2. BIK3, 4, and 5 are fields of the farms B3, B4 and B5, respectively. The soils were classified as silty loams. Annual mean temperature of the region is 9.0°C (1981-2010) and annual precipitation is 1129 mm. In the analysis years of this study (2017-2019), annual mean temperatures were above, and precipitation was below average, with the year 2018 being especially warm and dry.

The fields were part of the initial nitrate project of the canton Solothurn which was established in the year 2000 with the goal to decrease nitrate leaching to the groundwater. Thus, the fields had been managed according to the guidelines of the project, namely reduced tillage, and soil cover during the winter. Furthermore, the farmers adjusted their crop rotations to reach a Nitrate Index of 23. Fertilization was not an influencing factor in the Nitrate Index. To evaluate a potential future inclusion of this factor, different fertilization treatments were implemented in 2019 on the fields HYD2 and 4 (Table 2). The largest area of the fields was fertilized as usual (control), while on one strip (M1), the fertilization rate was reduced by around 20%. On the second strip (M2) of HYD2, fertilization was further reduced by 54% compared to the control. On the M2-strip of HYD 4, CULTAN fertilization (Controlled Uptake Long Term Ammonium Nutrition) was tested. CULTAN was first described by Sommer (2001) as a method where the required N fertilization for a crop is given as one application in the beginning of the vegetation period in form of an ammonium depot at the root zone.

Table 2. Applied amount of nitrogen fertilizer on fertilization treatments (Control, M1 and M2) on the fields HYD2 and HYD4 in 2019 in kg available N $ha^{-1}$.

| Field | Control | M1 | M2 |
|---|---|---|---|
| HYD2 | 138 | 110 | 64 |
| HYD4 | 140 | 109 | 100 (CULTAN) |

### 2.1.3. Field and laboratory methods

Nitrate leaching was monitored using Self-Integrating Accumulators (SIA), $N_{min}$ sampling and suction cups. SIA are cylinders containing an anion exchange resin developed by Terraquat. They are placed at the side of an excavated pit under undisturbed soil at a depth of roughly 1m. The anion exchange resin adsorbs and immobilizes the target solute from the seepage passing through the cylinder (Bischoff, 2007). In this project, three soil pits were established per field and strip, each containing four SIA which remained in the soil for approximately one year (Figure 4). They were changed between harvest of the previous and sowing of the next crop. After their excavation, the leaching rate was determined in the laboratory by desorbing nitrate from the exchange resin and measuring its concentration using the 'Smartchem 450 Discrete Analyser'. The results were then converted to nitrate load per year (kg $NO_3$-N $ha^{-1}$ $a^{-1}$) based on the surface area of the SIA. On the fields HYD2 and 4, suction cups (SIC20 from UMS Meter) were installed and samples for determination of nitrate concentration in seepage were collected monthly from May 2018 onwards.

Soil samples were taken at ten sites per field at a depth of 0-30 cm, 30-60 cm and 60-90 cm in October and February each year, except February 2018 when the soils were too wet. From the samples, mineral nitrogen ($N_{min}$), in form of nitrate, nitrite and ammonium, was extracted using 0.01M $CaCl_2$ and its concentration determined using the 'Smartchem 450 Discrete Analyser'. Additionally, water content and bulk density of the samples were ascertained and used to convert the $N_{min}$ concentration to $N_{min}$ content (kg N $ha^{-1}$). In October 2019, the soil samples were used for additional soil analyses. For each horizon, a CN-analysis by direct combustion (Vario Max Cube C/N Analysator) was conducted, quantifying total soil carbon, soil organic carbon and total soil nitrogen content. Additionally, the soil texture was evaluated using laser diffraction (Mastersizer 2000, Malvern). On the fields HYD2 and 4, bulk density was also determined using additional cylindric soil samples.

Crop yields were determined by manually harvesting either a certain number of plants (in the case of maize) or harvesting a certain area, analyzing the dry matter content, and extrapolating the results to one hectare. Furthermore, the N content of the sampled plants was determined by dry combustion. In the case of grass clover leys, fractions of grasses, legumes and herbage were separated, and their individual N contents determined. Biological nitrogen fixation (BNF) of the legumes was estimated using two assumptions. The first was that 86% of the legumes' N content originated from atmospheric $N_2$-fixation (Oberson et al., 2013) and secondly, that below ground biomass was roughly 70% of above ground biomass. Additionally, manure samples were taken from the farms and their dry matter content, pH, organic carbon and nutrient composition were determined. These values, along with data on mineral fertilization by the farmers, were used to summarize the fertilization management of each field for the analyzed period (2017-2020).

## 2.2. Nitrogen Budgets: Suisse Balance and Farm Gate Balance

For this project, the Suisse Balances (SB) of the selected farms were collected. They serve as a planning tool for farmers and a regulatory instrument for the controlling services (Bosshard et al., 2012). As mentioned earlier, an even SB in nitrogen and phosphorus is needed to receive direct payments. Therefore, SB is calculated annually for each farm. It considers nutrient imports and exports to and off the farm, as well as on-farm nutrient flows. The principle of the SB is to estimate availability of on-farm manure according to animal numbers and subtract from it the nutrient demand of the crop production. This interim balance shows the farm's nutrient self-sufficiency and the amount of nutrients that should be imported (or exported) in form of organic, mineral, and recycling fertilizers. The imports and exports of fertilizers are then taken into account for the total balance and the overall relative nutrient supply of the farm (Agridea and BLW, 2015).

In order to estimate the availability of on-farm manure, the number of animals, divided into different age groups and level of productivity, are linked to reference values of excretion according to Richner and Sinaj (2017). The availability of manure is corrected for the time the animals spend outside either in a yard or on pasture. Here it is assumed that 95% of the fraction of manure produced in the yard and 30% of manure produced on pasture is available for fertilization. The nitrogen from on-farm manure is further corrected for inevitable losses from the livestock housing and manure storage. Then, the farm-specific nitrogen utilization level is calculated from a basic utilization level of 60%, the farm-specific percentage of open crop land and the fraction of solid manure, resulting in available manure-N which is later used in the calculation of the balance. Animal numbers are also used to estimate feed demand of the farm, which is compared to on-farm feed production corrected for imported and exported feedstuff. Concentrate feed is generally only considered for dairy cows. The nutrient demand for the crop production is estimated according to area and yield of the different crops and their nutrient demand according to Richner and Sinaj (2017). The crop production's nutrient demand has a margin of error of 10%, which is included in the total balance. Relative nitrogen supply is then calculated as the ratio between N surplus and N demand (Agridea and BLW, 2015).

Most values are self-declared estimates by the farmer, such as yields, animal numbers, and imported fertilizers. Reference values from Richner and Sinaj (2017) are used to estimate nutrient content of manure, digestate and nutrient demand of crops. For some values, especially the correction factors and the margin of error, there are no references known (Bosshard et al., 2012).

The farm gate balance is a nutrient budget that uses the farm gate as its system boundary. The nutrient content of the inputs entering and outputs leaving the farm are considered in the calculation. On-farm nutrient flows are not considered. Main inputs include seeds, imported fertilizers, biological nitrogen fixation, N deposition, animals, feedstuff, and straw. Main outputs include sold plant and animal products and exported fertilizers. Nutrient output is subtracted from nutrient input for the balance (Oenema et al., 2003).

For this work, the farms' SBs were 'converted' to FGB as this is seen as a more comprehensive balance (Bosshard et al., 2012). For additional information, the farms' plot sheets of the analyzed fields and years were collected. They contain the dates of all soil cultivation measures, as well as of sowing and harvesting and dates, amounts and types of fertilizers and pesticides applied for each crop. The farm gate balance of the analyzed farms was calculated using the Excel-tool 'NutriGadget' (Reimer et al., 2020b). Values such as import of organic and mineral fertilizer and crop yields were derived from the farms' Suisse Balances and plot sheets. The rest of the entries, such as import of concentrate feedstuff and purchases and sales of animals were inquired from the farmers in personal correspondences. Nitrogen content of the inputs and outputs were derived, if not already incorporated in the program, from references such as the Gruber feeding tables (LfL, 2021) and mineral fertilizer nutrient contents. The NutriGadget estimates BNF according to standard values for different types of legumes and their yield levels. For legume mixtures, such as grass clover leys, the share of legumes is another considered factor. Inputs and outputs, as well as the N balances of the farms' SBs and FGBs were compared and presented graphically using R (R Core Team, 2020). For the comparison, the results of the SB were restructured to fit an input-output representation. Inputs included nitrogen from on-farm organic and imported fertilizers. Outputs were crop N demand and N from exported organic fertilizer.

## 2.3. Nitrate Leaching Models

### 2.3.1. Farm Model

The Farm Model (FM) is a Life Cycle Assessment (LCA) model in development at FiBL Switzerland. It is an Excel tool, assessing a farm's impact on the environment using 13 indicators, such as greenhouse gases (GHG), terrestrial, marine, and freshwater eutrophication and acidification. Both, the crop, and animal production of the farm are taken into account (Figure 5).

There are six sub models calculating the plants' phosphorus (P), nitrogen (N), carbon dioxide ($CO_2$) and heavy metal emissions, as well as the livestock's nutrient requirements, and emissions from enteric fermentation and manure management. Basis for these calculations are the user's data inputs and aligned reference data, such as nutrient compositions of organic and mineral fertilizers. The results of the sub models, as well as reference data from the ecoinvent 3.5 inventory (Frischknecht et al., 2004, ecovinvent, N.A.) are then used for the life cycle impact assessment.

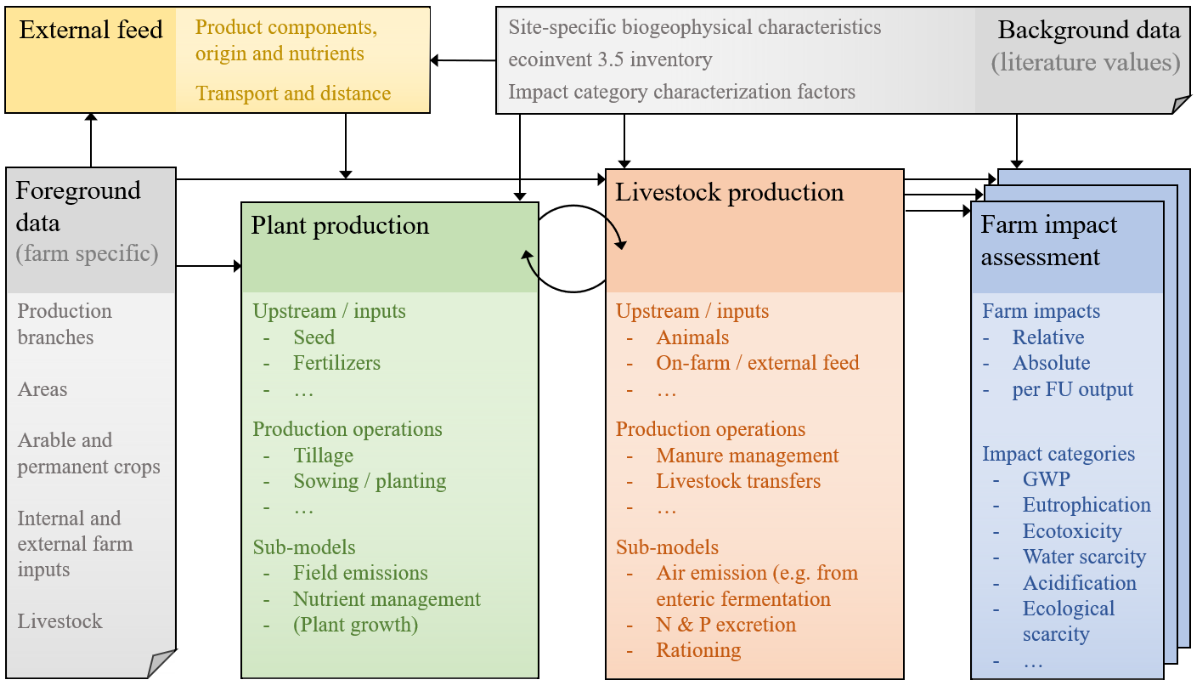


Figure 5. Schematic overview of the Farm Model. Source: FiBL, unpublished

At the center of data entry, there are two interconnected modules, namely the animal and the plant production. The connecting factors are the on-farm manure used as fertilizer for the crop production, and the animal feed, which is produced on the farm. These factors are automatically allocated to the other production cycle. Their quantity is determined by reference values on crop and animal nutrient requirements. Under- or oversupply of nutrients in either production cycle needs to be compensated by import or export of nutrients in form of fertilizers or feedstuff.

In this study, the animal husbandry module was excluded from the simulation. Nitrate leaching was estimated using the nitrogen model. Data entries include information on nutrient inputs from mineral and organic fertilizers, grazing, atmospheric N deposition and from BNF. Outputs mainly stem from nutrient removal from harvest. Nitrogen emissions are calculated based on Meier et al. (2012) and Meier et al. (2014). Apart from the N inputs and N exports, the model also considers the nitrogen fluxes in the soil (Figure 6).

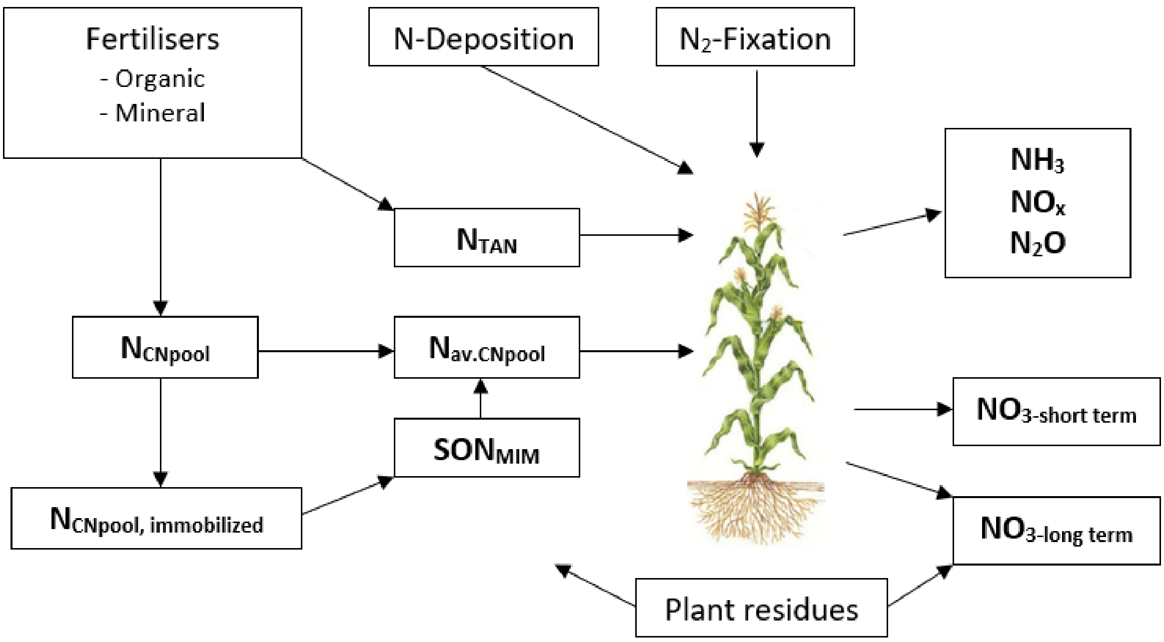


Figure 6. Nitrogen cycle considered in the Farm Model. $N_{TAN}$ = total ammoniacal nitrogen, $SON_{MIM}$ = management induced mineralization of soil organic nitrogen, $N_{CNpool}$ = nitrogen in C-N pool, which can be divided into $N_{av.CNpool}$ = nitrogen in short-term available C-N pool, and $N_{CNpool,\ immobilized}$ = immobilized nitrogen. Maize drawing: https://phys.org/news/2016-06-amazing-genetic-diversity-maize.html

Nitrogen inputs include fertilizers, BNF, and N deposition. N deposition is set at 25 kg N $ha^{-1}$, as suggested in (Rhim and Achermann, 2016). BNF is estimated depending on legumes grown and their respective reference rates of fixation. Mineral fertilizers are recorded by amount of N applied. Organic fertilizers can either be allocated according to availability of on-farm manure, as described above, or entered manually. In that case, the total amount of manure in $m^3$ or tons is entered, and nitrogen content is calculated according to a reference nutrient composition of the manure. The composition is influenced by the animal production cycle but can also be changed manually. Nitrogen from organic fertilizers is divided into total ammoniacal N ($N_{TAN}$), which can be taken up by the crop and N which is not readily available for plant uptake. Mineral fertilizers only contain $N_{TAN}$.

Nitrogen, which is not readily available for plant uptake, is assumed to enter the C-N pool. From there, the model differentiates two pathways based on a soil organic carbon sequestration model by Favoino and Hogg (2008). They suggest two pools, one of short-term available C and N and one containing the immobilized fractions. N immobilization is closely related to the change in soil organic carbon. Both processes have not yet been implemented in the model. Management induced mineralization of soil organic nitrogen is calculated according to Brock et al. (2012). Plant nitrogen uptake is estimated according to yield and reference N content of above- and below-ground biomass of the particular crop based on IPCC (2019). In the model, the harvest is further differentiated into main and by-product and respective N content. Nitrogen not taken up by plants and removed from the field by harvest, can potentially be lost from the system, either by volatilization or leaching.

Gaseous emissions include ammonia ($NH_3$), nitrogen oxides ($NO_x$) and nitrous oxide ($N_2O$) emissions. $NH_3$ emissions occur from the $N_{TAN}$ – fraction of fertilizers and were calculated here using the amount of fertilizer and their type specific emission factors of IPCC (2019). The Farm Model calculates direct and indirect $N_2O$ emissions and differentiates between emissions from $N_{TAN}$ and from the available C-N pool. The emission factors are based on the 2018 reporting tables (CRF) of the Swiss Greenhouse Gas Inventory (BAFU, 2020). Nitrate leaching is differentiated into short-term and long-term losses from the nitrogen fraction $N_{TAN}$ and from the available C-N pool respectively, where long-term losses can occur over a period of several years. A description of the N cycle including the equations can be found in Appendix 2.

The FM was used to model nitrate leaching from the five selected fields during 2018 and 2019. On the fields HYD2 and 4, the additional mitigation measures were also modeled. For each field, information on the crops grown, such as product use (food, animal feed or seed production), number of harvests per year and yield of the main and the by-product was entered. In a next step, fertilization was described. The model differentiated between liquid and solid manure, mineral fertilizers, and nutrient input from grazing. Grazing was not applicable on the selected fields. Farm-specific nitrogen composition of the organic fertilizers was derived from the manure analyses. BIK5 is the only farm importing all of its organic fertilizers. Information on their nutrient composition were taken from the farm's SB. Amount of fertilization was taken from the plot sheets, while crop yields were derived from the yield survey or in the case of maize on BIK4 and 5 from the farms' SBs, as the values of the yield survey were very high.

BNF was estimated according to the yield survey. The model evaluates emissions from each crop individually.

### 2.3.2. DAISY Model

DAISY is a mechanistic soil-plant-atmosphere system model, first developed at the Royal Veterinary and Agricultural University (now Faculty of Life Sciences, University of Copenhagen) in the late 1980s (Hansen et al., 1990). It can model water, heat, carbon, and nitrogen balances in agricultural systems, as well as pathways of pesticides. For these purposes, the model simulates plant growth, biogeochemical processes in the soil, and the bioclimate. The simulation is driven by weather and management data and is typically applied at field scale, as this is the fundamental management unit in crop production (Hansen et al., 2012) (Figure 7). DAISY consists of four major, interconnected models, namely the hydrological, soil organic carbon, nitrogen and crop model (Jabloun et al., 2018) which are shortly described below.

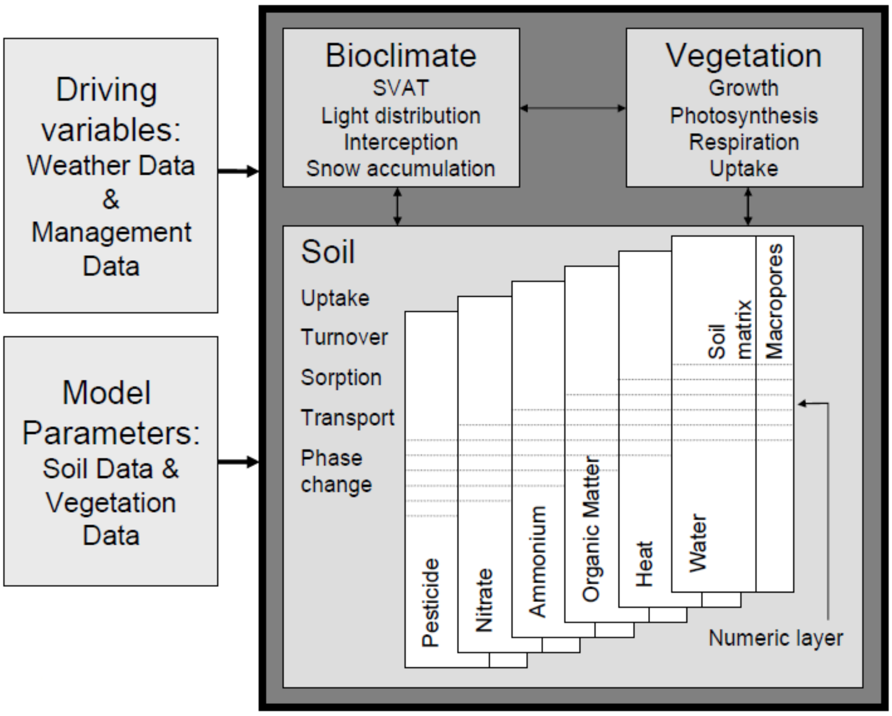


Figure 7. Schematic overview of the DAISY model. Source Hansen et al. (2012).

#### *Hydrological model*

DAISY simulates the hydrological processes of a crop production system (Figure 8). The water balance is fed by precipitation and irrigation and depleted by evapotranspiration. Precipitation is separated into snow- and rainfall. Snow can accumulate in a snowpack from where water can percolate further towards the soil. Rainfall can accumulate as ponded water on the soil surface if precipitation exceeds infiltration and evaporation. The rainfall can be intercepted by the canopy from where it can drip off when its capacity is exceeded. Canopy structure is also simulated in DAISY (see below). Throughfall and drip off can again be intercepted by a litter layer before reaching the soil surface (Hansen et al., 2012).

Once infiltrated into the soil, soil water can be stored in the soil matrix and in macropores. Water dynamics in the soil matrix are described using Richard's equation, while water flow and transfer between macropores and soil matrix is simulated by Darcy's law. The rate of water entering and leaving macropores depends on the surrounding soil's capacity to supply and receive water (Hansen et al., 2012, Rasmussen et al., 2015). Water may evaporate from any of the given stages (snowpack, canopy, litter, soil surface, and soil, including transpiration from plants). With daily weather data, DAISY chooses a model for the simulation of evapotranspiration which relies on potential (maximum) and reference evapotranspiration of a given crop (Hansen et al., 2012). Water uptake by vegetation is simulated using a water extraction model with a single root approach as described in Hansen and Abrahamsen (2009). The premise is that uptake is governed by water flow toward the root surface. The lower boundary of the soil system is defined by the depth of groundwater. A fixed or fluctuating groundwater table can be defined or free drainage conditions are assumed (deep groundwater) (Hansen et al., 2012).

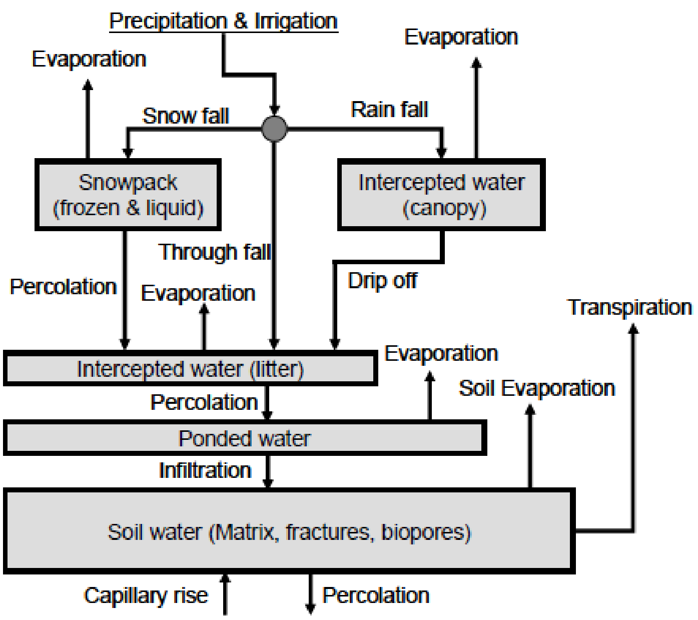


Figure 8. Schematic overview of the hydrological model of DAISY. Source*:* Hansen et al. (2012).

### ***Soil organic carbon model***

DAISY distinguishes between three main types of soil organic carbon: the soil microbial biomass (SMB), responsible for turnover processes, the added organic matter (AOM), stemming from organic fertilizers or plant residues etc. and the soil organic matter (SOM), containing all other organic carbon. Each type is further divided into two pools, one with a relatively fast, and one with a slower turnover rate. For SOM, there is an additional inert pool considered. For each organic matter input, a new set of AOM pools is created (Jensen et al., 1997, Hansen et al., 2012).

Carbon can be lost as $CO_2$ from the SMB pools from maintenance respiration and during turnover processes. These processes depend on the substrate-specific utilization efficiency. Maintenance respiration rate, as well as decomposition rates of all pools depend on soil moisture content and soil temperature. In the slow and fast SOM pool, as well as the slow SMB pool, an additional influencing factor is clay content of the soil, representing a physical barrier against decomposition processes. Nitrogen flows are calculated according to the C flows and pool specific, fixed C/N ratios (Jensen et al., 1997, Hansen et al., 2012).

### ***Nitrogen model***

DAISY considers organic nitrogen in plant tissue, litter, organic fertilizers and as soil organic nitrogen. Ammonium ($NH_4^+$), and nitrate ($NO_3^-$) are the mineral forms considered, present in atmospheric deposition, fertilizers, and in the soil solution. Ammonium can additionally by sorbed to soil particles (Hansen et al., 2012) (Figure 9). Main nitrogen inputs are atmospheric deposition, fertilization, BNF, and addition of organic matter. Atmospheric N deposition, BNF and fertilization will be described later, along with the weather data, crop calibration and management data. Organic matter from plant residues and organic fertilizers on the soil surface can be incorporated into the AOM pools either by tillage operations (see below) or by biological activities. Bio-incorporation rate is influenced by upper soil temperature and the C/N ratio of the organic substrate. In the process, carbon is lost as $CO_2$. Crops can take up ammonium and nitrate from the soil solution, thus being dependent on water flow towards the root surface. N uptake, as well as water uptake follows the single root concept with the main mechanisms being convection and diffusion (Hansen et al., 2012).

The processes of mineralization and immobilization of N are closely related to carbon turnover. N pools are adjusted along with their corresponding C pools according to a pool-specific C/N ratio. Net immobilization and net mineralization are then calculated from the overall N balance. Mineralization and immobilization processes are dependent on N demand of the biomass for growth and on the C/N ratio of AOM, with a low C/N ratio initializing N mineralization and vice versa. Turnover processes inherently depend on soil temperature and moisture content, as well as clay content, as described above (Jensen et al., 1997, Hansen et al., 2012).

Furthermore, DAISY considers nitrification and denitrification processes. The nitrification rate is estimated using the Michaelis-Menten-kinetics, describing enzymatic activity according to substrate availability ($NH_4^+$) where the maximum nitrification rate depends on soil temperature and water content. Soil water content is used as an indicator for oxygen concentration in the soil. Denitrification is first calculated as the potential denitrification rate at optimal, anoxic conditions and with sufficient nitrate availability. This rate is then corrected for actual oxygen-content in the soil, estimated according to soil water content. It is then further reduced according to nitrate availability, which is proportional to nitrate concentration in the soil. Solute transport, and therefore leaching of ammonium and nitrate is simulated in the solute transport model using the convection-dispersion equation (Hansen et al., 2012, Manevski et al., 2014). DAISY assumes that ammonium is sorbed strongly to clay particles and thus its leaching rate is very low (Hansen et al., 1990).

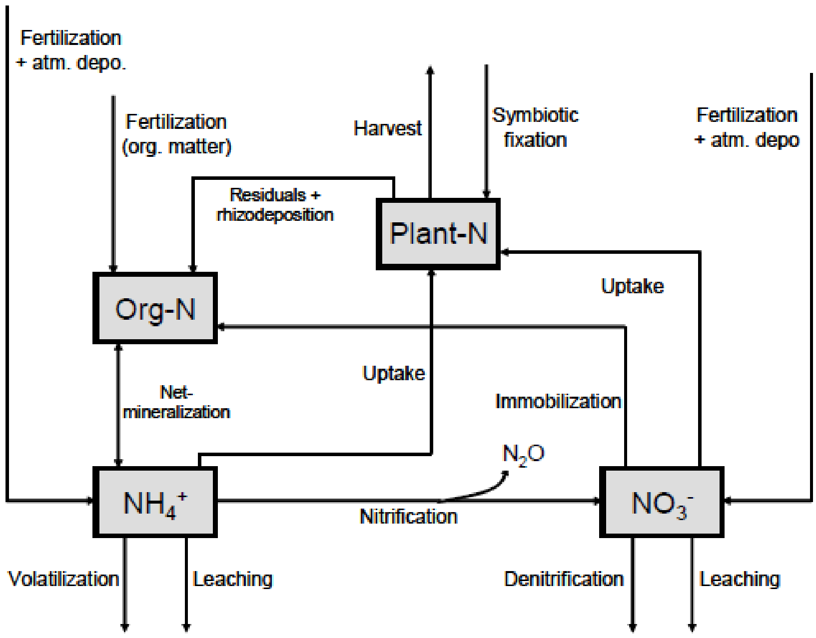


Figure 9. Schematic overview of the nitrogen model of DAISY. Source: Hansen et al. (2012).

### *Crop Model*

In the crop model (Figure 10), photosynthesis is the main driver for energy production in the crop and is described using a simple light response curve. Its rate depends on bioclimatic factors, namely temperature and light availability. Additionally, it is influenced by the crop's canopy structure, and by matter loss due to senescence and stress factors such as nitrogen and water deficiencies. The canopy structure is described by the leaf area distribution (LAD) which is dependent on plant height. This, in turn, depends on development stage and leaf area index (LAI). The LAI describes leaf area per ground area [$m^2\ m^{-2}$] and is an important measure for light interception. In DAISY, it is calculated using the specific light area index (SpLAI) and leaf weight. SpLAI represents the LAI per leaf dry mass [$m^2\ g\ DM^{-1}$]. In the case of intercropping, a composite canopy LAD is calculated using the individual crops' canopy LAD values. Assimilate obtained from photosynthesis is partitioned to the different plant organs, namely leaf, root, stem, and storage organ (grains and tuber) (Hansen et al., 2012). Canopy structure, nitrogen stress, partitioning, senescence, as well as leaf and root death are influenced by the development stage (DS) of the crop. DS represents the phenological development, which is divided into three main stages, emergence (DS=0), flowering (DS=1) and maturation (DS=2). The rate of development in the crop model is influenced by temperature and day length (Hansen et al., 2012).

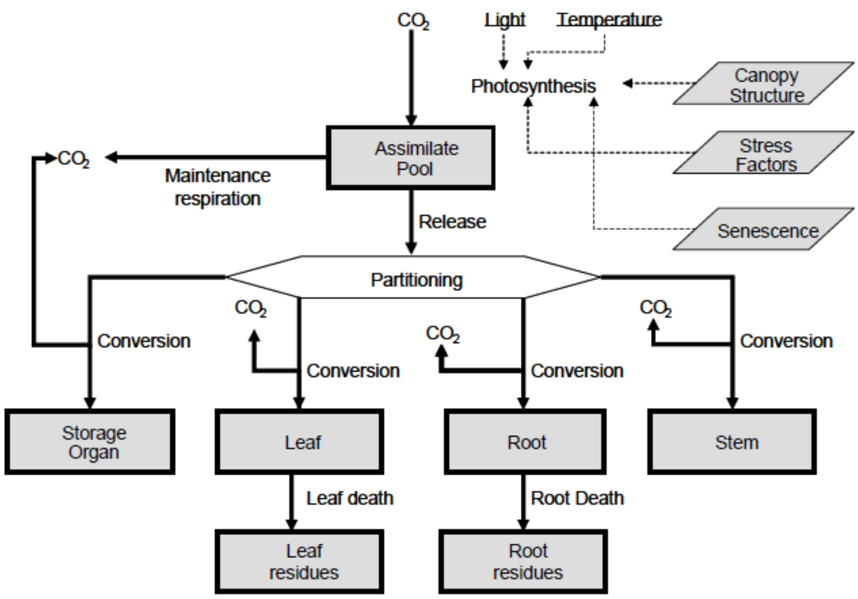


Figure 10. Schematic overview of the crop model of DAISY. Source*:* Hansen et al. (2012).

### *Application of the DAISY model*

In order to run a simulation with the DAISY model, the minimum data requirements of the driving variables, namely weather and management data, as well as of the parameters soil and vegetation need to be met. Background data on commonly used crops, tillage operations, and fertilizers are included in DAISY's data set. These background data can be changed, and calibrated, or new crops, tillage operations or fertilizers can be defined to better represent the actual conditions. Additionally, the simulation needs a time frame, meaning a start and end date. Lastly, simulation outputs need to be defined which, depending on the simulation purpose, can for example include results on harvest and the C- and N-balance at daily, monthly, or annual resolution (Hansen et al., 2012, Abrahamsen, 2020, Hansen and Abrahamsen, 2020).

In this study, the DAISY model was used to estimate nitrate leaching on the selected fields BIK3, 4, 5 and HYD2 and 4 between October 2017 and October 2019. The simulation was run with an extended warm-up period (starting in 2011 on BIK3, and 4, 2012 on BIK5 and 2013 on HYD2 and 4), which depended on available information. This is common practice, when using DAISY, although the extend of the warm-up period is not consistent among studies. It can reach from 4 years (Rasmussen et al., 2015) up to 10 (and more) years (Manevski et al., 2014). The general introduction manual (Hansen and Abrahamsen, 2020) suggests using one full crop rotation, at least however 4 years, as a warm-up period. The purpose is to make the simulation less sensitive to the initial soil conditions (Hansen and Abrahamsen, 2020).

The minimum requirement of meteorological data are daily values of average temperature, precipitation, and solar radiation (Hansen et al., 2012). The closest weather station to the selected fields was located in Wynau, canton Bern (47.255025 / 7.787475, MeteoSchweiz (2018)), around 4 to 8km beeline from the fields. It is located in a basin at 422 m above sea level and is part of the automatic monitoring network of MeteoSchweiz. Data for this study covered daily values of the time span between 17.12.2010 and 15.12.2020. Apart from average temperature, precipitation and solar radiation, the data also comprised wind speed, vapor pressure, and relative humidity. For the years of 2017, 2018, and 2019, reference evapotranspiration and minimum and maximum daily temperature, were supplied as well. There were three timespans (20.06.-04.07.13, 02.04.-04.04.19, and 14.07.-26.07.17), where precipitation values were missing. These were substituted by the subsequent values.

Soil properties in DAISY can be distinguished for different depths which can then be defined as horizons in a soil column. In this study, three horizons, 0-30 cm, 30-60 cm, and 60-90 cm, were defined according to sampling depth. Soil texture, namely clay, silt and sand fractions were used according to the analyses from the laser diffraction. Additionally, C/N ratio and

humus fraction were included. Humus fraction was calculated by multiplying the analyzed organic C content with the factor 1.72. On the fields HYD2 and 4, bulk density had also been analyzed and their values were included in the soil properties. On the BIK fields, bulk density from another field in close proximity was used, as no field specific values were available. On HYD2, hydraulic parameters for the two upper horizons were available.
In the soil column, the horizons were defined, as well as the lower boundary of the soil system, and the initial annual carbon input. On all fields free drainage was assumed, as the groundwater table is low (Hunkeler et al., 2015). An initial annual carbon input can be defined to improve the initial soil conditions. To estimate this value, an initial simulation with the given crop rotation was run without an initial carbon input. The resulting carbon balance estimated the total carbon input over the simulated period. This was divided by the number of years and given as initial annual carbon input in the final simulation run.

DAISY uses the manager model to define direct management actions, such as sowing, harvesting, fertilizing, or ploughing. Tillage operations, e.g. ploughing or disk harrowing, are further defined in a reference file. For each operation, working depth and the fraction of incorporation of organic matter from the surface are set. The action ploughing, includes the additional parameter ‘swap’ where two soil layers are swapped according to their depths (Hansen et al., 2012). For this study, a field cultivator action (‘grubber’) was added to the references and defined according to its working depth (~20 cm) and its incorporation rate (0.9). Several commonly used fertilizers with Danish reference values are also included in reference files. As the nutrient composition of organic fertilizers can vary greatly, and the mineral fertilizers used on the selected fields were not included in the reference file, fertilizers were newly defined. Mineral fertilizers are defined according to their ammonium fraction, while the rest of nitrogen is assumed to be nitrate. Organic fertilizers are parameterized by their dry matter fraction, total N and C fractions and the ammonium fraction of total N. If available, these values were derived from the manure analyses. Imported organic fertilizer parameters could be derived from the farms’ Suisse Balances or plot sheets, or from reference data, such as Richner and Sinaj (2017).
Management actions were added according to their date of application. Crop-specific management action can be defined and summarized in an activity. Activities of different crops can then be added up to a crop rotation. For this study, information on the fields’ crop rotation were collected from the farmers (Appendix 1). Exact data, in form of the plot sheets of 2014-2019 were retrieved for the fields BIK5, HYD2 and 4. For the fields BIK3 and 4, plot sheets of the years 2018 and 2019 were collected and information on crop rotation was given in personal

correspondence. Missing information of the plot sheets, such as exact dates, could usually be substituted by data from the yield survey or the farms' Suisse Balances.

Commonly used crops are also defined in reference files. Crops are described using several characteristics including development rate, photosynthesis, canopy structure, root development, partitioning and crop nitrogen. Each characteristic is defined by several parameters. These are calibrated for Danish conditions and often did not suit the conditions in this study. Therefore, crops were calibrated according to harvest and N content data from the yield survey. As substitute for grass clover leys, the crops ryegrass and white clover are both sown at the same time. Thus each crop needed to be calibrated individually while tracking the interactions between them. Spelt, grown on HYD4 did not have a reference file either, thus it was substituted with winter barley. Generally, six parameters concerning different characteristics were adjusted to calibrate the crops (Table 3).

Table 3. Overview of the parameters used for crop calibration in DAISY.

| **Parameter** | **Description** | **Unit** |
|---|---|---|
| DSRate | Development stage rate is the rate of phenological development, divided into DSRate 1 (development between emergence (0) and flowering (1)) and DSRate 2 (development between 1 and maturation (2)) | fraction |
| $F_m$ | $F_m$ is the photosynthetic rate at saturated light intensity, described by a function of temperature | g $CO_2$ $m^{-2}$ $h^{-1}$ |
| Qeff | Quantum efficiency is the light use efficiency at low light intensity | g $CO_2$ $m^{-2}$ $h^{-1}$ $(W\ m^{-2})^{-1}$ |
| SpLAI | Specific Leaf Area Index is a function of DS and is part of the description of the crop's canopy | $m^2$ g $DM^{-1}$ |
| Partit | Partitioning of assimilate defined for each plant compartment (storage organ, leaf, stem, root) depending on DS | fraction |
| CrpN | Crop nitrogen, potential, critical and non-functional limits of N concentration in each of the plant compartments | g N g $DM^{-1}$ |

The crops were calibrated individually for each field according to the yield survey. $F_m$, Qeff and SpLAI were the parameters used to adjust crop yield. There was generally a trend that the yields of cereals, in this case winter wheat (WW) and spelt/winter barley, were overestimated, while yield for silage maize and winter rapeseed were underestimated. The crop yield parameters were adjusted accordingly. Within the yield survey, dry matter yield and N content of the different plant parts, i.e. grain or tuber and vegetative material, were recorded. According to these values, partitioning (Partit) and crop nitrogen (CrpN) were adjusted. In the case of silage maize, the crop did not reach maturity in the suggested growing season. Therefore, DSRate was increased to better fit the actual phenological development.

Grass clover leys, as mentioned before, did not exist in DAISY as such. Ryegrass and white clover were sown at the same time, and interactions between the crops were considered in the simulation. The interactions complicated the calibration of the crops. They were calibrated according to the grass and legume fraction in the yield survey. Yields of both crops were higher than expected, especially when grown together, therefore the yield regulating parameters were decreased. Additionally, CrpN was adapted to fit N content of the yield survey and for white clover, the BNF factor was adjusted to 0.86, as used in the yield survey and suggested by Oberson et al. (2013). For crops which are harvested several times a year, there is a cut delay defined. This parameter was lowered for white clover as the crop did not recover the way it did on the field.

### 2.3.3. Comparison of the Results: SIA, Farm Model, DAISY

The results of the simulated nitrate leaching from the Farm Model and DAISY were compared to the measurements of the Self-Integrating Accumulators (SIA). These measured nitrate loads (kg $NO_3$-N $ha^{-1}$) of one SIA period. The first SIA period (2018) started in October 2017 with the installment of the SIA on the fields and ended depending on harvest time between August and November 2018. The SIA period 2019 followed the first and ended in August or September 2019 (Figure 4).

In DAISY, the output of the simulation was defined to contain N balances at field level on a monthly resolution. The results of nitrate leaching were summarized according to the SIA periods for each field to allow a comparison. The Farm Model estimated nitrate leaching for the individual crop and could therefore not be aligned with the SIA periods. Instead, the short-term nitrate leaching under the main crop of the SIA period was used for further analyses. Results of all three methods were presented graphically using R (R Core Team, 2020).

## 2.4. Extrapolation of the SIA Results to Regional Level

The SIA results from all fields of the NitroGäu project were extrapolated to the arable area that is part of the original nitrate project. Data on land use of all land under contract of the year 2020 was obtained from the Amt für Umwelt (Bureau for the Environment) Solothurn. The total arable land (including grass clover leys) made up 919ha of the total agricultural and horticultural area of 1394 ha. The NitroGäu project analyzed nitrate leaching under six of the main crops grown in the region, namely winter barley, winter wheat, spelt, silage maize, winter rapeseed, and grass clover leys. These crops covered an area of 796 ha in 2020 and thus made up 87% of the arable land. SIA results were grouped by crop and average nitrate leaching per crop was determined. Average nitrate leaching was multiplied with the total area of the crop, resulting in total nitrate leaching per crop. For each crop, its share of the total area, as well as of the total nitrate leaching was calculated. Additionally, the weighted average of nitrate leaching per hectare of the six crops was calculated. Along with the average seepage of roughly 470 mm $a^{-1}$ (Hunkeler et al., 2015), the nitrate concentration of the seepage under arable land was estimated.

# 3. Results

## 3.1. Nitrogen Budgets

The Suisse Balance (SB) and the Farm Gate Balance (FGB) differ in their methodology and thus in the nitrogen inputs and outputs included in the calculation (Figure 11 and Figure 12). The SB considers organic and mineral fertilizers for the N input. Here, organic fertilizers are divided into on-farm and imported fertilizers. The output consists of exported organic fertilizers and the nitrogen demand of the crop production. On the organically managed farm B3, N input consisted entirely of on-farm slurry and manure. Organic fertilizer was also exported from the farm. N inputs of all other farms included a combination of on-farm and imported organic fertilizers, as well as mineral fertilizers as the largest input factor. The farm B3 and B5 in 2019 showed negative N balances between 37 and 48 kg N $ha^{-1}$. N balances of the other farms were relatively even.
For the FGB, the inputs included bought-in live animals, imported feedstuff, straw, seeds, organic and mineral fertilizers, and biological nitrogen fixation (BNF). For the farm's outputs animal and plant products were considered, as well as the export of organic fertilizers. On all farms the nitrogen inputs of straw and seeds were marginal, together making up less than 5% of total N input. BNF contributed less than 10% of total N input, except on the farm H2, where it made up 17 and 12% in 2018 and 2019, respectively. On the farm B3, the main nitrogen input in the FGB was imported feedstuff, including concentrate feed, as well as grass silage and hay. Animal products and manure made up most of the farm's output, nearly to equal parts, while very little plant products were sold. On the other farms, mineral fertilizer made up a substantial part of the nitrogen inputs with at least 30% (B4, 2019) and up to 70% (B5, 2019) of total N input. On these farms, at least 50% of their output consisted of plant products with the rest being animal products. Organic fertilizers were not exported. The farm B4 changed their type of production from dairy to cattle fattening from 2018 to 2019, which could be observed in the changing composition of the inputs and outputs. In 2019, the share of imported feedstuff, as well as the export of plant products increased. N balances of the farms B4 and H2 were positive in both analysis years. The farm B3 showed a positive N balance in 2018 and a negative one in 2019, while results on B5 were the other way around, with a negative N balance in 2018 and a positive in 2019.

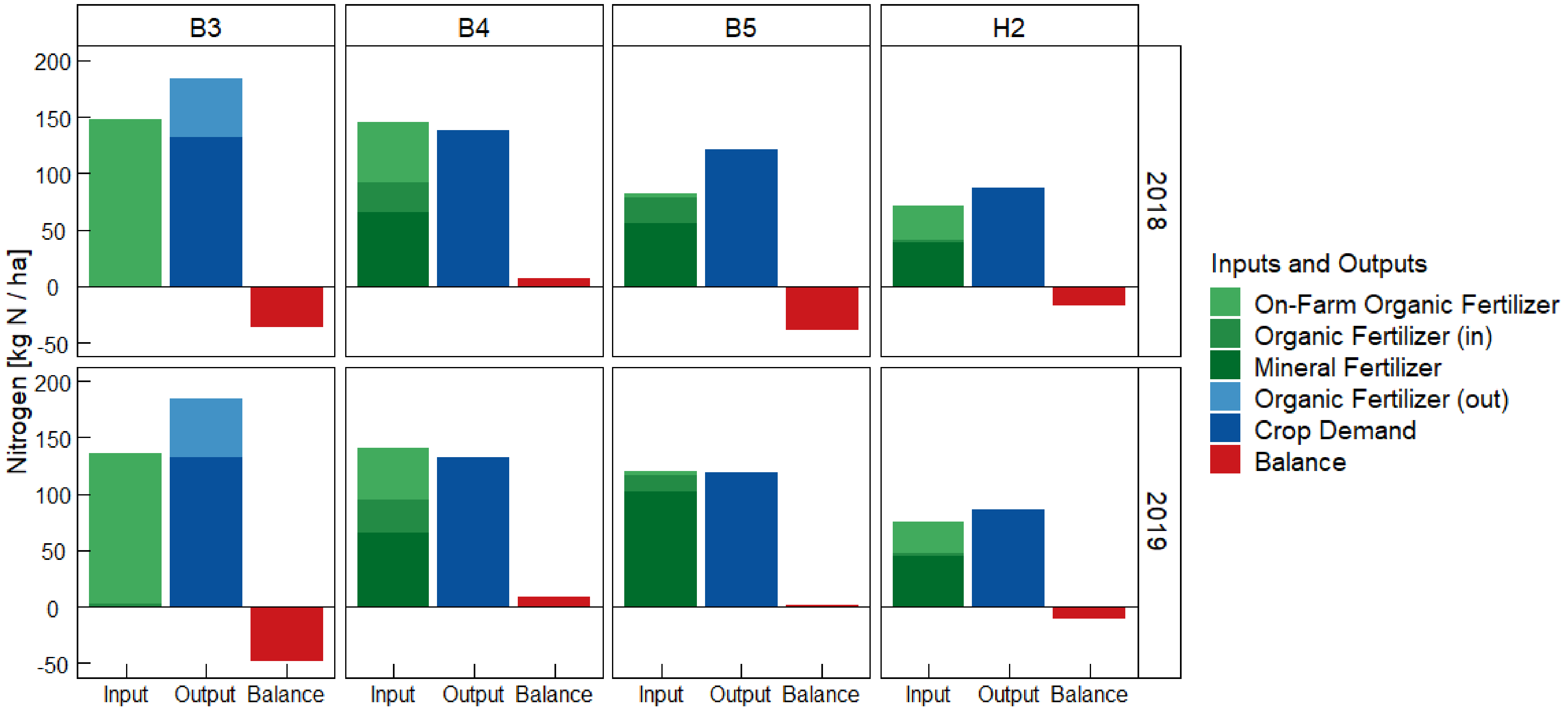


Figure 11. Nitrogen inputs, outputs, and balance of the Suisse Balances of the farms B3, B4, B5 and H2 in the years 2018 and 2019.

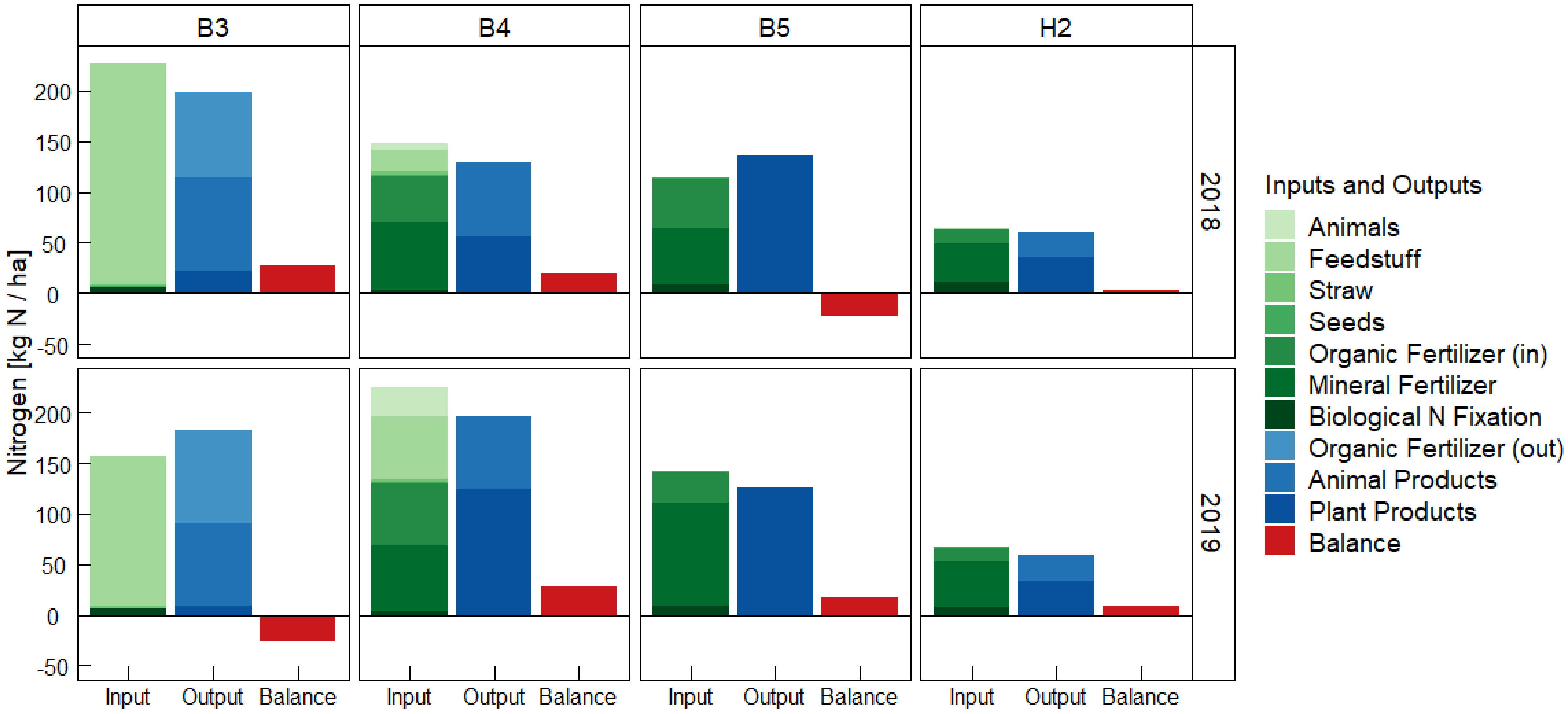


Figure 12. Nitrogen inputs, outputs, and balance of the Farm Gate Balances of the farms B3, B4, B5 and H2 in the years 2018 and 2019 calculated using NutriGadget.

The FGB generally showed more positive nitrogen balances and higher relative nitrogen supply compared to the SB results (Table 4). Altogether five out of eight SBs showed negative N balances, while the FGBs were negative only twice. Contrasting results of the two budget types were found on the farms B3 in 2018 and on H2 in both years. The largest difference between N balances of the FGB and the SB was found on B3 in 2018 (65 kg N ha$^{-1}$). On the other farms, the FGB, on average, showed N balances around 18 kg N ha$^{-1}$ higher than the SB. On all farms, except B4, the relative N supply calculated by the FGB was more than 10 % higher than that of the SB.

Table 4. Nitrogen Balance [kg N ha$^{-1}$] and Relative Nitrogen Supply [%] of the farms B3, B4, B5 and H2 in the years 2018 and 2019 from the Suisse Balances and the Farm Gate Balance calculations.

| **Year** | **Farm** | **Nitrogen Balance [kg ha$^{-1}$]** | | **Relative Nitrogen Supply [%]** | |
|---|---|---|---|---|---|
| | | Suisse | Farm Gate | Suisse | Farm Gate |
| 2018 | B3 | -37 | 28 | 72 | 114 |
| | B4 | 8 | 19 | 106 | 115 |
| | B5 | -39 | -22 | 68 | 84 |
| | H2 | -17 | 4 | 81 | 106 |
| 2019 | B3 | -48 | -26 | 64 | 86 |
| | B4 | 8 | 28 | 106 | 114 |
| | B5 | 2 | 17 | 102 | 113 |
| | H2 | -11 | 8 | 87 | 114 |

Relative Nitrogen Supply [%] shows the relationship between the nitrogen balance and the crop demand (SB) or output (FGB). Relative nitrogen supply above 100% corresponds to a nitrogen surplus (positive N balance), while coverage below 100% shows a nitrogen deficit (negative N balance).

## 3.2. Crop Calibration in DAISY

For winter wheat, spelt and the grass clover ley, yields and N contents simulated by DAISY were very similar to those determined in the yield survey (Table 5). Discrepancies between simulated and measured yields and N content arose in silage maize on all fields and winter rapeseed on HYD 4. Measured silage maize yields on BIK4 and 5 were above the Swiss average of 185 dt ha$^{-1}$ and 218 kg N ha$^{-1}$ nitrogen removal (Richner and Sinaj, 2017) which was not reached by the DAISY simulation. DAISY also registered that silage maize on BIK3 and 4 and HYD2_M2 suffered from nitrogen deficiency for around 21, 3.5 and 17 days, respectively. Noticeably, based on the yield survey, HYD 2 showed higher yield and N content on the M1 and M2 strips with lower fertilization levels than on the control strip. This reaction was not shown in DAISY, where yield and N content decreased with decreasing fertilization. Measured winter rapeseed yields on HYD4 were also above the Swiss average of 35 dt $ha^{-1}$ and 102 kg N $ha^{-1}$ (Richner and Sinaj, 2017). Again, yield and N content were higher on the treatment strips M1 and M2 compared to the control. Simulated results by DAISY were below Swiss average and did not differ between the fertilization treatments.

Table 5. Yield [dt DM $ha^{-1}$] and N content [kg N $ha^{-1}$] of the fields BIK3, BIK4, BIK5, HYD2 and HYD4 in the years 2018 and 2019 determined in the yield survey from the NitroGäu project and simulated by DAISY.

| Year | Field | Crop | Yield [dt DM $ha^{-1}$] | | N content [kg N $ha^{-1}$] | |
|---|---|---|---|---|---|---|
| | | | Yield survey | DAISY | Yield survey | DAISY |
| 2018 | BIK3 | Silage Maize | 192 | 145 | 180 | 126 |
| | BIK4 | Silage Maize | 277 * | 165 | 304 * | 156 |
| | BIK5 | Silage Maize | 218 * | 171 | 269 * | 168 |
| | HYD2 | Grass Clover Ley | 128 | 136 | 357 | 354 |
| | HYD4 | Spelt | 45 * | 44 | 72 * | 68 |
| 2019 | BIK3 | Winter Wheat | 49 | 50 | 117 | 113 |
| | BIK4 | Winter Wheat | 58 | 58 | 137 | 135 |
| | BIK5 | Winter Wheat | 51 | 51 | 121 | 124 |
| | HYD2_C | Silage Maize | 167 | 165 | 181 | 148 |
| | HYD2_M1 | Silage Maize | 186 | 164 | 202 | 136 |
| | HYD2_M2 | Silage Maize | 179 | 133 | 185 | 101 |
| | HYD4_C | Winter Rapeseed | 48 * | 29 | 163 * | 89 |
| | HYD4_M1 | Winter Rapeseed | 58 | 29 | 193 | 86 |
| | HYD4_M2 | Winter Rapeseed | 49 | 29 | 167 | 85 |

Yield and N content of winter rapeseed, spelt, and winter wheat are given as grain yield and grain N content.
* Values from the yield survey were substantially higher than Swiss averages from GRUD 2017 (Richner and Sinaj, 2017) and values from the respective farms' Suisse Balances (SB). For the crop calibration target, values of yield were derived from the SBs and target N content was calculated according to N content per dt dry matter yield [kg N $dt^{-1}$ DM] from Richner and Sinaj (2017).

## 3.3. Nitrate Leaching: SIA, Farm Model, DAISY

Nitrate leaching was measured by SIA (data supplied by the NitroGäu project) and modelled using the Farm Model or the DAISY model. The fields BIK3, 4, and 5 had a similar crop rotation during the analysis period, with BIK3 and 4 growing grass clover leys for 2 years and 1 year respectively, and BIK5 growing alfalfa for 3 years before silage maize (2018) and winter wheat (2018/19) on all fields (Figure 4). DAISY results were simulated for the SIA periods, while the Farm Model results represent the potential nitrate leaching from silage maize in 2018 and winter wheat in 2019. The alfalfa or grass clover leys that were still present until April 2018 were not considered by the Farm Model.

The SIA measurements showed lower nitrate leaching in the SIA period 2018 compared to 2019 on all fields (Figure 13). DAISY results showed this trend for BIK3 and BIK4 as well. For BIK5, however, DAISY showed very high leaching in 2018 and lower leaching in 2019. The Farm Model's results exhibited higher leaching in the first compared to the second time period across all fields. The results simulated by DAISY showed lower nitrate leaching compared to the SIA measurements over both time periods on all fields, except for BIK5 in 2018. Here, the DAISY result of 169 kg $NO_3$-N $ha^{-1}$ was higher than both other methods. In 2018, the Farm Model's results were generally higher than the SIA measurements. In 2019, there was no trend visible.

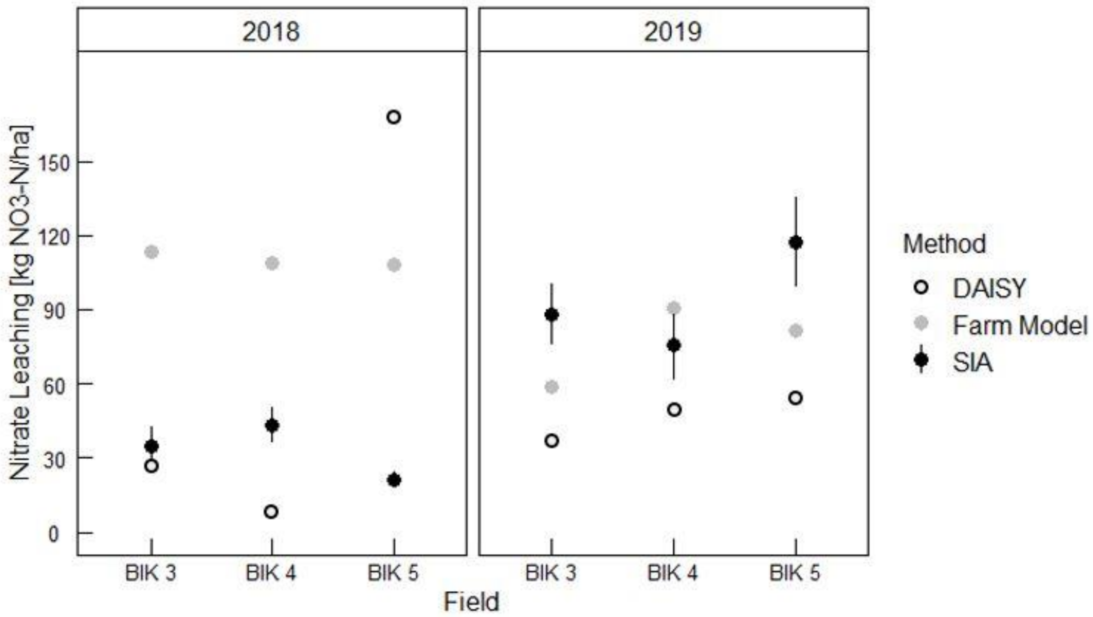


Figure 13. Nitrate leaching [kg $NO_3$-N $ha^{-1}$] of the fields BIK3, BIK4 and BIK5 in the SIA periods 2018 and 2019, measured by Self-Integrating Accumulators (SIA) and modelled by the Farm Model and by DAISY. Values measured by the SIA are presented along with their respective standard error.

On the fields HYD 2 and 4, fertilization was adjusted on two strips (M1 and M2) in the SIA period 2019. In 2018, the SIA were already placed on these strips and thus measured the nitrate leaching of the strips and of the control. The Farm Model and DAISY did not simulate differences in 2018, as the input variables did not change (Figure 14 and Figure 15).

On HYD2, the SIA measured nitrate leaching under a two-year grass clover ley in 2018, which was followed by silage maize in 2019. The SIA detected slightly lower nitrate leaching on strip M1, compared to M2 and the control in 2018. In 2019, this trend was still visible, however, nitrate leaching on M2 had decreased to a level only slightly above M1. Nitrate leaching over all strips was lower in 2019 compared to 2018. In 2018, the simulated results of the Farm Model and DAISY were compared to the SIA measurement under the control strip. The Farm Model's estimation was very close to the SIA value (44 and 45 kg $NO_3$-N $ha^{-1}$, respectively), while DAISY estimated lower nitrate leaching (14 kg $NO_3$-N $ha^{-1}$). In 2019, the Farm Model's results were considerably higher than the SIA measurements on all strips, with M1 showing higher leaching than M2 and the control strip. DAISY results were higher than the SIA measurements, and lower than the Farm Model's estimations and did not show a difference between the fertilization treatments.

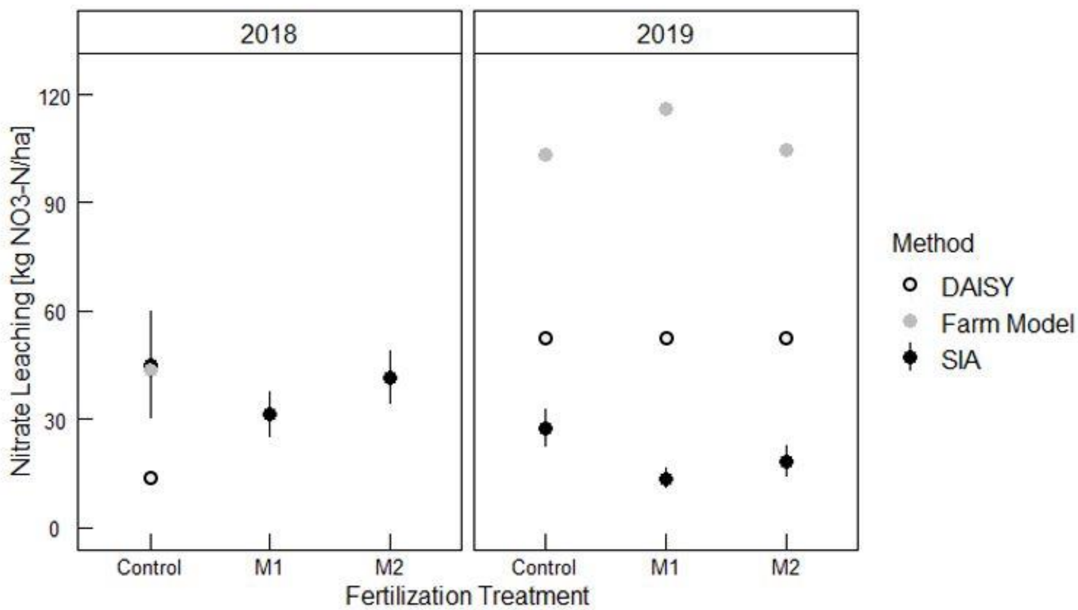


Figure 14. Nitrate leaching [kg $NO_3$-N $ha^{-1}$] of the fertilization treatment strips Control, M1 and M2 of the field HYD2 in the SIA periods 2018 and 2019, measured by Self-Integrating Accumulators (SIA) and modelled by the Farm Model and by DAISY. Values measured by the SIA are presented along with their respective standard error. Fertilization was adjusted in 2019. SIA measured nitrate leaching in 2018 on the three strips. The models only show one value for 2018, as no input variables changed between the strips.

On HYD4, spelt was grown during the SIA period 2018, followed by winter rapeseed in 2019. In 2018, the SIA measurements indicated considerably lower nitrate leaching under the M1 strip compared to the control and again lower leaching under M2 compared to M1. In 2019, the SIA results were considerably lower than those of 2018 and leaching under M2 was slightly higher than under M1 and under the control. In 2018, the simulated results of the Farm Model were lower than the SIA measurements under the control, and DAISY's results were lower than those of the Farm Model. In 2019, the Farm Model estimated higher nitrate leaching than the SIA measurements, with a decline in leaching from the control to M1 and further to M2. DAISY's simulated results were below the SIA measurements and did not show a difference between the fertilization treatments.

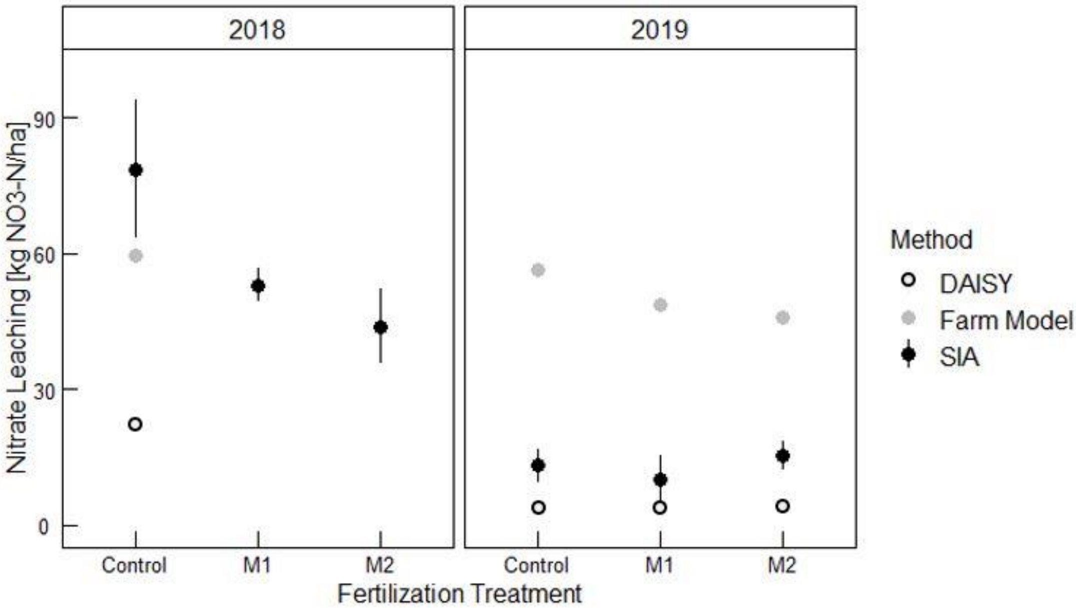


Figure 15. Nitrate leaching [kg $NO_3$-N $ha^{-1}$] of the fertilization treatment strips Control, M1 and M2 of the field HYD4 in the SIA periods 2018 and 2019, measured by Self-Integrating Accumulators (SIA) and modelled by the Farm Model and by DAISY. Values measured by the SIA are presented along with their respective standard error. Fertilization was adjusted in 2019. SIA measured nitrate leaching in 2018 on the three strips. The models only show one value for 2018, as no input variables changed between the strips.

The Farm Model overestimated nitrate leaching under silage maize on all fields and over all treatments on HYD2. The same applied to winter rapeseed on HYD4. DAISY underestimated nitrate leaching under winter wheat on all fields, as well as under winter rapeseed on HYD4. In general, DAISY tended to underestimate leaching in most cases, while the Farm Model tended to overestimate it (for both models, in 10 out of 14 values).

## 3.4. Extrapolation of the SIA Results to Regional Level

The nitrate leaching results from the SIA measurements under all fields included in the NitroGäu project were extrapolated to the arable area that is part of the original nitrate project. The SIA results of nitrate leaching per hectare of all fields were grouped per crop and extrapolated to the total area of each crop (Table 6). Most abundantly grown crops were grass clover leys, winter wheat and silage maize, frequently in a crop rotation similar to those of BIK3 and 4. Their combined area made up 82% of the total area considered here. Nitrate leaching per hectare was highest under winter wheat, followed by spelt and winter barley. Silage maize and winter rapeseed showed the same nitrate leaching levels, only slightly higher than grass clover leys. Noticeably, the share of total nitrate leaching of winter wheat exceeded its share of the area. All other crops either had a similar share of both or even a lower share of nitrate leaching. The weighted average of nitrate leaching of the six crops was 72 kg N $ha^{-1}$. From this value, the nitrate concentration of the seepage water under the arable area of the Gäu was estimated to be 67 mg $NO_3$ $L^{-1}$.

Table 6. Extrapolation of the Self-Integrating Accumulator (SIA) results of nitrate leaching per hectare to the crops' total area in the Gäu region. Area, nitrate leaching per hectare, total nitrate leaching per crop, share of area and share of nitrate leaching of the crops winter wheat, winter barley, spelt, silage maize, winter rapeseed and grass clover leys.

| Crop | Area [ha] | Share of area [%] | $NO_3$ per ha [kg N $ha^{-1}$] | $NO_3$ total [kg N] | Share of $NO_3$ [%] |
|---|---|---|---|---|---|
| Winter Wheat | 223 | 28 | 133 | 30665 | 54 |
| Winter Barley | 76 | 10 | 77 | 5839 | 10 |
| Spelt | 10 | 1 | 78 | 763 | 1 |
| Silage Maize | 167 | 21 | 44 | 7326 | 13 |
| Winter Rapeseed | 59 | 7 | 44 | 2562 | 4 |
| Grass Clover Leys | 261 | 33 | 38 | 10007 | 18 |
| Total | 796 | 100 | 72 | 57162 | 100 |

Values need to be interpreted according to the crop's position in the crop rotation, e.g. winter wheat is usually grown after grass clover leys, followed by silage maize or after winter rapeseed.

# 4. Discussion

## 4.1. Nitrogen Budgets

The relative nitrogen supply and the nitrogen balance calculated with the farm-gate budget yielded higher results compared to those from the Suisse balance. The applied inputs and outputs, as well as the system boundaries differed substantially between the methods. The FGB considered inputs of imported nitrogen on farm level, while the SB's inputs included the on-farm organic and imported organic and mineral fertilizers. Biological nitrogen fixation was included in the FGB, while it was not considered in the SB. Atmospheric nitrogen deposition was not included in either balancing method. Other inputs, such as feedstuff, not including concentrates, were considered indirectly in the SB when calculating the fodder production of the farm. Regarding the outputs, FGB considered all exported nitrogen on farm level, while in the SB, crop production and exported manure were considered. For the crop production, the SB included the N demand of the total crop production, while the FGB considered the N removal of the exported crops. N removal is generally higher than the N demand. The discrepancy between them depends on the crop but is especially high for grain and forage legumes (Richner and Sinaj, 2017). Another difference in methodology between the two balances is that the SB uses the available N fraction from organic fertilizers, while in the FGB, total nitrogen is used for the calculation. Therefore, best correlations between FGB and SB are usually achieved on arable farms without grain legumes (Bosshard et al., 2012), where inputs for both balances include the imported organic and mineral fertilizers and outputs include the entire crop production, where the non-existence of grain legumes minimizes the discrepancy between N removal and N demand. Most accurate correlations should be achieved with low amounts of imported organic fertilizers, due to the different N fractions considered by the two balancing types.

In this study, B5 was the only arable farm. In both years, the N balances were about 16 kg N ha$^{-1}$ higher in the FGBs, compared to the SBs. Thus, it was lower than the average difference in N balance over all farms of 18 kg N ha$^{-1}$. The only better correlation of N balance was found on B4 in 2018, where the N balance of the FGB was 11 kg N ha$^{-1}$ higher than that of the SB. The influence of intensive animal husbandry can be seen in the balance of B4 in 2019, compared to 2018. In 2019, due to the change in production from dairy to cattle fattening, higher inputs of feedstuff, live animals and organic fertilizers lead to a higher amount of inputs and an N balance of 20 kg N ha$^{-1}$ higher in the FGB, compared to the SB. The poorest correlation was achieved on B3 which was the only organically managed farm. Inputs and outputs differed between the balancing methods, as the main input in the SB was on-farm organic fertilizer, which was not considered in the FGB. Here, imported feedstuff was the main input. Most of the crop production was used as on-farm feedstuff, thus, it was not considered in the FGB. Animal products, such as milk, meat and offspring made up around half of the outputs, the other half was export of organic fertilizers, which in turn differed in amount in the SB due to the different N fractions considered. The results of this study comply with Bosshard et al. (2012) in terms of intensive animal husbandry with higher import of feedstuff and export of animal products leading to increased differences between the inputs and outputs, as well as the N balances of the two budgeting methods.

Errors in the nitrogen budgets can stem from farm-specific values estimated by the farmers. The amounts of imports and exports in the FGB and values such as animal numbers, consumption and import and export of feedstuff, crop yields, and cultivated area in the SB can be difficult to estimate and when the balance is used as a regulatory tool, these values can be prone to manipulation (Oenema et al., 2003, Bosshard et al., 2012). Uncertainties in the nitrogen budgets can also arise from assumptions of standard values for N contents of inputs and outputs (Oenema et al., 2003, Zikeli et al., 2017). For the calculation of the FGB in this study, exact information on nutrient contents could not always be obtained. Especially for feedstuff, animal products and imported organic fertilizers, N contents had to be estimated according to the farms' SBs or information given by the farmers. In the SBs, N contents of fertilizers, available N from on-farm manure and N demand of crops are based on the reference values of Richner and Sinaj (2017) and can be adjusted if farm-specific values are known to deviate from those. Another high degree of uncertainty in the FGB lies in the estimation of BNF (Oenema et al., 2003, Quemada et al., 2020, Reimer et al., 2020a). For grass clover leys, the NutriGadget differentiated between different percentages of white clover (between 10 and 40%) and used reference fixation rates to estimate total BNF. Ratios of clover were merely estimated and were not measured on the farms. Additionally, BNF is highly variable and dependent on yield, environmental factors, and soil conditions, such as moisture and N content (Anglade et al., 2015). The NutriGadget only considered yield level in the estimation. The SB considers BNF only indirectly via the lower N demand of leguminous crops. In the SB, sources of uncertainty arise not only from standard values of N contents, but also from standardized correction factors. For instance, deduction of available manure due to grazing of the animals and the basic N utilization rate to calculate available N fraction from manure were derived from discussions of experts leading to consensus values which are prone to high variability among farms. Correction factors for inevitable N losses from livestock housing and manure storage are standardized but can differ substantially depending e.g. on type of housing and type of manure (Bosshard et al., 2012).

The SB has the dual purpose of being a planning aid for farmers and a regulatory tool for the cantonal and environmental agencies. As an aid for fertilization planning, a field-specific approach could be more effective. It has also been criticized that the SB does not consider soil nutrient stocks in the crop nutrient demand (Bosshard et al., 2012), which goes against the 'good agricultural practice' for fertilization planning described by Richner and Sinaj (2017). The combination of a field-based fertilization plan, including soil nutrient stocks, could lead to a more accurate nutrient management and with it a decrease in harmful nutrient emissions to the environment (Bosshard et al., 2012, Richner and Sinaj, 2017). Alternatively, using FGBs instead of SBs could improve balance accuracy and yield higher environmental benefits. However, they have little to no planning value for the farmer (Bosshard et al., 2012). Oenema et al. (2003) suggested monitoring soil nutrient stocks along with FGBs as well, especially immobile nutrients like P, in order to assess the nutrient budget's accuracies.

## 4.2. Nitrate Leaching Models

### 4.2.1. Farm Model

The Farm Model is a life cycle assessment model, evaluating a farm's impact on 13 environmental indicators. In this study, the field nitrogen sub model was used to assess nitrate leaching from the analyzed fields. Input parameters included the type of crop, its yield, fertilization rate and BNF if applicable. Simulations were run for the main crops grown in the SIA periods 2018 and 2019 on the selected fields and results were compared to the SIA measurements. The SIA periods vary slightly in duration (SIA changes occurred between August and November) depending on time of harvest of the current and sowing of the subsequent crop (Figure 4). As main nitrate leaching takes place during the winter (Wey et al., Unpublished Manuscript) and therefore after the current SIA period, SIA results do not necessarily observe the nitrate leaching of the main crop of the SIA period, but rather of the previous crop. The FM does not consider time or crop rotation in the nitrogen sub model, but calculates nitrate leaching for a single crop. This aspect needs to be considered in the interpretation of the results. For example, on the BIK fields in 2018, FM seems very high, as it calculated leaching from maize, while the SIA most likely detected the winter leaching from the previous leys. 2019 SIA results were closer to FM results of 2018, as leaching from maize also occurred in winter 2018, observed in SIA period 2019. The same situation occurred on HYD2 in 2019. Direct comparison is therefore difficult, as the SIA give a cumulative leaching value for the entire SIA period, thus not observing the leaching of just one crop. On HYD2 in 2018, simulated and observed nitrate leaching was very similar. Here, both methods represented nitrate leaching from grass clover leys and no crop change occurred.

In general, FM results were grouped together for each crop. This would suggest that the type of crop has a large influence on nitrate leaching in the FM. The type of crop has an impact on harvested and residual biomass and its N content, which in turn influences the amount of N entering the available and the immobilized CN pool, and the amount of soil N being mineralized (Appendix 2). Another impact on the potential nitrate leaching in the FM is the amount of fertilizer applied. On the fields HYD2 and HYD4, different fertilization treatments (control, M1, M2; Table 2) were tested on the main crop in 2019 (HYD2: maize, HYD4: winter rapeseed). The SIA were already placed underneath the different fertilization strips in 2018 and recorded spatial differences in nitrate leaching. The FM was run once in 2018, as no input variables changed. In 2019, fertilization was adjusted, and the model was run once for each treatment. On HYD2, the SIA detected the same pattern between the three strips in 2018 and 2019, with leaching being lowest on M1 and M2 showing slightly lower results compared to the control. In 2019, contrary to the SIA results, FM showed higher nitrate leaching on M1, compared to M2 and the control. Again, most of the leaching detected by the SIA was probably lost in the winter under the grass clover ley, not necessarily picking up the change in fertilization yet, while the FM showed a reaction to the fertilization treatments. On HYD4, the SIA measurements in 2018 showed substantially lower nitrate leaching on M1 and M2 compared to the control, even though the management did not differ between the strips. This could suggest possible differences in soil properties, such as texture or hydraulic factors. However, these differences were not found in 2019, where nitrate leaching was slightly higher on M1, compared to M2 and the control. The FM showed a decline in potential nitrate leaching with decreasing amount of N fertilizer. On M2, CULTAN fertilization was applied, for which there is no reference values in the FM. Therefore, the results may not be accurate.

Another aspect of the FM results is that they represent the total potential nitrate leaching of a crop. The N model is based on a soil system budget, where gaseous losses in form of $N_2O$, $NH_3$ and $NO_x$, as well as nitrate leaching are quantified, while accounting for N turnover from the soil C-N pools (Meier et al., 2014). Apart from nitrate availability, the main influences on nitrate leaching include vegetation cover, soil properties and weather conditions, especially precipitation (Meier et al., 2014). Climatic conditions are partly taken into account in the FM by the assignment of production zones, as defined by BLW (2020). Improvements of the model could include the definition of some soil properties of importance for nitrate leaching, such as texture and humus content. Another aspect could be the inclusion of mineralization processes in the crop rotation, especially in the case of leguminous leys. For this, it might be necessary to use a monthly resolution.

There is no standard method for LCA modeling, therefore choice of the implemented N model, and its accuracy vary among studies. Therefore, Andrade et al. (2021) assessed performance and suitability of four different N models for LCA purposes, including DAISY and SALCA-$NO_3$ according to criteria from UNFCCC (2004). SALCA-$NO_3$ was developed by Agroscope in Switzerland for LCA studies (Richner et al., 2014). It is similar to the N model of the FM, as it estimates nitrate leaching from the field's N balance, also taking mineralization processes into account. However, it works on a monthly resolution and takes crop rotation and other factors, such as soil humus and clay content, into account (Richner et al., 2014). In Andrade et al. (2021), DAISY performed best of the four models, while SALCA-$NO_3$ came joint second with the mechanistic model ANIMO. The authors concluded, that although mechanistic models have the potential for higher accuracy, they are also less user-friendly compared to the simpler models, such as SALCA-$NO_3$. These findings suggest that the N model of the FM can be a useful tool for LCA studies. It has not yet been validated in other studies. In this study, the validation of the Farm Model's N model was difficult, as the results could not be aligned properly with the SIA measurements.

### 4.2.2. DAISY Model

DAISY is a process-oriented soil-plant-atmosphere simulation model. To model carbon and nitrogen cycles accurately, a precise simulation of the crop rotation is important (Kollas et al., 2015). For this, good parameterization of the single crops and their interactions within the crop rotation is required. Winter wheat for example is often simulated with good accuracy (Kollas et al., 2015, Yin et al., 2020) as it has been modeled frequently and is thus well parameterized across Europe (Palosuo et al., 2011, Yin et al., 2020) . On the contrary, Kollas et al. (2015) and Groenendijk et al. (2014) found difficulties simulating maize with good accuracy in DAISY, possibly due to less experience of the modelers with this crop and its wide range of varieties.

In this study, the cereals winter wheat and spelt showed high accuracy of simulated yield and N content with little calibration needed. Simulation of maize was not as accurate, with yield and N content often being underestimated (Table 5). Maize was calibrated with the recommended fertilization rate from Richner and Sinaj (2017), but target N content of the harvested biomass was only met on the fields BIK3 and 5. On BIK4 and HYD2, N content was substantially lower and could not be raised with reasonable changes of the crop parameters. On all fields, except for HYD2, the actual fertilization was lower than the recommended rate as maize followed leguminous leys and N mineralization from legume residues was assumed to replace part of the conventional fertilization. Therefore, yield and N content of maize dropped on these fields in the actual simulation runs. It seems that mineralization of the ley residues did not supply sufficient N to the maize (more detail below). The lower simulated N content of maize could also stem from suboptimal parameterization. On HYD2, recommended N fertilization was applied, but N content of maize was still substantially lower than the observed values. Simulated yield and N content also reacted differently to the fertilization treatments. Observed yield and N content was higher at lower fertilization, with highest values on M1. In DAISY, yield and N content decreased with decreasing fertilization.

The leguminous leys were especially challenging to calibrate. On BIK5, alfalfa was cultivated for three years before sowing maize. Alfalfa has not yet been parameterized in DAISY. The closest approximation of a parameterized crop was white clover which was used in the simulation runs. There are, however, major physiological differences between these two legumes. Alfalfa grows as an erect, leafy stem up to 120cm in height and develops a taproot that can reach a depth of two meters, while white clover is a stoloniferous plant which grows close to the ground. They also have different effects on the following crop. For example, N fertilizer replacement values of white clover can be around 100 kg N ha$^{-1}$ (Eriksen et al., 2008), while alfalfa can supply 100-200 kg N ha$^{-1}$ to the following crop (Bruulsema and Christie, 1987, Ballesta and Lloveras, 2010) and can still have a significant effect on the second following crop (Cela et al., 2011). Residue mineralization can vary as well, with alfalfa usually needing more time to decompose as its stem has higher lignin content than the leafier white clover (Baddeley et al., 2017). Therefore, white clover was a rather poor substitution for alfalfa, but the scale of this master thesis did not allow for new crop parameterization.

Grass clover leys were approximated in DAISY by intercropping ryegrass and white clover. The individual crops were calibrated while accounting for their interactions on the field, such as light interception and nutrient uptake. For the fields BIK3 and 4, the crops were only calibrated to roughly fit the total yield of the spring harvest in 2018. For HYD2, data on yield, N content, and grass to legume ratio were available for four cuts in 2018 and a single spring harvest in 2019. After calibration, the results corresponded well to the total harvested biomass and N content of the four cuts in 2018 and represented the grass to legume ratio reasonably well. However, the simulated development of the two crops in DAISY did not correspond to observed development on the field. Here, the first and second cut in 2018 yielded higher biomass than the third and fourth cut, while simulated yields in DAISY increased with each cut. The fourth cut showed the highest yield, also exceeding any of the observed yields from the field. For the single cut in 2019, the field observations showed biomass more than twice as high as that simulated in DAISY. Correspondingly, N content of the harvested biomass differed among the cuts between field measurements and the simulation.

Within the crop rotation, each crop has an influence on the following, due to e.g. N mineralization from harvest residues and effects on soil water content. Simulation of these carry-over effects can be challenging (Kollas et al., 2015). Especially, N mineralization from harvest residues is difficult to model, as it is affected by their composition and decomposition processes, which in turn depend highly on the quantity and C/N ratio of the residues (Gabrielle et al., 2002, Beaudoin et al., 2008). The simulation of soil N processes is generally difficult, due to spatial and temporal variation (Kersebaum et al., 2002) and close interaction with soil moisture and water balance (Jing et al., 2017).

In this study, maize followed leguminous leys on four of the five fields. Its N content and yield, as mentioned above, were not accurately simulated by DAISY. Apart from a suboptimal parameterization, as discussed above, another reason could be that the simulation of the N fluxes within the crop rotation was not accurate. Simulated residual N from the leys ranged between 50 and 60 kg N $ha^{-1}$ on the fields BIK3, 4 and HYD2, while on BIK5 152 kg N $ha^{-1}$ remained on the field. Residual N on BIK5 was particularly high because there was no spring harvest in 2019 and because of the high N content of the pure legume stand. On all fields, mineralization was the largest N source ranging from 150 to 230 kg N $ha^{-1}$ during the cultivation periods of maize. In the DAISY output, it was not possible to determine the source of mineralized N, but the trend showed higher mineralization rates on BIK5 and lowest rates on HYD2, where residual N was lowest. Crop uptake ranged from 150 to 200 kg N $ha^{-1}$. The other main pathway of nitrogen were losses due to denitrification, estimated to be 100 to 125 kg N $ha^{-1}$ during the maize cultivation period. These pathways were not measured in the field experiments of the NitroGäu and can therefore not be validated. However, DAISY has shown high denitrification estimates in another study (Groenendijk et al., 2014), where other models, as well as corresponding literature suggested negligible losses due to denitrification. Therefore, it is possible that denitrification was overestimated, leading to lower N availability for maize.

Nitrate leaching is highly dependent on soil hydraulic factors, such as field capacity and water saturation (Jabloun et al., 2018), as well as soil C and N fluxes, especially the long-term net N mineralization rate (Yin et al., 2020). These complex processes make the simulation of nitrate leaching challenging. In this study, DAISY tended to underestimate nitrate leaching compared to the SIA measurements. Contrary to the results of the FM, DAISY results could be compared directly to the SIA data, as their time frame was adjusted to the SIA periods.

On the fields BIK3, 4 and 5, the crop rotations during the analysis period were similar, with maize in 2018 and winter wheat in 2018/19. However, prior to maize different leys were grown on the fields. Grass clover leys were cultivated for two years and one year on BIK3 and BIK4, respectively. On these fields, DAISY picked up the trend of the SIA, where leaching in 2019 was higher than in 2018. In both years, DAISY simulated lower nitrate leaching compared to the SIA measurements. It is possible that, similar to HYD2, the crop development of ryegrass and white clover in DAISY, compared to the grass clover leys differed which could explain some of the variation in nitrate leaching. On BIK5, three years of alfalfa were grown. Here, DAISY showed very high leaching during the winter, but also during spring under alfalfa, totaling 169 kg $NO_3$-N $ha^{-1}$ in the SIA period 2018. This does not correspond to SIA measurements of only 21 kg $NO_3$-N $ha^{-1}$ in 2018. Neither does it correspond to Julier et al. (2017), stating that leaching under alfalfa is usually very low. It is rather known as a crop taking up nitrate from deep soil layers due to its deep taproot (Julier et al., 2017). In 2019, SIA measured comparably high nitrate leaching, while DAISY estimated a lower amount. As mentioned above, alfalfa had to be substituted by white clover. Alfalfa residues usually mineralize more slowly than white clover (Julier et al., 2017). The different trends of the simulation compared to the SIA measurements between 2018 and 2019 could partly stem from these different mineralization rates and N retention during winter.

On HYD2 and HYD4, different fertilization treatments were applied in 2019. DAISY was run once in 2018, as no parameters changed between the strips. On HYD2, fertilization of maize was adjusted in 2019 and DAISY was run once for each fertilization treatment. Other parameters, e.g. relating to soil or crops and crop rotation, were not changed. DAISY did not detect a change in nitrate leaching between the treatments. The reason for this is that DAISY estimated main leaching from December to March, with very little to no nitrate leaching during the cultivation of maize in the summer. Therefore, lower fertilization did not affect leaching in the SIA period 2019. Differences could arise in the next SIA period, which was, however, not included in this study. Furthermore, DAISY estimated lower nitrate leaching in 2018, compared to 2019, while SIA results showed an opposite trend. A possible explanation here is the different development of the ryegrass and white clover crops in DAISY compared to the observed development of the grass clover leys, resulting in temporal and possibly spatial differences in the soil N fluxes. On HYD4, DAISY results showed a slight increase of leaching on M2 in 2019, compared to the control. This resulted from higher leaching in March, after the application of 100 kg N $ha^{-1}$ in form of CULTAN fertilizer. DAISY, however, does not have an option for this kind of fertilization. Furthermore, crop simulation of winter rapeseed in DAISY did not pick up the changes in yield and N content observed in the fields.

In general, DAISY did not perform well in this study. DAISY underestimated nitrate leaching in most simulations compared to the SIA measurements and did not reliably reproduce the trend of leaching between the years and the crops. Similar to most process-oriented simulation models, DAISY runs on a broad set of parameters, many of which interact with each other and thus have a nonlinear effect on the simulation results (Jabloun et al., 2018). Therefore, it was difficult to find the source of the uncertainties. Jabloun et al. (2018) found 34 out of 128 crop and soil parameters strongly influencing DAISY outputs under winter wheat and maize. Considered outputs included evapotranspiration, nitrate leaching, grain yield and N content. Parameters influencing yield and N content related to the crop physiology and development. For the crop parameters, there was little information available from the field experiments, as only yield biomass and N content were observed. Physiological properties, such as the leaf area index, and phenological development were not recorded within the project. This left room for assumptions. Parameterization in general was found to be highly subjective to the modeler and their experience and perspective (Groenendijk et al., 2014, Kollas et al., 2015, Yin et al., 2020). In this study, the modeler did not have any previous experience with DAISY.

Most influential parameters of nitrate leaching related to soil water characteristics, such as field capacity and conductivity at saturation. In this study, data on the soils was available from the NitroGäu field experiments. Detailed hydraulic parameters were available for HYD2. On the other fields, soil texture, C/N ratio, humus content and soil bulk density were used by DAISY to estimate the hydraulic properties of the soils. Bulk density had not been measured on the fields BIK3, 4 and 5, instead values from BIK1 were used. DAISY can run simulations without specified bulk density, but then uses a pedotransfer function (Cosby et al., 1984), developed in North America. This, however, did not yield acceptable results in this study. The substitution of bulk density might not have been accurate but was a closer approximation than the pedotransfer function.

Furthermore, Jabloun et al. (2018) found that nitrate leaching of a crop was influenced by the parameterization of the previous crop. Therefore, accurate simulation of the crop rotation is important when analyzing N fluxes (Kollas et al., 2015, Jabloun et al., 2018, Yin et al., 2020). In this study, every field’s crop rotation included at least one crop which was not or not well parameterized in DAISY. Especially, the parameterization of the leguminous leys was challenging and affected four of the five fields (except HYD4), leading to high uncertainties of the simulated N fluxes. Simulation of N dynamics in plant and especially soil is generally challenging, due to the complex underlying processes. In order to decrease uncertainty of the simulations, several authors suggested a multi-model approach (Kollas et al., 2015, Yin et al., 2020). Both studies have found higher accuracy when using results from multiple models, both in crop and nitrogen simulation.

## 4.3. Extrapolation of the SIA Results to Regional Level

The extrapolation of the SIA measurements to the Gäu region showed that the nitrate concentration in seepage water under arable land (67 mg $L^{-1}$) was still higher than the target value of 60 mg $L^{-1}$ (Hunkeler et al., 2015). The calculated nitrate concentration stems from the six crops which were grown on 87% of the arable land. On the remaining 123 ha, the main crops were other cereals (38 ha), grain maize (38 ha), and sugar beet (22 ha). There was no information on nitrate leaching under these crops from the Gäu region. However, sugar beet was found to generally have a relatively low nitrate leaching potential (Bünemann-König, 2021) and in this study, nitrate leaching under maize was also below the six crops' average of 72 kg N $ha^{-1}$. Therefore, the nitrate concentration of the entire arable land of the Gäu could be lower than the calculated value of the six main crops.

The extrapolation of the SIA results to the total area of the analyzed crops showed the highest share of nitrate leaching under winter wheat with 54% (Table 6). Its share of the total area with 28% is the second largest after grass clover leys (33%). For all other crops, shares of nitrate leaching were similar or lower than their share of the area. As previously discussed, the SIA periods did not reflect the leaching effects of the main crop, but rather that of the previous crop. Therefore, crop rotations need to be taken into account. In a typical crop rotation of the Gäu region, winter wheat is grown after winter rapeseed or after maize which often follows grass clover leys. Hülsbergen et al. (2017) found high $N_{min}$ values in autumn after maize and winter rapeseed, which is at high risk of leaching, especially due to low N uptake of winter wheat in autumn. They suggested to reduce the share of maize and winter rapeseed or replacing winter wheat with winter barley, as it can take up higher amounts of N in autumn. In the NitroGäu project, SIA results under winter barley, grown after maize or winter rapeseed, did show lower nitrate leaching than those under winter wheat. It does seem to be a possible strategy to decrease nitrate leaching. However, there were only two observations under winter barley, which was not enough to draw reliable conclusions.

On the area under contract of the original nitrate project, a comprehensive set of mitigation strategies has already been implemented since the year 2000. Soil cover during the winter was implemented using cover crops or winter varieties of cash crops. Another strategy was reduced tillage, including no ploughing in late autumn or winter and early seeding of winter crops. Furthermore, the crop rotations were adjusted according to the Nitrate Index, e.g. by reducing areas of crops with high nitrate leaching potential, such as potatoes. Additionally, 136 ha were converted to extensive grassland (Hunkeler et al., 2015). These measures already covered some of the main target areas of mitigation strategies, such as crop rotation, land use and soil conservation.

However, fertilization management has not been targeted in the nitrate project, as it was not included in the Nitrate Index. In comparable projects, such as Hülsbergen et al. (2017) and Osterburg et al. (2007), optimizing fertilization management was one of the key concepts. As mentioned earlier, field specific fertilization planning in addition to the commonly used Suisse Balance could be an efficient way to decrease the farm's N balance (Bosshard et al., 2012). Additionally, $N_{min}$ sampling in spring, N analyses of manure, as well as a realistic crop yield estimation could help improve the fertilization planning (Osterburg et al., 2007, Hülsbergen et al., 2017). Furthermore, precision farming in form of variable rate application of N fertilizer was suggested in the other projects. However, this technique is costly and difficult to implement on small field sizes, which are predominant in the Gäu region. A reduction of fertilization rate can also be an efficient way to reduce nitrate leaching, as long as nutrient stocks are not depleted, and yield is not depressed substantially (Osterburg et al., 2007). It has been tested in the NitroGäu project, but for conclusive results, the SIA measurements of 2019/2020 need to be analyzed, which was not part of this study.

# 5. Conclusion

The N balances calculated by the farm-gate balance were on average 18 kg N $ha^{-1}$ higher than that of the Suisse Balance. Thus, confirming the first hypothesis of this study. The SB and the FGB differ in their methodology and thus in their suitability for different applications. The FGB is a widely used tool and can serve as an agri-environmental indicator. However, there is no standard methodology and applications can vary in considered inputs and outputs and system boundaries. This can complicate comparison between studies. The SB has the dual purpose of serving as a planning tool for farmers and a regulatory instrument of agri-environmental policies. Improvements to the balance are evaluated according to both purposes. Generally, the SB is viewed as an efficient and effective method and is a broadly accepted regulatory instrument.

Both the Farm Model and DAISY did not yield accurate nitrate leaching results when compared to the SIA measurements. The FM is a simple model with low levels of manual data input which makes it user-friendly. However, some important influencing factors, such as soil properties are not included in the estimation of nitrate leaching. Furthermore, the FM estimated for nitrate leaching for a single crop which made the alignment with the SIA measurements difficult and hindered validation of the simulated results. Therefore, the second hypothesis of this study, assuming that the FM would overestimate nitrate leaching compared to the SIA measurements, could not be answered with certainty. DAISY on the other hand is a complex soil-plant-atmosphere simulation model which requires a large amount of input data to parameterize the soil and the individual crops. It has been described as being over parameterized, as many parameters affect the output only marginally. In this study, crop calibration was problematic, as several crops had not been parameterized in the reference files of the model or did not fit well to the Swiss conditions. Therefore, the crop growth and the effects of the crop rotation were not simulated accurately, and neither was nitrate leaching. The simulated N fluxes, especially the mineralization and denitrification rates did not seem to match those on the field. The third hypothesis of this study assumed that nitrate leaching estimated by DAISY would correlate with the SIA measurements, when the model was calibrated. This could not be confirmed. A better parameterization of the crops as well as of the initial soil conditions could improve the simulation of the crop development and the N fluxes. The extrapolation of the SIA measurements to the Gäu region showed that the nitrate concentration in seepage water under arable land (67 mg $L^{-1}$) was still higher than the target value of 60 mg $L^{-1}$. Highest leaching was found under winter wheat after maize and winter rapeseed. These crops are characterized by high mineral N levels left in the soil after harvest.

However, winter wheat has a relatively low N uptake in autumn. Adjustments to the crop rotation, such as decreasing the share of maize and winter rapeseed or replacing winter wheat with winter barley could potentially decrease nitrate leaching, as assumed in the fourth hypothesis of this study. An additional mitigation strategy could be a field specific fertilization planning, including $N_{min}$ sampling in spring and taking mineralization of previous crops into account.


## Acknowledgements

I would like to thank Hannah Wey for providing and explaining all data and information I needed from the NitroGäu project. I would also like to thank Simon Moakes, Catherine Pfeifer, and Michael Thompson for helping me get started with the Farm Model and answering any questions I had along the way. Additionally, I would like to thank Marie Reimer for providing many useful insights into the DAISY model set up and the crop calibration. And I would like to thank Else Bünemann-König for helping me with any questions I had.

Thank you also to Christa, Louise and Birte for many walks and game nights and generally making my time at FiBL a lot of fun.

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# Appendix

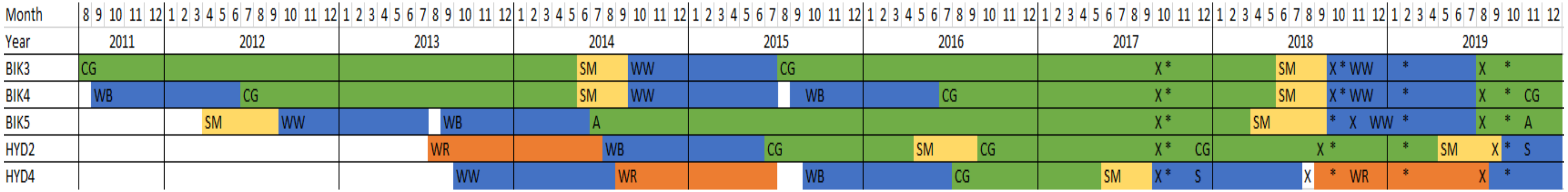
## Appendix 1. Soil Properties and Crop Rotations of the Selected Fields for the DAISY Simulations

Appendix 1.1. Soil properties of the fields BIK3, BIK4, BIK5, HYD2, and HYD4, including soil texture (content of sand, silt, and clay), humus content, C/N ratio and bulk density.

| Field | Horizon | Clay | Silt | Sand | Humus | C/N | Bulk Density |
|---|---|---|---|---|---|---|---|
| BIK3 | 1 | 14 | 56 | 30 | 4 | 9.42 | 1.45* |
| BIK3 | 2 | 12 | 59 | 29 | 2.41 | 8.81 | 1.57* |
| BIK3 | 3 | 12 | 49 | 39 | 1.34 | 9.03 | 1.56* |
| BIK4 | 1 | 13 | 58 | 29 | 3.6 | 9.06 | 1.44 |
| BIK4 | 2 | 14 | 56 | 30 | 2.49 | 8.84 | 1.57* |
| BIK4 | 3 | 11 | 56 | 33 | 1.34 | 8.84 | 1.56* |
| BIK5 | 1 | 15 | 53 | 32 | 3.5 | 9.13 | 1.45* |
| BIK5 | 2 | 11 | 54 | 35 | 2.65 | 8.94 | 1.57* |
| BIK5 | 3 | 10 | 47 | 43 | 1.26 | 8.95 | 1.56* |
| HYD2 | 1 | 11 | 53 | 36 | 2.24 | 8.81 | 1.68 |
| HYD2 | 2 | 10 | 53 | 37 | 1.05 | 8.43 | 1.76 |
| HYD2 | 3 | 10 | 61 | 29 | 0.73 | 8.4 | 1.78 |
| HYD4 | 1 | 12 | 65 | 23 | 2.73 | 8.87 | 1.55 |
| HYD4 | 2 | 12 | 66 | 22 | 1.09 | 8.36 | 1.65 |
| HYD4 | 3 | 14 | 70 | 16 | 0.95 | 8.17 | 1.66 |

* bulk density was not measured on these fields. Values were substituted with values from the field BIK1.

Appendix 1.2. Crop rotation of the fields BIK3, BIK4, BIK5, HYD2, and HYD4 for the complete period simulated in DAISY. Additionally, X represents change of Self-Integrating Accumulators (SIA) and * represents Nmin sampling. The crops are Alfalfa (A), Grass Clover Leys (CG), Spelt (S), Silage Maize (SM), Winter Barley (WB), Winter Rapeseed (WR), and Winter Wheat (WW).



# Appendix 2. Nitrogen Cycle of the Farm Model

Nitrogen from organic fertilizers is divided into total ammoniacal N ($N_{TAN}$), which can be taken up by the crop and N which is not readily available for plant uptake. Mineral fertilizers only contain $N_{TAN}$. Nitrogen, which is not readily available for plant uptake, is assumed to enter the C-N pool ($N_{CN\text{-}pool}$). From there, the model differentiates two pathways based on a soil organic carbon sequestration model by Favoino and Hogg (2008). They suggest two pools, one of short-term available C and N ($N_{av.CN\text{-}pool}$) and one containing the immobilized fractions ($N_{CN\text{-}pool,\ immobilized}$). The fractions $N_{CN\text{-}pool}$, $N_{CN\text{-}pool,\ immobilized}$ and $N_{av.CN\text{-}pool}$ are calculated as shown in Equations 1, 2 and 3, respectively.

$$N_{CN\text{-}pool} = (N_{tot} - N_{TAN})\ [+N_{TAN} * 0{,}3] \qquad \text{(Eq. 1)}$$

$$N_{CN\text{-}pool,\ immobilised} = F_{immo.} * (N_{CN\text{-}pool} - SON_{MIM} * NUR_{SONMIM} + N_{PRag} + N_{PRbg}) \qquad \text{(Eq. 2)}$$

$$N_{av.CN\text{-}pool} = N_{CN\text{-}pool} + SON_{MIM} * (1\text{-}NUR_{SONMIN}) + N_{PRag} + N_{PRbg} - N_{CN\text{-}pool,\ immobilised} \qquad \text{(Eq. 3)}$$

where
$N_{tot}$ is total nitrogen supplied to the soil,
$F_{immo.}$ is the immobilized fraction (not yet included in model),
$SON_{MIM}$ is the management induced mineralization of soil organic nitrogen (see below),
$NUR_{SONMIM}$ is the nitrogen utilization rate of $SON_{MIM}$,
$N_{PRag}$ is nitrogen from above ground plant residues,
$N_{PRbg}$ is nitrogen from below ground plant residues.

$N_{CN\text{-}pool,\ immobilized}$, however, is not yet implemented in the Farm Model, as N-immobilization is closely related to change in soil organic carbon (SOC). C-flows, however, are not yet included in the calculations, therefore $F_{immo.}$ cannot be determined, rendering $N_{CN\text{-}pool,\ immobilized}$ zero for the moment.

The model also considers management induced mineralization of soil organic nitrogen ($SON_{MIM}$). The calculation is based on Brock et al. (2012) and shown in Equation 4.

$$SON_{MIM} = \frac{N_{\text{PB}} - \text{N}_{Fix} - N_{Dep} * NUR_{Dep} - \sum N_{tot,Fert} * NUR_{Fert}}{NUR_{SONMIM}} + \Delta N_{min} \qquad \text{(Eq. 4)}$$

where

$N_{PB}$ is nitrogen from plant biomass (kg N),

$N_{Fix}$ is nitrogen input from atmospheric $N_2$-fixation (kg N),

$N_{Dep}$ is nitrogen input from atmospheric deposition (kg N),

$N_{tot.Fert}$ is total amount of N input from fertilizers (kg N),

NUR is the nitrogen utilization rate of the specific pools,

$\Delta N_{min}$ is N-mineralisation due to mechanic disturbance of the soil (kg N).

Plant nitrogen uptake is estimated according to yield and reference N-content of above- and below-ground biomass of the particular crop based on IPCC (2019). In the model, the harvest is further differentiated into main and by-product and respective N-content. Nitrogen not taken up by plants and removed from the field by harvest, can potentially be lost from the system, either by volatilization or leaching.

Gaseous emissions include ammonia ($NH_3$), nitrogen oxides ($NO_x$) and nitrous oxide ($N_2O$) emissions. $NH_3$ emissions occur from the $N_{TAN}$ – fraction of fertilizers and were calculated here using the amount of fertilizer and their type specific emission factors of IPCC (2019).

$NO_x$ emissions from $N_{TAN}$ are calculated as shown in Equation 5 (emission factor from ART, 2013).

$$NO_x\text{-}N_{TAN} = 14/30 * (0.007 * N_{tot}) \qquad \text{(Eq. 5)}$$

The Farm Model calculates direct and indirect $N_2O$ emissions and differentiates between emissions from $N_{TAN}$ and from $N_{av.CN\text{-}pool}$. Equations 6-9 show the applied calculations. The emission factors (EF) are based on the 2018 reporting tables (CRF) of the Swiss Greenhouse Gas Inventory (BAFU, 2020).

$$N_2O_{direct}\text{-}N_{TAN} = EF1\_N_2O * N_{TAN} \qquad \text{(Eq. 6)}$$

$$N_2O_{indirect}\text{-}N_{TAN} = EF4\_N_2O * (NH_3\text{-}N_{av.} + NO_x\text{-}N_{av.}) + EF5\_N_2O * NO_3\text{-}N_{short\text{-}term} \qquad \text{(Eq. 7)}$$

$$N_2O_{direct}\text{-}N_{av.\ CNpool} = EF1\_N_2O * N_{av.\ CNpool} \qquad \text{(Eq. 8)}$$

$$N_2O_{indirect}\text{-}N_{av.\ CNpool} = EF4\_N_2O * NO_x\text{-}N_{av.\ CNpool} + EF5\_N_2O * NO_3\text{-}N_{long\text{-}term} \qquad \text{(Eq. 9)}$$

where

$EF1\_N_2O$ equals 0.01, $EF4\_N_2O$ equals 0.03, and $EF5\_N_2O$ equals 0.01.

Nitrate ($NO_3$) leaching is differentiated into short-term and long-term losses from the nitrogen fractions $N_{TAN}$ and $N_{av.\ CNpool}$ respectively, where long-term losses can occur over a period of several years. The Farm Model estimates the potential $NO_3$ leaching, as shown in Equations 10 and 11.

$$NO_3\text{-}N_{short\ term} = (\sum N_{TAN,\ Fert.} * (1\text{-}NUR_{TAN,\ Fert.}) + (SON_{MIM} - \Delta N_{min}) * (1\text{-}NUR_{SONMIM}) +$$

$$N_{Dep.} * (1\text{-}NUR_{Dep.}) - NH_3\text{-}N - N_2O_{direct}\text{-}N -$$

$$(N_2O_{direct}\text{-}N_{av.\ CNpool} - EF1\_N_2O * (N_{PRag} + N_{PRbg})) \qquad \text{(Eq. 10)}$$

$$NO_3\text{-}N_{long\ term} = (\sum N_{tot,\ org.\ Fert.} - \sum N_{TAN,\ org.\ Fert.} - N_{CNpool,\ immobilised} + N_{PRag} + N_{PRbg} + \Delta N_{min}) * Frac_{Leach} \qquad \text{(Eq. 11)}$$

where

$Frac_{Leach}$ equals 0.18.

# Appendix 3. Nitrate Leaching: SIA, Farm Model, DAISY

Appendix 3. Nitrate leaching [kg $NO_3$-N $ha^{-1}$] of the fields BIK3, BIK4, BIK5 and of the fertilization treatment strips Control, M1 and M2 of the fields HYD2 and HYD4 in the years 2018 and 2019, measured by Self-Integrating Accumulators (SIA) and modelled by the Farm Model and by DAISY.

| **Year** | **Field** | **Nitrate Leaching [kg $NO_3$-N $ha^{-1}$]** | | |
|---|---|---|---|---|
| | | SIA | DAISY | Farm Model |
| 2018 | BIK3 | 35 | 27 | 113 |
| | BIK4 | 43 | 9 | 109 |
| | BIK5 | 21 | 169 | 108 |
| | HYD2 | 45 | 14 | 44 |
| | HYD2_M1 | 31 | - | - |
| | HYD2_M2 | 42 | - | - |
| | HYD4 | 79 | 22 | 59 |
| | HYD4_M1 | 53 | - | - |
| | HYD4_M2 | 44 | - | - |
| 2019 | BIK3 | 88 | 38 | 59 |
| | BIK4 | 76 | 50 | 91 |
| | BIK5 | 117 | 54 | 81 |
| | HYD2_C | 27 | 52 | 103 |
| | HYD2_M1 | 14 | 52 | 116 |
| | HYD2_M2 | 18 | 52 | 105 |
| | HYD4_C | 13 | 4 | 56 |
| | HYD4_M1 | 15 | 4 | 49 |
| | HYD4_M2 | 10 | 4 | 46 |

Fertilization on the fertilization treatment strips of HYD 2 and HYD 4 was adjusted in 2019. SIA measured Nitrate leaching in 2018 on the three strips. The models only show one value for 2018, as no input variables changed between the strips.