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– AN EMPIRICAL MODEL FOR PREDICTING NITRATE LEACHING FROM THE ROOT ZONE OF AGRICULTURAL LAND IN DENMARK

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Preface

The model NLES5 is the fifth version of an empirical model for prediction of nitrate leaching from arable lands. The first version was published by Simmelsgaard et al. (2000) and the previous version (NLES4) was described by Kristensen et al. (2008). The model predicts the nitrate leaching from the root zone based on nitrogen inputs and crops in the year of leaching, the crops in the previous year, the average nitrogen inputs through the last two years and information on soil type and drainage during the last two years. The model is developed in cooperation between Department of Agroecology (AGRO) and Department of Bioscience (BIOS), both Aarhus University.

The development of NLES5 was initiated in 2013 by AGRO and BIOS. In 2014, the Ministry of Food and Agriculture (MFVM) requested AGRO and Danish Centre for Food and Agriculture (DCA, AU) to update the NLES4 model. A scientific working group established for this purpose consisted of three members from AGRO, one from BIOS, two from SEGES (only in the period 2014-May 2019) and a consulting statistician (Kristian M. Kristensen, who also was involved in developing previous versions of the NLES model). The work has been part of the contract for policy advice provided by DCA for MFVM.

The Ministry of Food and Agriculture nominated an advisory board to follow the progress of the model development. The following institutions were invited to participate in this board: The Danish Agricultural Agency (Landbrugsstyrelsen, part of MFVM); The Environmental Protection Agency (Miljøstyrelsen, part of MFVM); The Nature Agency (Naturstyrelsen, part of MFVM); Knowledge Center of Agriculture (today SEGES, Landbrug og Fødevarer); University of Copenhagen (Department of Plant an Environmental Sciences); Aarhus University (AGRO, BIOS; DCA – Danish Centre for Food and Agriculture and DCE - Danish Centre for Environment and Energy).

During the project the advisory board had a number of meetings to monitor the progress of the model development. At these meetings, data used in the calibration and validation was presented and discussed, preliminary results of the model development was discussed, and requirements for model calibration, validation and uncertainty assessments were presented and discussed. A public workshop on modelling of nitrate leaching, was organized on 1st March 2018 in Emdrup, Copenhagen. All these discussions provided valuable inputs to the model development, and the authors gratefully acknowledge these inputs.

SEGES has provided measured nitrate-N concentration data from a number of field trials with variation in N fertilization levels, crops and soil types covering several years. Moreover SEGES provided information on soil texture and crop management for the modelling. Swedish University of Agricultural Sciences (SLU, Skara) has delivered nitrate-N concentration data from field trials with increasing fertilizer N rates. AGRO has modelled the water balances and calculated the N leaching for these external data that were used in the model calibration dataset. Two specialised advisors from SEGES participated in discussions on results of different model parametrisation as part of the analysing group that conducted the data analyses from 2014 until May 2019. This participation by SEGES ensured that the data provided by SEGES were accurately interpreted and applied and that relevant aspects of contemporary farming was properly reflected in the modelling. SEGES provided suggestions for model structure; however, although many of these suggestions were tested, the final choice of variable and the parametrisation of the model is the sole responsibility of the authors. Moreover, SEGES has commented on earlier versions of the report up until May 2019 (see link to details inside cover).

The authors thank SEGES for supplying the field experimental data for the calibration and suggestions for interpreting these field experiments. We also thank SLU for delivering nitrate concentration and weather data from the Swedish field trials.

Niels Halberg,

Director DCA – Danish Centre for Food and Agriculture

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Summary

NLES5 is an empirical model for predicting annual nitrate-N leaching, accounting for effects of nitrogen (N) inputs, crop sequences, autumn and winter soil cover, soils and weather conditions. The NLES5 model has been developed and calibrated based on nitrate leaching data, primarily from Denmark. The annual predicted nitrate leaching is defined for the period from April to March in the following year (leaching year), since the major part of the leaching takes place from October to March during the period of net precipitation surplus. The model takes into account effects of the main crops and winter vegetation in the year of leaching and in the previous year. Effects of N input in the leaching year and the average for the two previous years are also included in the model. N inputs include mineral N in fertilizers and manures, organic N in manures, mineral and organic N from grazing animals and biological N fixation. The model distinguishes mineral N applied in spring and autumn. Long-term effects of N input are accounted via an effect of total N in the topsoil. In addition, the model includes effects of water percolation in the leaching year and in the previous year, as well as the effects of soil clay content in the topsoil.

The model was calibrated against two datasets: Cal1 with 2053 observations of annual nitrate leaching from Denmark and Sweden during the period 1991 to 2017, and Cal2 with 54 observations of marginal N leaching from field experiments during 1976 to 2017. Marginal N leaching is defined here as the increase in N leaching per extra mineral N added in spring. The model was first estimated using the Cal1 dataset. Subsequently, the response of N leaching to spring applied mineral N fertiliser, which is referred to as the marginal N response, was recalibrated using the Cal2 dataset. The calibration procedure ensured no overall bias for the Cal1 dataset. Thus, the model both describes responses to crop and vegetation cover as well as representing experimental data on the average marginal N leaching rate. For the calibration of marginal N leaching, we used observed marginal N leaching rates at N rates near the crop economic optimal N application rate. The marginal N leaching at standard N rate in the calibration dataset varied from -6% to 76% and the average was around 17%. The model predicted the average annual marginal N leaching well, but captured only a small part of the variation in observed marginal N leaching. Long-term effects (>3 years) were not included in the dataset on N leaching and marginal N leaching (Cal2).

Cross validation showed that the model parameters were robust, giving nearly the same predictions using different subsets of the calibration dataset as found for the full calibration dataset. By the cross validation 10 different sub datasets was setup (90% of the data for calibration and 10% for validation) The mean bias error for the cross validation was less than 1 kg N/ha and the RMSE (Root Mean Square Error) was at the same level as found for the NLES5 model (app. 31 kg N/ha).

The NLES5 model includes a linear trend in N leaching representing a decline in N leaching of 0.11 kg N/ha/yr. This effect was in previous versions of the NLES model referred to as a "technology effect". This trend was calibrated for the period 1991-2017, and extrapolation of this effect outside this period should be considered with caution.

NLES5 predictions for a subset of the calibration data from monitoring on farmer fields (LOOP data), showed good correspondence between predicted and observed N leaching and flow weighted N concentrations for each of the five LOOP catchments located in northern, eastern and southern Jutland, Funen and Lolland. The NLES5 capture the variation between different soils and climate zones in Denmark.

A validation test using 856 independent observations of N leaching from three experiments showed a mean bias error of 1.7 kg N/ha, but with large variations between the experiments. The RMSE for the validation was 30.8 kg N/ha, which is at the same level as found for the calibration dataset (Cal1). The validation showed that the model predicted the effect of cover crops on N leaching at cropping system level well using data from a long-term crop rotation experiment. The validation also tested the ability to predict the marginal N leaching. Whereas the overall average marginal N leaching was well predicted, the model largely failed to capture the inter-annual variation in marginal N leaching. The model was also validated against a dataset with a large variation in cropping systems, for which the model captured the variation in most, but not all, systems.

Uncertainty analysis was conducted at both field and national scales. A Monte Carlo approach with 1000 parameter sets derived from the model covariance matrix was used to assess the uncertainty of the model parameters. The parameters sets were limited to be in the range of +/- 3 times the standard deviation for each parameter (>99% of the range of the parameter) and defined by the corresponding covariance matrix. The N leaching was predicted for each of the 1000 parameter sets, which allowed calculation of the standard deviation of model output. The uncertainty increased with N leaching level and therefore the uncertainty is higher for sandy soils under wet climate, compared to loamy soils under dry climate. The level of uncertainty as quantified by the coefficient of variation is app. 10%.

Scenario analyses for Denmark were used to predict mean N leaching and mean marginal nitrate leaching for the whole country. The inter-annual variation in average N leaching level for farmland in Denmark was predicted in the range between 40 kg N/ha and 92 N/ha with an average of 61 kg N/ha (for the climate period 1991-2010). The average marginal N leaching for farmland in Denmark was predicted to be on average 17% with an uncertainty of 2.5%-points. This is close to the 18% marginal N leaching previously predicted by the NLES4 model for Denmark. In the annual model predictions, the marginal N leaching varied between 10% and 25% over the years 1991 to 2010. The regional variation in N leaching over the farmland in Denmark (10×10 km grid scale) showed a variation in marginal N leaching of <5% to 25%. The uncertainty was app. 1%-points for farmland with low leaching levels up to 4%-points for areas with high leaching levels.

The model provides estimates of average N leaching for the most important agricultural crops grown in Denmark. Compared with the NLES4 model, the NLES5 model includes a better representation of crop sequences and winter vegetation cover, which is of great importance for application of the model for exploring cropping systems with low N leaching rates.

Future work should focus on enhancing knowledge on crops that are currently scarcely represented in the datasets, e.g. maize after grass, maize after maize, and potatoes. Effects of changes in autumn vegetation cover, such as early sowing of winter cereals should also be included. These effects has to be documented in a number of representative field experiments before the model can include these effects. There is also a need to consider long-term effect of changes in soil organic N, how this affects N leaching, and how such effects can be included in the model.

Dansk sammendrag

NLES5 er en empirisk baseret model, som beregner den årlige nitrat-N udvaskning fra rodzonen af landbrugsarealer og inddrager effekten af kvælstof (N) tilførsel, afgrøderækkefølge, efterårs- og vinterjorddække samt jordbund og vejrforhold. NLES5 modellen er udviklet og kalibreret på baggrund af primært danske data. Den årlige nitratudvaskning beregnes fra april til marts i det efterfølgende år (udvaskningsåret) hvor den største andel af udvaskningen sker i perioden fra oktober til marts, hvor der er et nedbørsoverskud. Modellen tager højde for såvel hovedafgrødens som vintervegetationens indflydelse i udvaskningsåret samt effekten af foregående års afgrøde. Effekten af N-tilførslens baseres både på N tilførsel i udvaskningsåret samt tilførslen i de to foregående år. N-tilførsel består både af mineralsk N tilført i form af kunstgødning og husdyrgødning, organisk N fra husdyrgødning, mineralsk og organisk N afsat fra græssende dyr og den biologiske N-fiksering. Modellen skelner mellem N tilført i henholdsvis forår og efterår i det første år. Langtidsvirkningen af det tilførte kvælstof beregnes ved hjælp af virkningen af den samlede kvælstof i det øverste jordlag. Endvidere omfatter NLES5 modellen vandgennemstrømningen indflydelse i udvaskningsåret og i det foregående år, samt betydningen af ler indholdet i det øverste jordlag.

NLES5 modellen er kalibreret mod to sæt data: Cal1 med 2053 observationer af årlig nitratudvaskning i Danmark og Sverige i perioden 1991-2017 og Cal2 med 54 observationer af marginal nitratudvaskning fra markforsøg med varierende N tilførsel udført i perioden 1976-2017. Den marginale N-udvaskning er her defineret som stigningen i N-udvaskning per ekstra kilo mineralsk N tilført om foråret. Modellen er først kalibreret til Cal1 datasættet. Dernæst blev den resulterende marginaludvaskning af nitrat-N, som følge af ekstra tilført mineralsk gødning tilført om foråret, kalibreret til Cal2 datasættets marginaludvaskning ved N tilførselsniveau tæt på den økonomisk optimale kvælstof norm for pågældende afgrøde. Ved kalibreringen af modellen sikredes, at der ikke skete skævvridning i forhold til Cal1 datasættet. Modellen beskriver således effekten af afgrøde, plantedække i efteråret/vinteren, tilført N med handels- og husdyrgødning, samtidig med at modellen repræsenterer den marginale N-udvaskning fundet i forsøg med stigende N gødning. Den marginale N-udvaskning ved standard N-tilførsel (økonomisk optimale N norm) i datasættet (Cal2) varierede mellem -6% og 76%, og gennemsnittet var ca. 17%. Modellens estimater stemmer med den målte gennemsnitlige marginale N-udvaskning over kalibreringsperioden, men modellen fangede kun en lille del af den observerede variation i marginal N-udvaskning mellem år og jordtyper/afgrøder.

En krydsvalidering viste, at modelstrukturen er robust, da krydsvalideringen gav næsten identiske prædiktioner af nitratudvaskningen som den samlede NLES5 model, der bygger på det samlede kalibreringsdatasæt. Ved krydsvalideringen blev anvendt 10 forskellige del-datasæt (10% af data udelades til validering og modellen kalibreres på de resterende 90% af data). Krydsvalideringen viste en gennemsnitlig afvigelse på mindre end 1 kg N/ha, og at RMSE (Root Mean Square Error, gennemsnitlig kvadratafvigelse) var på samme niveau som NLES5 modellen for det fulde datasæt (ca. 31 kg N/ha).

NLES5 modellen medregner en lineær udvikling i N-udvaskningen, svarende til et fald i N-udvaskningen på 0,11 kg N/ha/år. I tidligere versioner af NLES-modellen kaldes denne effekt en "teknologi effekt". Denne udvikling er kalibreret for perioden 1991-2017, og ekstrapolering uden for denne periode skal tages med forbehold.

Ved brug af en del af kalibreringsdatasættet fra monitorering af landbrugsjord (LOOP data – landovervågningsoplande) viste NLES5 god overensstemmelse mellem den gennemsnitlige prædiktion og den gennemsnitlige målte N-udvaskning samt gennemsnitlig målte afstrømningsvægtede N-koncentrationer for perioden 1991-2014 for hvert af de fem LOOP-oplande i Nordjylland, Østjylland, Sønderjylland, Fyn og på Lolland. NLES5 evner således at repræsentere den overordnede variation i nitratudvaskning mellem forskellige danske jorde og klimazoner.

En validering baseret på 856 uafhængige observationer af N-udvaskning fra fire forsøgsserier viste en gennemsnitlig afvigelse på 1,7 kg N/ha, men med stor variation mellem forsøgene. RMSE for valideringen var ca. 31 kg N/ha, hvilket er på samme niveau som for kalibreringsdatasættet (Cal1). Valideringen viste endvidere, at NLES5 modellen prædikterer effekten af efterafgrøder på N-udvaskningen med god præcision, når der ses på dyrkningssystemer i et længere tidsperspektiv. Valideringen testede også NLES5-modellens evne til at prædiktere marginaludvaskningen. Den gennemsnitlige marginaludvaskning blev prædikteret med god præcision, men modellen var ikke i stand til at fange variationen i marginaludvaskningen fra år til år. Endelig valideredes modellen mod et datasæt med en stor variation i dyrkningssystemer, hvor modellen opfangede variationen i de fleste systemer, men ikke alle.

En usikkerhedsanalyse af NLES5 modellen blev gennemført på både mark og landsskala. En såkaldt "Monte Carlo analyse" er gennemført ved at prædiktere 1000 parameter datasæt, der efterfølgende bruges som input til modellen. Parametrene ligger i intervallet +/- 3 gange standardafvigelsen (>99 % af udfaldsrummet for parameteren) og er defineret af en tilhørende kovarians-matrice. Usikkerhedsanalysen giver således et estimat på usikkerheden af modellens prædiktioner. Kvælstofudvaskningen blev prædikteret for hvert af de 1000 parametersæt, således at standardafvigelsen i modelestimaterne kunne beregnes. Usikkerheden øgedes i takt med N-udvaskningsniveauet, og derfor er usikkerheden højere for sandede jorde under våde klimaforhold sammenlignet med lerede jorde under tørre klimaforhold. Usikkerheden for hele landet er kvantificeret med en variationskoefficient på ca. 10%.

Scenarie-analyser for Danmark er gennemført for at kvantificere middel N-udvaskning og en gennemsnitlig marginaludvaskning for landet som helhed. År til år variation i gennemsnitligt nitratudvasknings niveau for landbrugsarealer i Danmark blev beregnet til at ligge mellem 40 kg N / ha og 92 N / ha med et gennemsnit på 61 kg N / ha (klimaperioden 1991-2010). For Danmark blev den gennemsnitlige marginal nitratudvaskning fra landbrugsjorde prædikteret med NLES5 til at være 17% med en usikkerhed på 2,5 procentpoint. Den regionale variation i marginaludvaskning fra landbrugsjorde i Danmark (opgjort for 10x10 km gridceller) blev estimeret til <5% op til 25%. Usikkerheden var ca. 1 procentpoint for landbrugsjord med lav udvaskning og op til 4 procentpoint for områder med høj udvaskning.

Modellen kan beregne den gennemsnitlige nitrat-N udvaskning for de vigtigste afgrøder i danske dyrkningssystemer. Sammenlignet med den tidligere NLES4-model har NLES5 en bedre repræsentation af afgrøderækkefølge og vinterplantedække, og dette har stor betydning, når modellen anvendes til at evaluere effekten af dyrkningssystemer.

Der bør fremover være særligt fokus på at opbygge viden om afgrøder, som for nuværende er begrænset repræsenteret i de tilgængelige datasæt, f.eks. majs efter græs, majs efter majs samt kartofler. Ligeledes kunne der med fordel ses på virkningen af ændringer i efterårsplantedækket som f.eks. tidlig såning af vinterkornsorter. Disse effekter skal dokumenteres i et antal repræsentative markforsøg, før modellen kan inkludere disse effekter. Endelig er der et behov for at se på langtidsvirkningen af tiltag i dyrkningen, der ændrer den organiske N pulje i jorden, samt hvordan sådanne ændringer påvirker N-udvaskningen på længere sigt.

1 Introduction

Nitrate leaching is considered the dominant nitrogen (N) loss pathway in from Danish agricultural systems (Pugesgaard et al., 2017; Blicher-Mathiesen et al., 2019). Nitrate leaching contributes to enhanced nitrate concentrations in groundwater and to N loadings of freshwater, coastal and marine ecosystems. Considerable political and regulatory efforts have been undertaken since 1985 to reduce nitrate leaching for improving quality of groundwater and surface water systems (Dalgaard et al., 2014). This has resulted in considerable reductions of the N surplus of Danish agricultural systems and in reduced nitrate leaching losses. However, there are still agricultural areas in Denmark, which based on modelling are considered to contribute with nitrate leaching losses that exceed N loadings required to achieve good environmental status in many coastal and marine ecosystems (Andersen et al., 2019).

Achieving good ecological status of aquatic ecosystems as stipulated by the EU Water Framework Directive and protection of vulnerable groundwater is expected to require spatial targeting of measures, if these are to be economically viable (Jacobsen and Hansen, 2016). There is a range of mitigation measures and these will vary in efficiency across farming systems and soils (Hashemi et al., 2018a). Such measures target various parts of the flow pathway of the nitrate lost through leaching from the bottom of the root zone. Measures may attempt to reduce the leaching directly or by enhancing the reduction of nitrate through denitrification in the subsoil or in wetlands (Hashemi et al., 2018b).

Regulations that involve spatial targeting will most likely require the ability to account for a portfolio of potential measures for reducing nitrate leaching, so that these can efficiently be integrated into current and future farming systems. Since measurements of nitrate leaching at field scale are costly, there is a need for simplified approaches for estimating nitrate leaching losses for application at both farm scale and for assessing losses at catchment and national scales. In Denmark, measurements of nitrate leaching have been largely based on measured nitrate content in soil water sampled from about 1 m depth using suction cells combined with modelling of the water balance to calculate the percolation of water at the suction cell depth, and the leaching is calculated as product of nitrate concentration and the amount of percolated water. Plants may have roots deeper than 1 m, resulting in potential overestimation of nitrate leaching with the method applied. This overestimation depend on soil and crop type, but has been estimated to be relatively small in common Danish cropping systems (Sapkota et al., 2012).

Process-based simulation models have the ability to simulate N turnover and loss processes at multiple scales (e.g., Doltra et al., 2019). However, such models require extensive calibration and detailed information in soils and crop management (Yin et al., 2017). Such detailed information is rarely available beyond research sites, and therefore scaling approaches are required to estimate inputs to these models or, alternatively, a simplified model can be applied. Simplified regression-based models have been developed and applied in Denmark (Simmelsgaard and Djurhuus, 1998; Simmelsgaard et al., 2000). These empirical models have been developed and calibrated based on measured nitrate leaching from experiments and monitoring networks. The latest version of these models is called NLES4 and was based on observational data from 1972 to 2004 (Kristensen et al., 2008). NLES4 models annual nitrate leaching as an effect of crops, N inputs, soil type and percolation. The NLES models have been extensively applied for supporting evaluation of policies for meeting nitrate leaching reduction targets. One of the major measures to reduce nitrate leaching from Danish agriculture has been reduction in the allowable N fertilizer rates, and the effect of N fertilization on nitrate leaching depends on how much of the extra added N fertilizer results in leaching, the so-call marginal N leaching. The marginal N leaching is thus the proportion of added extra N in fertilizer that is lost by nitrate leaching. This parameter has been greatly discussed in Denmark in connection to changes in governance structure for managing nitrate leaching. We have therefore given this issue particular attention.

Given the need for accurate prediction of the efficiency of measures that farmers can apply to reduce nitrate leaching, there is a need for a revised NLES model that reflects current cropping practices. There is also a need to validate the model predictions and obtain associated uncertainties (Larsen and Kristensen, 2007). This report describes the development of the NLES5 model using available data from 1991 to 2017, and the validation of the model using data from 2005 to 2017. The development of the model aimed to achieve the following effects on nitrate leaching: 1) Ability to simulate representative nitrate leaching across typical cropping systems, soil and climate conditions in Denmark, 2) Ability to simulate effects of autumn and winter vegetation characteristics on nitrate leaching, and 3) Ability to simulate effect of changes in N fertilization level on nitrate leaching.

This report presents results of the development, calibration, validation and uncertainty evaluation of NLES5. The data sets for calibration and validation are presented in Chapter 2. Chapter 3 describes the model structure, the statistical calibration procedures and the final model parameters. The model performance on different subsets of the calibration dataset are shown in Chapter 4, and the model performance for independent validation data are presented in Chapter 5. The uncertainty of model predictions for different scenarios at both field and national scale are presented in Chapter 6. The effect of N inputs on both the N leaching level and the specific effect of adding more mineral N in spring is exemplified and discussed in Chapter 7. An overall discussion of the model is given in Chapter 8. Appendix 1, 2, 3 and 4 includes detailed descriptions of data sets used in the calibration and validation, including other data referred to in Chapters 7 and 8.

2 Model variables and datasets on nitrate leaching

This study uses data from nitrate leaching measurements from field experiments in Denmark and Sweden (section 2.2) and from monitoring stations on farmer's fields in five catchments in Denmark (section 2.3). In general, these data have been collected from fields with the most common water flow situations in Danish agriculture having free draining conditions and where only limited nitrate reduction occurs through denitrification in the root zone.

Data of full year (April to March to cover the hydrological year) coverage of measurements of the nitrate-N flux concentration in the soil water at the lower depth of the root zone (typically 1 m) were collected, from experiments and monitoring where sampling had been conducted at regular intervals throughout the year. In most cases these measurement of soil water nitrate concentrations were taken from suction cups installed in the soil. However, in few cases samples drainage water were taken from drainage pipes from defined fields or plots. These concentrations were interpolated using percolation weighting (Lord and Shepherd, 1993) between measurement days and multiplied by model calculated daily percolation to obtain daily nitrate leaching, which were subsequently cumulated to annual values.

2.1 Overview of datasets

The data originate from different experiments and monitoring sites in Denmark and one experiment from Sweden (Table 2.1). Figure 2.1 shows the locations of the experimental and monitoring sites in Denmark. Most data are from dedicated field experiments covering different treatments from experimental research stations and field plots on farmers' fields. However, LOOP data consists of data from 29 actual fields on farms monitored from 1991-2014 for nitrate-N leaching losses.

The climatic conditions of the different locations are shown in Table 2.1. The average annual temperatures are within a range of 1°C among all Danish locations, and mainly determined by a north-south gradient. The variation in precipitation is greater with a maximum average annual precipitation around 1000 mm per year at the south-western part of Jutland and a minimum of around 710 mm at Lolland (Højvads Rende). The mean temperature for Skara (Sweden) is 6.9°C, which is lower than for sites in Denmark, but the precipitation is within the range for sites in east Denmark. The highest precipitation is found in the western part of Denmark, where sandy soils dominate.

Table 2.2 gives an overview of the monitoring sites (LOOP 1 to 6) and field experiments (101 to 226). These experiments are described in more detail in Appendix 1. The data divided into three different sets (*Cal1*, *Cal2* and *Val*), which were used for three different purposes:

Cal1: Development and calibration of the statistical model of nitrate leaching using the measured annual N leaching data. This covers data from 1991 to 2017 (see chapter 3)

Cal2: Subsequent (after *Cal1*) calibration of two parameters in the statistical model defining the marginal N response to applied mineral N fertilizer. Here derived marginal N response curves were used (see section 2.3). This dataset contains data from *Cal1* plus additional data from 1976-1988.

Val: Data used for model validation, which are independent from data for *Cal1* and *Cal2*, some of which are from some of the same sites and experiments as *Cal1*; however, with different crop combinations and different time periods.

Figure 2.1. Locations of experimental and monitoring sites with measurement of nitrate leaching.

Table 2.1. Location and site information on experimental and monitoring sites for measurement of nitrate leaching. Soils are categorized as LS (loamy soil), SL (sandy loam) and S (sand). Mean temperature and precipitation (corrected to soil surface) for sites in Denmark are average for 1990-2016 based on DMI 10 km grid values (precipitation) or 20 km grid (temperature). Precipitation is corrected to soil surface based on daily corrections.

Site	Longitude (°E)	Latitude (°N)	Soil type	Soil C (%)	Mean temperature (°C)	Mean precipitation 1990-2016 (mm)
Højvads Rende	11.29	54.87	SL	1.07	8.9	707
Odderbæk	9.52	56.75	LS	2.69	8.2	848
Horndrup Bæk	9.85	56.00	SL	1.35	8.3	845
Lillebæk	10.77	55.12	SL	1.26	9.0	803
Bolbro Bæk	9.09	55.06	LS	2.90	8.7	1002
Store Jyndevad	9.12	54.90	S	1.30	8.7	1020
Tylstrup	9.95	57.19	LS	1.90	8.2	881
Agervig	8.61	55.64	LS	4.10	8.4	1010
Lunding	9.56	55.22	SL	1.30	8.7	839
Foulum	9.57	56.50	SL	2.00	8.2	826
Ødum	10.13	56.30	SL	1.60	8.2	764
Aarslev	10.44	55.31	SL	1.50	8.9	784
Flakkebjerg	11.39	55.32	SL	1.20	8.8	710
Silstrup	8.64	56.93	SL	2.30	8.4	961
Borris	8.63	55.96	SL	1.40	8.6	990
Askov	9.11	55.47	SL	1.00	8.7	957
Tystofte	11.33	55.25	SL	1.60	8.9	643
Roskilde	12.05	55.62	SL	1.80	8.6	730
Aabenraa	9.36	55.02	L	2.50	8.7	997
Rønhave	9.77	54.96	L	1.50	9.0	819
Sdr. Stenderup	9.63	55.45	L	1.40	8.7	839
Løgumkloster	9.14	55.06	S	1.22	8.7	880
Bolderslev	9.24	55.02	S	1.22	9.0	983
Jyderup	11.37	55.58	LS	1.30	8.6	712
Holstebro	8.44	56.38	S	3.29	8.3	974
Guldborg	11.73	54.85	L	0.94	9.0	744
Skara (Sweden)	13.43	58.37	LS	1.60	6.9*	795*

*: Values based on annual data from 2006-2010

*Table 2.2. Monitoring data (LOOP 1, 2, 3, 4, and 6) and field experiments with data on nitrate leaching from different sites and different years. The number of observations used for model calibration (Cal1 and Cal2) and validation (Val) are shown. * marks sites where nitrate concentration was measured in samples from drainage pipes; in all other cases nitrate concentration was sampled from suction cups.*

No.	Years	Site	Cal1	Cal2	Val
LOOP 1	1991-2014	Højvads Rende	108		
LOOP 2	1991-2014	Odderbæk	137		
LOOP 3	1991-2014	Horndrup Bæk	96		
LOOP 4	1991-2014	Lillebæk	139		
LOOP 6	1991-2014	Bolbro Bæk	149		
101	1991-2004	Lunding, Næstved, Silstrup, Aabenraa	33		
102	1991-1993	Sdr.Stenderup, Silstrup, Askov, Agervig, Borris, Rønhave, Tylstrup, Jyndevad, Foulum, Ødum, Roskilde, Aarslev, Tystofte	48		
103	1976-1988	Agervig*, Sdr. Stenderup*		88	
104	1991-1994	Foulum, Jyndevad	25		
105	1991-1992	Ødum	8		
106	1991-1992	Jyndevad	10		
112	1994-1996	Jyndevad	23		
113	1991-1992	Jyndevad, Foulum, Ødum	36		
114	1991-1992	Jyndevad	20		
115	1991-2003	Foulum	12		
117	1997-2016	Flakkebjerg, Foulum, Jyndevad	270		751
118	1991-2001	Foulum	168		
119	1998-1999	Foulum	36		
122	1997-2001	Silstrup*	31		
216	2002-2012	Flakkebjerg, Foulum	240		
217	2010-2012	Foulum, Jyndevad, Rødekro	16		
220	2007-2011	Foulum	231		
221	2006-2009	Skara	21	19	
223	2012-2014	Foulum, Løgumkloster, Bolderslev	80		
224	2015-2016	Guldborg, Holstebro, Jyderup	35	34	4
225	2013-2016	Jyndevad, Foulum, Flakkebjerg			39
226	2014-2017	Foulum, Flakkebjerg	81	64	62
Total	**1976-2017**		**2053**	**235**	**856**

2.2 Measurement and calculation of nitrate leaching

For each of the observational datasets the annual water balance was simulated using the Daisy root zone model (version 4.01). Daisy is a one-dimensional soil-plant-atmosphere model designed to simulate the crop production as well as the water and N balance in the agro-ecosystems (Abrahamsen and

Hansen, 2000). Soil water dynamics include water flow described by the Richards equation in the soil matrix, uptake and evapotranspiration by plants and soil. The calibration of the water balance model in Daisy is described by Børgesen et al. (2013).

The Daisy model calculates the water balance on a daily time step using daily data of precipitation, air temperature and global radiation. The precipitation is based either on direct observations from local meteorological stations or for the LOOP monitoring and SEGES data on interpolation of the measured precipitation to a 10×10 km grid using data from the Danish Meteorological Institute (DMI) measurement network. If a LOOP catchment is represented in more than one 10×10 km grid, the mean of two grids is used. The precipitation data is corrected on a daily basis for the under-catch of wind and wetting according to guidelines from DMI (Refsgaard et al., 2011).

The reference evapotranspiration was calculated using the local data on global radiation and temperature using the Makkink equation adjusted for Danish conditions. For LOOP data (LOOP1-6) and SEGES data (Experiment 224), calculation was based on DMI 20×20 km grid data. Mean daily temperature were for most experiments based on local observations, whereas data from LOOP 1-6 and experiment 224 was based on 20 km grid scale values delivered by DMI. The calculation of potential evapotranspiration from the reference evapotranspiration followed recommendations in Refsgaard et al. (2011). Soil crop cover, which influence the crop transpiration and hereby the overall water balance, is based on sowing and harvesting day information from the field experiment. Crop biomass development and Leaf Area Index, which affect the transpiration is simulated on basis of standard Daisy parameters (Styczen et al., 2006) and the weather data (precipitation, air temperature and global radiation).

Data on soil texture and hydrological parameters used by the Daisy model to simulate water transport and actual evapotranspiration were based on local soil measurements from Jacobsen (1989) for most experiments and local soil data for LOOP monitoring stations and experiments 221 and 224. Field management data on crop types, soil tillage, sowing and harvest dates, irrigation and N fertilization from the experiments, was included in the Daisy water balance simulations. Daisy simulations was conducted for the entire crop rotation in one continuous model run with a 4 year “warm up period” to ensure that initial soil water content is based on the effect of actual soil, crop and weather conditions.

Calculation of nitrate leaching over time is based on multiplying modelled water transport at a certain depth under the root zone (depth were soil water nitrate concentrations are sampled, typically 1 m, or from drainage pipe at drainage depth) and the measured nitrate concentration in the soil water sampled.

Measurements of nitrate concentrations in soil water are in most experiments conducted every two weeks during the drainage season for the fields in experiments 101-226. The calculation of nitrate leaching was based on the simulated daily drainage by interpolating nitrate-N concentration between sampling dates according to cumulated drainage flow, assuming that nitrate concentrations in the extracted soil water represents flux concentrations on the observation dates. The minimum number of nitrate samplings was set to 6 times during a percolation season for inclusion in the dataset.

For the monitored fields (LOOP1-6), the soil water samples were collected by having under-pressure in the suction cells for a week. The concentration in the soil water for the whole period, from day of start of collecting soil water until next time the measurement starts (approx. 7 days during the drainage season and two monitoring periods (7 days) during summer). For LOOP data the calculation of nitrate leaching was based on the simulated drainage for the period between two start measurement days, and assuming that the measured nitrate concentrations in the extracted soil water represents mean flux concentrations for the period.

The cumulated annual leaching was obtained from 1th April to 31th March in the following year. The average annual percolation for the involved sites are shown in Table 2.3.

Table 2.3. Mean annual precipitation (observations corrected to soil surface) and mean annual percolation (modelled by using the Daisy model) during the measurement periods for the Cal1 dataset.

Experiment	Start year	End year	Precipitation (mm)	Percolation (mm)
LOOP 1	1991	2014	710	202
LOOP 2	1991	2014	848	363
LOOP 3	1991	2014	841	349
LOOP 4	1991	2014	808	309
LOOP 6	1991	2014	1002	509
101	1991	2004	986	484
102	1991	1993	895	495
104	1991	1994	1015	606
105	1991	1991	734	299
106	1991	1991	959	482
112	1994	1996	916	494
113	1991	1992	841	427
114	1991	1992	940	540
115	1991	1992	835	369
117	1998	2004	905	420
118	1995	2001	760	284
119	1998	1999	870	367
122	1997	2000	1183	719
216	2003	2012	715	257
217	2010	2011	1061	642
220	2007	2010	792	234
221	2006	2009	780	288
222	1991	1991	960	483
223	2012	2014	996	533
224	2014	2016	882	373
226	2015	2017	844	440
All data	**1991**	**2017**	**858**	**416**

2.3 Calculation of marginal N leaching rate from experimental data

The response of nitrate-N leaching to increasing N application is an important output from the NLES5 model as this response is used to evaluate the environmental effects of the regulation of N application rates. Therefore, we paid special attention to the calibration of the response of N leaching to variation in N application rate. Unfortunately, we found very few recent empirical data from experiments with measurements of N leaching for several different N fertilization rates in the same experiment. Especially, we could not identify Danish N leaching experiments with at least four different N input rates performed in the period 1989 to 2014. From 2015 new N response experiments were established, and most of these data were used in the calibration of the NLES5 model.

The marginal N response was obtained for all available annual datasets from *Cal2* dataset. The marginal nitrate leaching was only estimated from the field trials with at least four N application rates using an exponential function:

$$\mathrm{L} = \alpha \cdot e^{\beta \cdot N}$$

where L is the nitrate leaching rate (kg N ha/y), N is the mineral N applied in spring in the actual year (kg N ha/y), and α and β are estimated parameters.

The marginal N leaching rate (M_N, %) is calculated from this function as

$$M_N = \beta \cdot \alpha \cdot e^{\beta \cdot N} \cdot 100\%$$

where N is the N rate at which the marginal N leaching rate is estimated.

The NLES5 model was calibrated to the estimated marginal N response of nitrate leaching by using all available data from experiments with at least four different N application rates (dataset *Cal2* in Table 2.2.). Statistics and parameter values for these data are found in Appendix 1 Table A.4.1. The *Cal2* dataset includes experiments with variable N application rates repeated in several years as well as single year experiments (Appendix 1 Table A1.3). We have included a short description of these experiments in Appendix 3. The harvested crop and the following winter crop for each of the experiments are shown in Appendix 4 Table A.4.1. Data include experiments from Sdr. Stenderup and Agervig (tile drains, used only in *Cal2*) and Skara (Sweden, suction cups used in both *Cal1* and *Cal2*). Other data from exp. 224 (SEGES data used in *Cal1*) and from new leaching experiments with variable N application rates (exp. 226) are also shown. The predicted marginal N leaching used in the calibration of the NLES5 model is shown in Appendix 4 Table A4.2. Tables A4.1 and A4.2 also include marginal N leaching results from the Broadbalk long-term wheat experiment in the UK, measured using a combination of tile drains and suction cups, and from Askov (lysimeters) where response to long-term N application was measured. However, these two experiments did not fulfil the selection criteria for inclusion in *Cal1* or *Cal2*. For the Broadbalk experiment, we did not have the required meteorological data, and the nitrate leaching level in lysimeter studies may be biased compared with field measurements due to boundary effects.

Figure 2.1 shows two examples from exp. 226, where the exponential function is optimized to applied mineral N fertilization in spring. Only data in the range 25 - 150% of the recommended N rate were used for the optimization, treatments with fertilizer-rate = 0 kg N/ha were excluded, because there is often an observed drop in N leaching at very low N application rates. The parameters α and β and the R^2 values for all field trials included in the *Cal2* dataset are shown in Appendix 4 A.4.1. The crops included in these N response experiments consisted of cereals, oilseed rape, grass in rotation, grass for seed and fodder beets (Table A3.2), and by far the majority of the observations are from experiments with cereals, which does not fully represent the average composition of crops in Denmark.

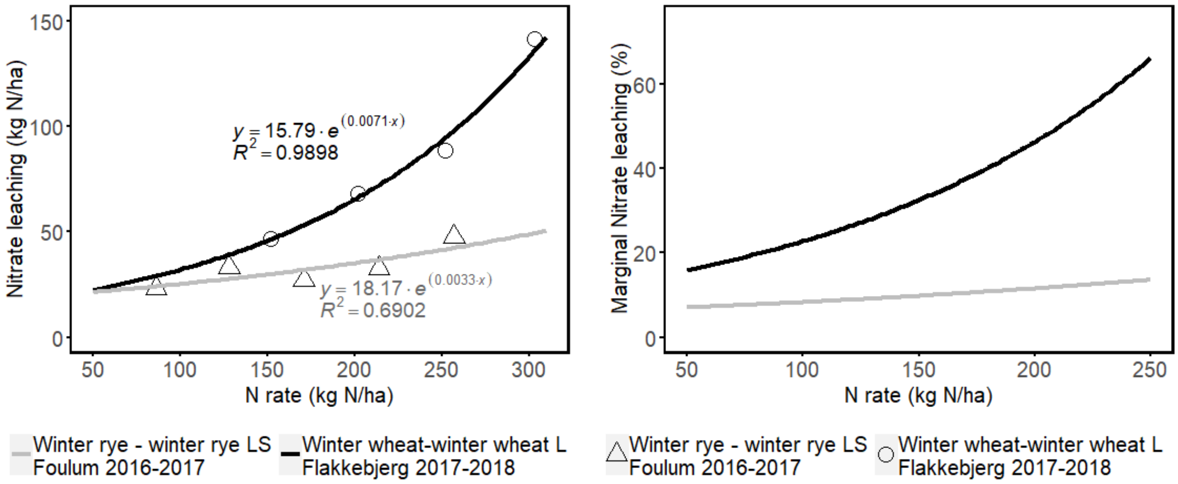

Figure 2.1. Exponential functions fitted to nitrate leaching observations from two different years placed at two sites (Flakkebjerg and Foulum) (left graph). The marginal N leaching is the slope of the marginal leaching curves (right graph).

2.4 Classification of crops, soil and nitrogen management

Crops were classified in relation to growing season and crop type. Since the nitrate leaching was calculated for the period April to March, covering the main crop growing period (main crop) and the following autumn and winter period (winter cover), we differentiated the vegetation cover of these two periods. In NLES5 we also included the vegetation cover of the previous year (previous main crop, and previous winter cover as illustrated in Figure 2.2).

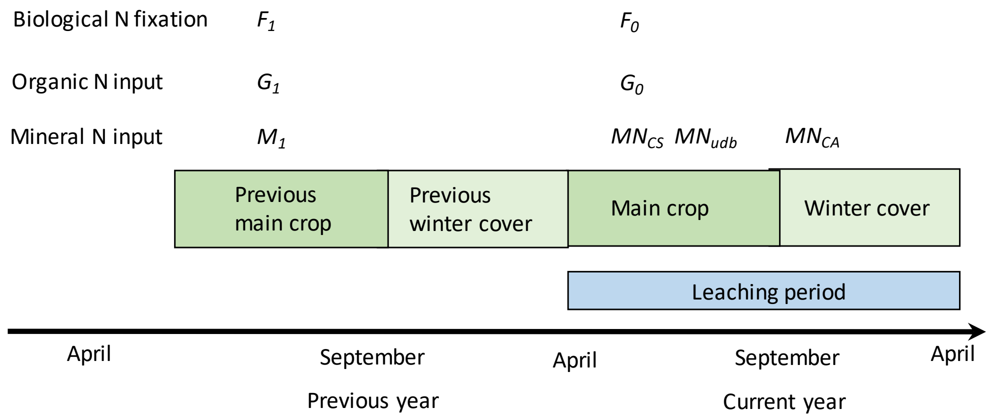

Figure 2.2. Timing of the crop and winter cover periods relative to the period defined for the nitrate leaching. The timing for N input in mineral and organic form from fertilization and biological N fixation is also shown for the current and previous year. In addition, NLES5 includes the N inputs from the year prior to the previous year (not shown in the graph).

The main crops were grouped into 13 categories, mainly based on their growing periods as well as characteristics in terms of residual N effects:

M1. *Winter cereals* comprise winter wheat, winter rye and winter barley, but not winter cereals after a grass or grass-clover (see M10).

M2. *Spring cereals* comprise spring barley, spring wheat and spring oats, but not spring cereals after grass or grass-clover (see M12).

M3. *Grain legume-cereal mixtures* comprise crops of mixtures of grain legumes (e.g. peas and lupin) with spring cereals (e.g. oats and spring barley). This includes crops grown for whole-crop silage and for maturity.

M4. *Grass-clover and grass* may have varying proportions of forage legumes in the stand. It may also comprise other perennial forage crops such as lucerne.

M5. *Grass for seed* production.

M6. *Set-aside* is an unfertilized grass without legumes, typically cut once during summer, but without removal of cuttings.

M7. *Beets and hemp*. Beets include both sugar beets and fodder beets.

M8. *Maize and potato* include both silage maize and potato, but not maize after grass or grass-clover (see M11). Potato was merged with maize, because there were only few observations on potato in the calibration dataset.

M9. *Winter oilseed rape*.

M10. *Winter cereal after grass* is a winter cereal established in the autumn after ploughing of a grass, set-aside, grass for seed and grass-clover.

M11. *Maize after grass* is a silage maize established in spring after a grass, set-aside, grass for seed and grass-clover that would typically be ploughed in spring.

M12. *Spring cereal after grass* is a spring cereal sown in spring after a grass, set-aside, grass for seed or grass-clover that is ploughed in spring or late autumn.

M13. *Grain legume and spring oilseed rape* include faba bean, lupin, soybean, peas grown for maturity in pure stands and spring oilseed rape.

The winter cover was grouped in 8 categories based on their vegetation cover and potential mineralization from the previous crop:

W1. *Winter cereals* comprise winter wheat, winter rye or winter barley. This includes winter cereals not following grass (see W7), and there is no accounting for time of sowing.

W2. *Bare soil* cover conditions following an autumn harvested crop, no establishment of winter cereals or winter oilseed rape, and where there is no information on soil cultivation or chemical weed control, i.e. there may actually be a stand of volunteers or weeds (see W5). However, this does not cover situations after maize or potato (see W3).

W3. *Autumn cultivation* is the situation, where the soil (stubble) was cultivated after an autumn harvested crop. It also covers situations with chemical weed control in autumn to remove weeds and volunteers, and following a late harvested potato or maize where there is no known stand of weeds or volunteers (see W5).

W4. *Cover crop* is either an undersown grass or other types of cover crop (catch crop) established by undersowing in the main crop or sown after harvest of the main crop. This may cover many different species of cover crops (e.g. fodder radish, winter rye, ryegrass or chicory). The cover crop is followed by a spring sown crop, whereas situations where an undersown grass continues as a grass in the following year is covered in W6.

W5. *Weeds and volunteers* cover situations where there is known stand of weeds or volunteers after an autumn harvested crop.

W6. *Grass-clover, grass for seed, beet, winter oilseed rape. Grass clover* are crops of either grass-clover that continues until the following year (see also W7). Grass for seed also continue till the next year.

Sugar beet or fodder beet as main crop have long growing season, and winter oilseed rape are established in autumn.

W7. *Winter cereal after grass* are winter wheat, winter rye or winter barley sown in autumn after a grass or grass-clover main crop.

W8. Grass ploughed late autumn or winter before sowing a spring crop.

For the previous main crop only four categories were used, again considering growing periods and residual N effects:

MP1. *Winter cereals* comprise winter wheat, winter rye and winter barley, but not winter cereals after grass or grass-clover (see MP4).

MP2. *Other crops* comprise all other crops than winter cereals, but not grass and grass-clover (MP3) or crops established after grass-clover and fodder grass (see MP4).

MP3. *Grass or grass-clover in rotation.*

MP4. *Spring or winter crops grown* after grass or grass-clover.

For the previous winter cover 10 different categories was used:

WP1. *Winter cereals* comprise winter wheat, winter rye or winter barley. This includes winter cereals not following grass or grass-clover (see WP9 or WP10).

WP2. *Bare soil* include conditions following an autumn harvested crop, no establishment of winter cereals or winter oilseed rape, and where the field either has been sprayed to remove weeds or there no information on soil cultivation, i.e. there may actually be a stand of volunteers or weeds.

WP3. *Grass or grass-clover* include grass, lupin or grass-clover main crops that are continued to the next year.

WP4. *Cover crops* in the previous winter.

WP5. *Grass for seed and set-aside*. Set-aside is an unfertilized grass without legumes, typically cut once during summer, but without removal of cuttings.

WP6. *Beets and hemp.* Beets is a main crop of sugar beets or fodder beets. Both beets and hemp are late harvested crops that prohibit use of cover crops.

WP7. *Bare soil after maize* or potatoes is a bare soil after the harvest of the crops.

WP8. *Winter oilseed rape.* Winter oilseed rape sown in the previous autumn.

WP9. *Bare soil or winter cereal following grass or grass-clover ploughed in the previous spring*.

WP10. *Bare soil or winter cereal following grass or grass-clover ploughed in autumn (before 1 November).*

In addition to this grouping, autumn and winter crop-cover in the leaching year were grouped into two categories for determining the nitrate leaching response to increasing N input. These two categories differentiate crops with and without a large N uptake during autumn:

WC1: *Crops with large N uptake in autumn*. Grass, grass-clover, sugar beet and fodder beet as main crop and grown in autumn, and winter oilseed rape sown in autumn.

WC2: *Crops with low or moderate N uptake in autumn*. All other crops and autumn vegetation cover situations.

Soils are classified based on their topsoil (0-25 cm) texture. The clay content (%) and the total N in the topsoil (Mg N/ha) is required. Soils are also grouped into sandy soils and loamy soils. The sandy soils were defined at sandy soils with coarse soil texture, i.e. less than 10% clay and less than 40% fine sand (JB1 and JB3) in the Danish soil classification. Other soils are classified as loamy.

The N input is divided into the N input in the current year and for the previous two years (all in kg N/ha/yr). The following N inputs are considered in the current year:

- MN_{CS} is the mineral N applied in fertilizer or manure in spring (kg N/ha/yr)
- MN_{CA} is the mineral N applied in fertilizer or manure in autumn (kg N/ha/yr)
- MN_{Udb} is the N deposited by grazing livestock (kg N/ha/yr)
- F_0 is the biological N fixation (kg N/ha/yr)
- G_0 is the organic N applied in manure in spring (kg N/ha/yr)

The following **average** annual N inputs are considered for the two previous years (1 and 2 are indices referring to each to the two previous years):

- M_1 and M_2 are mineral N applied in fertilizer or manure (kg N/ha/yr)
- G_1 and G_2 are organic N applied in manure (kg N/ha/yr)
- F_1 and F_2 are biological N fixation (kg N/ha/yr)

The biological nitrogen fixation (BNF) was estimated for main crops and cover crops (Appendix 1 Table A.1.2). BNF in LOOP 1 to 6 was calculated using the Danish farm planning program "Grønt Regnskab" from the Danish Agricultural Advisory Service (Hvid 1999). The BNF was calculated according to Høgh-Jensen et al. (2004) for the other datasets. The latter method requires information on dry matter yield of harvested legumes, which was available from most experiments. Where no information on dry matter were available, mean dry matter yields for similar crops from experiments with measured dry matter yields was used. It should be noted that there is considerable uncertainty in estimated BNF due to uncertainties in legume biomass and BNF efficiency as affected by soil N supply.

2.5 Calibration data

Table 2.4 shows the number of observations for combinations of main crop and winter cover. The dataset includes a total of 2053 observations. The dominating crops are winter and spring cereals. However, grass-clover and grass are also strongly represented. The winter cover is dominated by winter cereals, grass-clover as well and bare soil and cover crops. There were fewer observations with specific observations that allow the winter cover to be characterized as autumn cultivation or weeds/volunteers.

Table 2.4. Number of observations of combinations of main crops and winter cover for the calibration data (Cal1).

	W1. Winter cereal	W2. Bare soil	W3. Autumn cultivation	W4. Cover crop	W5. Weeds, volunteers	W6. Winter oilseed rape, grass-clover	W7. Winter cereal after grass	W8. Grass ploughed late autumn or winter	Total
M1. Winter cereal	191	171	15	20	8	37			442
M2. Spring cereal	96	125	53	111	46	176			607
M3. Grain legume –cereal mixtures	8		3	33	19	19			82
M4. Grass and grass-clover						274	2	46	322
M5. Grass for seed	1			3		11	4	4	23
M6. Set-aside	1					6			7
M7. Beet and Hemp	8					77			85
M8. Maize and potato	6		68	67					141
M9. Winter oilseed rape	40		1						41
M10. Winter cereal after grass	13	16	6	18	22	8			83
M11. Maize after grass			7	12		1			20
M12. Spring cereal after grass	21	7	1	51	14	24			118
M13. Grain legume and spring oilseed rape	41	3	5	12	21				82
Total	**426**	**322**	**159**	**327**	**130**	**633**	**6**	**50**	**2053**

Table 2.5 shows the number of observations for combinations main crop and previous winter cover. The winter previous crop is dominated by winter cereals, bare soil and grass-clover/cover crops.

Table 2.5. Number of observations of combinations of main crops and previous winter cover for the calibration data (Cal1).

	WP1. Winter cereal	WP2. Bare soil	WP3. Grass-clover and cover crops	WP4. Grass for seed	WP5. Set-aside	WP6. Beets	WP7. Bare soil after maize	WP8. Winter oilseed rape	WP9. Bare soil after spring ploughed grass	WP10. Bare soil after autumn ploughed grass	Total
M1. Winter cereal	442										442
M2. Spring cereal	23	349	19	136	2	60	18				607
M3. Grain legume –cereal mixtures	3	26	5	39		4	5				82
M4. Grass-clover		2	315	1	1	1			2		322
M5. Grass for seed		1	11		9				2		23
M6. Set-aside		2		1	4						7
M7. Beet and Hemp	1	62	14	8							85
M8. Maize and potato		30		48		3	60				141
M9. Winter oilseed rape								41			41
M10. Winter cereal after grass									75	8	83
M11. Maize after grass										20	20
M12. Spring cereal after grass									3	115	118
M13. Legume crops and spring oilseed rape		49	3	28		2					82
Total	**461**	**529**	**367**	**261**	**16**	**70**	**83**	**41**	**82**	**143**	**2053**

The average, minimum and maximum rates of N fertilization and N fixation are shown in Appendix 1 Table A1.2 for the different experiments and monitoring sites in the calibration data (Cal1). In most cases differences in N fertilization rate is driven by crop types and whether the cropping system is under organic or conventional management. In general, the highest N fertilization rates are found among the data from the LOOP sites on commercial farms (LOOP 1-6), and the lowest mean N application rates are found within experiment 117, which includes organic arable cropping systems. More detailed information on the LOOP data is given in Appendix 2.

To provide an impression of the variability in the N fertilization rates over the period (1991-2017) and within the years, Figures 2.3 and 2.4 show the spring and autumn mineral N application rates, respectively. The figures show that spring application accounts for the main N inputs and that large variation in N application is found for all years within the periods. The dots in Figures 2.3 and 2.4 shows that there are a few observations with very high N fertilization rates. These high mineral N application rates are more pronounced in the start of the period. The average autumn mineral N applications are low compared with the spring mineral N application for all years.

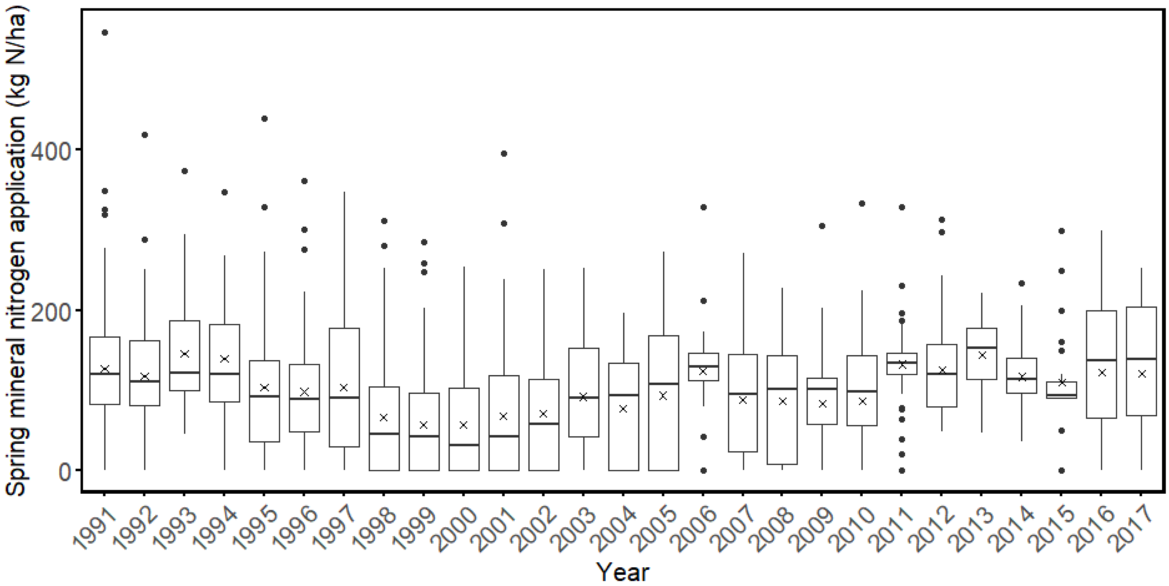

*Figure 2.3. Box plot of the mineral N application rates in spring (kg N/ha). Mineral N includes both the mineral part in manure and the total N in the mineral fertilizers. Boxes indicate the 25 to 75 percentile. Horizontal line within the box is the median. The upper and lower vertical lines from the hinge indicate the largest and smallest values at 1.5 * IQR, where IQR is the inter-quartile range, or distance between the first and third quartiles, a roughly 95% confidence interval for comparing medians. Dots show observations outside the mean plus/minus the 95% confidence interval. × marks the mean value.*

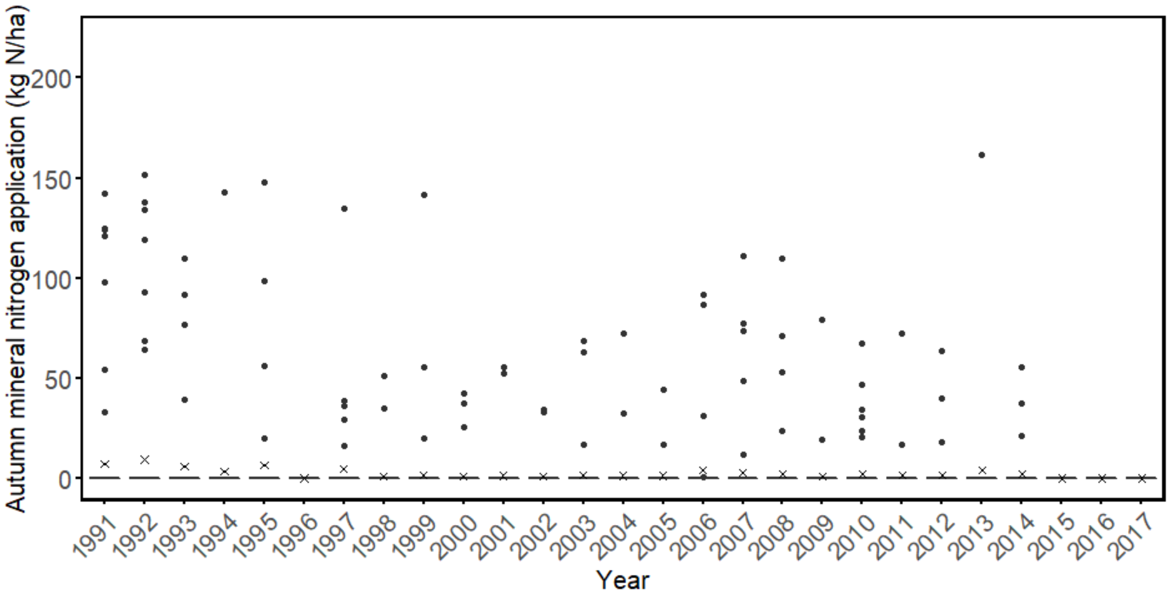

*Figure 2.4. Box plot of the mineral N application rates in autumn (kg N/ha). Mineral N includes both the mineral part in organic manure and the total N in the mineral fertilizers. Boxes indicate the 25 to 75 percentile. Horizontal line within the box is the median. The upper and lower vertical lines from the hinge indicate the largest and smallest values at 1.5 * IQR, where IQR is the inter-quartile range, or distance between the first and third quartiles, a roughly 95% confidence interval for comparing medians. Dots show observations outside the mean plus/minus the 95% confidence interval. × marks the mean value.*

Figure 2.5 shows a boxplot of the application rates of organic N in manures, which refers to the organic N of organic fertilizers only. Data from 1991 to 2014 include organic fertilizers whereas the data in 2015, 2016 and 2017 does not include organic fertilizers. This is because the data from 2015-2017 does not contain observations from the LOOP stations.

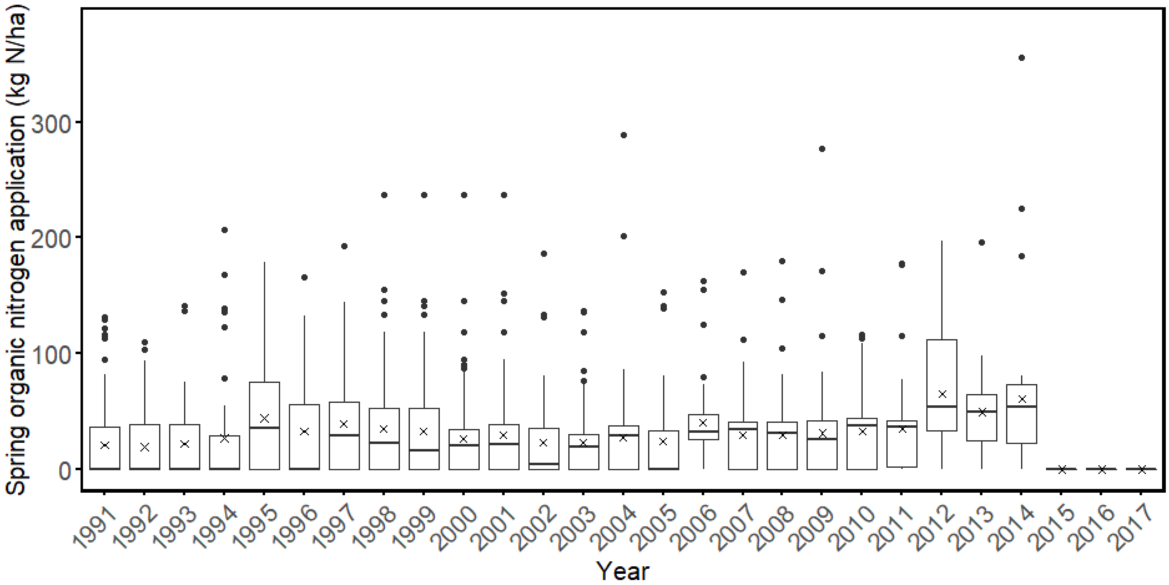

*Figure 2.5 Box plot of the spring organic N application rate with manure (kg N/ha). Only the organic part of the organic fertilizers. Boxes indicate the 25 to 75 percentile. Horizontal line within the box is the median. The upper and lower vertical lines from the hinge indicate the largest and smallest values at 1.5 * IQR, where IQR is the inter-quartile range, or distance between the first and third quartiles, a roughly 95% confidence interval for comparing medians. Dots are observations outside the mean plus/minus the 95% confidence interval. × is the mean value.*

Table 2.6 shows the number of combinations of main crop and winter crops represented in *Cal2* that includes the data of marginal N leaching. This dataset is partly a subset of *Cal1*, supplemented with data previously used for the calibration of the NLES4 data set (Kristensen et al., 2008). Nitrogen fertilization rates for *Cal 2*, are shown in Appendix 1 Table A.1.3. Data consist of 22 experiments with N fertilization levels in the previous three years similar to the actual N fertilization level in the leaching year. Other data have a shorter history with high, recommended and low N rates. Thus, the effects of long-term (>3 years) differences in N fertilization is partly represented in the *Cal2* data set.

Table 2.6. Number of marginal N leaching observations in the Cal2 dataset for main crop and winter vegetation cover combinations. Each observation consists of 4-7 sets of observations of N application rates and measured N leaching, from which the marginal N leaching rate was estimated. In total 235 annual nitrate leaching data (Table 2.1 and in appendix 4 Table A4.1) were available to provide 54 marginal N response observations.

	W1. Winter cereal	W2. Bare soil	W3. Autumn cultivation	W4. Cover crop	W5. Weeds, volunteers	W6. Winter oilseed rape, grass-clover	W7. Winter cereal after grass	W8. Grass ploughed late autumn or winter	Total
M1. Winter cereal	15	2							17
M2. Spring cereal	3	4	6	4	4	4			25
M3. Grain legume –cereal mixtures									
M4. Grass and grass-clover						4			4
M5. Grass for seed						1	1		2
M6. Set-aside									
M7. Beet and Hemp						2			2
M8. Maize and potato									
M9. Winter oilseed rape									
M10. Winter cereal after grass		1							1
M11. Maize after grass									1
M12. Spring cereal after grass		1				1			2
M13. Grain legume and spring oilseed rape	1								1
Total	**19**	**8**	**6**	**4**	**4**	**12**	**1**		**54**

2.6 Validation data

A total of 856 observations were included in the dataset for validation (Table 2.7). The data consist of a broad combination of main crops and winter crops. This dataset includes the main combinations of crops used in Denmark, but does not fully represent the crop distribution for the Danish agricultural land.

Table 2.7. Number of observations of combinations of main crops and winter vegetation cover for the validation data (Val).

	W1. Winter cereal	W2. Bare soil	W3. Autumn cultivation	W4. Cover crop	W5. Weeds, volunteers	W6. Winter oilseed rape, grass-clover	W7. Winter cereal after grass	Total
M1. Winter cereal	35	1	11	34	20	3		104
M2. Spring cereal	13		30	152	56	94		345
M3. Grain legume –cereal mixtures			3	23	13			39
M4. Grass-clover	1	81	1			33	1	117
M5. Grass for seed								
M6. Set-aside								
M7. Beet and Hemp								
M8. Maize and potato	4	20	2		20	1		47
M9. Winter oilseed rape	68		35	34				137
M10. Winter cereal after grass						1		1
M11. Maize after grass	2		1					3
M12. Spring cereal after grass			2	8	4			14
M13. Grain legume and spring oilseed rape			4	30	15			49
Total	**123**	**102**	**89**	**281**	**128**	**132**	**1**	**856**

The validation data consists of observations from 2005 to 2017. The average, minimum and maximum of the N fertilization and N fixation in the validation data are shown for the different experiments in Appendix 1 Table A.1.4. In general, the mineral N application rates are 16 kg N/ha lower in the validation data compared with the calibration data (Figure 2.6). Autumn mineral N fertilization is not included in the validation data set. Organic manure N application (Figure 2.7) is on average 33 kg N/ha lower in the validation data, whereas the N fixation is on average 6 kg N/ha lower compared with the calibration data set. The validation data set is dominated by low N input systems (experiment 117), but includes also very high N fertilization rates (experiments 224 and 225).

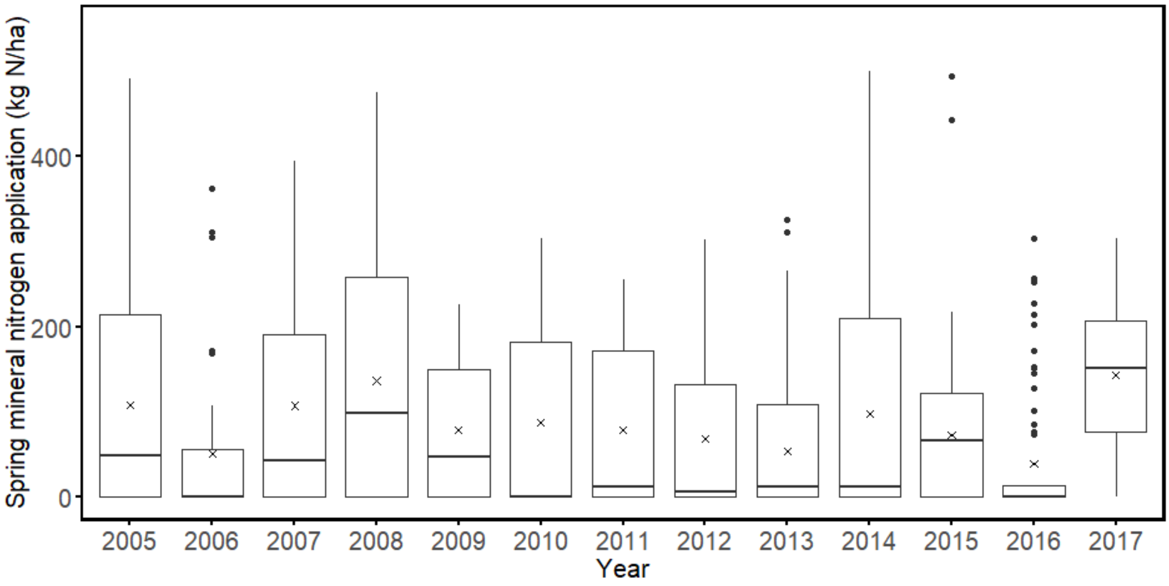

*Figure 2.6. Mineral N application rates for the validation data set. Vertical lines indicate the standard deviation. Boxes indicate the 25 to 75 percentile. The horizontal line within the box is the median. The upper and lower vertical lines from the hinge indicate the largest and smallest values at 1.5 * IQR, where IQR is the inter-quartile range, or distance between the first and third quartiles, a roughly 95% confidence interval for comparing medians. Dots are observations outside the mean plus/minus the 95% confidence interval. × is the mean value.*

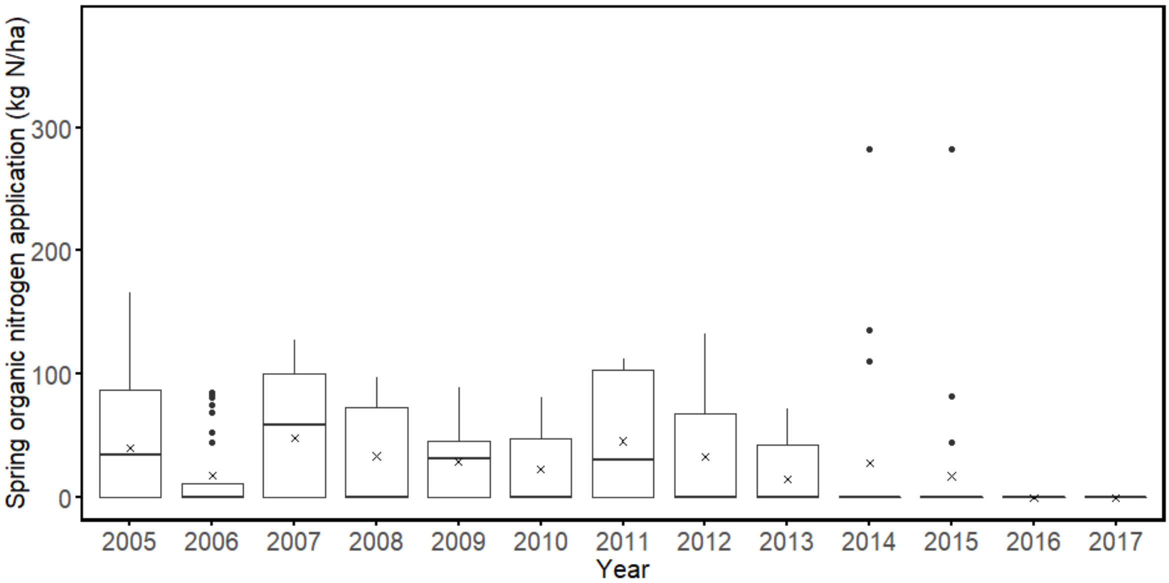

*Figure 2.7. Organic manure N spring application rates used in the validation data set. Vertical lines indicate the standard deviation. Boxes indicate the 25 to 75 percentile. The horizontal line within the box is the median. The upper and lower vertical lines from the hinge indicate the largest and smallest values at 1.5 * IQR, where IQR is the inter-quartile range, or distance between the first and third quartiles, a roughly 95% confidence interval for comparing medians. Dots show observations outside the mean plus/minus the 95% confidence interval. × is the mean value.*

3 Model description, parameterization and cross-validation

The model structure of NLES5 follows the same overall structure as previous NLES models (Simmelsgaard et al., 2000; Kristensen et al., 2008). However, changes have been made to how N inputs and crops and cropping sequences are defined in the model. A large number of different model formulations using different input variables have been tested prior to the final formulation of NLES5. Some of the different model formulations tested are presented in Table 3.1.

Table 3.1 Examples on how variables have been transformed and used as predictors, in a large number of tests of different model formulations during the NLES5 model development.

Variables	Model formulation tested during the model formulation process.
Nitrate leaching	Log10, Square root.
Mineral N effects	Mineral N split up in autumn and spring application; total N on annual basis; spring N rate effects scaled to crop recommended N rates using an exponential function and a power function.
Organic N effects	Mineralization during year 1 and following years of N from different types of organic fertilizers (Slurry from pigs and cattle, and solid manure) using an empirical model by Sørensen et al. (2017); total N in organic fertilizers; total N split up into a mineral and an organic part.
Crop effect	Mineralization from crop residues modelled using expert assessments. Previous main crop and main crop type classifications within a number of classes (4-14 different classes). Winter cover split up into different classes (4-12).
Mixed Crop and N effects	Introducing a scaling factor dependent on winter crop cover.
N yield	N in the harvested (removed) biomass.
Percolation	Annual percolation, seasonal percolation (April-August, September-December, January-March). Parameters independent or dependent of soil type.
Soil	Clay content in top-soil, clay content in sub-soil, organic C content, organic N content in top-soil or top- and sub-soils within the root zone.

These different model formulations were made following intensive analyses of the calibration data described in Chapter 2, discussion among the analysis group on how effects could be implemented in the model, and statistical analyses of how changes in model structure affects model performance. During model development the model performance was evaluated in several ways:

1. Ability to predict the data used for calibration (*Cal1* dataset), evaluated as R^2, *Mean Bias Error (MBE)* and Root Mean Square Error (RMSE) (Section 4).
2. Ability to predict effects of changes in crop rotations, crop management (e.g. cover crops) and fertilization management (fertilizer type and rate) using standardized scenarios (Chapter 6.1).
3. Ability to predict the marginal N leaching rate (Chapter 5.2).
4. Ability to predict independent data using a cross-validation approach using the Cal1 dataset (Chapter 4.3)
5. Ability to predict entirely independent data (*Val* dataset, Chapter 5).

Points 1 to 3 in the list above was part of the model development process, whereas points 4 and 5 were conducted after choosing the final model and its parameterization. The model was parameterized by minimizing the sum of squared differences using the square root transformed annual N leaching rates in an iterative procedure based on the *Cal1* dataset (Section 3.2). However, results showed that this procedure resulted in underestimation of the marginal N leaching compared to experimental data. Therefore, an additional model parameterization procedure was performed using the *Cal2* dataset, where only the model intercept and the parameter defining response to spring N application (MN_{CS}) in the current crop year was changed. In this case the model was optimized by minimizing the squared error of the marginal N leaching rate at standard N fertilizer rate (*Cal2* data), and at the same time achieving a zero mean bias error for the *Cal1* dataset.

3.1 Model description

The overall model structure of NLES5 is as follows:

$$L = \tau(Y - 1991) + \{(\mu + \theta_i N + C)^{\kappa}\}(P\ S)\rho \tag{1}$$

where L is the predicted annual nitrate leaching rate (kg N/ha/yr), is the effect describing trend over time (kg N/ha/yr), Y is year, μ is the intercept, Θ is a response factor to winter vegetation class (two classes WC1: grass-clover, grass, beets and winter oilseed rape; WC2: other, including bare soil and cover crops), κ is the power to which the effects of intercept+N+C is raised, N is the effect of N input (see below), C is the effect of crop and vegetation cover (see below), P is the effect of water percolation (see below), S is the effect of soil properties (see below), and ρ is a parameter that corrects for bias in the prediction due the use of square root transformed N leaching values. In the parameter estimation κ was fixed to 1.5 based on previous experiences (Kristensen et al., 2008).

The model has three major components:

- A linear trend in N leaching rate over time, which is additive to other effects.
- Effects of N input and crops (N+C), which can be viewed as the effect of crop and N input on effective nitrate concentration in the leachate.
- Effects of soil and percolation ($P\ S$) on the transport of nitrate, and this is multiplied with the effect of N input and crops.

The effects of N inputs on the N input factor (N) are described as:

$$N = \beta_t NT + \beta_{CS} MN_{CS} + \beta_{CA} MN_{CA} + \beta_{udb} MN_{udb} + \tag{2}$$

$$\beta_{m1} (M_1+M_2)/2 + \beta_{f0} F_0 + \beta_{f1} (F_1+F_2)/2 + \beta_{g0} G_0 + \beta_{m1} (G_1+G_2)/2$$

where β are effects of different types of N input, NT is the total N in the topsoil (0-25 cm, Mg N/ha), MN_{CS} and MN_{CA} are the mineral N in fertilizer and manures applied in spring and autumn (kg N/ha), respectively, MN_{udb} is the mineral N deposited by grazing animals (kg N/ha), M_1 and M_2 are the mineral N in fertilizers and manure applied in the two previous years (kg N/ha), F_0, F_1 and F_2 are the amount of biological N fixation in the current and the previous two years (kg N/ha), G_0 is the amount of organic N applied in manure in spring in the current year, G_1 and G_2 are the amount of organic N applied in manure in the previous two years (kg N/ha). The parameter (β_{m1}) for effect of mineral N (M_1+M_2)/2 and organic N (G_1+G_2)/2 in the previous two years were set to the same value, since initial model parameterization showed little difference.

The crop effects (C) are described as:

$$C = \eta_{mp} + \eta_{wp} + \lambda_{ma} + \lambda_{wa} \tag{3}$$

where η_{mp} is the effect of main previous crop, η_{wp} is the effect of previous winter vegetation, λ_{ma} is the effect of main crop in the actual year, and λ_{wa} is the effect of winter vegetation cover in the actual year.

The soil effects (S) are described as:

$$S = \exp\,(\zeta\, Clay) \tag{4}$$

where ζ is a parameter that quantifies the effect of clay content in the top soil (0-25 cm) ($Clay$, %).

The effects of percolation (P) are described as:

$$P = [1 - \exp(-\delta_{1s} A_{Aa} - \delta_{2s} A_{Ab})]\, \exp(-v_{2s} A_{Pb}) \text{ for sandy soils} \tag{5}$$

$$P = [1 - \exp(-\delta_{1c} A_{Aa} - \delta_{2c} A_{Ab})]\, \exp(-v_{2c} A_{Pb}) \text{ for loamy soils} \tag{6}$$

where δ's and v's are the effects of water percolation (Daisy model simulation ver. 4.01; Hansen et al., 2012) for different periods and soil groups. A_{Aa} is the percolation (mm) from April to August in the current year, A_{Ab} is the percolation (mm) from September to March in the current leaching year, and A_{Pa} is the percolation (mm) from September to March in the previous leaching year. For details see Chapter 2.2 and Figure 2.2. Sandy and loamy soils are defined in Chapter 2.

The non-linear relationship between nitrate leaching and the N input and crop term (N+C) is accounted for by raising the sum of these effects by the power of κ. However, this term does not fully account for variation among crops and autumn vegetation cover on the nitrate leaching response to N input, which was revealed during model development. The model therefore distinguishes the response of different vegetation types on nitrate leaching by multiplying the N term in eq. (1) by θ.

Both percolation and clay content will affect nitrate leaching by scaling with the factor (S and P), where S is the effect of clay in the soil and P is the effect of percolation. The effect of clay content relates to the nitrogen (primarily nitrate, but also ammonium) retention and transformation properties of soils, whereas the percolation reflects a simple nitrate transport effect.

3.2 Model parameterization

A two-step approach (A and B) (Figure 3.1) was applied for model parameterization. This approach was also applied for the model cross-validation reported in chapter 4.

In the first step all data in the Cal1 dataset were used to estimate model parameters using the non-linear parameter optimization of the square root transformed annual nitrate leaching using Gauss Newton method as implemented in the procedure Nlin of SAS (SAS Institute Inc. Cary NC). This means that we assume that all observations are independent. However, there are probably some correlations between observations from the same year and observations from the same field/plot. As this is ignored the estimated uncertainty on estimated parameters could be biased. Square root transformation was used to obtain observations that could be assumed to be normally distributed. Three model parameters (the power „ the trend , and the scaling parameter) were estimated separately in this procedure since they could not be properly estimated with the NLIN procedure. Therefore the following four sub-steps were applied in the first step of parameter estimation (A):

1. The power κ was fixed before the iterative process was started. We tested a number of different values, but ended at 1.5 as also used in the NLES4 model (Kristensen et al., 2008). The model parameters was obtained without any trend over years.
2. The trend over years (τ) was estimated from average annual model transformed residuals (sub-step 1) to calculate a trend. The trend was converted to un-transformed values by multiplying the estimating trend by 2 (the derivative of x^2).
3. Parameters (except κ, *and* τ) were estimated simultaneously using data from the Cal1 dataset.
4. The scaling parameter ρ was calculated to make the mean of all predicted leaching data equal to the mean of all observed leaching data. This accounts for the bias of back-transformation of the square root transformed estimated nitrate leaching values.

The following two sub-steps were applied in the second step of parameter estimation (B):

1. The parameter β_{CS} was re-calibrated to ensure that the marginal N response was in accordance with observed mean marginal nitrate leaching giving similar weight to each observation of marginal

nitrate leaching. This was done by minimizing the squared error of the marginal nitrate leaching rate at standard N fertilization rate using the Cal2 dataset. Negative marginal nitrate leaching values was set to null.

2. In order to ensure that this did not lead to overall model bias, the μ parameter was simultaneously changed so that the mean of all predicted values still was equal of the mean of all observed values in the Cal1 dataset. This procedure potentially also affects the uncertainty of model parameters in Tables 3.1 and 3.3. However, this was ignored and the reported SE values are therefore those from the SAS NLIN procedure from the first calibration step.

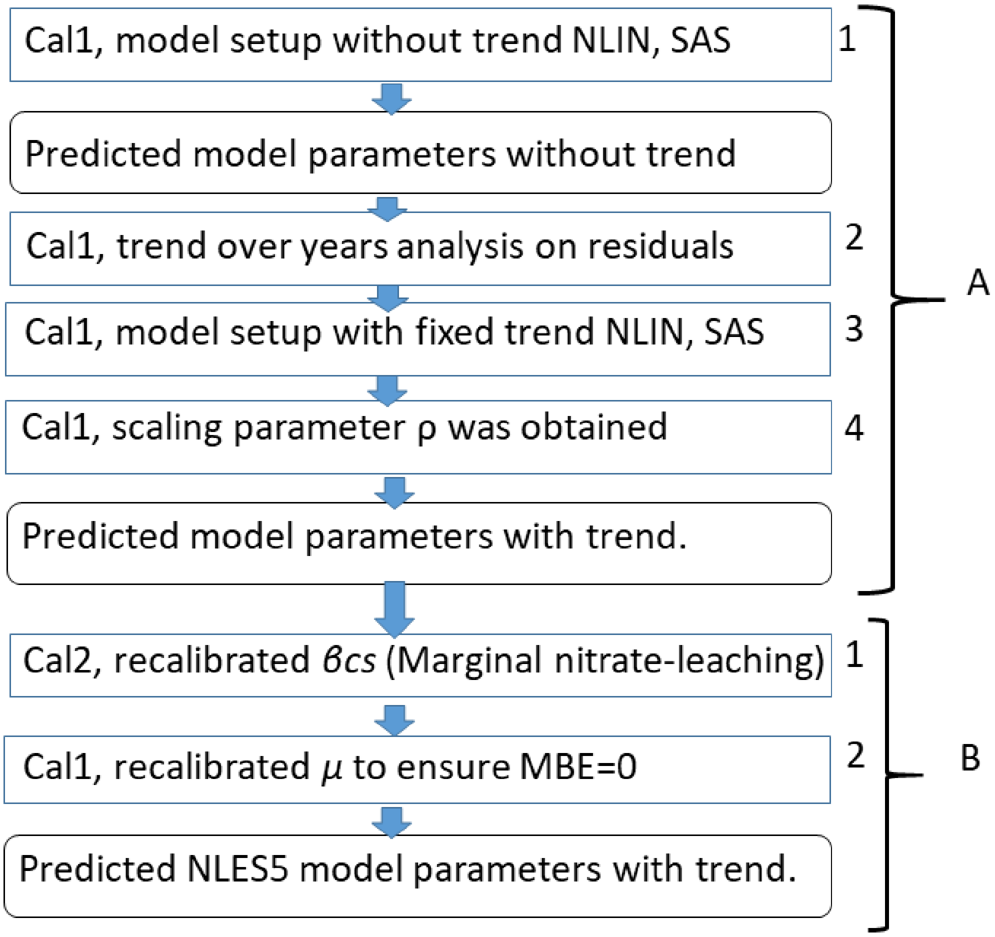

Figure 3.1. Steps (A and B) and sub-steps in the model parameterization procedure of the NLES5 model.

3.3 Model parameters

The estimated model parameters are shown in Table 3.2 and 3.3. All parameters related to crop and vegetation parameters are shown in Table 3.3, whereas other parameters are shown in Table 3.2.

Table 3.2. Estimated model parameters related to responses to nitrogen, soil and percolation responses in the NLES5 model. Both the estimate and the standard error (SE) of the estimate is shown.

Parameter	Description	Estimate	SE
τ	Effect of leaching trend over years (kg N/ha/yr)	-0.1108	-
κ	The power to which the effect of N input and crops is raised	1.5	-
ρ	A scaling factor to account for bias from back-transformation	1.085	-
μ	Intercept	23.51000	4.341800
β_{NT}	Total N in the top 25 cm soil layer (Mg N/ha)	0.456793	0.202200
β_{CS}	Mineral N application in spring in current year (kg N/ha)	0.049570	0.007000
β_{CA}	Mineral N application in autumn in current year (kg N/ha)	0.157044	0.034257
β_{udb}	Mineral N deposited by grazing animals in current year (kg N/ha)	0.038245	0.011056
β_{m1}	Effect of mineral and organic N, incl. N deposited by grazing animals) in the previous two years (kg N/ha)	0.026499	0.006121
β_{f0}	Biological N fixation in the current year (kg N/ha)	0.016314	0.005530
β_{f1}	Biological N fixation in the previous two years (kg N/ha)	0.026499	0.006121
β_{g0}	Organic N in animal manure in current year (kg N/ha)	0.014099	0.008799
θ_1	Winter crop group 1 (WC1)	1.000000	
θ_2	Winter crop group 2 (WC2)	1.205144	0.110679
ζ	Soil clay content in the topsoil (0-25 cm) (%)	0.001849	0.004557
δ_{1s}	Percolation in the period April-August on sandy soils (mm)	0.001194	0.000437
δ_{2s}	Percolation in the period September-March on sandy soils (mm)	0.001107	0.000306
v_{2s}	Percolation in the period September-March in the previous leaching year on sandy soils (mm)	0.000856	0.000163
δ_{1c}	Percolation in the period April-August on loamy soils (mm)	0.000798	0.000233
δ_{2c}	Percolation in the period September-March on loamy soils (mm)	0.000745	0.000180
v_{2c}	Percolation in the period September-March in the previous leaching year on loamy soils (mm)	0.000638	0.000144

Table 3.3. Crop and vegetation cover parameters in the NLES5 model. Winter cereal is used as standard reference with a parameter value of 0. Negative values indicate lower leaching and positive values increased leaching compared to the reference crop or vegetation cover. The effects can be compared relatively within each group: Main crop (M), winter vegetation cover (W), previous main crop (MP), previous winter vegetation cover (WP). Both the central estimate and the standard error (SE) of the estimate is shown.

Crop code		Estimate	SE
Main crop			
M1	Winter cereal	0	
M2	Spring cereal	-6.744	2.725
M3	Grain-legume mixtures	-7.279	3.089
M4	Grass or grass-clover	-13.493	4.183
M5	Grass for seed	-17.478	5.388
M6	Set-aside	-11.192	4.821
M7	Sugar beet, fodder beet	-0.640	3.196
M8	Silage maize and potato	3.534	2.973
M9	Winter oilseed rape	-7.319	2.295
M10	Winter cereal after grass	-1.248	8.049
M11	Maize after grass	19.524	9.745
M12	Spring cereal after grass	-6.229	9.154
M13	Grain legumes and spring oilseed rape	-2.866	3.201
Winter vegetation cover			
W1	Winter cereal	0	
W2	Bare soil	-2.055	1.185
W3	Autumn cultivation	-0.456	1.499
W4	Cover crops, undersown grass and set-aside	-15.959	2.674
W5	Weeds and volunteers	-3.792	1.700
W6	Grass and grass-clover	-14.596	2.569
W7	Winter cereal after grass	-1.049	0.000
W8	Grass ploughed late autumn or winter	-21.060	6.208
Main previous crop			
MP1	Winter cereal	0	
MP2	Other crops than winter cereals and grass or grass-clover	2.847	1.031
MP3	Grass or grass-clover	0.664	2.000
MP4	Spring or winter crops after grass or grass-clover	1.160	9.838
Winter previous crop			
WP1	Winter cereal	0	
WP2	Bare soil	9.704	2.864
WP3	Grass-clover	10.601	3.447
WP4	Cover crops	9.354	2.902
WP5	Grass for seed and set aside	13.241	5.101
WP6	Beets and hemp	5.483	3.094
WP7	Bare soil after maize or potatoes	-1.572	2.963
WP8	Winter oilseed rape	7.413	0.000
WP9	Bare soil or winter cereal following grass-clover ploughed in spring	7.396	7.976
WP10	Bare soil or winter cereal following grass-clover ploughed in autumn	10.975	9.318

4 Model performance on calibration data

Figure 4.1 shows the predicted and observed nitrate leaching over the period of calibration data (*Cal1*) from 1991 to 2017. Overall, the model predicts the observed nitrate leaching with good precision for this dataset (2053 observations). There is no mean bias due the correction by the ρ factor*.* On the annual basis model average and median predictions mostly follows the year to year variation in observed nitrate leaching. Figure 4.2 shows the residuals obtained for the different years. In some years with extreme weather conditions, the model cannot capture the observed nitrate leaching. An example is 1992, where the model underestimates the observed nitrate leaching. This year had a severe drought period in spring, resulting in very low yields and low crop N uptake. Such effects of extreme weather conditions are not captured by the NLES5 model. In 2017 the model under-predicted nitrate leaching due to a very wet summer and autumn, which resulted in high observed leaching rates in September- December.

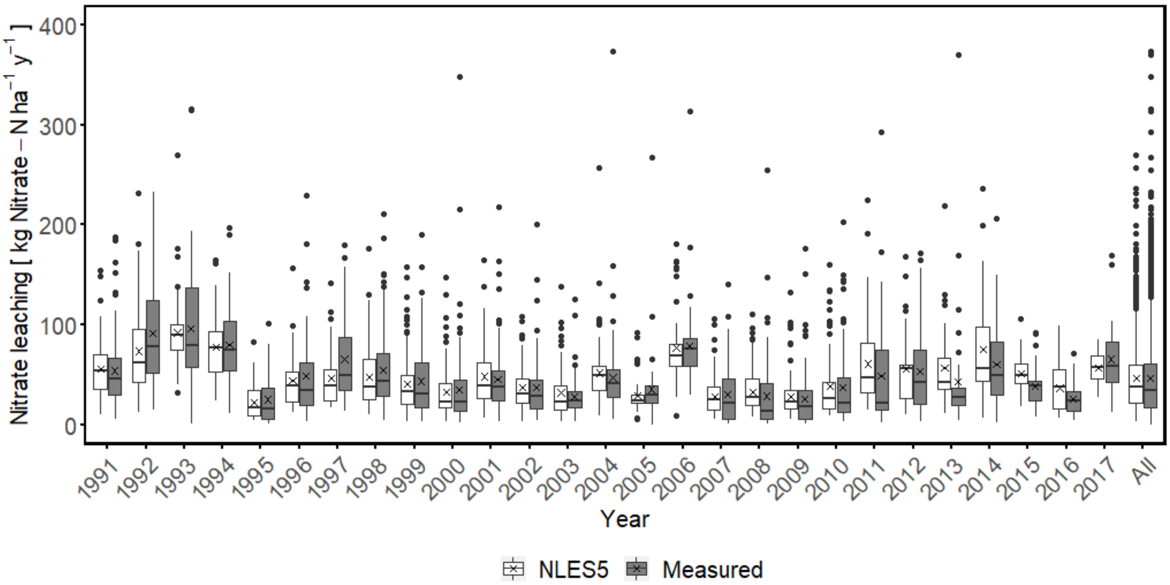

*Figure 4.1. Observed and model predicted nitrate leaching over the period 1991-2017 (Cal1 dataset). The horizontal lines in the box indicate the median values, and the lower and upper hinges correspond to the first and third quartiles (the 25th and 75th percentiles). The upper and lower vertical lines from the hinge indicate the largest and smallest values at 1.5 * IQR, where IQR is the inter-quartile range, corresponding to the 95% confidence interval. × shows the mean.*

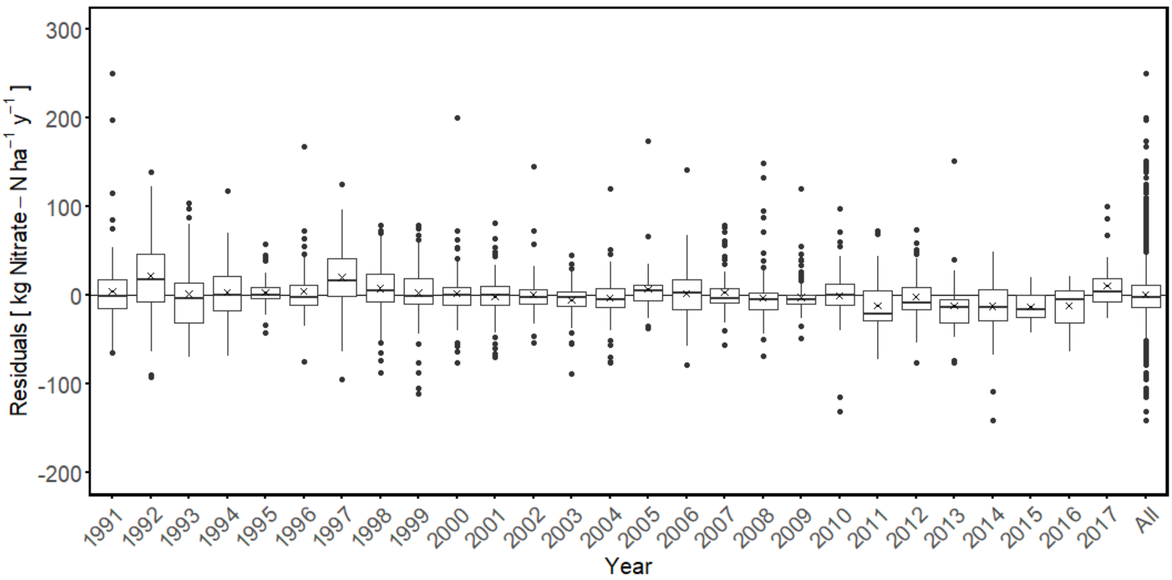

*Figure 4.2. Residuals (observed minus model predicted) nitrate leaching over the years 1991-2017 (Cal1 dataset). The horizontal lines in the box indicate the median values, and the lower and upper hinges correspond to the first and third quartiles (the 25th and 75th percentiles). The upper and lower vertical lines from the hinge indicate the largest and smallest values at 1.5 * IQR, where IQR is the inter-quartile range, corresponding to the 95% confidence interval. × shows the mean.*

Table 4.1 shows average NLES5 model predictions (P) together with the observed nitrate leaching (M). The number of observations used in the calibration for each combination of main crop and winter crop are shown in Table 2.4. For each column, the same winter vegetation cover parameter (Table 3.2) is used for the predictions, and in each row, the same main crop parameter are used in the predictions. Where a low number of observations (Table 2.4) of a certain combination of main crop and winter cover, there can be a high mean residual between predicted and observed. For grain legumes as main crop and bare soil as winter cover there were only 2 observations in the calibration, resulting in a high deviation.

Table 4.1. Average nitrate leaching (kg N/ha) obtained for combinations of main crop (rows, M1-M13) and winter crop (columns, W1-W8). Measurements (M) and predictions (P).

	W1		W2		W3		W4		W5		W6		W7		W8		All	
	M	**P**	**M**	**P**	**M**	**P**	**M**	**P**	**M**	**P**	**M**	**P**	**M**	**P**	**M**	**P**	**M**	**P**
M1	48	51	43	48	55	66	30	19	22	30	39	29					44	47
M2	42	44	52	50	55	54	35	34	50	53	27	26					40	40
M3	37	52			66	90	30	36	45	41	55	50					41	44
M4											30	28	27	43	70	54	36	32
M5	37	36					19	8			21	27	23	19	40	35	25	25
M6	66	61	31	46							29	16					33	31
M7	21	40									45	45					43	44
M8	92	126			96	108	62	54									80	83
M9	56	64			151	79											58	65
M10	77	91	91	91	84	61	25	27	44	47	105	88					63	63
M12					231	214	128	141			107	154					163	167
M13	74	76	110	105	186	118	21	20	90	57	33	38					48	44
All	50	54	51	53	84	87	40	39	51	49	33	32	24	27	68	53	47	47

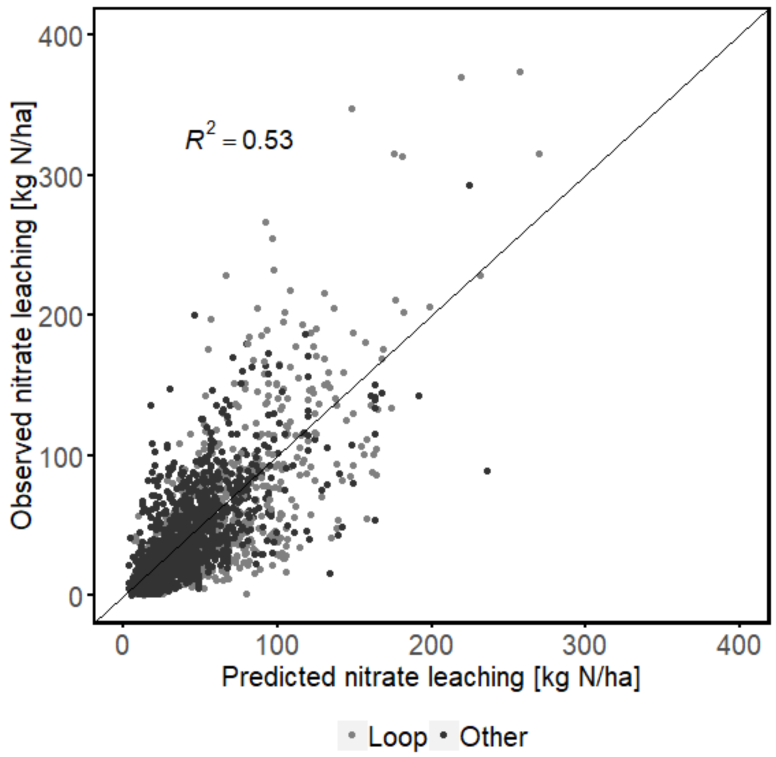

Figure 4.3. Observed versus model predicted annual nitrate leaching for the Cal1 dataset shown separate for the LOOP monitoring sites and the data from experiments. The line shows the 1:1 relation.

The predictions and observations are compared in Figure 4.3. Overall, there is a good correspondence for nitrate leaching below app. 100 kg N/ha, whereas the model under-predicts at high leaching rates above 150 kg N/ha. This tendency is particularly evident for observed nitrate leaching above 200 kg N/ha.

Table 4.2. Statistics on model prediction of nitrate leaching (kg N/ha) for the Cal1 dataset divided between data from the LOOP monitoring sites and the experimental sites. Root Mean Square Error (RMSE) and Mean Bias Error (MBE) of the residuals (measured-predicted) are shown along with the R^2 of the relation between observed and predicted values and the average nitrate leaching

Dataset	RMSE	MBE	R^2	Mean N leaching	Number of observations
Experimental	25.0	0.0	0.46	39	1424
LOOP	38.0	0.0	0.54	63	629
All	29.6	0.0	0.53	47	2053

Nitrate leaching from monitored farm fields in the LOOP network (29 fields, 629 observations) is on average 61% higher compared with average of the data from experimental sites (1424 observations) (Table 4.2). The RMSE of the model predictions was also greater for the LOOP than for the experimental datasets.

The R^2 of the NLES5 model is 0.53, which is the same as for the NLES4 model (Kristensen et al., 2008), but somewhat lower than for NLES1 and NLES2 models, mostly due to a broader coverage of crops and crop management in the data underpinning NLES5. The NLES5 model has as RMSE of 29.6 kg N/ha, which is lower than 33.6 kg N/ha for the NLES4 model (Kristensen et al., 2008).

4.1 NLES5 predictions for the LOOP monitoring sites

As mentioned in Chapter 2, data from the LOOP catchments are monitored on fields belonging to normal farming practice, which include a higher variation in the measured nitrate leaching compared to leaching from experiments plots. Data from the Loop catchments are therefore suitable to see how well the NLES5 model predict the measured leaching. Table 4.2 shows that the NLES5 model predicted the annual mean measured value of 63 kg N/ha with an R^2 of 0.54 for all 629 observations from the Loop catchments.

As often seen for empirical models, predicted leaching is less variable than observations from practical farming conditions, see for example NLES5 predicted and measured leaching for different categories of crop cover in Table 4.3. Here we see that the measured leaching have lower minimum and higher maximum leaching than predicted by NLES5. On the other hand, NLES5 well predicts averages for a number of observations in specific categories, which also is a natural performance of an empirical model. In the next section we will evaluated how well the NLES5 model predicts the average leaching for different combinations of crops, for the five individual LOOP catchments and for the annual values giving a trend in the leaching for the period 1991-2014.

Table 4.3 shows the measured and predicted nitrate leaching tabulated for the main crop and winter cover situation for the LOOP data. The model adequately predicts the large leaching when a grass field is ploughed in autumn and followed by a winter cereal. The average NLES5 predicted and measured leaching are 60 and 53 kg N/ha, respectively, when the main crop is forage grass or grass-clover and this crop is followed by grass, grass-clover or winter oilseed rape (62 observations). But the leaching increases to 108 and 114, respectively, when the grass is ploughed in autumn and followed by winter cereal (9 observations). We see some of the same effects for seed grass. The average model predicted and measured leaching are 27 and 21 kg N/ha, respectively, when the seed grass is followed by grass, grass-clover or winter oilseed rape (11 observations), but the average leaching increases when seed grass is ploughed and followed by winter cereal. In this situation, the average predicted and measured leaching are 35 and 40 kg N/ha, respectively (4 observations).

For the LOOP sites we measured very high nitrate leaching when maize was grown after ploughing of grass or grass-clover, and the NLES5 model can to a large extent predict this effect of crop sequences, even though the average NLES5 predictions for 3 observations is 225 kg N/ha against a measured average of 317 kg N/ha. When maize follow other crops than grass or winter cereal the average NLES5 predicted leaching of 107 kg N/ha is very close to the measured mean value of 104 kg N/ha (55 observations).

For beets mainly grown for sugar production in LOOP 1, the NLES5 predicted leaching of 43 kg N/ha is very close to the measured average of 44 kg N/ha for 30 observations.

For winter cereal followed by bare soil the NLES5 predicted a slightly lower leaching of 55 kg N/ha, than the measured average of 59 kg N/ha for 67 observations, and for winter cereal followed by winter cereal the NLES5 predicted an average leaching of 52 compared to the average measured of 52 kg N/ha/yr. Remarkably lower leaching is observed for winter cereal followed by cover crops, where the NLES5 predicted leaching of 30 kg N/ha is only slightly lower than the measured average of 36 kg N/ha for 7 observations. For winter cereal followed by grass or winter oilseed rape NLES5 predicted average of 36 kg N/ha is slightly higher than the measured average of 40 kg N/ha/yr for 23 observations. In conclusion, we see that the NLES5 model reasonably well predicts the average of the relative low measured leaching for forage grass followed by forage grass, and for seed grass or spring cereal followed by winter cereal, and for sugar beet or mixed grain legume cereal or winter cereal followed by bare soil or by winter cereal. The NLES5 model also fairly well predicts the relatively high average measured leaching for grain legume and spring seed rape, silage maize and spring crop, winter cereal or silage maize cropped after ploughed grass/grass-clover (Table 4.3).

Table 4.3. Measured and model predicted leaching as mean, min and max (kg N/ha) for the combinations of main crop and winter cover tabulated for the LOOP data in the Cal1 dataset. The number of observations (n) is also shown.

			Meas-ured	NLES5	Measured		NLES5	
Main crop	Winter cover	n	mean	mean	min	max	min	max
Forage grass and grass-clover.	Bare soil after grass	2	27	43	24	29	37	49
Forage grass and grass-clover.	Grass-clover. w. oilseed rape	62	53	60	1	194	10	131
Forage grass and grass-clover.	W. cereal after grass/ grass-clover	9	114	108	6	315	18	176
Grain legume and s. oilseed rape	Bare soil, stubble	3	137	84	118	152	60	119
Grain legume and s. oilseed rape	Winter cereal	12	96	79	3	185	5	174
Maize after grass/grass-clover	Bare soil, autumn tillage	3	317	225	207	374	199	257
Maize after grass/grass-clover	Grass-clover, w. oilseed rape	1	107	154	107	107	154	154
Mixed grain legume cereal	Bare soil, autumn tillage	1	55	158	55	55	158	158
Mixed grain legume cereal	Cover crops	16	37	53	9	109	14	106
Mixed grain legume cereal	Grass-clover, w. oilseed rape	15	61	60	18	197	27	149
Mixed grain legume cereal	Winter cereal	4	54	77	34	77	53	106
Oilseed rape	Bare soil, autumn tillage	1	151	79	151	151	79	79
Oilseed rape	Winter cereal	25	54	68	11	97	30	117
Seed grass	Bare soil after grass	4	23	19	8	29	7	33
Seed grass	Cover crops	3	19	8	4	42	6	12
Seed grass	Grass-clover. w. oilseed rape	11	21	27	3	50	9	63
Seed grass	Winter cereal	1	37	36	37	37	36	36
Seed grass	W. cereal after grass/ grass-clover	4	40	35	14	60	30	41
Set aside (green fallow)	Grass-clover, w. oilseed rape	6	29	16	6	57	9	28
Set aside (green fallow)	Winter cereal	1	66	61	66	66	61	61
Silage maize	Bare soil, autumn tillage	55	104	107	12	348	49	269
Silage maize	Cover crops	3	141	73	77	254	41	96
Silage maize	Winter cereal	4	116	119	36	169	60	168
Spring cereal	Bare soil, stubble	39	58	52	7	233	12	142
Spring cereal	Cover crops	31	63	56	11	218	10	139
Spring cereal	Grass-clover, w. oilseed rape	28	55	43	6	211	6	177
Spring cereal	Winter cereal	49	49	48	6	229	7	157
S. crops after grass/grass-clover	Bare soil, stubble	3	133	121	16	228	17	231
S. crops after grass/grass-clover	Grass-clover, w. oilseed rape	4	38	73	14	54	20	139
S. crops after grass/grass-clover	Winter cereal	7	114	102	59	178	52	145
Sugar beet, fodder beet	Grass-clover, w. oilseed rape	30	44	43	6	205	11	124
Sugar beet, fodder beet	Winter cereal	6	10	35	1	20	11	80
Winter cereal	Bare soil, autumn tillage	6	66	77	14	151	25	164
Winter cereal	Bare soil, stubble	67	59	55	9	202	7	181
Winter cereal	Cover crops	7	27	30	1	74	8	85
Winter cereal	Grass-clover, w. oilseed rape	23	40	36	12	123	15	85
Winter cereal	Winter cereal	61	52	59	8	167	13	161
W. cereal after grass/grass-clover	Bare soil, autumn tillage	1	77	58	77	77	58	58
W. cereal after grass/grass-clover	Bare soil, stubble	3	166	106	90	205	78	136
W. cereal after grass/grass-clover	Cover crops	1	94	62	94	94	62	62
W. cereal after grass/grass-clover	Grass-clover, w. oilseed rape	8	105	88	0	216	13	142
Forage grass and grass-clover.	Bare soil after grass	9	81	83	19	178	49	112

4.2 Variation between locations and annual trend

The average measured nitrate leaching for the five LOOP catchments are used to evaluate to what extent the NLES5 model is able to predict variation in leaching and in flow-weighted nitrate concentration between different regions in Denmark. Figure 2.1 shows that the five LOOP catchment are located both in the northern and southern part of Jutland as well as one catchment is located on Funen and one on Lolland (south of Zealand). The catchments also represent differences in farm practice as farmers in the loamy catchment LOOP 1 on Lolland mainly are arable farmers cropping cereals, beets for sugar production, grass for seed and winter oilseed rape. Crops grown in the loamy dominated soils in LOOP 3 and 4 are mainly covered by cereals and winter oilseed rape, but also grass and some maize as farmers in those catchments have some animal production. In contrast, the two sandy dominated catchments in northern and southern Jutland (LOOP 2 and 6) have intensive dairy production. The crop rotation in these catchments is dominated by grass-clover, maize and cereals with high input of fertilizer and manure, especially to the grasslands. The differences in farming are reflected in the use of mineral fertilizer and the application of manure with low total input for LOOP 1 and higher N input in LOOP 2 and 6 (Table 4.4). Also, precipitation and percolation differ between the five catchments with low precipitation and percolation in LOOP 1 and high precipitation and percolation in LOOP 6. Both differences in the farming system and in the level of precipitation and therefore also in percolation have substantial influence on the N leaching level with low average measured leaching of 31 kg N/ha for the arable farming in LOOP 1 and higher N leaching in LOOP 3 and 4 of 47 and 45 kg N/ha, respectively. Both catchments have more livestock and higher percolation than LOOP 1. The highest average leaching of 77 and 100 kg N/ha is observed for the two sandy dominated catchments, LOOP 2 and 6, respectively.

Table 4.4. Applied mineral fertilizer, applied manure and manure from grazing animals, harvest nitrogen and measured and NLES5 predicted nitrate leaching as well as average percolation tabulated for each of the five LOOP catchments as an average for the period 1991-2014.

LOOP	No of stations	n	Mineral N	Manure N	Grazing N	BNF	Harvest	Measured N leaching	NLES5 N leaching	Percolation
			(kg N/ha)							(mm/y)
1	3 or 4	108	118	11	0	9	121	31	28	202
2	6	137	66	150	7	20	128	77	79	362
3	4	96	122	60	28	22	137	47	50	350
4	6	139	89	107	6	10	123	45	46	307
6	7 or 8	149	96	137	35	24	160	100	93	512

The regional variation in average nitrate leaching between the five LOOP catchments is predicted well with the NLES5 model with an RMSE of 3.8 kg N/ha and an R^2 of 0.997 (Figure 4.4). To show that the NLES5 model does not only predict differences in the leaching due to variation in the percolation, we also tested how well the NLES5 model predicts the flow-weighted nitrate-N concentration. NLES5 predicted a slightly lower fit for the average flow-weighted nitrate concentration between the five LOOP catchments, but still fairly well with an RMSE of 1.4 mg N/L and R^2 of 0.840 (Figure 4.4). The NLES5 model is thus capable of predicting the average nitrate leaching and average flow-weighted nitrate concentration for the 629 observations in the five different LOOP catchments, but it has less skill in predicting leaching for single observations.

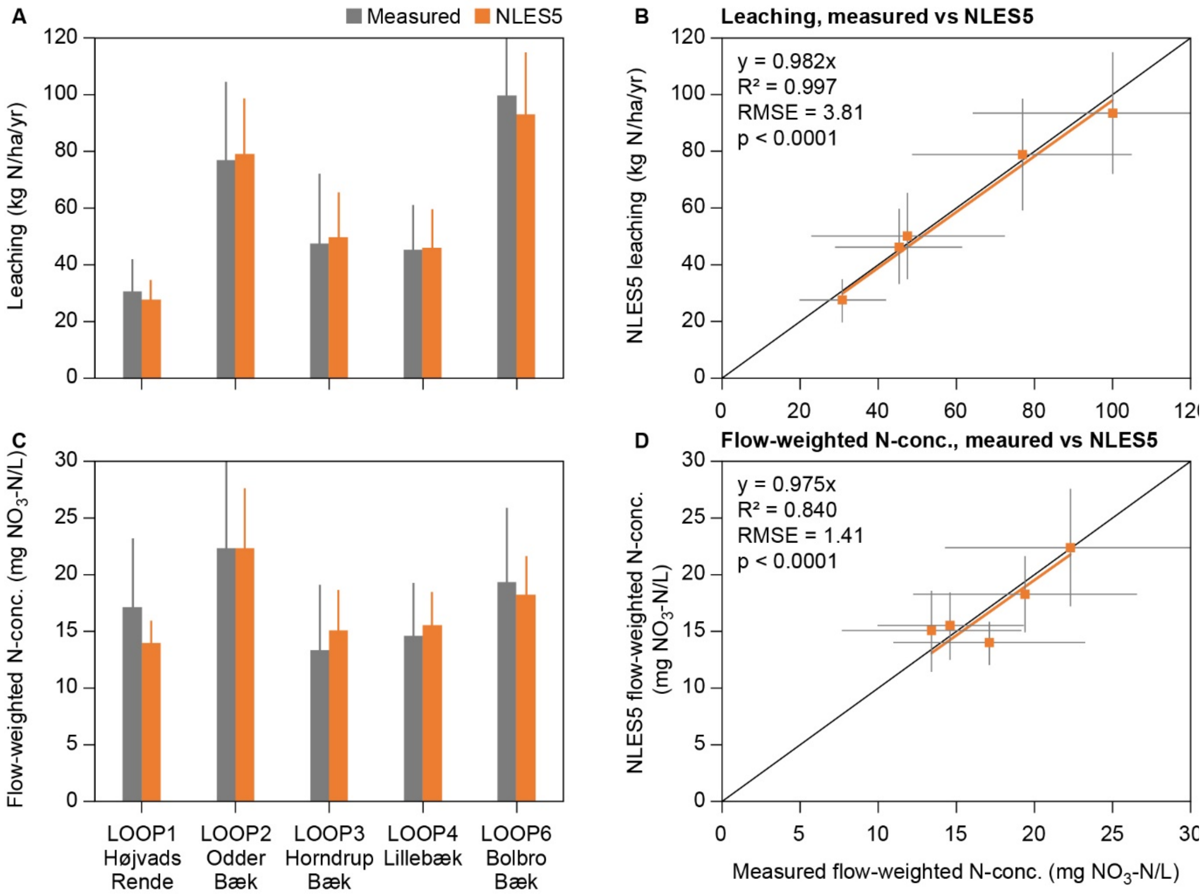

Figure 4.4. Average and standard deviation for measured and NLES5 predicted nitrate leaching (A) and (C) for each of the five LOOP catchments,x-y plot for leaching (B) and flow-weighted nitrate concentrations (D) for the average value calculated for the period 1991-2014.

4.3 Annual trend in nitrate leaching and flow-weighted nitrate concentrations

Farm practice and input of nitrogen to crops have been regulated due to several Actions plans in Denmark during the period 1987-2017 (Dalgaard et al., 2014). Since the LOOP measurements are monitoring data from fields belonging to practical farmers, the input of fertilizer and crop management follow the restrictions given in the governmental legislations. The question is therefore, whether the NLES5 model predicts the observed changes in the leaching recorded in the measured data for the monitored period 1991-2014.

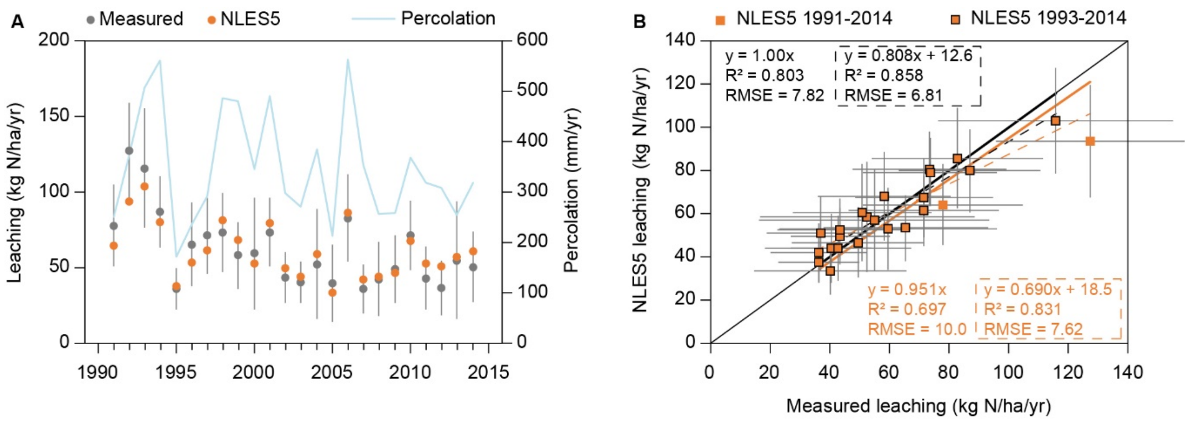

Figure 4.5. Measured and NLES5 predicted nitrate leaching as annual mean and standard deviation for the five LOOP catchments in the period 1991-2014, A) annual values, B) x-y plot. Annual percolation is shown in A.

The annual NLES5 predicted leaching follow to a great extent the variation in measured N leaching for the period, although with some differences. The NLES5 predicted annual average is lower than measured for 6 of 7 individual years until 1997 and after this year higher for 11 of 17 years. We added a trend in the model to address that not all changes in farm practice were able to be built into the NLES5 model. The model does not include yield as an influential factor, and we know that the yield for both cereals, maize and grass with the same level of fertilization has increased during the monitoring period. In addition, tillage practices have changed from early autumn to late November on loamy soils and to February on sandy soils in this monitoring period (Blicher-Mathiesen et al., 2019), and this may also have affected nitrate leaching.

As seen in Figure 4.5 the annual NLES5 predicted leaching rates are 12, 33 and 13 kg N/ha lower than the measured leaching in the first three years 1991, 1992 and 1993, respectively. In 1991 we measured very high leaching for a number of observations and the low average of the NLES5 prediction for this year is most pronounced in LOOP 2, 3 and 6. For station 104 in 1991 the grain legumes were followed by spring barley in 1992 and the measured leaching was 61 kg N/ha and the NLES5 predicted 39 kg

N/ha. On station 601 in 1991, the grain legumes were followed by winter wheat and the measured leaching was 184 kg N/ha and the NLES5 predicted 81 kg N/ha, a difference of 100 kg N/ha; this field also received manure of 24 kg N/ha in the spring a practice that is unusual because grain legumes have sufficient capacity to obtain N through BNF.

High measured leaching and relatively low NLES5 predictions were observed in 1991 for 3 stations with grazing cattle, which in some cases can give very high measured leaching due to high heterogeneity in deposition of urine and dung by the grazing animals.

Two observations for spring oilseed rape show high measured N leaching. On station 203 spring oilseed rape in 1991 was followed by bare soil (Table 4.3). The measured leaching was 162 kg N/ha and the NLES5 predicted is 107 kg N/ha. For the other observations on station 206 in 1991, spring oilseed rape is followed by winter wheat and the measured leaching is 151 kg N/ha, while NLES5 predicts 72 kg N/ha. We only had very few observations for spring oilseed rape for calibration, and this crop was pooled with grain legumes for the model calibration. Three fields had grain legumes in 1991 as mentioned above, and those three fields also have very high measured leaching, both in 1991 and 1992. Farmers are recommended to reduce fertilizer rate by 20-40 kg N/ha for crops following grain legumes, because of the residual N effect (NaturErhvervstyrelsen, 2013).

The very high measured N leaching compared to the NLES5 prediction in 1991 is for some of the LOOP stations caused by specific farming issues, such as grazing animals, high leaching from spring oilseed rape and from grain legume. The lower NLES5 predictions in 1991 are therefore not a general issue for all LOOP catchments and stations and most pronounced for the loamy catchment LOOP 3 and the two sandy catchments LOOP 2 and 6 (Figure 4.4).

For 1992 we observe high N leaching for fields with low yield. For all LOOP catchments in 1992, we had 25-60 kg N/ha lower N harvest in spring barley and winter wheat due to very dry conditions, and for some grass fields, the harvest in 1992 was 100 kg N/ha lower than in other years at similar N fertilizer rates (Blicher-Mathiesen et al., 2019). In LOOP 2 an especially low yield of 36 kg N/ha is observed for one station, but also a very high application of manure contributed to the high measured leaching level.

There were thus special farming and climatic conditions in 1991 and 1992 that results in deviations between observed and predicted N leaching, which cause a lower R^2 of 0.70 and RMSE of 10.0 kg N/ha for the relation between the annual measured and the NLES5 predicted leaching for the entire period 1991-2014, compared to these values for the period 1993 to 2014 having a fairly good prediction of the annual average values with R^2 of 0.83 and 0.86 and a slope of 0.81 and intercept of 12.6 kg N/ha (Figure 4.5B).

As mentioned above, the NLES5 model predicted the variation in the average flow-weighted nitrate concentration between the individual LOOP catchments fairly well, which means that the regional variation in the measured nitrate concentration is reasonably well predicted by the NLES5 model. For the flow-weighted concentration, the average NLES5 prediction for 1991 and 1992 was significantly lower than the average measured value (Figure 4.6A), due special farming issues for some observation fields with grain legumes, grazing animals and spring oilseed rape as described above. However, the annual NLES5 predicted nitrate concentration tends to be at a higher level than the measured in the years after 1997. Hence, in 1998, 2000, 2005, 2009 and 2010 the predicted concentrations are close to the measurements. Regression for the annual average of the NLES5 and measured flow-weighted concentration showed R^2 of 0.86 and 0.74 for the entire period 1991-2014 and without 1991 and 1992, respectively (Figure 4.6B).

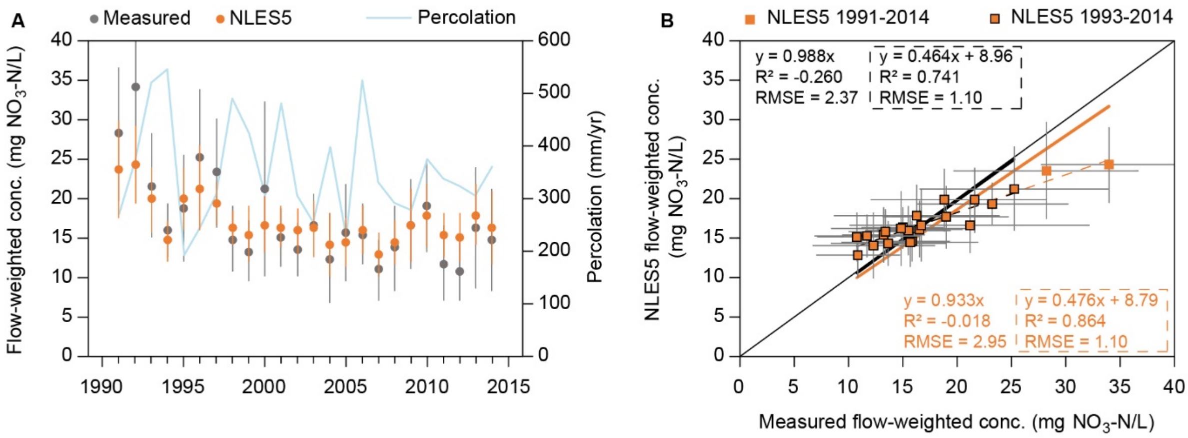

Figure 4.6. Measured and NLES5 predicted flow-weighted nitrate concentration as annual mean and standard deviation for LOOP data in the period 1991-2014; A) for the measured period, B x-y plot.

For individual LOOP catchments, the NLES5 model predicts fairly well the annual variation in leaching with R^2 between 0.43-0.79 and RMSE between 9.7 and 22.8 kg N/ha/yr (Figure 4.7 and Table 4.5). Also the NLES5 prediction of the average annual flow weighted nitrate concentration for the individually LOOP catchments was fairly good with an R^2 between 0.34 and 0.73 and RMSE between 1.5 and 3.1 (Figure 4.8 and Table 4.6).

Table 4.5. Statistics of slope, intercept, R^2, RMSE for NLES5 prediction of average yearly measured leaching for each of the five LOOP catchments.

LOOP	Slope	Intercept	R^2	RMSE (kg N/ha/yr)
1 Højvads Rende	0.516	11.7	0.431	9.72
2 Odder Bæk	0.510	39.7	0.579	15.7
3 Horndrup Bæk	0.485	27.1	0.584	14.3
4 Lillebæk	0.824	8.95	0.793	9.11
6 Bolbro Bæk	0.618	31.5	0.654	14.9

Table 4.6. Statistics of slope, intercept, R^2, RMSE for NLES5 prediction of average of flow-weighted yearly measured flow-weighted nitrate concentration for each of the five LOOP catchments.

LOOP	Slope	Inter-cept	R^2	RMSE (kg N/ha/yr)
1 Højvads Rende	0.154	11.4	0.351	1.53
2 Odder Bæk	0.467	12.1	0.729	3.09
3 Horndrup Bæk	0.225	11.3	0.339	2.39
4 Lillebæk	0.410	9.15	0.457	2.17
6 Bolbro Bæk	0.468	9.01	0.636	2.21

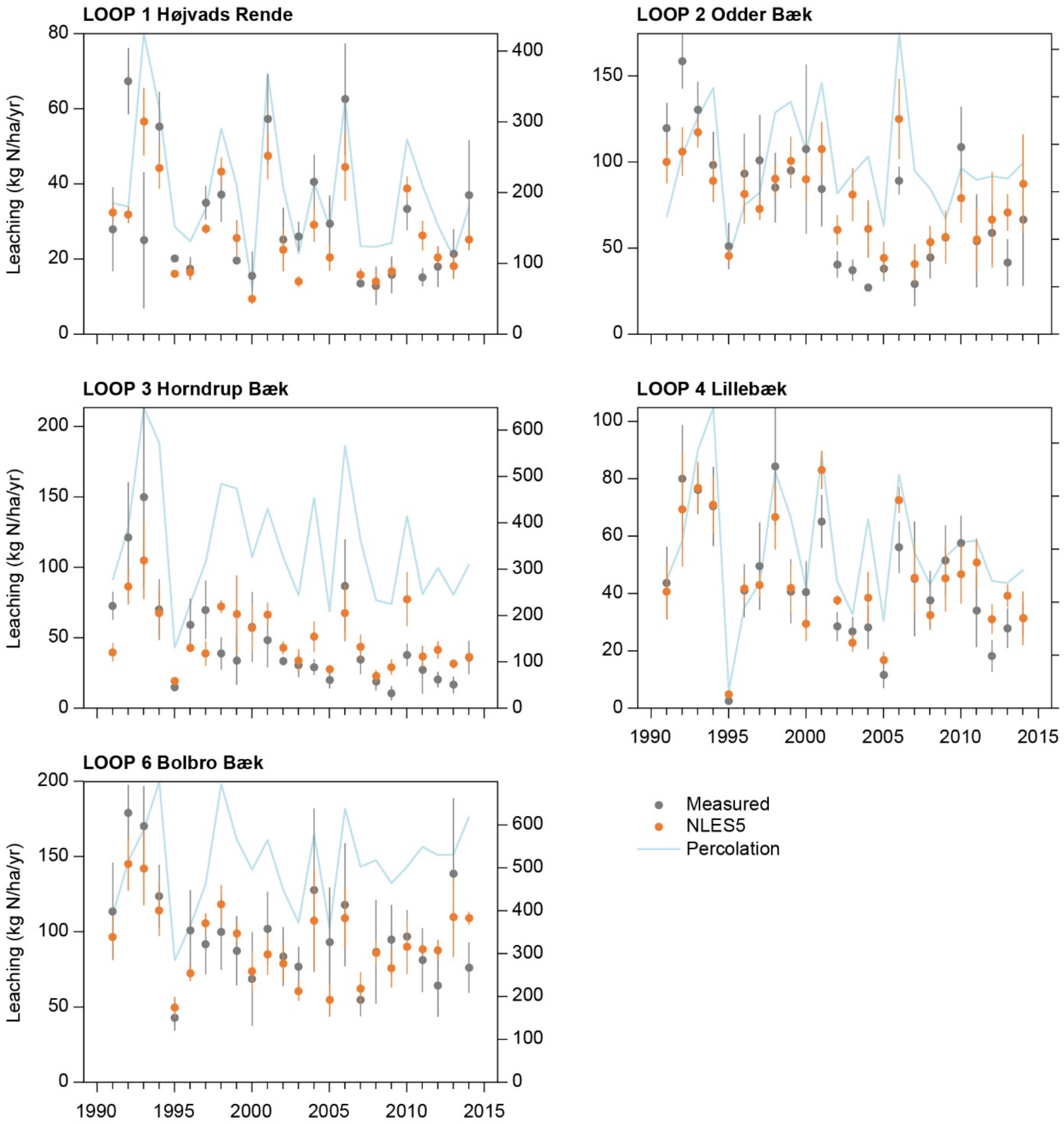

Figure 4.7. Measured and NLES5 predicted nitrate leaching (kg N/ha) as annual mean and standard deviation for each of the five LOOP catchments in the period 1991-2014. Note that the y-axes have different scales. The statistics of the relationship between observed and simulated mean annual N leaching is shown separately for each LOOP catchment.

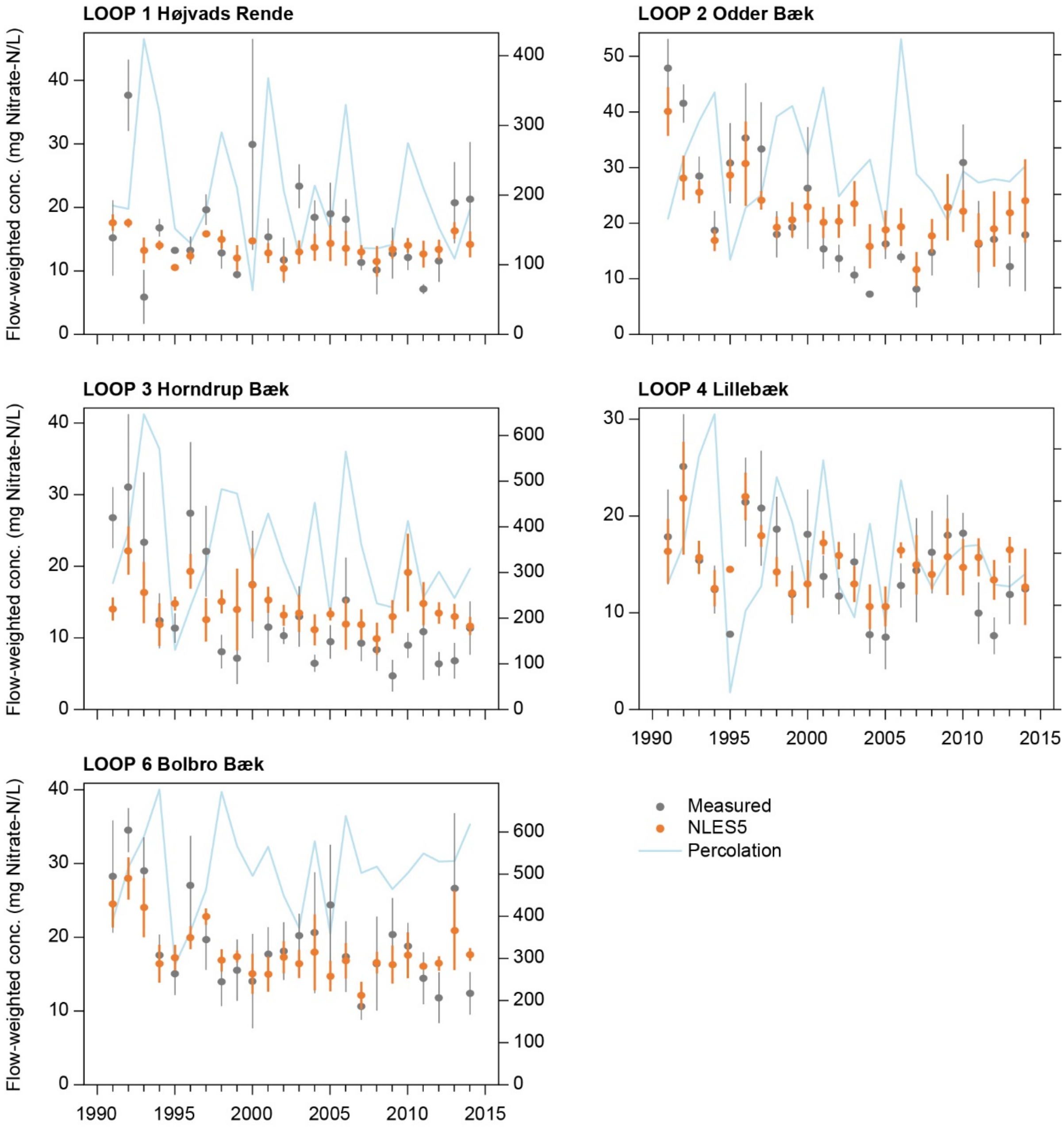

Figure 4.8. Measured and NLES5 predicted flow-weighted nitrate concentration and standard deviation for each of the five LOOP for the period 1991-2014. Note that the y-axes have different scale. The statistics of the relationship between observed and simulated mean annual N leaching is shown separately for each LOOP catchment.

4.4 Cross validation

A cross-validation of the model was performed by subdividing the *Cal1* dataset into 10 subsets with a total of 2046 observations (Table 4.5). Each subset consisted of 90% of the data used for model calibration according to the two-step procedure described in Chapter 3. After model calibration, the predictions were performed for the remaining 10% of the data. This was repeated for all 10 subsets, resulting in a total set of predicted and observed nitrate leaching values.

Table 4.5. Statistics on nitrate leaching (kg N/ha) from cross-validation. Root Mean Square Error (RMSE), Mean Bias Error (MBE, measured-predicted) and mean measured N leaching obtained for each of the ten subsets of the Cal1 dataset used for cross-validation as well as for the sets in the cross-validation.

Subset	Observations	MBE	Mean N leaching	RMSE
1	206	4.8	47.6	30.4
2	206	0.2	47.4	31.5
3	205	3.2	47.1	28.0
4	204	-2.5	45.7	32.3
5	204	-0.3	42.9	26.2
6	204	-1.8	47.9	32.0
7	204	-1.9	46.7	35.0
8	203	-4.6	49.6	32.8
9	205	-1.3	44.8	31.9
10	205	4.9	47.9	32.1
All	**2046**	**0.1**	**46.8**	**31.2**

The ten different validation subsets have a range in mean N leaching going from 42.9 to 49.6 kg N/ha. The mean bias error (predicted minus observed) was 0.1 kg N/ha, showing that the model tended to slightly overestimate the nitrate leaching when predicting beyond the datasets used for model calibration.

The RMSE calculated as the root means squared difference between observed and predicted values was 31.2 kg N/ha, which can be compared with the RMSE of 29.6 kg N/ha from the calibration of the full model (Table 4.2). The correlation between measures and predicted nitrate leaching was 0.69, corresponding to an R^2 of 0.48.

In addition to these validation statistics the index of agreement (IA) was calculated according to Willmott (1981) as a measure of model performance:

$$IA = 1 - \frac{\sum_{i=1}^{n}(O_i - P_i)^2}{\sum_{i=1}^{n}(\lceil P_i - \bar{O} \rceil + |O_i - \bar{O}|)^2} \tag{7}$$

where O_i and P_i are observed and predicted nitrate leaching values for observation i, respectively. $\bar{O}$ is the average observed nitrate leaching. IA is a standardized measure of the degree of model prediction error and varies between 0 and 1, where 1 indicates a perfect match, and 0 indicates no agreement at all. IA can detect additive and proportional differences in the observed and simulated means and variances. For our cross-validation an IA of 0.81 was obtained for the dataset *Cal1*, which indicates fairly good performance in prediction of nitrate leaching beyond the calibration data.

The results of the cross-validation was subdivided between the LOOP and experimental data in the *Cal1* dataset (Table 4.6). Generally, the difference in mean bias error (MBE) was app 6.8 kg N/ha for the two subsets (LOOP and experimental). The RMSE was greater for the LOOP than for the experimental dataset, as also seen for the model calibration (Table 4.2). However, both subsets showed higher RMSE for the cross-validation than from the calibration. Overall there was a good correspondence between observed and predicted N leaching in the cross-validation (Figure 4.9).

Table 4.6. Statistics on model prediction of nitrate leaching (kg N/ha) from cross-validation of the Cal1 dataset divided between data from the LOOP monitoring sites and the experimental sites. Root Mean Square Error (RMSE) and Mean Bias Error (MBE) of the residuals (measured-predicted) are shown along with the R^2 of the relation between observed and predicted values and the average measured nitrate leaching.

	Observations	**R^2**	**MBE**	**RMSE**	**Mean N leaching**
LOOP	629	0.48	-4.7	40.6	63
Experimental	1424	0.43	2.1	25.8	39
All	2053	0.48	0	31.3	47

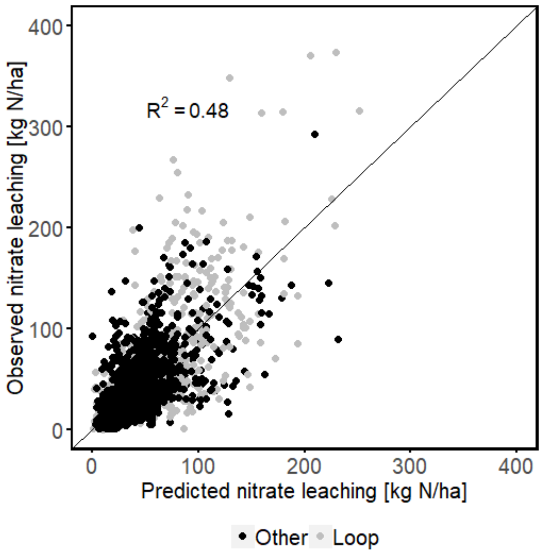

Figure 4.9. Plot of predicted and observed annual nitrate leaching from the cross-validation using the Cal1 dataset.

5 Model validation

5.1 Validation of all datasets

The validation dataset (*Val*) included results from four experiments as shown in Table 2.2, and this include a total of 856 observations (Chapter 2.6). The main part of the observations comes from experiment 117, which is a long-term crop rotation experiment with arable organic and conventional farming systems conducted at three locations: Jyndevad, Foulum and Flakkebjerg (Pandey et al., 2018; de Notaris et al., 2018a). The data for validation from this experiment covered the period 2005-2016, whereas data from this experiment from 1997 to 2004 was included in the *Cal1* calibration dataset. This experiment included different treatments and a range of different crops, but in particular it allows the prediction of effect of cover crops to be assessed.

Experiment 225 compared nitrate leaching from a range of different cropping systems for optimised biomass production at two locations, Jyndevad and Foulum, from 2013 to 2016 (Manevski et al., 2018). This dataset allows the model to be assessed for a range of different crop types.

Experiment 226 covers data on N leaching from spring barley and winter wheat with increasing N fertilizer rate from the VIRKN project during 2014-2017 (Hansen and Thomsen 2019). Data from this experiment was also used for model calibration as part of both the *Cal1* and *Cal2* datasets. However, data with early sowing of winter wheat and spring barley with cover crops were not included in the calibration and are used here for model validation. This dataset allows the model prediction of marginal N leaching to be assessed.

The validation showed variation in model performance among the four datasets (Table 5.1). Overall, the model bias was 1.7 kg N/ha, but with large variations among the datasets and a bias of 13.2 kg N/ha for experiment 226. The RMSE was 30.8 kg N/ha, which is close to the value of 29.6 kg N/ha found for the model calibration (Table 4.2). The RMSE was greatest for experiment 117, which covered experimental cropping, some of which were not well captured by the model.

Table 5.1 Statistics on model prediction of nitrate leaching (kg N/ha) from validation divided between data from the four experiments included in the Val dataset. Root Mean Square Error (RMSE) and Mean Bias Error (MBE) of the residuals (measured-predicted) are shown along with the R^2 of the relation between observed and predicted values and the average measured nitrate leaching. IA is the index of agreement according to Willmott (1981).

Experiment	RMSE	MBE	R^2	IA	Mean N leaching	Observations
117	30.4	0.6	0.37	0.77	39	751
224	20.1	19.7	0.98	0.65	75	4
225	14.7	8.8	0.70	0.98	71	39
226	25.8	13.2	0.34	0.69	26	62
All	30.8	1.7	0.40	0.91	40	856

The model fairly well captured the inter-annual variation in nitrate leaching in the validation dataset (Figure 5.1). The largest deviations were seen for 2007 and 2014. Overall, there was quite some scatter between model-predicted versus observed N leaching (Figure 5.2). However, as indicated by the statistics in Table 5.1, there was no general bias in the model estimates.

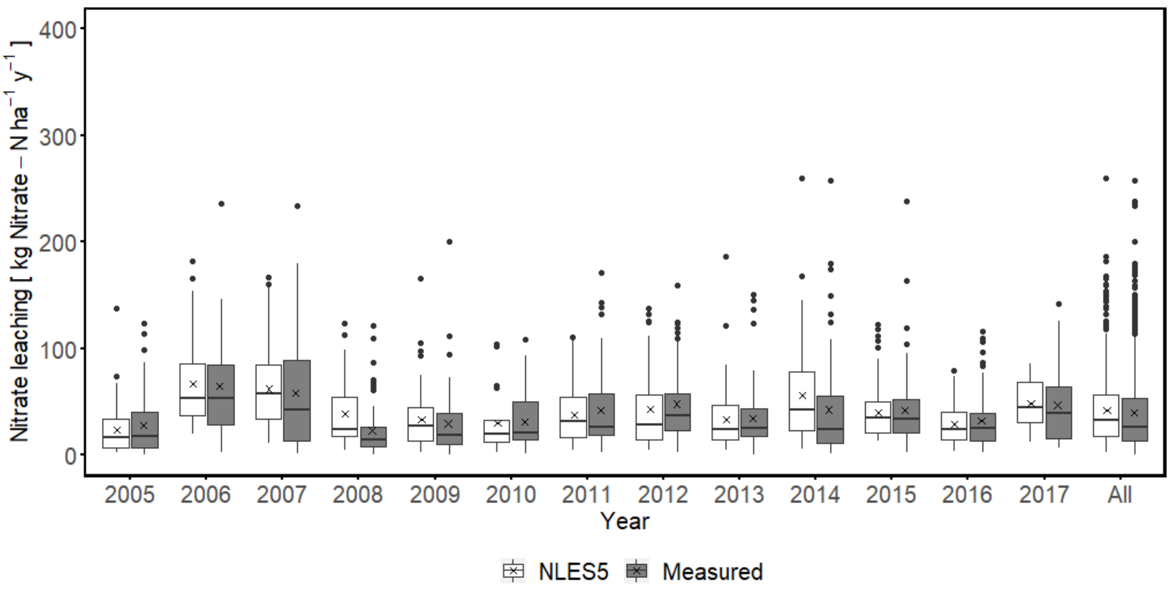

*Figure 5.1. Observed and model predicted nitrate leaching over the period 2005-2017 for model validation (Val dataset). The horizontal lines in the box indicate the median values, and the lower and upper hinges correspond to the first and third quartiles (the 25th and 75th percentiles). The upper and lower vertical lines from the hinge indicate the largest and smallest values at 1.5 * IQR, where IQR is the inter-quartile range, corresponding to the 95% confidence interval. × shows the mean.*

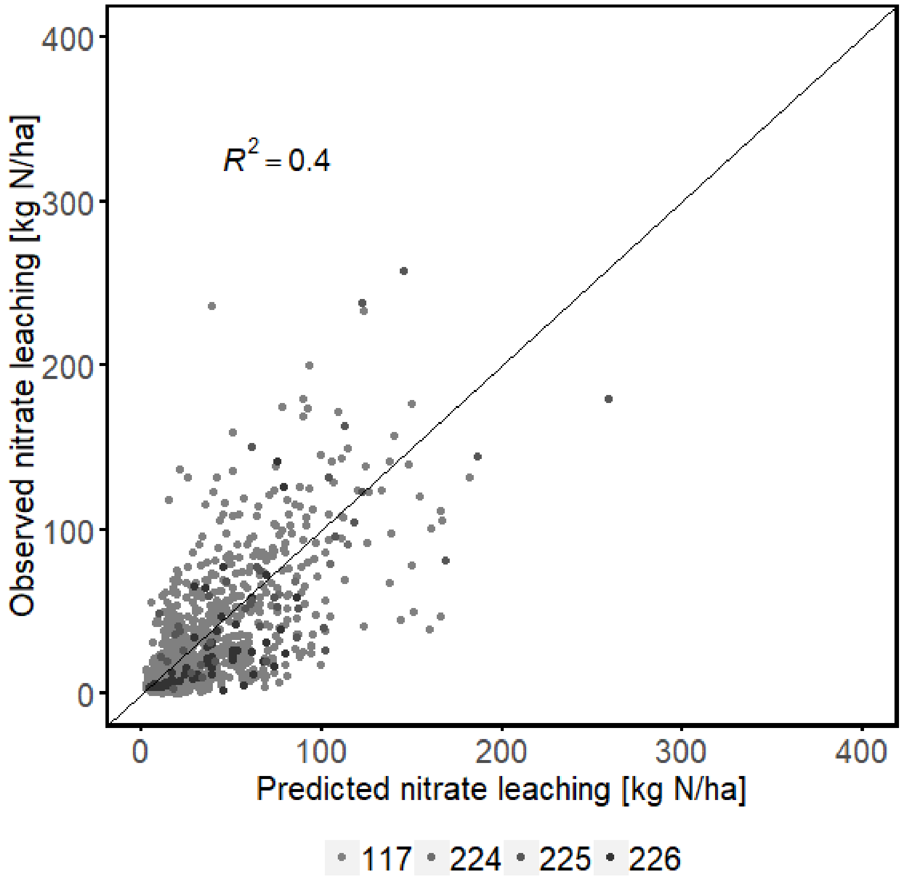

Figure 5.2. Observed versus model predicted annual nitrate leaching for the validation (Val) dataset shown separate for the four experiments. The line shows the 1:1 relation.

5.2 Validation on a long-term arable organic farming experiment (exp. 117)

The data from the long-term experiment on arable organic and conventional cropping systems covered two different periods. The period 2005-2009 included data from all three sites (Jyndevad, Foulum and Flakkebjerg), whereas data from 2010-2016 only included Foulum. Here data from full crop rotations were used to calculate average nitrate leaching at cropping system level for the periods 2005-2008 and 2011-2014.

Figure 5.3 shows that the model well captures location differences in nitrate leaching level. However, treatment differences are not well captured at Jyndevad, whereas better model skill is found at Foulum and Flakkebjerg. For the period 2011-2014 at Foulum measurements were available from a larger number of plots, and here model predictions agreed reasonably well with observations (Figure 5.4).

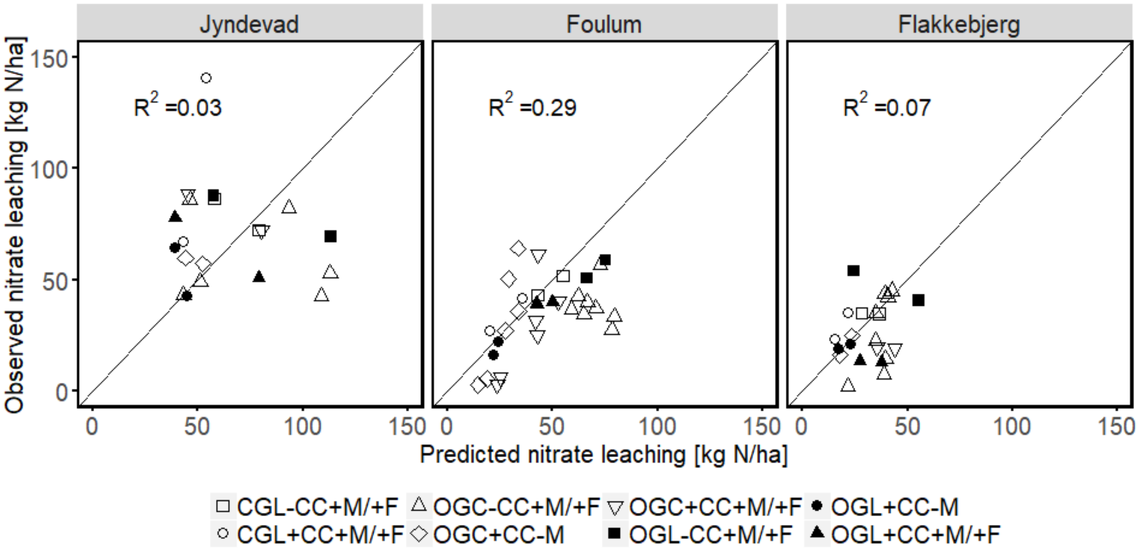

Figure 5.3. Observed versus predicted nitrate leaching as average over the period 2005-2008 from experiment 117 for three different locations. The long-term field experiments included (1) rotations with grass-clover in organic farming(OGC) or grain legumes in organic farming (OGL) or conventionally managed (CGL) systems, (2) with (+CC) and without (−CC) cover crops, and (3) with (+M) and without (−M) animal manure (in OGC and OGL), and with (+F) mineral fertilizer (in CGL). For details see *Pandey et al. (2018).*

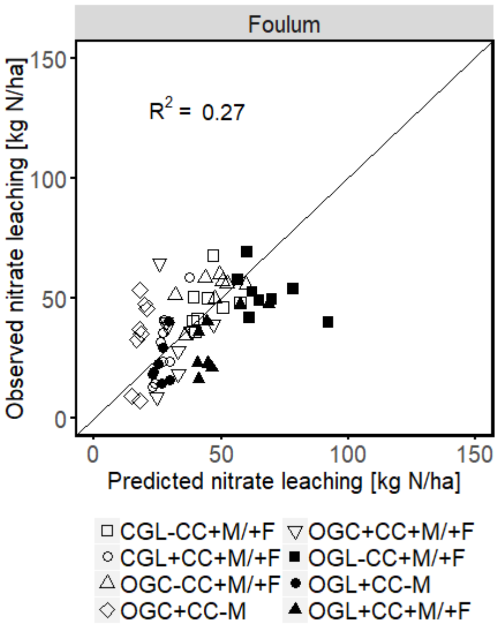

Figure 5.4. Observed versus predicted nitrate leaching as average over the period 2011-2014 from experiment 117 for Foulum. The long-term field experiments included combination of (1) rotations with grass-clover in organic farming (OGC) or grain legumes in organic farming (OGL) or conventionally managed (CGL) systems, (2) with (+CC) and without (−CC) cover crops, and (3) with (+M) and without (−M) animal manure (in OGC and OGL), and with (+F) mineral fertilizer (in CGL). For details see de Notaris et al. (2018a).

The experiment included treatments with (+CC) and without (-CC) cover crops. This allowed treatment effects of cover crops to be calculated at cropping systems level. Figure 5.5 compares the cover crop effect at the three locations. The cover crop effect was reasonably well estimated with the model for Foulum and Flakkebjerg, whereas it was overestimated at Jyndevad. This is due to negative effects of cover crops in some systems at Jyndevad, largely due to issues related to success of cover crop establishment (Pandey et al., 2018). For the period 2011-2014 with more replications in the experiment at Foulum, there was a good agreement between observed and simulated effects of cover crops on nitrate leaching.

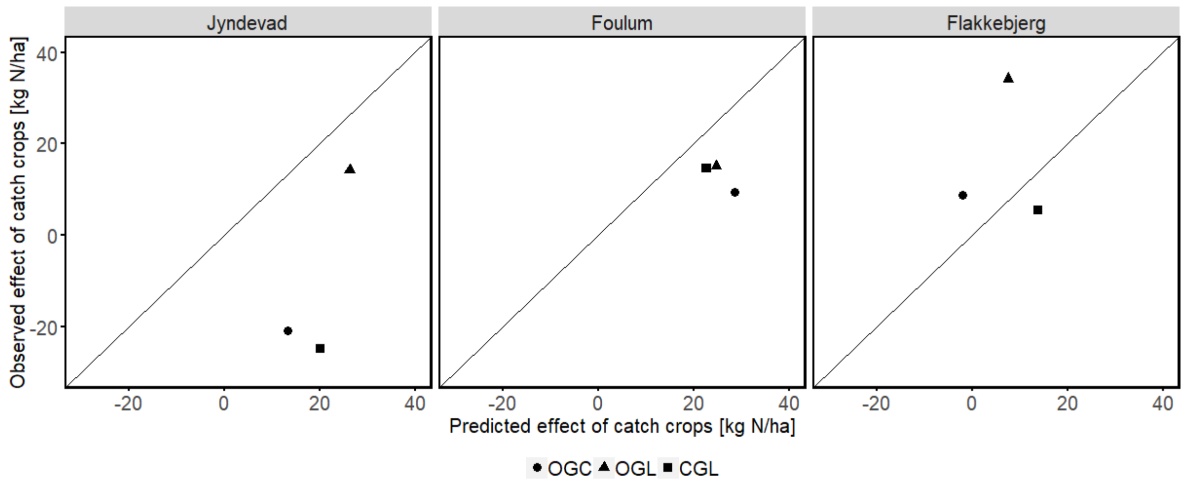

Figure 5.5. Observed versus predicted nitrate leaching effects of cover crops at cropping system level for 2005-2008 from experiment 117 for three different locations. The symbols refer to the different cropping systems as defined by Pandey et al. (2018).For details see caption of Figure 5.3. Cover crops in OGC and OGL included a mixture of perennial ryegrass and clover (at the sites with coarse sand and sandy loam soils) or winter rye, fodder radish and vetch (at the site with loamy sand soil), and cover crops in CGL included only perennial ryegrass at all the sites.

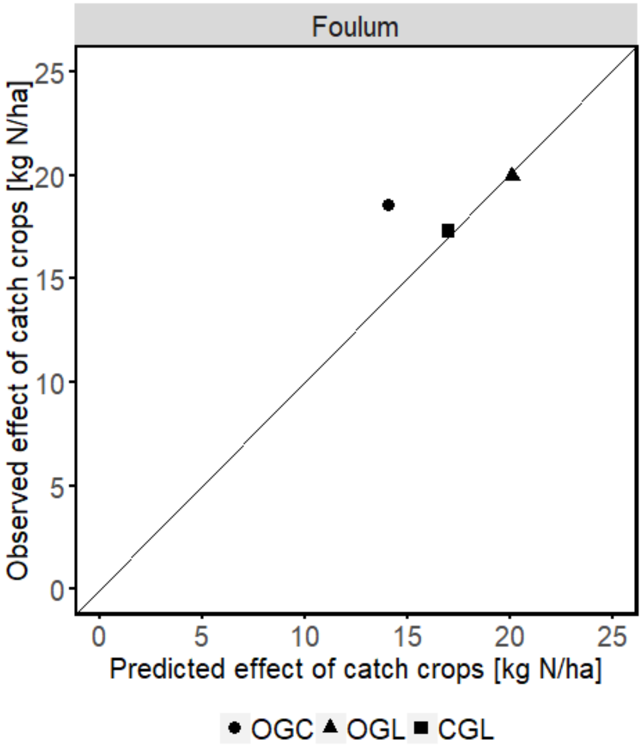

Figure 5.6. Observed versus predicted nitrate leaching effects of cover crops at cropping system level for 2005-2008 from experiment 117 for three different locations. The symbols refer to the different cropping systems as defined by de Notaris et al. (2018a). See caption for Figure 5.4.

5.3 Validation on data from optimized biomass cropping systems (exp. 225)

The average N leaching over the period 2013-2016 was calculated for individual cropping systems at Jyndevad and Foulum. The results in general show a good correspondence between observed and model predicted values (Figure 5.7).

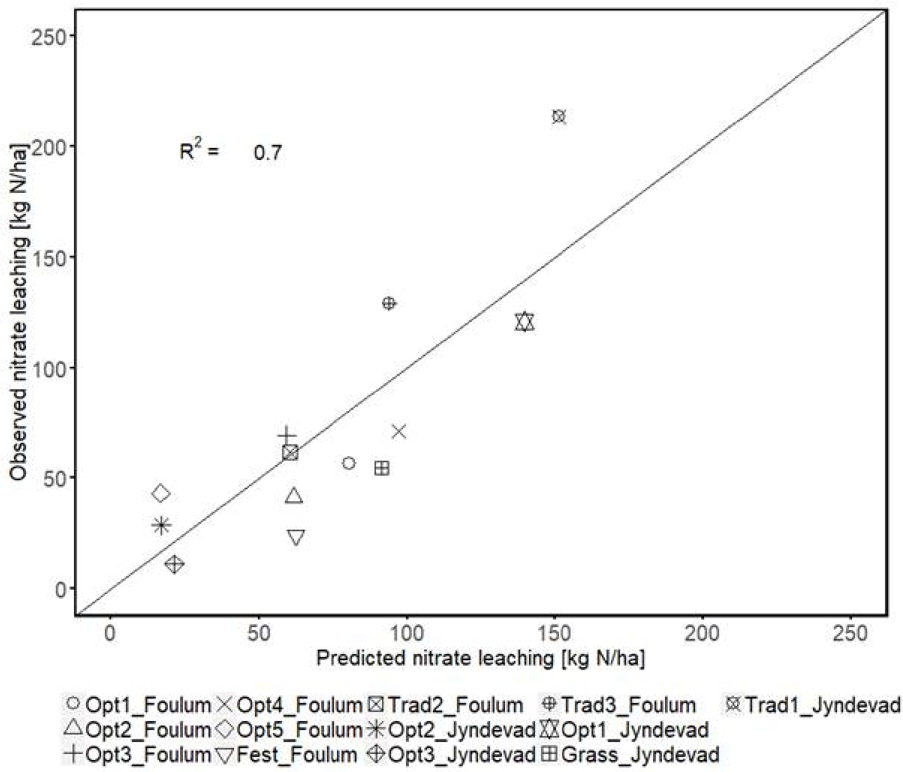

Figure 5.7. Observed versus predicted nitrate leaching as average over the period 2011-2014 from experiment 225 for Jyndevad and Foulum. Opt1..Opt5: cropping systems optimised for maximum biomass production (maize, beet, hemp/oat, triticale as main crops, winter rye or winter oilseed rape as harvested cover crop), Grass: (grass-legume mixtures), Traditional systems: (Trad1, Trad2 and Trad3 are continuous maize or triticale, and a cereal crop rotation respectively). The symbols refer to the different cropping systems as defined by Manevski et al. (2018).

5.4 Validation of the marginal N leaching rate (exp. 226)

Experiment 226 included treatments with increasing N fertilizer rates conducted at Foulum and Flakkebjerg. The marginal N leaching rate at standard fertilizer rate was calculated for both observed and model predicted values using the method described in Section 2.3. There was a large variation in the observed marginal N leaching, which only to a minor extent was captured by the model, although the model captured the average marginal N leaching.

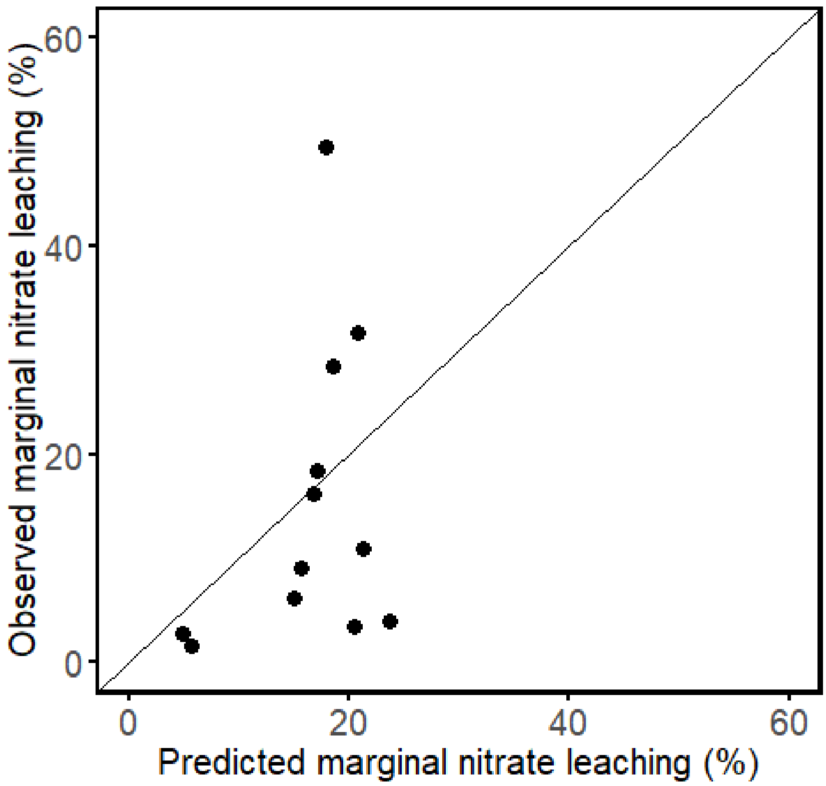

Figure 5.8. Observed versus model predicted marginal N leaching at standard fertilisation rate using data from experiment 226 for two different locations in the validation dataset (Val). Spring barley with cover crop and early sown winter wheat (Flakkebjerg) and winter rye (Foulum).

6 Uncertainty and scenario analysis

The data from the model calibration was used to assess the uncertainty of the NLES5 model. The uncertainty of a model is both relevant when looking on single field model predictions (Section 6.1) and on higher scale which includes many field predictions obtained by aggregation (Section 6.2). The calibration of the NLES5 model resulted in estimated model parameters and a covariance matrix of the model parameters. The covariance matrix and the optimized parameter values including standard deviations were used to randomly generate 1000 parameter sets by using the R software (R Foundation for Statistical Computing 2018) applying the tmvtnorm package (Wilhelm and Manjunath, 2015). The parameter sets were sampled from a truncated multivariate normal distribution, with the lower and upper truncation point set at 3 times the standard deviation from the predicted parameter value. This method to simulate a large number of parameter sets gives an output distribution that follows approximately a normal distribution that covers the whole parameter space between the lower and upper truncation point while maintaining the correlation between the parameters. All thousand parameter sets were used as input to the NLES5 model structure to generate a thousand separate nitrate leaching predictions. For the 1000 parameters sets, the parameters β_1 and μ were adjusted with the same scaling factor for β_1 and the same value for μ as obtained in calibration step five (Section 2.3) The annual trend parameter τ was not varied for the 1000 sets of parameters, but held constant to the initial value of -0.1105 kg N/ha/yr obtained for the calibration data set (*Cal1*).

6.1 Uncertainty based on field scale predictions

To exemplify the uncertainty of model parameters on the N leaching on field scale level, three common crops sequences representing spring cereal and winter cereal grown on three different typical soils in Denmark under dry and wet weather conditions was set up to exemplify the NLES5 model predictions. Table 6.1 shows the different cropping systems and N fertilization rates. Three soils represent loam (L, equivalent to Danish soil class JB7), loamy sand (LS, equivalent to Danish soil class JB4) and sand (S, equivalent to Danish soil class JB1). The clay contents was 15.5% (L), 8.9% (LS) and 3.9% (S). Organic N content in the top soil was 2.14, 2.18 and 3.29 Mg N/ha for the soils L, LS and S, respectively. These soil types were taken from soil data at the experimental sites at Jyndevad (S), Foulum (LS) and Flakkebjerg (L).

Table 6.1. Crop rotations and N fertilization used in calculation of uncertainty in Fig. 6.1.

Previous crop	Previous winter crop	Main crop	Winter crop	Code	Mineral N spring application (kg N/ha)
Spring Barley	Bare soil	Spring Barley	Bare soil	SB_B	140
Spring Barley	Catch crops	Spring Barley	Catch crops	SB_CC	140
Winter wheat	Winter wheat	Winter wheat	Winter wheat	WW_WW	200
Maize	Bare soil	Maize	Bare soil	M_B	190
Grass	Grass	Maize	Bare soil	MG_B	190

Two different weather conditions were used in the predictions with annual percolation of 240 mm (dry, low percolation) and 610 mm (wet, high percolation). The same percolation values were used for all tree soil types to neutralize differences in percolations due to differences in soil hydraulic parameters and crops.

Figure 6.1 shows that the leaching for spring barley with bare soil (SB_B) is simulated to be nearly the same for soil types L and LS, whereas leaching is higher for the sandy soil (S). This is due to the effects of both clay content and total soil N content. Also, the percolation parameters for sand are higher than for LS and L soils (Table 3.2). The nitrate leaching for winter wheat (WW_WW) is predicted to be slightly higher compared to spring barley. We assumed that these crops have similar percolation; however, the percolation from a field with winter vegetation cover (e.g. WW_WW and SB_CC) will be lower compared with spring cereal followed by bare soil (SB_B). Accounting for such effects would reduce the difference in predicted leaching rates between SB_B and WW_WW.

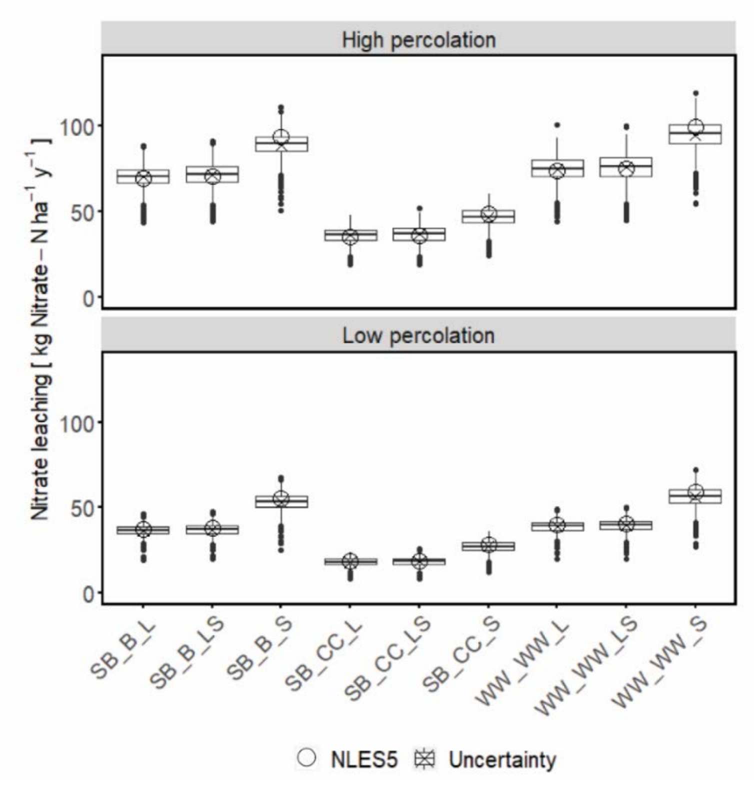

*Figure 6.1. Field scale simulated nitrate leaching for three continuous crop rotations (SB_B, spring barley followed by bare soil; SB_CC, spring barley followed by catch crop; and WW_WW, winter wheat followed by winter wheat). Three soil types L (loam), SL (sandy loam) and S (sand). The uncertainty range is based on 1000 realisations of the NLES5 model reflecting the parameter uncertainties using a Monte Carlo approach. Boxes indicate the 25 to 75 percentile. Horizontal line within the box is the median. The upper and lower vertical lines from the hinge indicate the largest and smallest values at 1.5 * IQR (where IQR is the inter-quartile range, or distance between the first and third quartiles, a roughly 95% confidence interval for comparing medians). Dots are observations outside the mean plus/minus the 95% confidence interval. × is the mean value.*

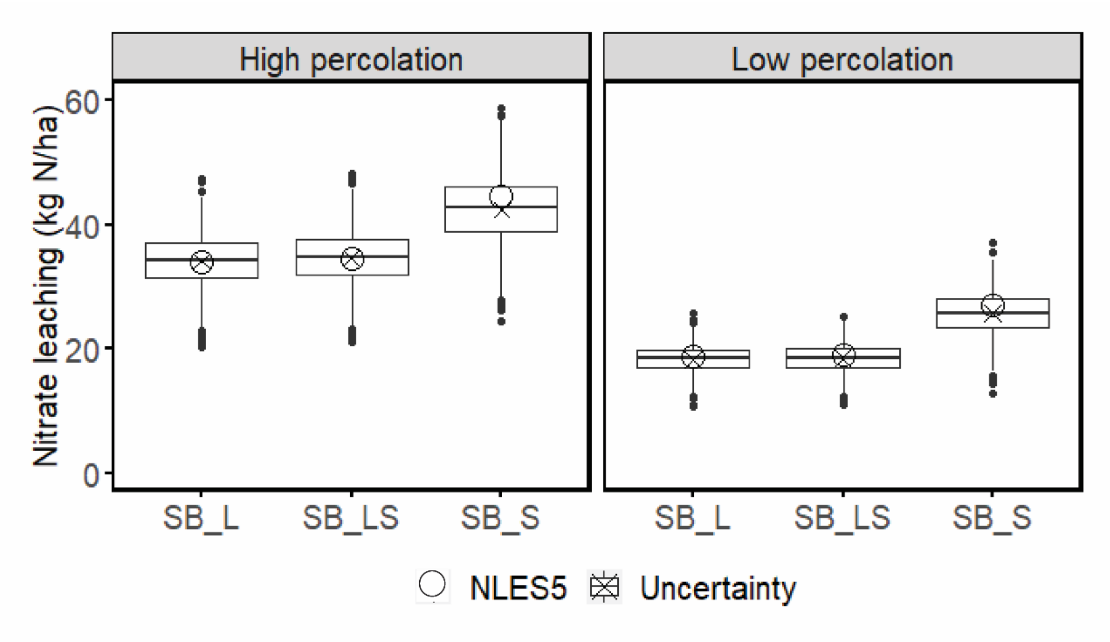

*Figure 6.2. Effects of cover crops (SB_B minus SB_CC) obtained for the three soil types under two different percolation regimes. Boxes indicate the 25 to 75 percentile. Horizontal line within the box is the median. The uncertainty range is based on 1000 realisations of the NLES5 model reflecting the parameter uncertainties using a Monte Carlo approach. The upper and lower vertical lines from the hinge indicate the largest and smallest values at 1.5 * IQR (where IQR is the inter-quartile range, or distance between the first and third quartiles, a roughly 95% confidence interval for comparing medians). Dots are observations outside the mean plus/minus the 95% confidence interval. × is the mean value.*

The effect of cover crops can be calculated by subtracting the leaching of spring barley after bare soils and the leaching of spring barley after a cover crop (Figure 6.2). The effect of a cover crop is highest under high percolation rates, as leaching increases with percolation to a certain extent (eqn. 1, 5 and 6, section 3.1). As percolation is a multiplicative effect in NLES5, the effects and the uncertainty of the cover crop effect will also be greater with high percolation rates. The effect of cover crops is higher for sandy soils than found for loamy soils. This is also found in field experiments and is also included in the Danish catalogue of nitrogen mitigation measures (Eriksen et al., 2014), although this effect was not found in the validation dataset (Figure 5.5). The effect for sandy soils varies between 34-46 kg N/ha and for loamy soils between 16-28 kg N/ha (Figure 6.1). The effect of cover crops estimated by NLES5 is within the range of estimates in the Danish catalogue of nitrogen mitigation measures.

Figure 6.3 shows the uncertainty and mean marginal nitrate leaching of the three different cropping systems, simulated using the three soils under the different percolation regimes. The marginal nitrate leaching increases with higher percolation. The marginal nitrate leaching is also generally higher for sandy soils.

The modelled marginal N leaching of winter wheat (WW_WW) and spring barley with bare soil (SB_B) is at the same level and has the same uncertainty. The marginal N leaching of spring barley with cover crops (SB_CC) is generally lower. The long-term effects of increased mineralization from cover crops is not fully included in the NLES5 as only the previous year's winter cover is included as variable in the model. Therefore, the model only accounts for residual N mineralized in the first year after having a cover crop and long-term effect may be different.

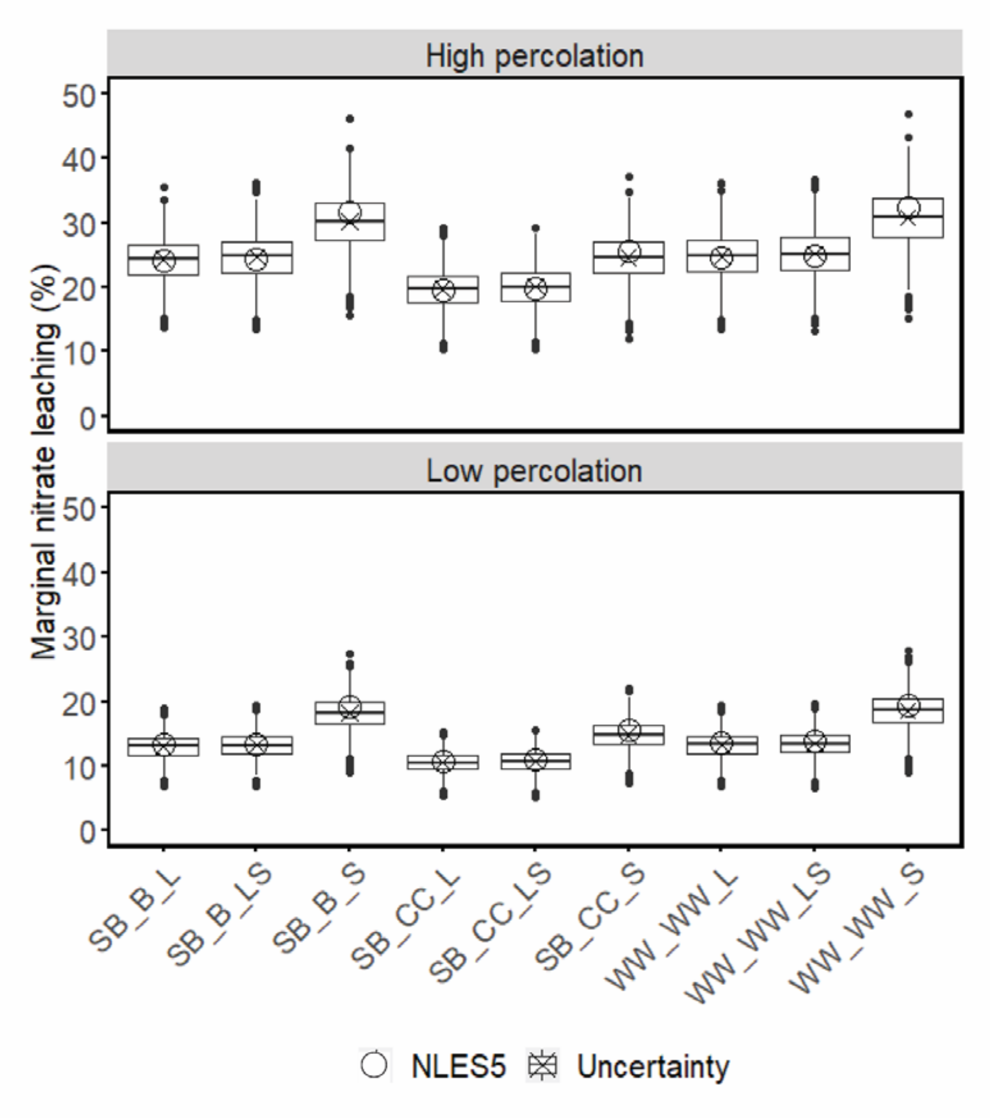

*Figure 6.3. Marginal N leaching obtained for the different cereal crop, soils and percolation regimes. The uncertainty range is based on 1000 realisations of the NLES5 model reflecting the parameter uncertainties using a Monte Carlo approach. Boxes indicate the 25 to 75 percentile. Horizontal line within the box is the median. The upper and lower vertical lines from the hinge indicate the largest and smallest values at 1.5 * IQR (where IQR is the inter-quartile range, or distance between the first and third quartiles, a roughly 95% confidence interval for comparing medians). Dots are observations outside the mean plus/minus the 95% confidence interval. × is the mean value.*

The effects of grass-clover as previous crop on N leaching are exemplified by comparing the leaching of maize grown as continuous maize with maize grown after spring ploughed grass or grass-clover (Figure 6.4). The results show an increase in N leaching of 78-95 kg N/ha with high percolation and 38-55 kg N/ha at low percolation from having grass-clover prior to a maize crop. The uncertainty is greater for maize after grass than for maize, and the uncertainty also increases with percolation rate. N leaching for the maize after ploughed grass obtained as average of the 1000 sets of parameters is lower than the NLES5 model using the standard parameters. This is not seen for maize after maize (M_B) where the model predictions of the 1000 parameter sets on average is at the same level as the NLES5 model. The NLES5 model prediction is within the 95% confidence interval.

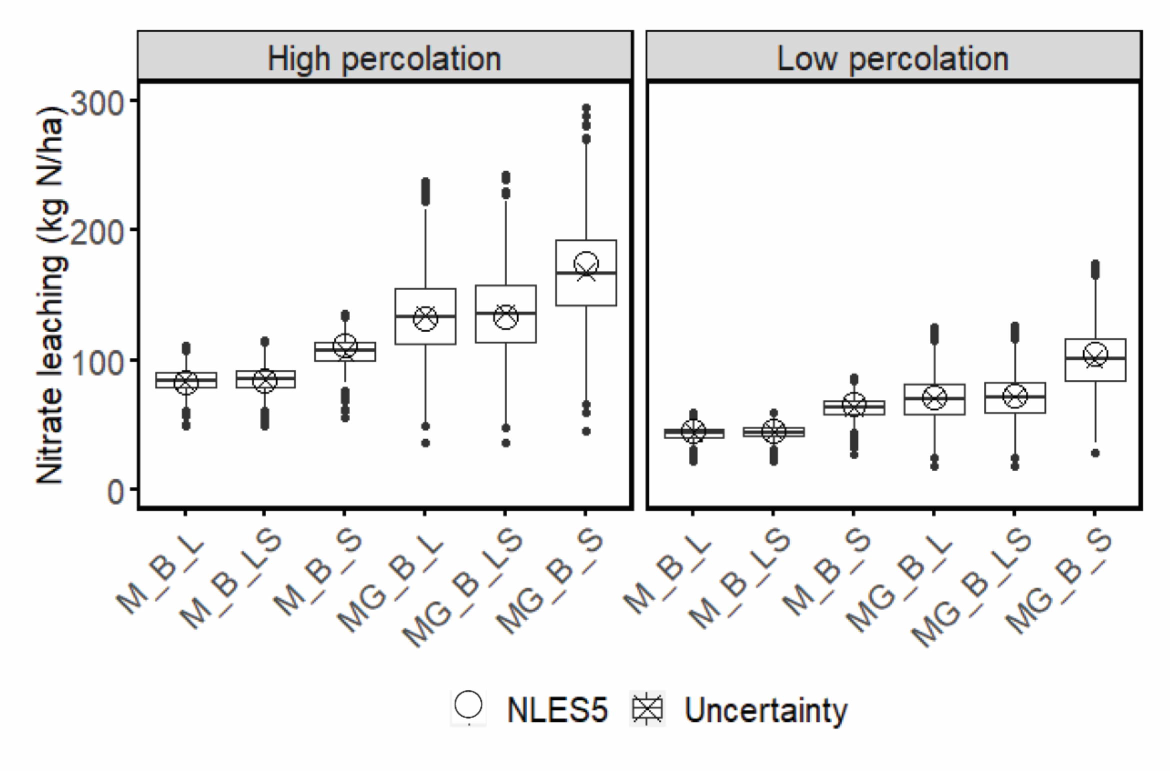

*Figure 6.4. Field scale simulated nitrate leaching for two continuous crop rotation systems (M_B, maize followed by bare soil; and MG_B, maize after grass or grass-clover ploughed in spring followed by bare soil. Three soil types L (loam), SL (Sandy loam) and S (sand). The uncertainty range is based on 1000 realisations of the NLES5 model reflecting the parameter uncertainties using a Monte Carlo approach. Boxes indicate the 25 to 75 percentile. Two weather condition (High percolation and low percolation). The horizontal line within the box is the median. The upper and lower vertical lines from the hinge indicate the largest and smallest values at 1.5 * IQR (where IQR is the inter-quartile range, or distance between the first and third quartiles, a roughly 95% confidence interval for comparing medians). Dots are observations outside the mean plus/minus the 95% confidence interval. × is the mean value.*

6.2 Uncertainty and marginal N leaching at 10 km grid scale

The NLES5 model is used for national upscaling and scenario analyses to study effects of changes in cropping systems and fertilisation rates. These approaches typically use an upscaling approach where information on crop and fertiliser management at individual farmer fields are combined with soil and climate data to estimate nitrate leaching (Børgesen et al., 2013). There are several uncertainties associated with the estimation of nitrate leaching at national and sub-national scales. Two important sources of uncertainty relate to the estimation of input data for the modelling of N leaching and to the parameters of the NLES5 model. Here, we address the effects of parameter uncertainty on the modelled national scale N leaching level and marginal nitrate leaching rate.

6.2.1 Input data for the model predictions

Input data for the model analysis were adapted from a previous study (Børgesen et al., 2015). In our study only predictions for the scenario projections for 2021were used, with the same farmland area and cropping systems as in the year 2011. The adopted scenario from Børgesen et al., (2015) includes an increase in the use of mineral N fertilizer application with 69.500 ton N compared to fertilizer use in 2011, equal to a total use of 274.000 ton N applied with mineral N fertilizers in 2021. Fertilization on organic farms (6% of the area) was kept constant in this scenario, and manure application was also kept constant. This gives the opportunity to compare the NLES5 predictions of N leaching and marginal nitrate leaching with the previous NLES4 model predictions as similar N inputs and crops are used in the two studies. These two studies do not reflect the actual changes in fertilizer use and crop distribution that has taken place in Denmark up until today, but is only a comparison study of the two models.

6.2.2 NLES5 model setup for the uncertainty analysis on regional and national scale.

Model simulations were conducted for all Danish farm fields included in the national databases (>600.000 fields) using the farmland and crop distribution in 2011. The nitrate leaching and marginal nitrate leaching were predicted on sub-field scale level to be able to include the effects of soil type distribution within the field. Weather data for the period 1990-2010 (21 years) was used for creating a database of monthly simulated percolation using the Daisy model. The percolation database consist of representative combinations of soils, crop-sequences and weather data sets obtained for 609 locations distributed in a 10 km grid covering Denmark. The trend (year) used for both NLES4 (Technology effect) and for NLES5 (Annual trend) was fixed to the year 2011. The basic setup of the model was adapted from Børgesen et al. (2013).

To be able to compare results between NLES4 and NLES5, a number of model assumptions in relation to crops, cropping systems and nitrogen fertilizers were made. For most input data to NLES5 the same assumptions as for NLES4 were used. However, NLES4 and NLES5 differ in model structure (crop classes and N fertilization); therefore, we revised some assumptions. The NLES5 model contains an effect of a cover crop in the previous winter (previous crop). This is not included in the NLES4 model. The two models use different classifications for main crops, which give different crop effects in the two models. The most important changes included in NLES5 is the effect of ploughing of grass in the previous year (previous winter crop) before sowing of winter cereals or before sowing of spring crops (silage maize and spring cereals). On farm scale level the grass in rotation was on average ploughed every 3 years (adopted from the NLES4 simulation (Børgesen et al., 2013)) and hereby 1/3 of the grass area in rotation was assumed as previous crop area to maize or cereals depending on the farm specific cropping system. This has led to new cropping sequences in the NLES5 modelling scenario described with the four cropping periods: main crop, winter crop, previous year main crop and previous years' winter crop.

6.2.3 Scenario analysis using the NLES5 model

Figure 6.5 shows the mean nitrate leaching estimated for different parts of Denmark, which depicts the same spatial variation as found using the NLES4 model. The highest leaching rates are found in the central and western part of Jutland, which are dominated by high livestock density, sandy soils and high percolation rates. These areas are also dominated by dairy farms with high proportion of grassland and a high share of silage maize in the cropping systems. Low leaching rates are found in the eastern part of Denmark with lower rainfall. These differences are in accordance with experiments (Hansen and Thomsen, 2017; Hansen et al., 2019).

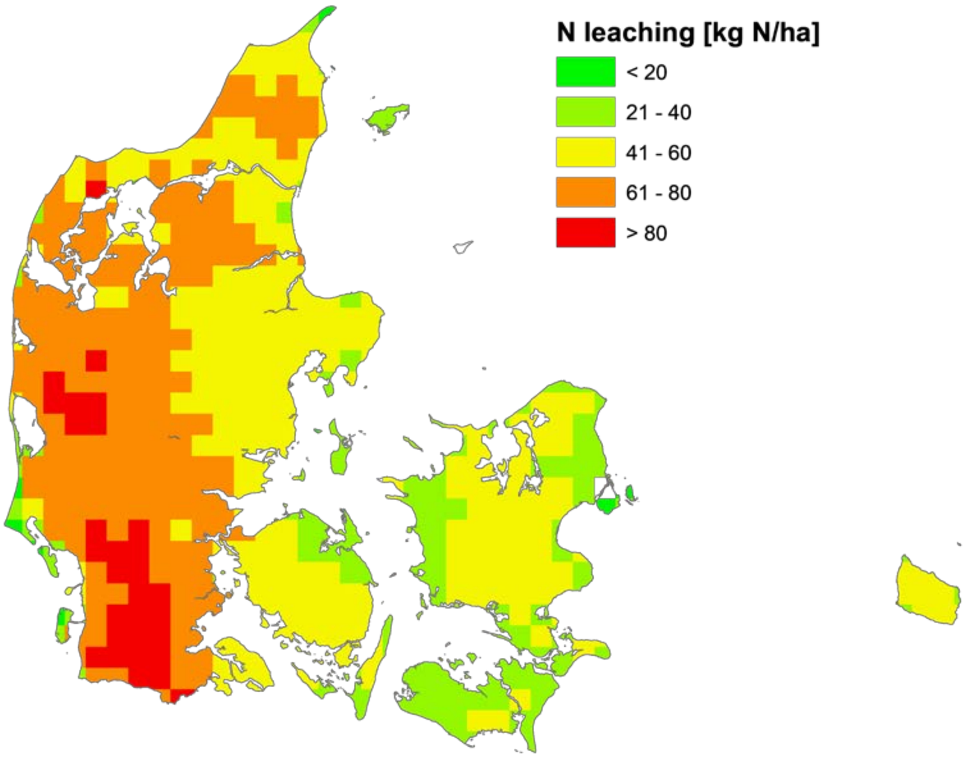

Figure 6.5. Mean nitrate leaching using the NLES5 model at the N level in Børgesen et al. (2015) based on land use in 2011 and N fertilization rate projected for 2021. The mean result is based on annual predictions using 21 years of observed weather data for the period 1990-2010.

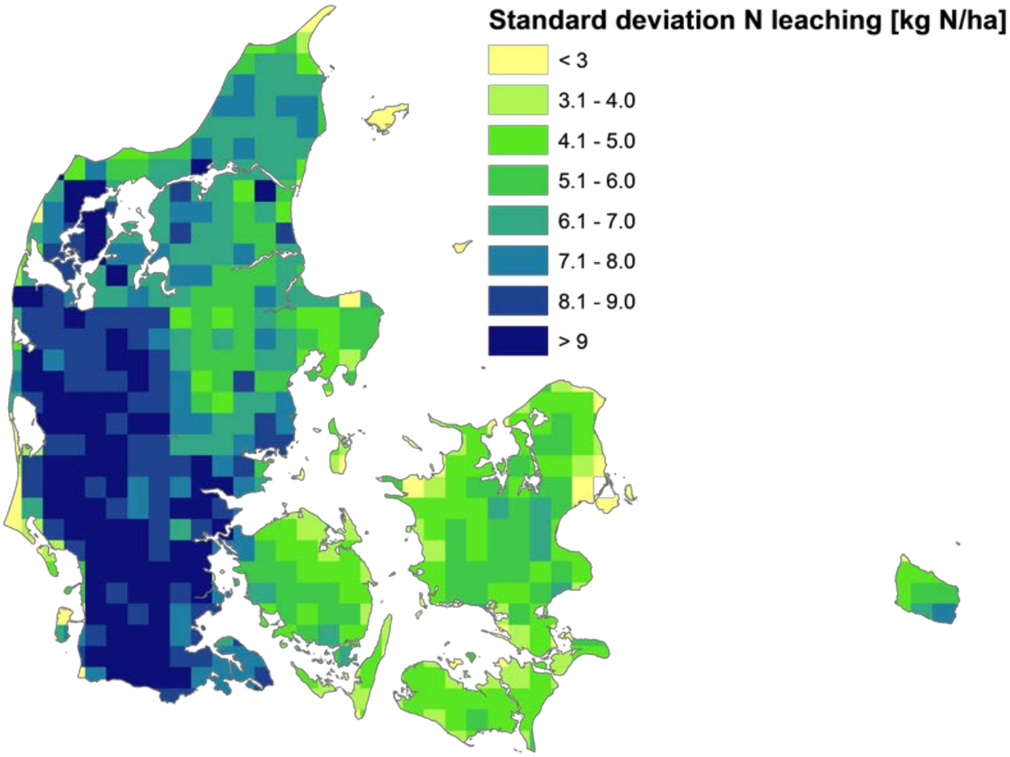

Figure 6.6. Standard deviation of the predicted nitrate leaching (kg N/ha) using the NLES5 at the N level in Børgesen et al. (2015) based on land use in 2011 and N fertilization projected for 2021. The mean nitrate leaching result is based on annual predictions using 21 years of observed weather data for the period 1991-2010. The uncertainty range is based on 1000 realisations of the NLES5 model reflecting the parameter uncertainties using a Monte Carlo approach.

The uncertainty expressed by the standard deviation (kg N/ha) obtained from the 1000 sets of parameters (Figure 6.6) follows the same spatial pattern as the N leaching level in Figure 6.5. This accords with findings at field level (Figure 6.1), where the uncertainty was highest at high percolation and high N leaching levels.

Figure 6.7 shows the spatial variation in modelled average marginal N leaching. In general, the highest marginal N leaching is found in the same areas that have high values for N leaching (compare Figures 6.5 and 6.7).

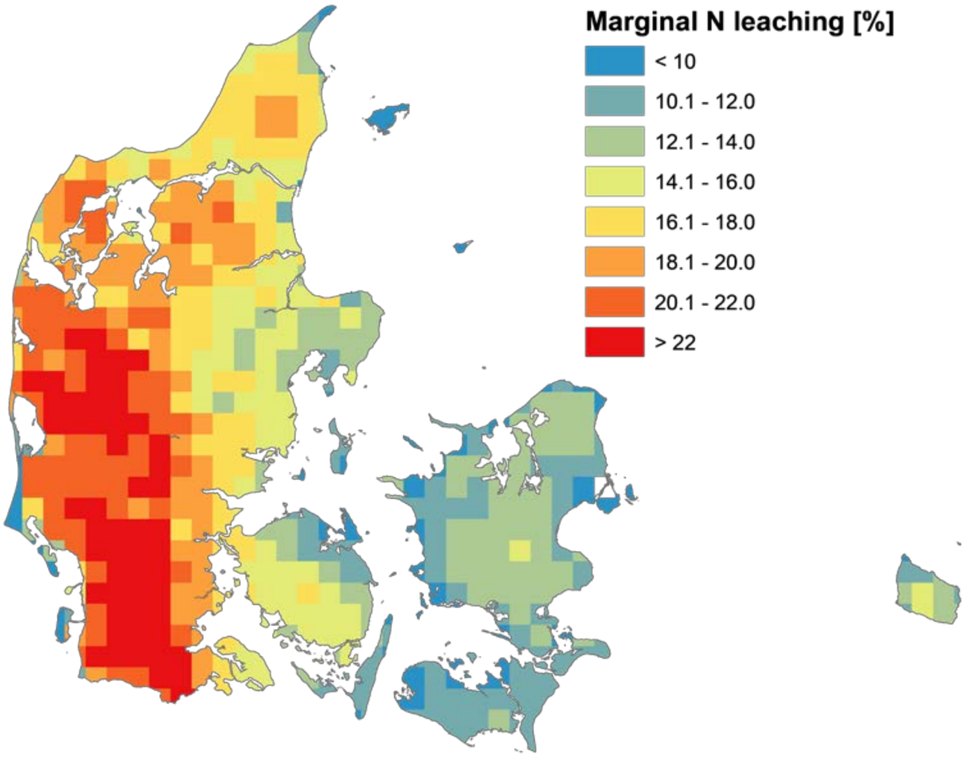

Figure 6.7. Marginal N leaching (%) at the N level that was projected for 2021 (Børgesen et al., 2015) calculated using the NLES5 model. The mean nitrate leaching result is based on annual predictions using 21 years of observed weather data for the period 1991-2010.

The uncertainty of the marginal N leaching is shown in Figure 6.8 and expressed as standard deviation in %-points. The uncertainty shows the same spatial variation as for the marginal N leaching rate (Figure 6.7). The standard deviation increases with the nitrogen leaching level as also seen in Figure 6.10. The standard deviation of marginal N leaching is within the range of 1 to 4 %-points. This uncertainty is only due to the uncertainty level of the NLES5 model parameters. There are other sources for uncertainty of the marginal N leaching such as the annual weather conditions and the historical N application levels on the fields. These are not included in this scenario analysis as only 2011 farm data were used and the results are presented as average of 21 years of simulations.

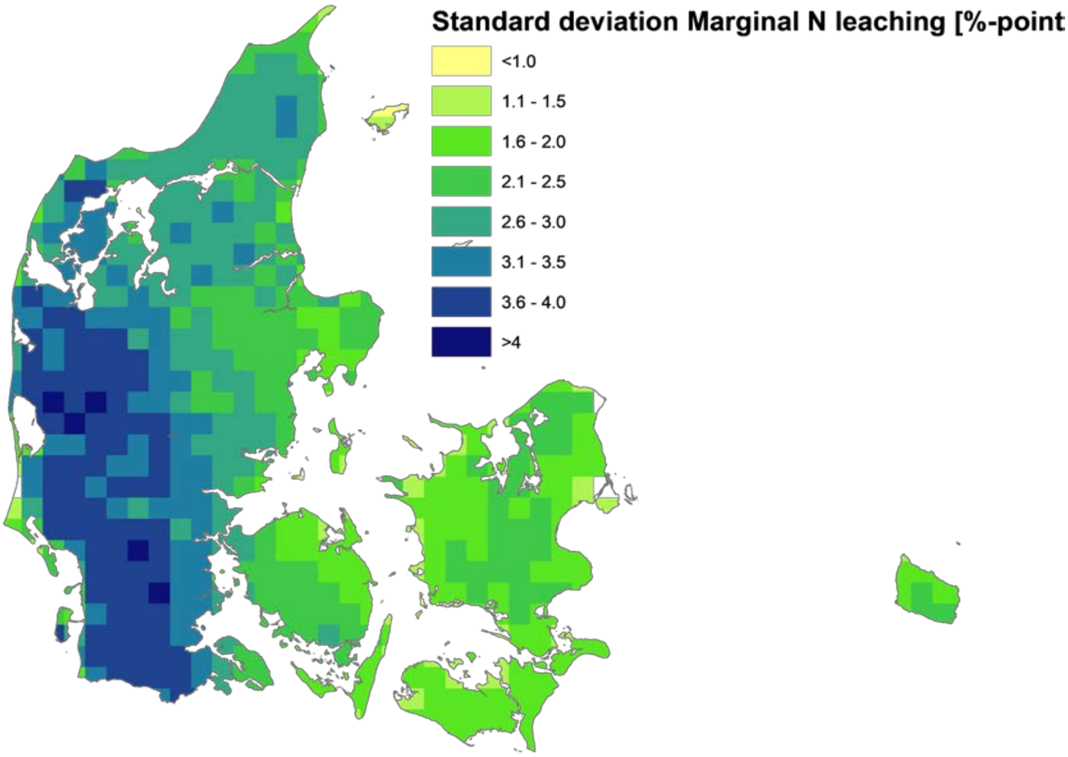

Figure 6.8. Standard deviation (%-point) obtained for the marginal N leaching based on model predictions using 1000 different sets of NLES5 parameters. The mean marginal N leaching result is based on annual predictions using 21 years of observed weather data for the period 1991-2010. The uncertainty range is based on 1000 realisations of the NLES5 model reflecting the parameter uncertainties using a Monte Carlo approach

Figure 6.9 shows the spatial variation in coefficient of variance (CV, %) for marginal N leaching. CV is the standard deviation as percent of the mean N leaching. There is very limited variation in the CV, since the standard deviation largely follows the marginal N leaching, which again follows the N leaching level (Figure 6.10). Figure 6.10 shows a high correlation between the marginal N leaching (right) and the N leaching level (left graph), and that the standard deviation of marginal N leaching increases with the N leaching. A large part of the variation in N leaching is caused by the variation in percolation rate.

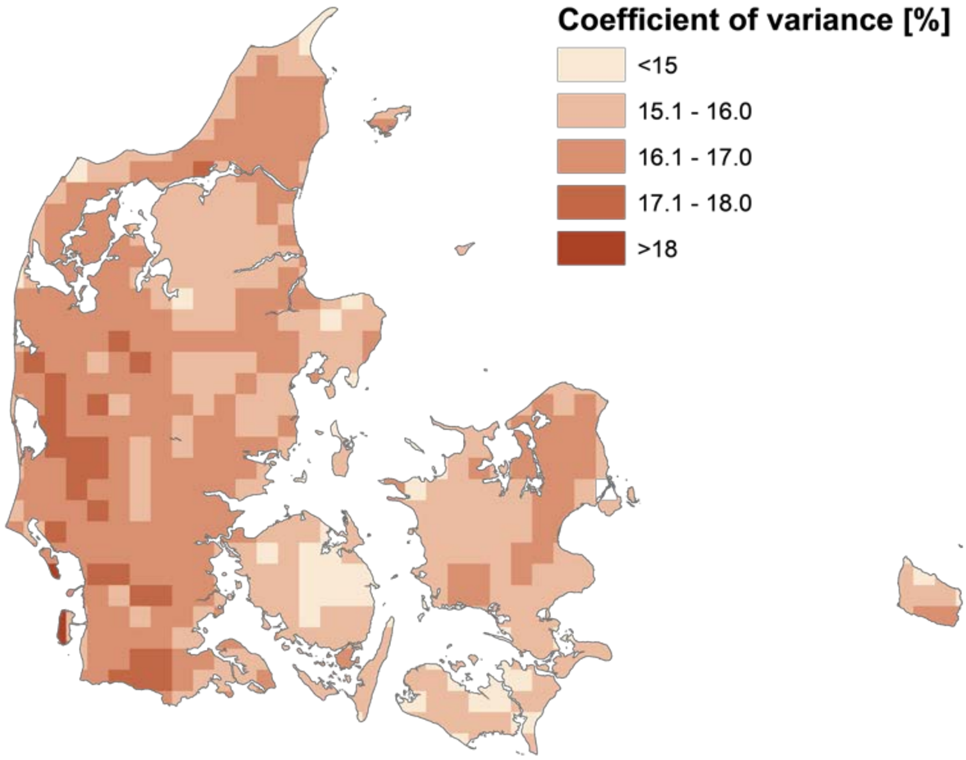

Figure 6.9. Coefficient of variance (%) of parameter uncertainty for the marginal N leaching based on model predictions using 1000 different sets of NLES5 parameter data sets. The uncertainty range is based on 1000 realisations of the NLES5 model reflecting the parameter uncertainties using a Monte Carlo approach.

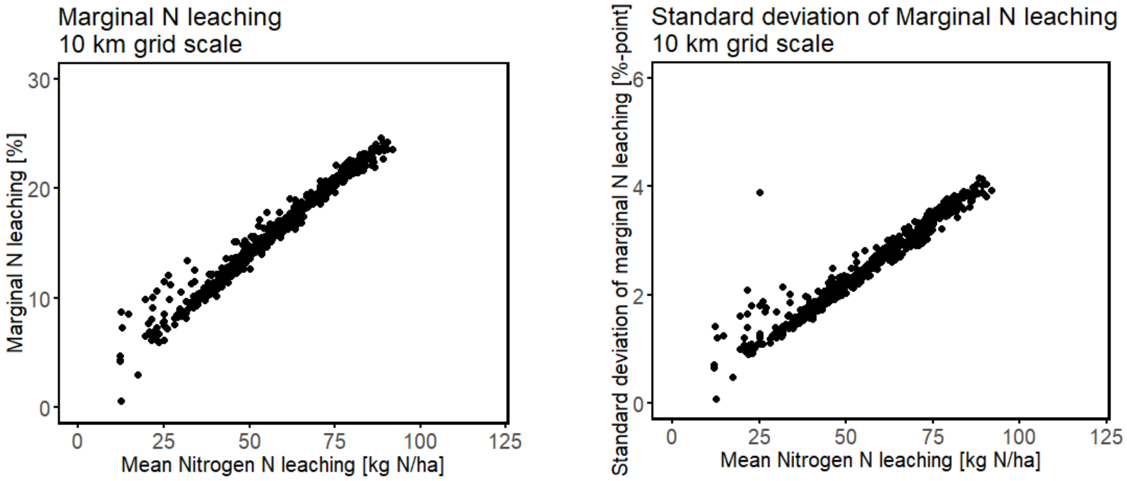

Figure 6.10. Marginal N leaching as function of N leaching level (left) and standard deviation of the marginal N leaching from parameter uncertainty as function of N leaching level (right)

6.3 Uncertainty and marginal N leaching at national scale

The predictions at national level are aggregated results based on the same results as described in section 6.2 and presented on the 10 km grid scale level. Figure 6.11 presents the annual results for the single years used to obtain the mean result. The estimated average leaching varies from year to year between 39 kg N/ha (minimum, 1997) and 92 kg N/ha (maximum, 1998). This variation is driven by differences in weather conditions (percolation) between the years. The average leaching across years is estimated to 61 kg N/ha. In Børgesen et al. (2015) the similar scenario was simulated with NLES4 to an average nitrate leaching of 67 kg N/ha. Thus, NLES5 predicts in general a lower nitrate leaching level of approximately 6 kg N/ha compared to NLES4. The uncertainty expressed by the standard deviation of the nitrate leaching is calculated to app. 6 kg N/ha for the mean result. The relative uncertainty at national scale is app. 10%, due to the NLES5 model parameter uncertainty. The difference between the two models (NLES4 and NLES5) is within the uncertainty range of NLES5.

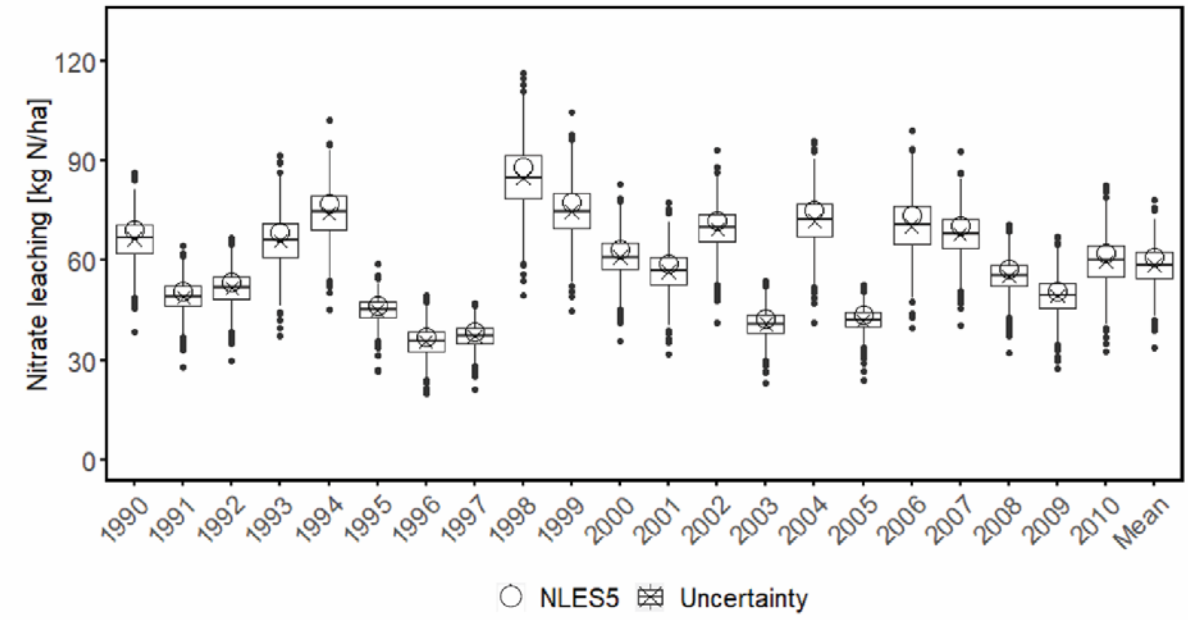

*Figure 6.11 Average nitrate leaching (kg N/ha) simulated using land use in 2011 and N use projected for 2021 (Børgesen et al., 2015). Results are calculated for weather data from individual years. The uncertainty represent 1000 realisations of NLES5 parameter uncertainty. Boxes indicate the 25 to 75 percentile. Horizontal line within the box is the median. The upper and lower vertical lines from the hinge indicate the largest and smallest values at 1.5 * IQR (where IQR is the inter-quartile range, or distance between the first and third quartiles, a roughly 95% confidence interval for comparing medians). Dots are observations outside the mean plus/minus the 95% confidence interval. × is the mean value.*

The mean marginal N leaching for the NLES5 model obtained for the 21 years is predicted to app. 17 % (Figure 6.12). The standard deviation obtained from the uncertainty analysis is app. 2.6 %-points. For the NLES4 model predictions in Børgesen et al. (2015), the marginal N leaching was 18%, which shows a marginal N leaching of the NLES5 model at the same level as NLES4. The NLES4 predictions is within the uncertainty range of the NLES5 model (app. 2.6 %-points). The year-to-year variation in the marginal N leaching (Figure 6.12) is between 10% and 25%, which shows the high impact of year-to-year variation of weather (percolation) impact on the predicted marginal N leaching. This dependence between marginal N leaching and percolation is partly seen in Figure 6.10, where also differences in soil, crops and N fertilization between the 10 km grid cells affects the variation in marginal N leaching. In the predictions on national scale of marginal N leaching (Figure 6.12) only the effect of percolation between the years is included as other factors are kept constant for the different years.

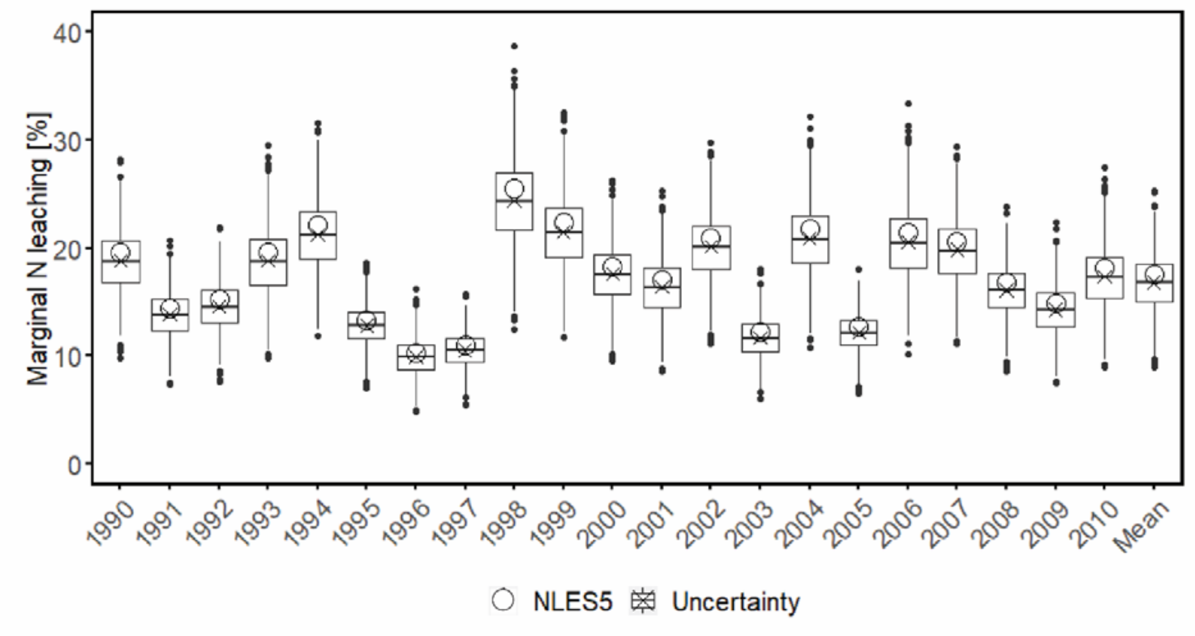

*Figure 6.12. Average marginal N leaching (%) simulated using land use in 2011 and N use projected for 2021 (Børgesen et al., 2015). Results are calculated for weather data from individual years. The uncertainty represent 1000 realisations of NLES5 parameter uncertainty. Boxes indicate the 25 to 75 percentile. Horizontal line within the box is the median. The upper and lower vertical lines from the hinge indicate the largest and smallest values at 1.5 * IQR (where IQR is the inter-quartile range, or distance between the first and third quartiles, a roughly 95% confidence interval for comparing medians). Dots are observations outside the mean plus/minus the 95% confidence interval. × is the mean value.*

7 Effects of N application rate on N leaching (marginal N leaching)

7.1 Short term effects (3 years N input)

The effect of N application rate on nitrate leaching is an important output from NLES5 as described in Chapter 6. NLES5 takes into account the N inputs in the predictions of N leaching (Chapter 3) based on the N inputs in the leaching year and in the two years preceding the leaching season. Farm N inputs to fields will often show correlation between years, e.g. on dairy farms the N input and the N removal in crops is generally higher than on many arable and pig farms. This correlation in N input between years in the calibration data may have affected how the model attributes the N effect between a first year effect and an effect of N input in the following years. Therefore, the effect of three years of N inputs should be considered as a whole, and the attribution of N effects between years may not be precise. The data on N inputs for calibration were limited to a three-year time span. In the calibration of the marginal N response of the model, both N inputs in the leaching year and in the preceding two years were used as predictors. However, in many of the experiments used for the calibration, the mineral N input only varied in the year of leaching, whereas some data came from long-term experiments (Agervig and Sdr. Stenderup exp. 103) where N input also varied in the preceding years.

Figure 7.1 shows mean annual marginal N leaching for the years 1976-2017 (data from Appendix 4 Tables A4.1 and A4.2) that were used for the calibration of the effect of additional applied mineral N in spring. The mean of all annual values is also shown for both the calibrated exponential models and the NLES5 estimates. Separate graphs of marginal N leaching are shown in Figure 7.1 for N rates below recommended rate (25-75%), at the recommended N rate (75-125%) and above the recommended N rate (125-150%). Most focus should be given to the results at the recommended rate, as the interval around optimum has the largest practical relevance, and only these data were used to calibrate marginal leaching response to mineral N application in NLES5.

The measured average marginal N leaching (fitted data) varied considerably from year to year (see Table A4.2), and the NLES5 model could not predict the same large annual variation in marginal leaching (Figure 7.1). Part of the inter-annual variation could be explained by differences in crop sequences used in the different years, but there were other factors than crops influencing profoundly the inter-annual variation, and these factors are not well described in the NLES5 model. This could be due to crop growth conditions or the timing of percolation between years and during the year that are not captured by NLES5. Other factors could be temperatures in the autumn and winter which affect the soil N mineralization processes. At the recommended N rate the average marginal N leaching response across the years 1976-2017 was 17% for the *Cal2* data and the NLES5 model was calibrated to give the same average marginal N response at the recommended N rate. Across the 2017 field data, the fitted marginal leaching was exceptionally high and above 35% at the recommended N rate, while it was about 5% in the previous year of 2016 (Figure 7.1). Other years with high marginal N leaching are 1980, 1985 and 2008. The *Cal2* dataset has relatively many data from 2016 and 2017, but each observation of marginal leaching counted similarly in the calibration. Anyway, the inclusion of field data from the exceptional year 2017 has a relative high influence on the average estimated marginal N leaching for the whole period.

The observed marginal N leaching for 2008 was also high, and this observation was based on one single treatment in one experiment with oats in Sweden ("Skara" experiment 221). Due to the limited amount of data available from experiments with variable N rates, and due to the high variation in marginal N leaching between years, the calibration included data for the entire period 1976-2017 giving similar weight to all available experimental data, although negative marginal nitrate leaching values was set to 0%.

The method to obtain the marginal N leaching in the NLES5 was by calculating the leaching at the N rate used in the experiment and subsequently calculating the leaching at a 1 kg N/ha higher N application rate. From these predictions the leaching increase is multiplied with 100 giving a marginal N leaching as %-points. In the single experiments the marginal N leaching was based on curve fitting to an exponential function using observed leaching at different N application rates. The more linear response of NLES5 compared to individual measurements in experiments (individual fields) is a result of the year to year variation in N responses due to many other factors that could not be included in NLES5 as well as the way the response to N input is formulated in the model. This resulted in a less dynamic marginal N leaching than the observed year to year variation in marginal N leaching and a more linear marginal N response between the different N rates. That means that the marginal N leaching is overestimated by low N application rates and under-estimated at N rates higher than the N recommendation.

It should be noted that only few of the experimental data used to calibrate the marginal nitrate leaching came from experiments performed on coarse sandy soils and no data from maize crops were available in the dataset (*Cal2*) used to calibrate marginal nitrate leaching. We expect a high marginal nitrate leaching on coarse sandy soils and in maize crops. Of the data used for calibration of marginal nitrate leaching (Figure 7.1), 41 experiments included cereals and winter crops.

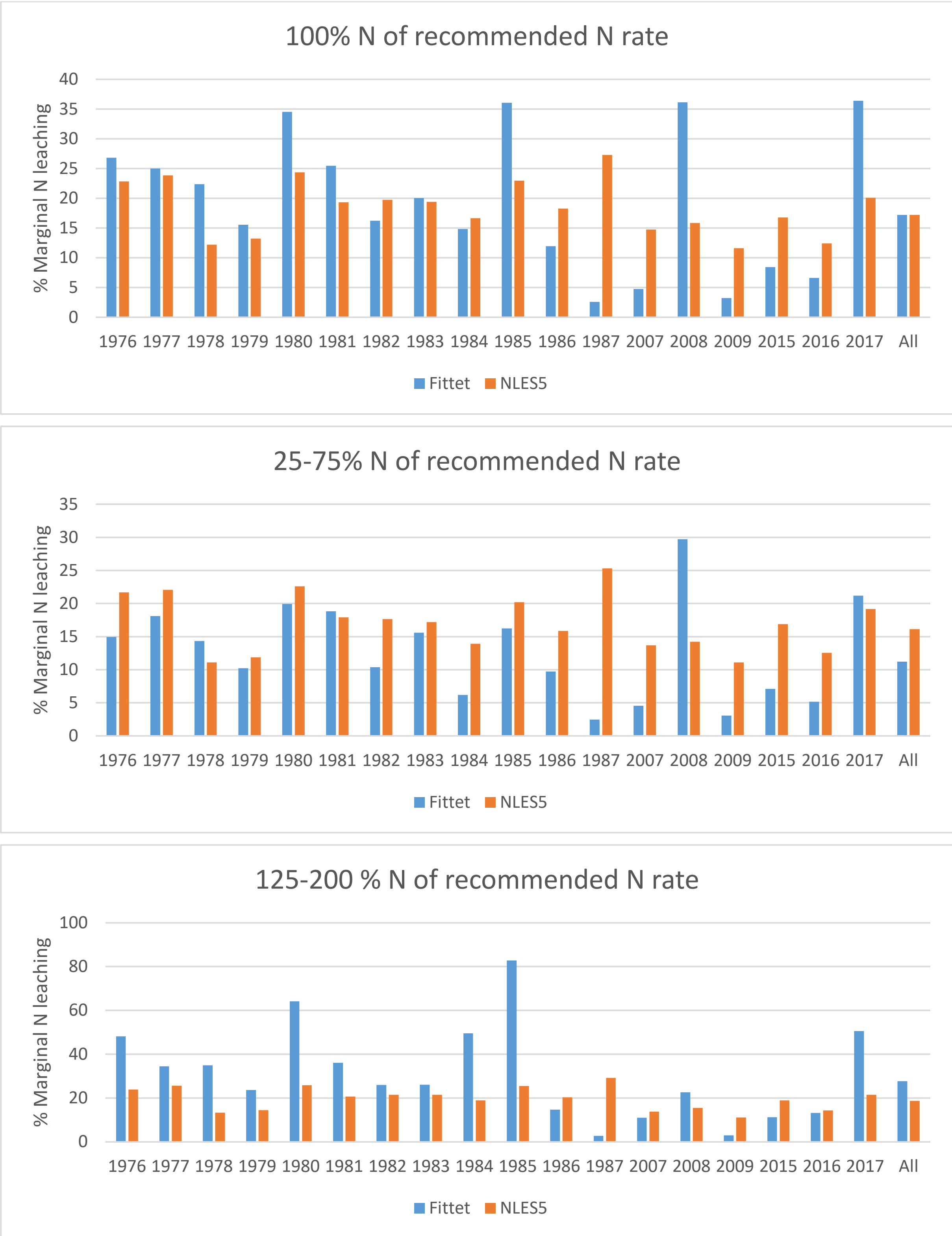

Figure 7.1. Annual mean marginal N leaching estimated using an exponential model fitted to leaching data (Appendix 1 Table A.3.2) and estimated for the same conditions with the NLES5 model. Results from 1976 to 1987 are data from experiment 103 (Agervig and Sdr. Stenderup), 2007-2009 are from Experiment 221 (Skara, Sweden) and 2015-2017 are from experiments 225 and 226 (SEGES and VIRKN).

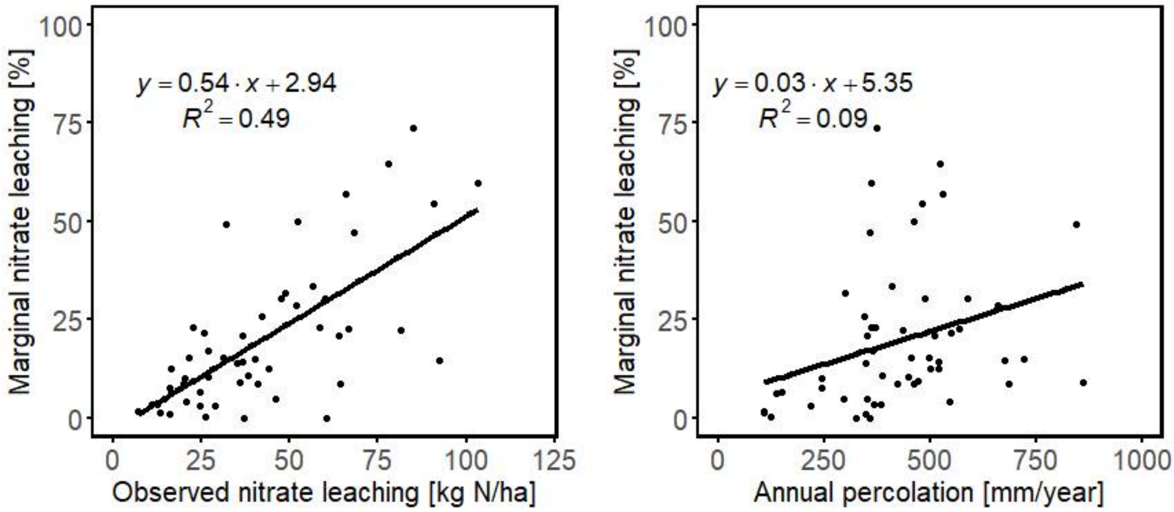

Figure 7.2. Marginal N leaching (at recommended N level) in cereals and winter crops estimated by exponential fitting to observations related to total nitrate leaching in the same experiment (a) and related to water percolation in the year of measured leaching (b).

The marginal N leaching predicted by an exponential function to the single field data sets (*Cal2*) from experiments were not significantly related to annual water percolation (Fig. 7.2b), but there was generally a positive relationship between nitrate leaching and the marginal N leaching (Fig. 7.2a).

7.2 Nitrogen leaching measured in other N response experiments

In the Broadbalk field experiment (Appendix 3) and the Askov lysimeter experiment (Appendix 3) variable N rates were applied repeatedly over a longer period and effects on N leaching were measured. These results were not included in the NLES5 calibration and in Figure 7.1, since these the setup of these experiments deviated from the standard setup of other experiments, and for the Broadbalk experiment (>150 years with variable continued N rates) the describing variables needed in the model were not available. A problem by the Askov lysimeter study was that the small lysimeters were surrounded by unplanted soil resulting in large border effects. This could result in larger plant growth and less nitrate leaching, especially at high N rates. On the other hand lysimeter studies are expected to better reflect leaching conditions in drained soils. The marginal N leaching estimated from the Broadbalk and Askov long-term experiments showed significant inter-annual variation.

Figure 7.3 shows the N leaching and marginal N leaching measured in the lysimeter experiment at Askov from 1974 to 1981. The application of variable N rates started in 1974 and was repeated until 1981. The average marginal leaching estimated by fitting to an exponential function was 10% at the normal N rate (110-150 kg N/ha) when including also two years with autumn application of mineral N, and only 7% when excluding the two years with autumn N application. The soil used in this experiment was loamy with 17% clay and annual precipitation was high at 927 mm on average.

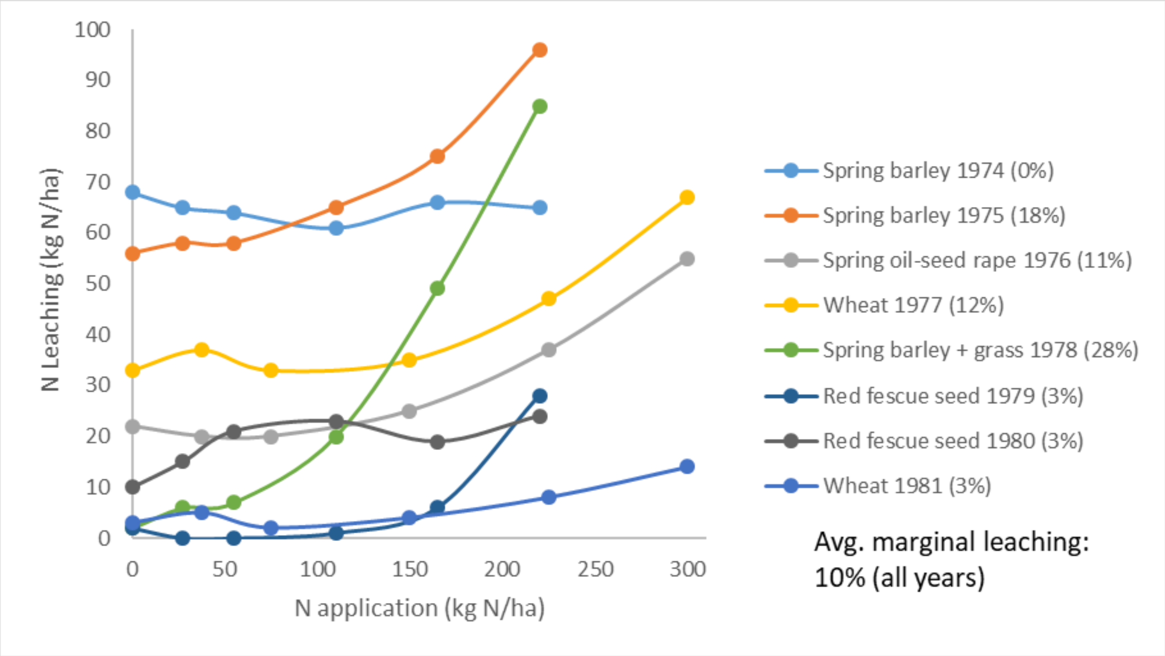

Figure 7.3. Nitrate leaching measured in the Askov lysimeter experiment with increasing mineral N application applied during a period of 8 years (data from Kjellerup and Kofoed, 1983). In 1978 and 1979 the plots received fertilizer in spring plus half of the N rate for the next grass seed crop applied in the autumn. The marginal leaching at normal N rate (1N=110 kg N/ha or 150 kg N/ha) was calculated by fitting an exponential function to data (excluding 0N) and shown in brackets as a percentage for each leaching period. The experiment is described in Appendix 3.

Figure 7.4 shows N leaching measured in the Broadbalk long-term experiment with continuous winter wheat. By application of 192 kg N/ha a very high marginal N leaching of 68% was estimated for the first year by fitting to an exponential function. The average marginal leaching across years at 192 kg N/ha was 19%, and 12% if excluding the exceptional first year. The soil is a clay loam with 18-27% clay and mean precipitation was 696 mm. This experiment illustrates that marginal N leaching on a specific location can be quite variable from year to year even with the same crop and very high in certain years (approximately one out of ten). Continuous cropping of winter wheat gives lower yields due to diseases, and it is uncertain how much this affected the marginal N leaching in this experiment, but it could potentially result in a higher marginal N leaching.

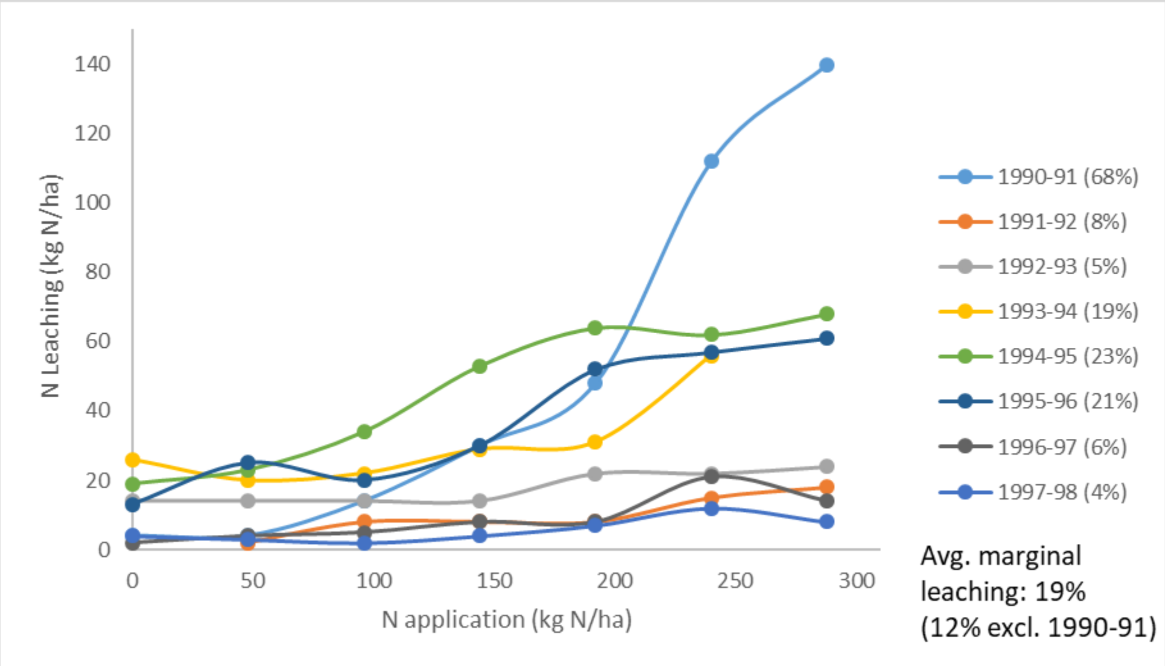

Figure 7.4. Nitrate leaching in the Broadbalk continuous wheat experiment between 1990 and 1998. The calculation assumes that 20% of the total leached through drains and 80% in groundwater (data from Goulding et al., 2000). The marginal leaching at 192 kg N/ha was calculated by fitting an exponential function to data (excluding 0N) and shown as a percentage for each leaching period in brackets. New tile drains were installed in autumn 1993. The experiment is described in Appendix 3.

In a long-term arable crop rotation experiment started in 1997 at Research Centre Foulum different crop rotations with variable N inputs were compared, including both inputs of mineral N fertilizers, animal manure and biological nitrogen fixation. De Notaris et al. (2018a) found a linear relationship between N input and N leaching when N leaching was analyzed separately for fields with and without cover crops. The average marginal N leaching in this experiment including long-term effects was 8%, both on plots with and without catch crops (de Notaris et al., 2018a). The soil was a loamy sand with 8% clay. All plots in this experiment received N rates below the economic optimum. So marginal N leaching measured in this experiments covers conditions below the optimum N application rate.

7.3 Coarse sandy soils and maize cropping

We only found few experiments with increasing N application in maize crops and also few experiments on coarse sandy soils. Results from Manevski et al. (2015) indicate that marginal leaching in maize can be high, especially in maize with grass as the previous crop. However, the marginal N response could not be estimated precisely from the study of Manevski et al. (2015) as only a limited number af N rates were included in the measurements. Table 7.1 shows the marginal N leaching estimated by repeated maize cropping on a coarse sandy soil in Northern Germany (Wachendorf et al., 2006). The marginal N leaching estimated by an available N rate of 173 kg N/ha (recommended N rate for maize in DK) was found to be 22% without a cover crop in the maize and 7% by continuous use of cover crops. In Denmark the use of cover crops in maize has increased over recent years due to legislation on use of cover crops. In some parts of Denmark cover crops established between continuous maize is not expected to perform so well as in Northern Germany.

Table 7.1. Marginal N leaching estimated in maize cropped on coarse sandy soil in Northern Germany with and without continuous use of grass catch crops (data from Wachendorf et al., 2006). Marginal N leaching was calculated from exponential response parameters estimated in a continuous 4 year experiment (average of 4 years). A fertilizer replacement value of 50% was assumed for the slurry N when estimating the recommended fertilizer rate (1N).

Slurry, kg total N/ha	Cover Crop	Mineral N fertiliser (1N), kg N/ha*	Marginal N leaching at 1N, %	Avg. marginal N leaching at 1N, %
0	No	173	11	22
62	No	142	37	
124	No	111	19	
0	with CC	173	5	7
62	with CC	142	10	
124	with CC	111	7	

* The recommended N rate on coarse sandy soils in DK for 2019 is 173 kg N/ha.

In another experiment in Northern Germany repeated on two soil types, either mineral fertilizers or mono-digested maize (digested slurry based on maize) were used in continuous maize cropping, and N leaching was related to the mineral N application in either manure or mineral fertilizer (Svoboda et al., 2013). Table 7.2 shows marginal N leaching estimated from exponential response parameters given by Svoboda et al. (2013) at the recommended N rate of 173 kg N/ha in Denmark. The estimated average marginal leaching on both locations was 30-31%.

Table 7.2. Marginal N leaching by continuous maize cropping without catch crops estimated from exponential response parameters in a two-year experiment at two locations in Northern Germany (data from Svoboda et al., 2013). The marginal N leaching was estimated at the recommended mineral N application rate for Denmark in 2019.

Site	Period	Mineral N fertiliser (1N), kg N/ha	Yearly drainage, mm	Marginal N leaching at 1N, %
Hohenschulen 12 % clay	2007/2008	173	358	35
	2008/2009	173	218	27
	Average			31
Karkendam 4% clay	2007/2008	173	527	42
	2008/2009	173	304	18
	Average			30

These measurements in maize crops show that a realistic average marginal N leaching in continuous maize without cover crops is in the range of 22-31%. Other studies indicate that marginal N leaching can be significantly higher in rotations with maize following a grass crop, if the residual N effect of grass is not accounted for by N application (Manevski et al., 2015). In a scenario analysis with the present NLES5 model we estimated a marginal N leaching at high percolation (610 mm) and optimal N rates of 31-38% with the highest rate on coarse sand. This was estimated for maize after grass, while the corresponding marginal N leaching for maize following other crops than grass was 23-29%. This is in fairly good accordance with the German measurements described above.

The German study by Wachendorf et al. (2006) also indicates that continuous use of grass as catch crops in continuous maize can reduce marginal N leaching to a level around 10% on coarse sandy soils, which is at the same level or lower than for cereal crops. In contrast to cereals, where cover crops has low influence on marginal N leaching (e.g. de Notaris et al., 2018a), the continuous use of grass cover crops in maize seems to significantly reduce marginal N leaching.

Another lysimeter study on Askov Experimental station was performed on a coarse sandy soil (5% clay). Three levels of mineral N (50%, 100% and 200% of recommended N rate) were applied repeatedly over a period of ten years (1974-83). The average (10-year) response of N rate on N leaching was linear up to 160 kg N/ha in spring barley with a marginal leaching of 13% and linear up to 320 kg N/ha in fodder beets with a marginal N leaching of 3% (Larsen and Kjellerup, 1989; Sørensen and Børgesen, 2015). The marginal leaching estimated in this experiment included residual effects on N leaching of 1-10 years variable N application and no cover crops were included.

7.4 Long term effects of N application rate

Experiments with ^{15}N-labelled fertilizers have shown that 21-25% of the applied N fertilizer is present in the topsoil three years after application to a spring cereal crop (Kjellerup and Kofoed, 1983; Sørensen, 2004). After application of ^{15}N-labelled fertilizers to winter wheat, Sørensen and Thomsen (2005) only found about half as much labelled N in the soil compared to spring barley. This is in accordance with English studies in winter wheat by Hart et al. (1993), who recovered 17% of the applied fertilizer N in soil after the first harvest which declines to about 12% after the third year. Experiments with ^{15}N isotopes should be interpreted with care as pool substitution effects may occur, which potentially could mean that more labelled N remains in soil than the true net N retention in soil (Jenkinson et al., 1985; Sørensen and Thomsen, 2005). However, the measured N uptake observed in a number of different field experiments with cereals performed under conditions with low N losses support that it is realistic that 20-25% of applied mineral N remains in soil after spring barley and about half of that remains after winter wheat (e.g. de Notaris et al., 2018b). This residual N in soil will be released/mineralized slowly over many years and contribute to both crop N uptake and to N leaching (Hart et al., 1993). The proportion of mineralized N that is leached is higher than from mineral N applied in spring as mineralization also takes place outside the growing season. The proportion of residual N that is leached is influenced by soil type, crop rotation, including the use of cover crops, and length of growing season. This also implies that future leaching from the residual N may change if cropping systems are changed.

An estimate of the long-term effect (within ca 10 years after N application) was given by Sørensen et al. 2019. They estimate an average cumulated additional leaching in year 4-10 after N application of 1-3% (average 2 %) of applied N. They assume that 12-25% of the applied mineral N remains in the soil 3 years after application (from plant and root residues and root exudates) and that 1/3 of the mineralized N is leached on average. Cumulated over 10 years this gives a marginal N leaching of about 2% in addition to the short-term effects estimated by the NLES5 model. As mentioned in Section 2.5 both experiments with short term (<3 years of relative N fertilization in cropping history) and longer term N fertilization were included in the *Cal2* calibration dataset. We consider the error caused by this in the calibration of marginal N leaching to be small, as the residual effects after 3 years are generally small and impossible to detect by leaching measurements. Other factors such as crop-sequences and weather have much higher effects than long-term effects of N application rates.

More N remains in soil after application of organic N in manures. About 50% of the organic N applied in pig and cattle slurry remains in soil after 3 years after application (Sørensen et al., 2017), meaning that organic manure N will also contribute more to a long-term effect.

8 Discussion

8.1 Crop effects

Crop sequences and plant cover during the autumn and winter period are very important for N leaching and NLES5 provides a good estimate of the average effect of the major crop types in Danish agriculture. NLES5 is structured with four separate cropping periods in relation to the estimated leaching: Main crop, winter crop (in the period of leaching) and previous main crop and previous winter crop (Figure 8.1). This structure was chosen despite weaknesses such as crop groups that are strongly related/confounded, e.g. a main crop of winter cereal will also have winter cereal as previous winter crop. This makes parameter estimates correlated, and great care had to be taken in the definition of crop groups to avoid excessive correlations that would greatly enhance model uncertainty.

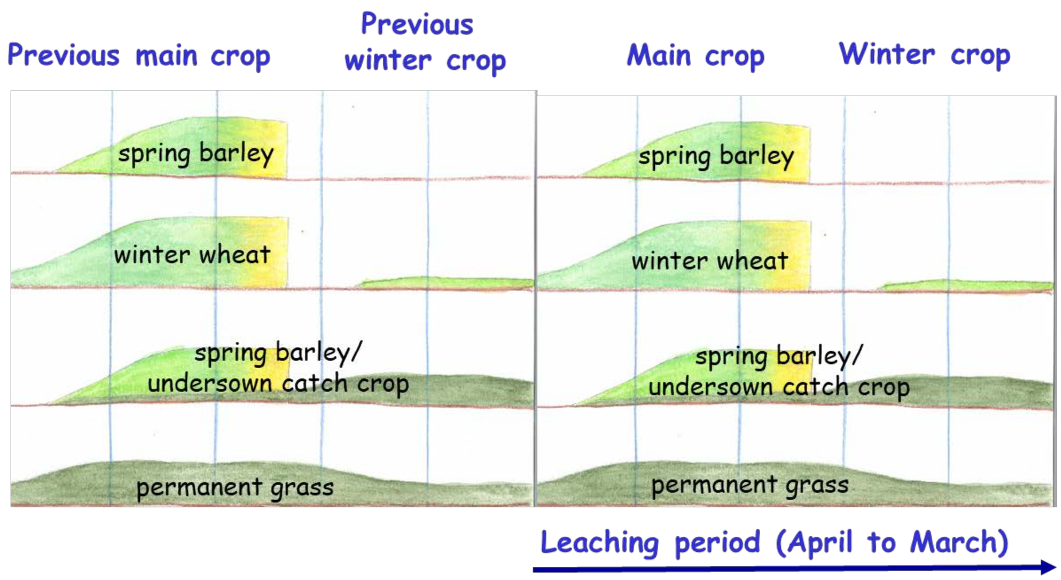

Figure 8.1. Illustration of the cropping periods and N uptake in crops influencing N leaching in the NLES5 model with four examples of crop rotations with different N uptake pattern.

Grass and grass-clover crops generally result in a low N leaching level during their growing period, but will release large amounts of mineral N during mineralization of crop residues in the years following break-up of these crops. The utilization of this residual N by crops depends on the type of crop grown and the fertilization rate of the following crop, and there can be interactions depending on the crop sequence. To estimate this effect the model is designed with separate main crops of winter cereal, spring cereal and maize, either with or without a previous grass/grass-clover crop. Especially for maize a previous grass crop increases N leaching significantly (Table 3.2 M11). The model captures only to some extent the mean effects of previous grass crop on the leaching the following year, but there are also observations with large deviations (e.g. maize after ploughed grass/grass-clover, Table A2.3).

Studies have shown that there can be a significant N mineralisation and risk of high N leaching also in the second year after ploughing grass crops (Simmelsgaard and Djurhuus, 1998). This second year effect is estimated in NLES5 by an effect from having 'previous main crop' groups with a previous grass crop (MP3 and MP4). The effect of grass in the previous year before the leaching season is accounted for by 'previous winter crop' (WP10, WP11), and special main crop groups (M10, M11 and M12). The previous crop effect is further complicated by interactions with the effect of previous N input (in the previous two years) in the model. A fodder grass crop will normally receive a large input of N by fertilizers and/or by symbiotic N fixation, and this N effect will also contribute to the residual effect of grass calculated by the model. This model structure has the advantage that it can include interactions between N input and crop sequence, but it also means that the estimate of the pure effect of a specific crop and effect of fertiliser cannot be directly derived from the model structure.

Potatoes is an important crop in some areas of Denmark, and it should be noted that the effect of potatoes on nitrate leaching is not well estimated by NLES5. This deficiency is due to lack of leaching data representing the diversity of potato cropping. Potatoes for direct human consumption can be harvested in early summer with a potential for large leaching losses during the following autumn, whereas potatoes for industrial use are growing until late in the autumn and can possibly be comparable with beets in regard to N leaching. Due to properties as late establishment in spring by row cropping and later growth, potatoes were grouped together with maize in the model.

8.2 Cover crop effects

Scenario analyses with NLES5 were set up for specific crop sequences, e.g. spring barley with or without a cover crop. The reduction in N leaching from growing the cover crop is estimated to be in the range of 34 to 46 kg N/ha under conditions with high percolation (610 mm) and 19 to 28 kg N/ha at low percolation (240 mm). The intervals indicate the effect of soil type with the lowest effect for more clayey soils (JB6) and the highest effect on coarse sand (JB1). These model estimated effects agree well with experimental data from Denmark (e.g. Thomsen and Hansen, 2014; de Notaris et al., 2018a). The net effect on N leaching of having cover crops in a crop rotation is estimated from a reducing effect in the leaching year and an extra leaching in the year after having a cover crop. The extra leaching after the cover crop is due to release of N from cover crop residues that can contribute to N leaching. To estimate the net effect of cover crops in the model it is therefore important both to account for the effect in the year with the cover crop and the effect in the following year, which is represented as the effect of previous winter crop in the model. The scenario analyses with NLES5 showed a reduction in marginal N leaching rate of 5 to 6%-points by use of cover crops in spring barley at high percolation (610 mm) and a reduction of 3 to 4%-points at low percolation (240 mm) with the highest reductions in the most sandy soils (all calculations at optimal N rate).

8.3 Effects of N inputs on estimated leaching

The effect of N inputs on N leaching is divided in a contribution from N inputs applied in the leaching year and a contribution from N inputs in the previous two years. The first year effect is divided into mineral N applied in spring, mineral N applied in autumn, organic N in manure applied in spring, mineral N deposited by grazing animals and N from BNF. Organic N applied with manure in autumn or by grazing is assumed to have no effect on N leaching in the year of application as net N mineralization from manure is normally below 0 until a few months after the application (Sørensen et al., 2017).

The effect of N input in the previous two years is divided into a pooled effect for mineral and organic N inputs from both mineral fertilizers, total N in organic manure and N deposited from grazing animals, and a separate effect from estimated N inputs from BNF. For simplicity, no distinction is made between timing of N inputs in the two previous years, even though a higher effect can be expected from inputs in the previous year compared to inputs made two years ago (Hart et al., 1993; Sørensen et al., 2017; Webb et al., 2013). In fact the mineralization of residual N is about twice as high in the second year than in the third year and, therefore, the contribution to leaching could also be about twice as high in the second year after application. The assumption made that the leaching rate in the second and third year after application is similar from both organic and mineral N sources is based on experiments with ^{15}N-labelled manures and fertilizers. Such experiments showed that in the second and third year after application the N release, calculated as percent of N input, is nearly the same for all input types (Jensen et al., 1999; Thomsen et al., 1997).

Long-term effects of N fertilization level are indirectly included in the nitrate leaching dataset *Cal1* and *Cal2* used for calibration, as the fields used in the experiments has been used in agricultural production for more than 100 years and have received N fertilizers for >50 years. This means that the soil nitrogen pool in the soil has been supplied with new organic N in crop residues and from organic fertilizers every year. Organic matter from the previous many years is slowly mineralized and thereby supplying nitrogen for crop growth. This is often referred to as background mineralization which also increases nitrate leaching due to high mineralisation outside the crop uptake period. Following this logic the long-term effects of nitrogen is captured by the effect of soil N concentration in the NLES5 model.

The *Cal2* dataset includes data from the Agervig and Sdr. Stenderup field trials (experiment 103). Here four N rates (0%, 50%, 100% and 150%) were applied over a longer period than the tree years accounted for in the model. If there is a residual effect of mineral N after the first 3 years this would mean that the effect of the first three years included in the model would be overestimated, and an increase in marginal leaching over time would be expected. Results in Table A4.1 does not show an increase in marginal N leaching over time. Probably the long-term effect of mineral N application was so low that it could not be detected, and this effect could be ignored in the calibration.

NLES5 calculates a higher effect of spring applied mineral N (parameter β_{cs}) compared to organic N applied with manure in spring (β_{cg0}). A number of leaching studies in lysimeters indicated that the short-term leaching from mineral N and organic N inputs in manure are similar (Sørensen and Børgesen 2015). One reason for this discrepancy could be that ammonia losses from manure are not considered in the model. Inputs of organic manure N and ammonia losses are correlated (Hutchings et al., 2001). Ammonia losses will reduce N leaching, and when ammonia losses occur from applied manure, organic N is also applied with the manure. This co-variation may give an underestimation of leaching losses from organic manure N, and the effect of ammonia losses may be implicitly included in the effect of organic N applied with manure. In the development of NLES5 we tested a correction of ammonia losses in the mineral N input with manures using a simple estimation of ammonia loss from manure. However, this calculation did not improve the performance of the model and we decided to ignore ammonia volatilisation in the model. The effect of ammonia loss is therefore expected to be included mainly in the model parameter for effect of organic manure N input in the year of application.

8.4 Effect of cropping year (technology improvements)

NLES5 has a time-trend correction corresponding to a yearly linear decrease of N leaching of 0.11 kg N/ha/yr with a starting point from year 1991. This trend was significant and could not be accounted for by any of the parameters in the model. This yearly trend in N leaching would have been significantly higher, if experimental data from 2017 were excluded from the calibration. In 2017 N leaching predictions were under-estimated significantly compared to observations and therefore the declining time trend in the model was reduced. When data were divided into on-farm data (LOOP) and data from experimental stations, the trend for 1991-2014 was nearly similar in both data sets. Several aspects in the farming system can have affected the declining N leaching from around 1990 to present such as: i) genetic improvement of crop varieties over time, ii) improvements in soil cultivation and crop establishment, iii) improved control of pests, diseases and weeds. However, not all these elements are expected to have an effect at the experimental stations as soil tillage and sowing technology has not changed significantly there in the period since 1991.

This time trend in the model implies that the model is expected to be best suited for estimations in the period 1993-2017. In practice, we expect that the model is also valid for use in projections for about a decade ahead. However, caution needs to be taken on accounting for the effect of future technology improvements when applying the model.

8.5 NLES5 and the N balance by additional N application

A simple N balance of extra applied mineral N in cereals is shown in Table 8.1. Some of the assumptions used for the N flows are taken from Petersen and Djurhuus (2004). In a recent field study presented by de Notaris et al. (2018b) a first year marginal N uptake in grain was found to be 46% for spring barley and 64% for winter wheat under nearly optimal conditions. The corresponding marginal N uptake in straw was found to be 15% in barley and 12% in winter wheat, which is in accordance with the assumptions by Petersen and Djurhuus (2004). The marginal N uptake in cereals is found to be nearly constant at different N rates, even at N rates that are significantly higher than the economical optimal N rate (e.g. de Notaris et al., 2018b). Denitrification varies greatly among different soil types and is influenced by precipitation, ground water level, soiltexture and soil structure. Under conditions with high denitrification, less N leaching can be expected. After application of ^{15}N-labelled mineral fertilizers to spring barley, 20-25% of the labelled N is recovered in soil after 3 years (Kjellerup and Kofoed, 1983; Sørensen, 2004). After application of labelled mineral N to winter wheat in spring, only about half of this amount is recovered in soil (Sørensen and Thomsen, 2005), corresponding to 10-12% remaining in soil after 3 years. This residual N is derived from roots and root exudates as well as other aboveground residues left in soil. The residual N in soil is expected to be released over a period of 100 years or more, and can contribute with some extra leaching in the long term. The variation in the total balance is less than indicated in Table 8.1 as high N leaching will be combined with lower N uptake in the crop and vice versa. The overall N balance indicated in Table 8.1 is close to 100%.

Table 8.1. Overview of estimated change in the N balance by application of additional mineral N to cereal crops three years after N application.

N component	Spring cereal (% of N input)	Winter cereal (% of N input)
N in grain	30-50	45-65
N in straw	15	12-15
Leaching (1-3 years)	5-25	5-25
Denitrification	5	5
Deposition	0	0
Ammonia loss	2	2
Residual soil N after 3 years	20-25	10-12
Total balance	77-122	79-121

In a previous assessment of the effects of N application on N leaching, Petersen and Djurhuus (2004) only assumed mineral N to contribute with 8-14% to the soil N pool, and that could justify a higher marginal N leaching rate from applied mineral N. However, we find this to be an underestimation of residual N remaining in soil. We expect that there is a general decline in the organic N pool that is independent of N application rate (Petersen and Djurhuus, 2004) due to the general decomposition of organic matter in soil. This decline is counter-balanced by a proportion of both applied mineral N and organic N in manures that remain in soil for a relatively long time. This retention of N in soil is nearly proportional to the N input, and may result in a positive net N accumulation in soil at high N inputs. When straw is not harvested, the straw N mainly contributes to a long-term accumulation of soil N.

8.6 Perspectives for further development

The NLES5 model presents an improvement over previous versions of the model in the sense that it better handles the effect of crop sequences and winter vegetation cover on nitrate leaching. However, the model still has weaknesses, and some of these are related to availability of data for calibrating the model. These weaknesses include novel mitigation measures such as effect of early sowing of winter cereals. There is also a need to obtain better information on the status of the autumn and winter vegetation cover. The data used with the model calibration did not fully allow us to separate between situations of bare soil and weeds/volunteers, which makes it difficult to adequately quantify effects of measures such as cover crops. There is also need to improve the calibration of some crops and cropping sequences that are poorly represented in the calibration datasets, e.g. maize after grass, maize after maize, and potatoes. There is also a need to focus on long-term effect of changes in soil organic N and how this affects N leaching, and how such effects can be better included in the model beyond having total soil N as a determining factor.

The current version of the model proved extremely difficult to calibrate, and a mixed approach for this calibration had to be implemented. There is a need in future studies to consider other statistical approaches for both model calibration and validation. However, such approaches should retain the functional aspects of the current model, i.e. it should be possible to estimate the effects on nitrate leaching of different crops and crop sequences as well as effects of variation in N application rates under varying soil and climate conditions.

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10 Appendix 1 Data overview

Table A.1.1. Experimental information and number of observations used in the calibration and validation

Exp. no.	Years	Experiment information	Site	Reference
LOOP 1	1991-2014	102-105 with 1995 out 103 until 2009 107 from 1996.	Højvads Rende	Blicher-Mathiesen et al., 2019
LOOP 2	1991-2014	201-206 all years 203 with 2011-2013 out 206 until 2010	Odderbæk	Blicher-Mathiesen et al., 2019
LOOP 3	1991-2014	301-304	Horndrup Bæk	Blicher-Mathiesen et al., 2019
LOOP 4	1991-2014	401-406 401,403-406 without 1995	Lillebæk	Blicher-Mathiesen et al., 2019
LOOP 6	1991-2014	601-605, 607, 608 605 until 2008	Bolbro Bæk	Blicher-Mathiesen et al., 2019
101	1991-2004	Crop rotation, drainage measurements	Lunding, Naestved, Silstrup, Aabenraa	Simmelsgaard, 1994 (Danish report)
102	1991-1993	Analyses of nitrate in drain-water from 16 fields at different sites	Stenderup, Silstrup, Askov, Agervig, Borris, Roenhave, Tylstrup, Jyndevad, Foulum, Oedum, Roskilde, Aarslev, Tystofte	Olsen, 1995 (Danish report)
103	1976-1988	Nitrate leaching at four N levels	Agervig, Sdr stenderup	Simmelsgaard and Djurhuus, 1998
104	1991-1994	Nitrate leaching following cultivation of clover at different times	Foulum, Jyndevad	Djurhuus and Olsen, 1997
105	1991-1992	Nitrate leaching, soil tillage, catch crop (Ødum)	Ødum	Hansen and Djurhuus, 1997a Hansen and Djurhuus, 1997b
106	1991-1992	Nitrate leaching, long time soil tillage, catch crop, N-rate (B-mark)	Jyndevad	Hansen and Djurhuus, 1997a Hansen and Djurhuus, 1997b
112	1994-1996	Nitrate leaching, continued B-mark, introduction or discontinuation of catch crop	Jyndevad	Hansen et al., 2000a Hansen et al., 2000b
113	1991-1992	Crop rotation, N-rate, organic matter application (Systemforskning)	Foulum, Jyndevad og Ødum	Hansen, 1994
114	1991-1992	Crop rotation, permanent pasture, 3xN (K-mark)	Jyndevad	Hansen 1992
115	1991-1992	Dairy crop rotation (S7 and S8)	Foulum	-
117	1992-2016	Organic and conventional grain crop rotations	Flakkebjerg, Foulum, Jyndevad	Askegaard et al., 2011 Pandey et al., 2018 de Notaris et al., 2018a
118	1995-2001	Grass and clover effects on leaching	Foulum	Eriksen et al, 1999 Eriksen et al., 2004a Eriksen et al., 2004b
119	1998-1999	Organic dairy (Burrehøjvej)	Foulum	Eriksen, 2001 Eriksen and Søegaard 2000

				Eriksen et al., 2015
122	1997-2001	Low input crop rotation with grazing	Silstrup	Kristensen et al., 2008
216	2003-2012	CENTS	Flakkebjerg, Foulum	Hansen et al., 2015
217	2010-2011	Maize experiment at Foulum and Jyndevad	Foulum, Jyndevad	Manevski et al., 2015
220	2007-2010	Organic dairy crop rotation	Foulum	Eriksen et al., 2015
221	2007-2009	Nitrogen leaching under 6 fertlilization levels in Skara (SW Sweden)	Skara (Sweden)	Delin and Stenberg, 2014
223	2012-2015	Maize and Catch crops (after maize)	Foulum, Løgumkloster, Bolderslev	Hansen et al., 2013. Hansen and Kristensen, 2014 Hansen and Kristensen, 2015 Hansen and Kristensen, 2016
224	2015-2016	Increasing nitrogen rates from national field trials (SEGES)	Guldborg, Holstebro, Jyderup	Piil, 2016 Piil, 2017 Piil et al., 2018
225	2014-2016	Energy crop experiments	Jyndevad, Foulum	Manevski et al., 2018
226	2015-2017	Cereal crops with catch crops, N fertilization and sowing dates (VIRKN)	Foulum, Flakkebjerg	Hansen and Thomsen, 2017 Hansen and Thomsen, 2019 Hansen et al., 2019

Table A.1.2. Nitrogen inputs of mineral N (Min N) and organic N (Org N) applied in the different experiments used for calibration of NLES5 (average, minimum and maximum). Calibration data (Cal1).

Type	Min N spríng			Min N autumn			Org N all year			N fixation		
	Mean	Min	Max	Mean	Min	Max	Mean	Min	Max	Mean	Min	Max
Exp. no	Kg N ha^{-1} year^{-1}											
1	125	0	234	2	0	72	3	0	35	6	0	239
2	139	0	349	11	0	148	67	0	164	23	0	304
3	152	0	320	5	0	119	43	0	288	56	0	457
4	138	0	288	16	0	226	43	0	347	9	0	284
6	162	0	547	5	0	151	80	0	337	48	0	476
101	115	0	246	5	0	121	50	5	176	56	0	471
102	109	0	250	0	0	0	19	0	102	21	0	362
104	113	92	150	0	0	0	0	0	0	0	0	0
105	120	120	120	0	0	0	0	0	0	0	0	0
106	90	60	120	0	0	0	0	0	0	0	0	0
112	89	60	120	0	0	0	0	0	0	0	0	0
113	92	39	162	0	0	0	19	0	54	0	0	0
114	62	0	216	0	0	0	11	0	41	46	0	297
115	198	181	221	0	0	0	92	51	152	0	0	0
117	18	0	68	0	0	0	14	0	37	70	0	799
118	35	0	140	0	0	0	71	0	178	73	0	410
119	48	0	97	0	0	0	67	0	133	0	0	0
122	36	20	135	0	0	0	36	0	92	57	0	156
216	130	0	187	0	0	0	27	0	49	9	0	176
217	137	20	230	0	0	0	14	0	55	0	0	0
220	43	0	118	0	0	0	48	0	125	168	0	655
221	76	0	135	0	0	0	0	0	0	0	0	0
222	120	120	120	0	0	0	0	0	0	0	0	0
223	117	0	300	0	0	0	57	0	157	0	0	0
224	124	0	300	0	0	0	0	0	0	0	0	0
226	112	0	257	0	0	0	0	0	0	0	0	0
All data	**95**	**0**	**547**	**3**	**0**	**226**	**38**	**0**	**347**	**46**	**0**	**799**

Table A1.3. Nitrogen inputs of mineral N (Min N) and organic N (Org N) applied in the experiments used in the calibration dataset for the marginal N response. Calibration data 2. (Cal2).

Type	Min N spríng			Min N autumn			Org N all year			N fixation		
	Mean	Min	Max	Mean	Min	Max	Mean	Min	Max	Mean	Min	Max
Exp. no	Kg N ha^{-1} $year^{-1}$											
103	117	0	495	13	0	235	11	0	636	26	0	186
221	76	0	135	0	0	0	0	0	0	0	0	0
224	122	0	300	0	0	0	0	0	0	0	0	0
226	119	0	303	0	0	0	0	0	0	0	0	0
All data	115	0	495	5	0	235	4	0	636	10	0	186

Table A1.4. Nitrogen inputs of mineral N (Min N) and organic N (Org N) used the different experiments used in the validation dataset (Val).

Type	Min N spríng			Min N autumn			Org N all year			N fixation		
	Mean	Min	Max	Mean	Min	Max	Mean	Min	Max	Mean	Min	Max
Exp. no	Kg N ha^{-1} $year^{-1}$											
117	72	0	491	0	0	0	6	0	44	46	0	416
224	200	100	300	0	0	0	0	0	0	0	0	0
225	195	0	499	0	0	0	0	0	0	0	0	0
226	127	0	303	0	0	0	0	0	0	0	0	0
Grand Total	82	0	499	0	0	0	5	0	44	40	0	416

11 Appendix 2 LOOP data

LOOP (Landovervågning) is the Danish Agricultural Monitoring Programme on nitrate leaching from agricultural soils. The programme was established during the winter 1989/90 based on the Action Plan for the Aquatic Environment passed by the Danish Parliament (Grant et al., 2011). The monitoring is carried out in six small agricultural catchments, which have been chosen to represent the main soil types and the variation in livestock density, crops and climatic conditions found in Denmark. The monitoring encompasses direct measurements of nutrient content in soil water in five of the six catchments (Figure 2.1). Hence, measurements are also performed in drainage water, upper groundwater and stream water. Information of crops and cover crops, the amount of applied chemical fertilizer and manure, dates of tillage and ploughing are collected annually at field level by interviews.

The catchments have different soil types ranging from USDA textural classes: sand (S), loamy sand (LS) and sandy loam (SL) (Table 2.1). Land use in the catchments is dominated by agriculture (70-98%) and forest (0-30%).

11.1 Soil water extraction

Soil water are collected from 10 suctions cups in each field installed in a V-shape-pattern. The description of materials and installation is given in Rasmussen (1996). The suction cups are installed below the root zone and at slightly different depth according to local soil texture, 96-122 cm below soil surface (Table A2.1).

Table A2.1. Approximate depth for suction cups for soil water extraction.

		Depth of installation ditch		App. total depth
LOOP	**Stnr**	**(m)**	**(cm)**	**(cm below surface)**
1	101-105	0.7-0.8	75	96
2	201-202	0.6-0-7	65	107
2	203-206	0.8	80	101
3	301-304	0.7-0.8	75	117
4	401-406	0.8	80	122
6	601-608	0.8	80	101

Soil water is extracted from the suction cups with a continuous tension system in which vacuum of 0.7 bar is applied immediately after the previous sampling, and the sampler is left a week with vacuum until next sampling. Advantage and disadvantages between the continuous and sudden tension system is described in a review of methods for in situ soil water extraction (Weihermüller et al., 2007). During the leaching season, weekly water samples from the 10 suction cups were pooled to one sample that was analysed for nitrate, total N and ammonium. At LOOP 6 soil water samplings were done all weeks in a year as this areas have high precipitation and some leaching in the summer as well. The chemical analyses were performed by certified laboratories in accordance with the EU directive concerning technical specifications for chemical analysis and monitoring of water status (EU, 2009). At the soil water stations, the groundwater table was measured in piezometers. The groundwater level were measured weekly in the runoff period and monthly in periods with no percolation. In the set-up of the lower boundary of the Daisy model used for calculating percolation, the Daisy parameters for drain depth, aquitard etc. was calibrated so the Daisy modelled groundwater table meet the measured values.

11.2 Leaching and percolation

Nitrate leaching was calculated by using a simple multiplication method, as sum of percolation between two sampling dates are multiplied with the measured nitrate concentration for the same sampling week. The amount of leached nitrogen (*L*, kg N/ha) between date 1 and date n was calculated as:

$$L = \sum_{i=1}^{n} Ci * Di \qquad (1)$$

Where C_i is the nitrate concentration (mg NO_3-N/L^{-1}) in the extracted soil water at date I, and D_i is the amount of percolation (L/m^2) during the two sampling dates (i, i+1). A flow weighted N concentration was calculated by dividing yearly N leaching with the percolation.

Percolation was calculated using the root zone model DAISY, which is a one-dimensional soil-plant-atmosphere model designed to simulate the crop production as well as the water and nitrogen balance in the agro-ecosystems (Hansen et al., 1991a; Abrahamsen and Hansen, 2000). Soil water dynamics include water flow described by the Richards equation in the soil matrix, uptake and evapo-transpiration by plants. The model calculates the water balance on a daily step using data for daily values of precipitation, air temperature and global radiation and prepared by the Danish Meteorological Institute. The data are based on interpolations of measured precipitation from local stations to a 10×10 km grid and 20×20 km grid for temperature and global radiation, respectively (Scharling, 2012). The precipitation data is corrected on a daily basis for effect of wind and wetting according to guidelines from the Danish Meteorological Institute (Refsgaard et al., 2011). If the catchment is represented in more than one 10×10 km grid a mean of two grids are used.

At suction cup installation, a soil profile was excavated next to each nest to characterize horizons, and the texture, density, carbon and nitrogen content, pH and water retention of each horizon down to the depth of the suction cups was measured. Furthermore, 258 soil samples at 100 cm^3 were taken to investigate soil water retention, which were used to fit the parameters n, α, and unsaturated hydraulic conductivity defined by van Genuchten (van Genuchten, 1980). Saturated hydraulic conductivity and the parameter l are defined from the texture and bulk density of the soil according to the European pedo-transfer function HYPRES (Wösten et al., 1999).

The lower boundary of the root zone is defined by the level of the groundwater. There are four different methods to simulate the groundwater level: i) Free drainage, with deep groundwater level, ii) Pipe, where the groundwater level is modelled with an impermeable layer beneath the pipes and the groundwater level is defined by the pipe parameters, iii) Fixed groundwater level, and iv) File with measured groundwater level is input to the simulation. For crop initialization and parameterization, we used standards described for crops and Danish soil types in Styczen et al. (2006).

The soil water stations in the five catchments represent very different groundwater conditions as the loamy dominated Højvads Rende and Lillebæk have relatively large areas with tile drain. About half of the sandy dominated Odderbæk has deep groundwater and the other half have high groundwater level drained by title drains. The loamy Horndrup Bæk does not have any title drains as this catchment have a high topographic gradient, but to model the level of groundwater for those sites we used the pipe set-up in the model (Table A2.1). In the Bolbro Bæk catchment, the groundwater level in some areas is only 1.5–2 m below soil surface. According to the very different conditions, the groundwater is handled specifically for each soil water station (Table A2.2).

Table A2.2. Method for simulation of groundwater level at 28 soil water stations placed the five catchments.

	Højvads Rende	**Odderbæk**	**Horndrup Bæk**	**Lillebæk**	**Bolbro Bæk**
Pipe	4 stations		4 stations	6 stations	
Pipe fixed deep		3 stations			
Groundwater table		3 stations			8 stations

11.3 Crop cover and consumption of fertilizer in LOOP

For each field hosting a soil water station the various crops and cover crops as well as the application of chemical fertilizer and manure data are based on an interview with the farmer.

Table A2.3. Average, minimum and maximum nitrate leaching measured and predicted by NLES5 for different combinations of main crop and winter cover from the LOOP catchments.

			Meas-ured	NLES5	Measured		NLES5	
Main crop	**Winter cover**	**obs**	**mean**	**mean**	**min**	**max**	**min**	**max**
Forage grass and grass-clover	Bare soil after grass ploughed in the previous spring	2	27	31	24	29	22	39
Forage grass and grass-clover	Grass, Clover	63	57	60	1	301	7	141
Forage grass and grass-clover	Winter cereal after grass	9	114	132	6	315	25	227
Grass for seed	Bare soil after grass ploughed in the previous spring	4	23	20	8	29	12	32
Grass for seed	First year undersown grass (ley), Catch crops	3	19	7	4	42	5	10
Grass for seed	Grass, Clover	11	21	24	3	50	10	73
Grass for seed	Winter cereal after grass	4	40	59	14	60	52	73
Legume crops, cere-als for green cut, crops with under-sown grass/clover	Bare soil, stubble	2	129	79	118	140	50	108
Legume crops, cere-als for green cut, crops with under-sown grass/clover	First year undersown grass (ley), Catch crops	21	60	58	18	197	29	127
Legume crops, cere-als for green cut, crops with under-sown grass/clover	Winter cereal	11	85	66	3	185	4	125
Maize after ploughed grass/grass-clover	Bare soil with autumn till-age	3	317	224	207	374	199	254
Maize after ploughed grass/grass-clover	Grass, Clover	1	107	172	107	107	172	172
Oil seed rape	Bare soil with autumn till-age	1	151	73	151	151	73	73
Oil seed rape	Bare soil, stubble	1	152	97	152	152	97	97
Oil seed rape	Winter cereal	24	65	78	16	163	33	179
Set aside (green fal-low)	Bare soil, stubble	4	31	53	13	42	44	68
Set aside (green fal-low)	First year undersown grass (ley), Catch crops	13	33	24	6	103	11	33
Set aside (green fal-low)	Grass, Clover	1	23	26	23	23	26	26
Set aside (green fal-low)	Winter cereal	4	46	42	33	66	23	68
Silage maize	Bare soil with autumn till-age	55	104	106	12	348	48	212
Silage maize	First year undersown grass (ley), Catch crops	3	141	75	77	254	42	106
Silage maize	Winter cereal	3	99	93	36	169	59	125
Spring cereal	Bare soil with autumn till-age	1	55	159	55	55	159	159
Spring cereal	Bare soil, stubble	37	64	55	7	261	12	160
Spring cereal	First year undersown grass (ley), Catch crops	57	56	54	8	218	10	204

Spring cereal	Grass, Clover	9	53	47	6	143	19	107
Spring cereal	Winter cereal	46	52	51	6	229	7	147
Spring crops after ploughed grass/grass-clover	Bare soil, stubble	3	133	87	16	228	18	124
Spring crops after ploughed grass/grass-clover	First year undersown grass (ley), Catch crops	6	106	99	14	216	50	154
Spring crops after ploughed grass/grass-clover	Grass, Clover	1	38	42	38	38	42	42
Spring crops after ploughed grass/grass-clover	Winter cereal	7	114	109	59	178	54	143
Beets	Grass, Clover	43	41	42	6	205	3	156
Beets	Winter cereal	5	9	27	1	20	7	60
Winter cereal	Bare soil with autumn tillage	6	66	75	14	151	25	159
Winter cereal	Bare soil, stubble	63	61	56	9	202	7	134
Winter cereal	First year undersown grass (ley), Catch crops	12	43	38	1	105	8	89
Winter cereal	Grass, Clover	14	33	47	12	123	29	73
Winter cereal	Winter cereal	61	54	59	8	167	13	153
Winter cereal after ploughed grass/ grass-clover	Bare soil with autumn tillage	1	77	69	77	77	69	69
Winter cereal after ploughed grass/ grass-clover	Bare soil, stubble	3	166	110	90	205	75	151
Winter cereal after ploughed grass/ grass-clover	First year undersown grass (ley), Catch crops	5	82	81	17	176	50	134
Winter cereal after ploughed grass/ grass-clover	Grass, Clover	1	0	18	0	0	18	18
Winter cereal after ploughed grass/ grass-clover	Winter cereal	9	81	81	19	178	33	127

12 Appendix 3 Short description of additional experiments

12.1 The Sdr Stenderup and Agervig experiments

The measurement were made in farmer's fields at Sdr. Stenderup (soil clay of 17%) and Agervig (soil clay of 5%). The nitrate leaching data were based on measurements in systematically drained fields with measurement of drainage from pipe drains and regular measurement of nitrate concentration in drainage water (Simmelsgaard, 1998). Crops rotations were decided by the farmers. Results from 1976 to 1988 were used here.

12.2 The Broadbalk/Rothamsted experiment (Goulding et al. 2000)

In the Broadbalk continuous wheat experiment variable N applications were used continuously since about 1850. Goulding et al. (2000) presented leaching data from plots with continuous wheat for the period 1990-98. The plots received variable N rates from 0 to 288 kg N/ha. The nitrate leaching from the plots is calculated by combining nitrate concentrations measured in drains and in suction cups in the same plots and by assuming that 20% of drainage goes to drains and 80% to groundwater (suctions cups). The study showed high variation in nitrate leaching between years and very high marginal leaching in one out of the nine years. The soil is a clay loam with 18-27% clay.

12.3 The Askov lysimeter experiment (Kjellerup and Kofoed, 1983)

An experiment was established with 6 different N rates (0 to 2 times normal rate) continuously applied to the same lysimeters at Askov over 8 growing seasons (Kjellerup and Kofoed, 1983). The lysimeters were cylindrical with a diameter of 1.03 m and a depth of 1.5 m. The soil is sandy loam (17% clay) and a rotation of different crops (Table A.3.1) was used over the 8 year period. The precipitation is high for Danish conditions with an average rainfall of 927 mm over the experimental period. Nitrate leaching was calculated based on measured nitrate concentration and drainage from lysimeters. In the years with red fescue half of the N rate was applied in the previous autumn. The soil around the lysimeters was unplanted, which gave less shade at the edge and thus better plant growth, especially at high N rates. On the other hand, lysimeters are expected to better mimic leaching conditions in drained soils than suction cups and the amount of drainage water can be measured directly.

Table A.3.1. Crop rotation and standard N rates used in a lysimeter experiment at Askov where different levels of mineral fertiliser N were applied repeatedly over the period 1974-1981 (Kjellerup and Kofoed, 1983).

Year	Crop	N rate, kg N/ha
1974	Spring barley	110
1975	Spring barley	110
1976	Spring oilseed rape	150
1977	Winter wheat	150
1978	Spring barley	110
1979	Red fescue	110
1980	Red fescue	110
1981	Winter wheat	150

12.4 The Skara experiment (Delin and Stenberg, 2014)

Nitrate leaching was measured in bi-annual trials started in each of 3 years (2007, 2008, 2009) in a field in south-west Sweden on a loamy sand soil (14% clay) (Delin and Stenberg, 2014). Nitrate leaching was calculated from nitrate concentrations measured in suction cups placed at 80 cm depth and calculated drainage. In the first year with variable N application and leaching measurement, the crop was a spring oats. The following crops were winter wheat (2008 and 2010) or spring barley (2009) receiving a similar N rate in all plots. This experiment does not include repeated variable N applications and only a 1-year effect of N application is measured.

13 Appendix 4 Marginal N response parameters calculated for different experiments

Table A4.1. Estimated parameters in exponential functions used to estimated N leaching in response to different N rates in response field trials, and correlation of fitted function to measurements.

Trial	Year	Soils type	Main crop	Winter crop	Parameters in exp. function		Correla-tion
		JB	Main	Win	α	β	R^2
Guldborg	2015	6	WW	WW	6.5	0.005	0.97
Guldborg	2016	6	WW	WW	5.0	0.002	0.57
Ytteborg	2015	1	WW	WW	52.8	0.002	0.69
Ytteborg	2016	1	WW	WW	15.4	0.004	0.86
Jyderup	2015	4	WW	WW	35.8	0.003	0.96
Jyderup	2016	4	WW	WW	47.3	-0.002	0.66
Flakkebjerg	2016	6	WW	WW	15.9	0.003	0.76
Flakkebjerg	2017	6	WW	WW	15.8	0.007	0.99
Flakkebjerg*	2016	6	WW	WW	2.6	0.004	0.58
Flakkebjerg*	2017	6	WW	WW	23.1	0.005	0.84
Flakkebjerg	2016	6	SB	CC	2.8	0.003	0.95
Flakkebjerg	2017	6	SB	CC	3.3	0.010	0.93
Flakkebjerg	2016	6	SB	BA	26.5	0.000	0.09
Flakkebjerg	2017	6	SB	BA	43.0	0.006	1.00
Flakkebjerg	2016	6	SB	TI	7.3	0.004	0.84
Flakkebjerg	2017	6	SB	TI	25.4	0.008	1.00
Foulum	2016	6	WR	WR	18.2	0.003	0.69
Foulum	2017	6	WR	WR	16.2	0.007	0.99
Foulum*	2016	6	WR	WR	3.7	0.008	0.82
Foulum*	2017	6	WR	WR	15.2	0.002	0.85
Foulum	2016	6	SB	CC	7.2	0.005	0.45
Foulum	2017	6	SB	CC	8.8	0.012	0.84
Foulum	2016	6	SB	BA	76.9	-0.001	0.85
Foulum	2017	6	SB	BA	57.1	0.003	1.00
Foulum	2016	6	SB	TI	8.8	0.003	1.00
Foulum	2017	6	SB	TI	20.4	0.007	0.96
Sdr. Stenderup	1976	7	SR	WW	10.7	0.008	0.98
Sdr. Stenderup	1977	7	WW	BA	30.5	0.004	0.99
Sdr. Stenderup	1978	7	SB	GR	13.9	0.007	0.99
Sdr. Stenderup	1979	7	Seed GR	Seed GR	9.4	0.008	0.99
Sdr. Stenderup	1980	7	Seed GR	WW	15.0	0.013	0.68
Sdr. Stenderup	1981	7	WW	BA	12.4	0.007	0.93
Sdr. Stenderup	1982	7	SB	BA	50.0	0.001	0.63
Sdr. Stenderup	1983	7	FB	BA	56.9	0.002	1.00
Sdr. Stenderup	1984	7	SB	WW	17.0	0.004	0.97

Sdr. Stenderup	1985	7	WW	WW	21.6	0.002	0.80
Sdr. Stenderup	1986	7	WW	WW	54.4	0.003	0.86
Sdr. Stenderup	1987	7	WW	BA	49.3	0.001	0.02
Sdr. Stenderup Mean leach*	**1976-1987**	**7**	**C.Rot**	**C.Rot**	**27.9**	**0.004**	**1.0**
Sdr. Stenderup All leach**	**1976-1987**	**7**	**C.Rot**	**C.Rot**	**27.2**	**0.004**	**1.00**
Agervig	1979	4	CL.GR	CL.GR	20.8	0.003	0.99
Agervig	1980	4	CL.GR	CL.GR	8.6	0.006	0.89
Agervig	1981	4	SB	BA	64.5	0.003	0.96
Agervig	1982	4	FB	FB	22.7	0.005	0.93
Agervig	1983	4	SB	CL.GR	28.6	0.005	1.00
Agervig	1984	4	CL.GR	CL.GR	1.0	0.009	0.98
Agervig	1985	4	SB	GR	4.1	0.029	0.98
Agervig	1986	4	CL.GR	CL.GR	12.5	0.001	0.98
Agervig	1987	4	SB	GR	8.9	0.000	0.97
Agervig	1988	4	FB	FB	25.9	0.004	0.96
Agervig Mean_leach *	**1979-1988**	**4**	**C.Rot**	**C.Rot**	**16.7**	**0.005**	**0.97**
Agervig All leach **	**1979-1988**	**4**	**C.Rot**	**C.Rot**	**30.4**	**0.001**	**0.05**
Skara	2007	6	OAT	WW	42.5	0.001	0.19
Skara	2008	6	OAT	BA	25.6	0.007	0.82
Skara	2009	6	OAT	WW	23.2	0.001	0.39
Lysimeters							
Askov	1974	6	SB	Ba	63.7	0.000	0.06
Askov	1975	6	SB	Ba	50.8	0.003	0.95
Askov	1976	6	SR	WW	17.8	0.003	0.88
Askov	1977	6	WW	Ba	28.9	0.002	0.79
Askov	1978	6	SB GR	GR	3.5	0.015	0.99
Askov	1979	6	GR	GR	0.8	0.013	0.48
Askov	1980	6	GR	WW	16.9	0.002	0.40
Askov	1981	6	WW	Ba	2.1	0.006	0.66
Askov Mean_leach*	**1974-1981**		**C.Rot**	**C.Rot**	**24.3**	**0.003**	**0.8712**
Askov All leach**	**1974-1981**		**C.Rot**	**C.Rot**	**14.2**	**0.004**	**0.09**
Broadbalk	1990	7	WW	WW	2.1	0.008	0.81
Broadbalk	1991	7	WW	WW	2.6	0.015	0.97
Broadbalk	1992	7	WW	WW	12.5	0.002	0.94
Broadbalk	1993	7	WW	WW	14.4	0.005	0.89
Broadbalk	1994	7	WW	WW	21.0	0.005	0.90
Broadbalk	1995	7	WW	WW	17.1	0.005	0.85
Broadbalk	1996	7	WW	WW	2.9	0.006	0.83
Broadbalk	1997	7	WW	WW	1.7	0.006	0.74
Mean_leach*	**1990-1997**	**7**	WW	WW	9.4	0.006	0.98

*Early sowing. SB: Spring barley, WW: Winter wheat, BA: Bare soil; SR: Spring oilseed rape; TI: Volunteers and weeds; CC: Catch crops; WR: Winter rye; CL.GR: Grass-clover; GR: Grass, SB _GR Spring barley with undersown grass, FB Fodder beet, C-rot: Crop rotation.

*Mean Leach: Mean of annual leaching for all years used for parametrization of exponential model (e.g. Experiment with 8 years and 5 N rates gives 1 observations at each of the five N rates total 5 observation).

**All leach: All annual leaching for all years used for parametrization of exponential model (e.g. Experiment with 8 years and 5 N rates gives 8 observations at each of the five N rates total 40 observation)

Table A4.2. Marginal N response from the field trials. For N level parameters of the different field experiments, see Table A4.1.

Trial	Year	Soil type	Main crop	Winter crop	Relative N Levels used to predict marginal N response				Marginal N response (%) at different N levels			
		JB	Main	Win	0%	50%	100%	150%	0%	50%	100%	150%
Guldborg	2015	6	WW	WW	0	100	200	300	3	6	10	17
Guldborg	2016	6	WW	WW	0	100	200	300	1	1	2	2
Ytteborg	2015	1	WW	WW	0	100	200	300	10	12	15	18
Ytteborg	2016	1	WW	WW	0	100	200	300	6	10	14	22
Jyndevad	2015	4	WW	WW	0	100	200	300	12	17	24	34
Jyndevad	2016	4	WW	WW	0	100	200	300	-9	-8	-6	-5
Flakkebjerg	2016	6	WW	WW	0	100	200	300	4	5	7	8
Flakkebjerg	2017	6	WW	WW	0	100	200	300	4	5	7	9
Flakkebjerg	2016	6	WW	WW	0	100	200	300	1	2	3	4
Flakkebjerg	2017	6	WW	WW	0	100	200	300	12	19	31	52
Flakkebjerg	2016	6	SB	CC	0	75	150	225	1	1	2	2
Flakkebjerg	2017	6	SB	CC	0	75	150	225	3	7	16	35
Flakkebjerg	2016	6	SB	BA	0	75	150	225	0	0	0	0
Flakkebjerg	2017	6	SB	BA	0	75	150	225	25	39	59	92
Flakkebjerg	2016	6	SB	TI	0	75	150	225	3	4	6	8
Flakkebjerg	2017	6	SB	TI	0	75	150	225	21	39	73	137
Foulum	2016	6	WR	WR	0	80	160	240	6	8	10	13
Foulum	2017	6	WR	WR	0	80	160	240	11	18	30	50
Foulum	2016	6	WR	WR	0	85	170	255	3	6	11	21
Foulum	2017	6	WR	WR	0	80	160	240	3	3	4	5
Foulum	2016	6	SB	CC	0	70	140	210	3	4	6	8
Foulum	2017	6	SB	CC	0	70	140	210	10	23	51	113
Foulum	2016	6	SB	BA	0	70	140	210	-8	-7	-7	-6
Foulum	2017	6	SB	BA	0	70	140	210	15	19	22	27
Foulum	2016	6	SB	TI	0	70	140	210	3	4	5	6
Foulum	2017	6	SB	TI	0	70	140	210	13	21	34	54
Sdr. Stenderup	1976	7	SR	WW	0	75	150	225	8	15	27	48
Sdr. Stenderup	1977	7	WW	BA	0	75	150	225	13	18	25	35
Sdr. Stenderup	1978	7	SB	GR	0	67.5	135	200	9	14	22	34
Sdr. Stenderup	1979	7	Seed	Seed	0	60	120	180	7	12	18	29

			GR	GR								
Sdr. Stenderup	1980	7	Seed GR	WW	0	27.5	55	82.5	19	28	39	56
Sdr. Stenderup	1981	7	WW	BA	0	80	160	240	8	15	25	43
Sdr. Stenderup	1982	7	SB	BA	0	55	110	165	3	4	4	4
Sdr. Stenderup	1983	7	FB	BA	0	46	92	138	9	10	11	11
Sdr. Stenderup	1984	7	SB	WW	0	69.2	138.4	207.6	6	8	10	14
Sdr. Stenderup	1985	7	WW	WW	0	76.55	153.1	229.65	4	4	5	5
Sdr. Stenderup	1986	7	WW	WW	0	78.5	157	235.5	15	18	22	28
Sdr. Stenderup	1987	7	WW	BA	0	75	150	225	4	5	5	5
Sdr. Stenderup Mean_leach*	**1976-1987**	**7**	**C.Rot**	**C.Rot**	**0**	**65.5**	**131**	**197**	10	13	17	21
Sdr. Stenderup All leach**	**1976-1987**	**7**	**C.Rot**	**C.Rot**	**0**	**65.5**	**131**	**197**	**9**	**12**	**15**	**20**
Mean_M#	**1976-1987**	**7**	**C.Rot**	**C.Rot**	**0**	**65.5**	**131**	**197**	**9**	**12**	**18**	**26**
Median_M##	**1976-1987**	**7**	**C.Rot**	**C.Rot**	**0**	**65.5**	**131**	**197**	**8**	**13**	**20**	**28**
Agervig	1979	4	CL. GR	CL. GR	0	119	238	357	6	9	13	18
Agervig	1980	4	CL. GR	CL. GR	0	150	300	450	5	12	30	72
Agervig	1981	4	SB	BA	0	35	70	105	21	23	26	29
Agervig	1982	4	FB	FB	0	115	230	345	10	17	29	48
Agervig	1983	4	SB	CL. GR	0	60	120	180	15	21	30	41
Agervig	1984	4	CL. GR	CL. GR	0	162.5	325	487.5	1	4	19	86
Agervig	1985	4	SB	GR	0	30	60	90	12	28	67	160
Agervig	1986	4	CL.GR	CL.GR	0	165	330	495	1	1	2	2
Agervig	1987	4	SB	GR	0	35	70	105	0	0	0	0
Agervig	1988	4	FB	FB	0	80	160	240	9	12	16	21
Agervig Mean_leach*	**1979-1988**	**4**	**C.Rot**	**C.Rot**	**0**	**95.5**	**191**	**287**	9	14	23	38
Agervig All leach**	**1979-1988**	**4**	**C.Rot**	**C.Rot**	**0**	**95.5**	**191**	**287**	**4**	**4**	**5**	**5**
Agervig Mean annual#	**1979-1988**	**4**	**C.Rot**	**C.Rot**	**0**	**95.5**	**191**	**287**	**8**	**13**	**23**	**48**
Agervig Median ann##	**1979-1988**	**4**	**C.Rot**	**C.Rot**	**0**	**95.5**	**191**	**287**	**8**	**12**	**23**	**35**
Skara	2007	6	OAT	WW	0	45	90	135	4	4	5	5
Skara	2008	6	OAT	BA	0	45	90	135	18	24	33	45
Skara	2009	6	OAT	WW	0	45	90	135	3	3	3	3
Askov	1974	6	SB	BA	0	55	110	165	0	0	0	0
Askov	1975	6	SB	BA	0	55	110	165	14	16	18	21
Askov	1976	6	SR	WW	0	75	150	225	6	8	10	12
Askov	1977	6	WW	BA	0	75	150	225	7	8	10	12
Askov	1978	6	SB GR	GR	0	55	110	165	5	12	28	64
Askov	1979	6	GR	GR	0	55	110	165	1	2	4	8
Askov	1980	6	GR	WW	0	55	110	165	3	3	3	3

Askov	1981	6	WW	BA	0	75	150	225	1	2	3	4
Askov Mean_leach*	**1974-1981**		**C.Rot**	**C.Rot**	**0**	**47**	**128**	**191**	7	8	10	12
Askov All leach**	**1974-1981**		**C.Rot**	**C.Rot**	**0**	**47**	**128**	**191**	**5**	**6**	**9**	**11**
Mean_M#			**C.Rot**	**C.Rot**	**0**	**47**	**128**	**191**	**6**	**6**	**10**	**15**
Medi. M##			**C.Rot**	**C.Rot**	**0**	**45**	**120**	**180**	**6**	**5**	**7**	**10**
Broadbalk	1990	7	WW	WW	0	100	200	300	4	17	75	328
Broadbalk	1991	7	WW	WW	0	100	200	300	2	4	8	17
Broadbalk	1992	7	WW	WW	0	100	200	300	3	4	5	6
Broadbalk	1993	7	WW	WW	0	100	200	300	7	12	20	32
Broadbalk	1994	7	WW	WW	0	100	200	300	10	15	24	38
Broadbalk	1995	7	WW	WW	0	100	200	300	8	13	21	35
Broadbalk	1996	7	WW	WW	0	100	200	300	2	3	7	13
Broadbalk	1997	7	WW	WW	0	100	200	300	1	2	4	8
Mean_leach*	**1990-1997**	**7**	WW	WW	0	100	200	300	5	10	19	36
All leach**		**7**	**C.Rot**	**C.Rot**	**0**	**100**	**200**	**300**	**4**	**7**	**14**	**26**
Mean_M#		**7**	**C.Rot**	**C.Rot**	**0**	**100**	**200**	**300**	**5**	**9**	**20**	**60**
Median_M##		**7**	**C.Rot**	**C.Rot**	**0**	**100**	**200**	**300**	**3**	**8**	**14**	**25**
All data					0	80	160	240				
Mean_M#					0	75	150	225	7	10	17	32
Median_M##					0	94	188	283	5	8	11	18
Crop specific												
Mean_M#			WW	WW	0	76	152	228	5	8	15	32
Mean_M#			WW	BA	0	66	132	198	7	10	14	20
Mean_M#			SB	BA	0	60	119	179	9	14	21	32

Crops: SB: Spring barley, WW: Winter wheat, BA: Bare soil; SR: Spring oilseed rape; TI: Volunteers and weeds; CC: Catch crops; WR: Winter rye; CL.GR: Grass-clover; GR: Grass, SB _GR Spring barley with undersown grass; FB Fodder beet; C-rot: Crop rotation; GR Seed grass.

*Mean Leach: Mean of annual leaching for all years used for parametrization of exponential model (e.g. Experiment with 8 years and 5 N rates gives 1 observations at each of the five N rates total 5 observation).

**All leach: All annual leaching for all years used for parametrization of exponential model (e.g. Experiment with 8 years and 5 N rates gives 8 observations at each of the five N rates total 40 observation)

#Mean_M: Mean of the annual marginal N leaching.

##Median M: Median of the annual marginal N leaching.

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SUMMARY

A new updated version of the empirical nitrate leaching model NLES is presented in this report. The NLES5 model is designed to estimate nitrate leaching from the root zone of agricultural land in Denmark. The previous version NLES4 was redesigned to better capture effects of nitrogen inputs in fertilizers, manure and biological N fixation as well as crop sequences and autumn and winter vegetation cover.

NLES5 is based on measured nitrate leaching in both experimental fields and farmer fields. 2053 field observations from 1991 to 2017 were used for the calibration of the model. The model is validated using data from independent field measurements (856 observations) and by cross validation. Uncertainty analysis and scenario analysis of both nitrate leaching and marginal nitrate leaching response to increased N application is presented.

The model can estimate average marginal nitrate leaching response to mineral nitrogen application, total nitrate leaching and the effects of a number of field N mitigation measures. Nitrate leaching depends on soil type, crop type and precipitation. The Marginal nitrate leaching was estimated at national scale with a mean of 17%.