Model-based quantification of nitrate-nitrogen leaching considering sources of uncertainty

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„Der Boden entkompliziert, so wie er das Wasser reinigt. […]
Das wirkliche Leben macht einfach.“

(Robert Musil, 1880–1942,
Der Mann ohne Eigenschaften)

Abstract

The European Water Framework Directive has demanded the implementation of key measures in Europe to pursue a good water quality for all water bodies since 2000. The present situation in Germany clearly highlights the need for further actions. Especially more precise determination of nitrate-N losses is still required because of high variations regarding inorganic and/or organic N fertilization, portions of harvest amounts and residues, and associated C and N transformations in soil and plant. The nitrate-N (NO_3-N) leaching in agricultural soils is, thus, the dominating process of an unwanted nitrogen loss, esp. under winter mild, humid climate and artificial drainage. Consequently, the question arose whether or not in-depth, realistic description of all relevant plant and soil-related processes may provide meaningful results on the NO_3-N leaching considering different sources of uncertainties.

In the course of this thesis, (I) the general applicability of the process-based model CoupModel (Jansson and Karlberg, 2010) was investigated at first by means of a baseline scenario in the form of a temporary red clover catch crop (undersown in winter wheat) without considering uncertainties arising from model parameterization. This investigation included beside the manual calibration based on observed water discharge and NO_3-N leaching in an artificial drainage system a comprehensive sensitivity analysis identifying important input parameters regarding N leaching. (II) Within different approaches of automated model optimization, a number of these sensitive parameters were selected to vary between predefined ranges. Both the formal Bayesian approach and the more informal Generalized Likelihood Uncertainty Estimation (GLUE) were tested on mown permanent grassland to evaluate both resulting parameter distribution and the uncertainty of N dynamics in soil. As one result, the GLUE approach was chosen because of its more universal applicability to investigate the impact of input-parameter uncertainties on (III) soil water balance and (IV) NO_3-N leaching under different silage maize cultivations. Furthermore, impact of undersown annual grass on the soil water balance and its efficiency to reduce the NO_3-N leaching under silage maize were evaluated.

The manual calibration of the baseline scenario resulted in plausible NO_3-N leaching, even though significant divergences between measured and modeled N leaching in drainage water were found temporarily for the red clover cultivation in periods with increased mineralization potential. Consideration of variations regarding particular input parameters by means of automated optimization also showed plausible but also highly variable NO_3-N leaching in the seepage water below the rooting zone under permanent grassland mainly determined by the applied N-fertilizer amount. By means of the GLUE approach, comprehensive evaluation of simulated soil water balance and NO_3-N leaching in silage maize cultivations confirmed both only minor water stress in case of bi-cropping with undersown grass and the strong relationship between N leaching and fertilization. General reduction of NO_3-N leaching could not be stated for undersown grass and was only found in and after periods with below-average precipitation and in case of high N fertilization (> 200 kg N ha^{-1} $year^{-1}$). Finally, the combination of uncertainties arising from measurements and model parameterization suggests that common guide values for the NO_3-N leaching are hardly reliable without considering tolerable variations.

Kurzfassung

Die Europäische Wasserrahmen-Richtlinie fordert seit ihrer Einführung im Jahr 2000 eine Umsetzung von Maßnahmen, um eine gute Wasserqualität in allen Wasserkörpern in ganz Europa zu erreichen bzw. sicherzustellen. Die derzeitige Situation in Deutschland zeigt deutlich, dass weitere Maßnahmen notwendig sind. Insbesondere eine genauere Bestimmung der Verluste an Nitrat-Stickstoff wird aufgrund der hohen Schwankungsbreite hinsichtlich mineralischer und/oder organischer Düngung, der Anteile von Erntemasse und -rückständen bzw. der damit verbundenen C- und N-Transformationsprozesse in Boden und Pflanze benötigt. Die Nitratauswaschung unter landwirtschaftlich genutzten Böden ist daher der dominierende Vorgang eines unerwünschten Stickstoffverlustes, insbesondere unter wintermilden, humiden Witterungsbedingungen und in künstlichen Drainagen. Daher stellte sich die Frage, ob eine fundierte, realitätsnahe Beschreibung aller relevanten Prozesse in Pflanze und Boden zu aussagekräftigen Resultaten für die Nitratauswaschung unter Berücksichtigung verschiedener Ursachen für Unsicherheiten führt.

Im Rahmen dieser Doktorarbeit wurde (I) die generelle Anwendbarkeit des prozessbasierten Modells CoupModel (Jansson und Karlberg, 2010) zunächst für ein Basisszenario in Form einer temporären Rotklee-Zwischenfrucht (eingesät in einen Winterweizen-Bestand) ohne die Berücksichtigung von Unsicherheiten hervorgerufen durch die Modellparametrisierung überprüft. Diese Untersuchung beinhaltete neben einer manuellen Kalibrierung gegen gemessenen Abfluss und Nitratauswaschung in einer künstlichen Drainage eine ausführliche Sensitivitätsanalyse zur Identifikation von wichtigen Modellparametern für die Nitratauswaschung. (II) Im Rahmen von verschiedenen Ansätzen zur automatischen Modelloptimierung wurden mehrere dieser sensitiven Parameter ausgewählt, welchen eine gewisse Unsicherheit innerhalb eines vorgegebenen Wertebereichs unterstellt wurde. Sowohl der formelle Bayes'sche Ansatz als auch der informellere Generalized Likelihood Uncertainty Estimation (GLUE) Ansatz wurde danach für ein Dauergrünland unter Schnittnutzung getestet, um die resultierende Parameterverteilung und die Unsicherheit der N-Dynamik im Boden zu bewerten. Basierend darauf wurde der GLUE-Ansatz aufgrund seiner universelleren Anwendbarkeit ausgewählt, um den Einfluss der Parameter-Unsicherheit auf (III) die Wasserbilanz im Boden und (IV) die Nitratauswaschung unter verschiedenen Silomais-Systemen zu untersuchen. Weiterhin sollten der Einfluss einer einjährigen Gras-Untersaat auf die Wasserbilanz im Boden und die Effizienz zur Verminderung der Nitratauswaschung unter Silomais bewertet werden.

Die manuelle Kalibrierung des Basisszenarios lieferte plausible Ergebnisse für die Nitratauswaschung, obwohl signifikante Abweichungen zwischen gemessener und simulierter N-Fracht im Drainagewasser unter der Rotklee-Nutzung in Perioden mit erhöhtem Mineralisierungspotenzial zeitweise auftraten. Die Berücksichtigung der Variabilität von bestimmten Modellparametern mittels einer automatischen Optimierung zeigte ebenfalls eine plausible jedoch stark schwankende Nitratauswaschung im Sickerwasser unterhalb der Hauptwurzelzone unter Grünland, hauptsächlich bestimmt durch die applizierte N-Düngung. Die ausführliche Bewertung der Wasserbilanz und der Nitratauswaschung im Silomaisanbau durch die Verwendung des GLUE-Ansatzes bestätigte sowohl den dominanten Einfluss der N-Düngung auf die auswaschbare N-Fracht als auch einen vernachlässigbaren Wasserstress durch

eine Grass-Untersaat. Eine generelle Reduktion der Nitratauswaschung durch eine Gras-Untersaat konnte jedoch nicht bestätigt, sondern nur in und nach Perioden mit unterdurchschnittlichem Niederschlag und gleichzeitig hoher N-Zufuhr (> 200 kg N ha^{-1} a^{-1}) eindeutig gezeigt werden. Schließlich konnte durch die kombinierte Betrachtung von Unsicherheiten bedingt durch Messungen und Modell-Parametrisierung gezeigt werden, dass allgemein gültige Werte für die Nitratauswaschung kaum anwendbar bzw. übertragbar sind ohne Berücksichtigung einer tolerierbaren Variabilität.

Preface

This thesis consists of the following five papers (Chapters 2–6) in addition to introduction (Chapter 1), detailed discussion (Chapter 7), and conclusions (Chapter 8):

1. **Conrad, Y.**, Fohrer, N., 2009a. Modelling of nitrogen leaching under a complex winter wheat and red clover crop rotation in a drained agricultural field. *Phys. Chem. Earth* **34**, 530–540, http://dx.doi.org/10.1016/j.pce.2008.08.003,
(Impact Factor: 1.477 (2014/15)).
2. **Conrad, Y.**, Fohrer, N., 2009b. Application of the Bayesian calibration methodology for the parameter estimation in CoupModel. *Adv. Geosci.* **21**, 13–24, http://dx.doi.org/10.5194/adgeo-21-13-2009, (Journal Impact: 1.31).
3. **Conrad, Y.**, Fohrer, N., 2009c. A test of CoupModel for assessing the nitrogen leaching in grassland systems with two different fertilization levels. *J. Plant Nutr. Soil Sci.* **172** (6), 745–756, http://dx.doi.org/10.1002/jpln.200800264, (Impact Factor: 1.459 (2014/15)).
4. **Conrad, Y.**, Fohrer, N., 2016. Simulating impacts of silage maize (Zea mays) in monoculture and undersown with annual grass (Lolium perenne L.) on the soil water balance in a sandy-humic soil in Northwest Germany. Agr. Water Manage. **178**, 52–65, http://dx.doi.org/10.1016/j.agwat.2016.09.005, (Impact Factor: 2.286 (2014/15)).
5. **Conrad, Y.**, Fohrer, N., xxx. Modeling the temporal dynamics of nitrate-nitrogen leaching under silage maize (Zea mays) in monoculture and bi-cropping with annual grass on a drained field considering model uncertainties. Submitted to Agric. Water Manage.
(20 September 2016, status: under review).

Contents

Abbreviations

ANOVA	Single factor analysis of variance
$Ca(NH_4NO_3)$, CAN	Calcium-ammonium-nitrate
C:N	Carbon nitrogen ratio
CV	Coefficient of variation
*CV**	Quartile coefficient of variation
Deep	Deep percolation
Drain	Drainage water
DW	Dry weight
E.C.	Electric conductivity
ETa, ETI	(Actual or real) evapotranspiration
ETp	Potential evapotranspiration
Evap	Evaporation
Intercep	Interception
GLUE	Generalized Likelihood Uncertainty Estimation
GSI	Growth Stage Index
LAI	Leaf Area Index
LogLi	LogLikelihood
mbs	Meters below surface
MCMC	Marcov-Chain-Monte-Carlo
NSE	Nash-Sutcliffe (model) efficiency
pF	Measure of soil water tension (pF = lg cm water column)
OF	Objective function
R^2	Coefficient of determination; squared Pearson's correlation
RUE	Radiation use efficiency
SMN	Soil mineral nitrogen
SO_4^{2-}	Sulfate ion
SOC	Soil organic carbon
SOM	Soil organic matter
SON	Soil organic nitrogen
SurfOutflow	Surface water outflow of water
SWP	Seepage-water period
SVAT	Soil-vegetation-atmosphere-transfer
TDR	Time-domain-reflectometry
Transp	Transpiration
R	Ch. 2: resulting term in the water balance equation Ch. 5 and 6: original parameter space of input parameter
*R**	Range reduction of accepted input parameter
P, Prec	Precipitation amount in the water balance equation
VP	Vegetation period

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Chapter 1 Introduction

1.1 Background, motivation and objectives

Nitrogen is an essential major plant nutrient that is often limited in natural ecosystems because of its high demand during plant growth. Therefore, optimum yields and soil fertility can only be maintained by sufficient N fertilization to agricultural land. The synthetic production of mineral-N fertilizer by artificial N fixation to ammonia (Haber and Bosch, 1910) followed by conversion into nitric acid (Ostwald, 1902) has provided the basis for intensified agriculture with increasing yields since the 1950s. Until then, agricultural production was highly dependent on small-scale nutrient cycles usually at farm scale where soil fertility was maintained by symbiotic-N fixation such as of legume plants and frequently applied organic-N fertilizers as farmyard and liquid manure, and guano. This management practice aiming at sustainable humus reproduction accompanied by the ban on synthetic-N fertilizers is applied in organic farming to date. Also as a result of intensified fertilization up to nearly 200 kg N ha^{-1} $year^{-1}$ in the 1970s and 1980s (Graeber et al., 2015), the chemical and biological quality of surface water and surface-near groundwater decreased dramatically because of high nitrate-nitrogen (NO_3-N) and phosphate concentrations until the 1990s (BMU, 2001).

The prevention of persistent and long-term hazards for humans, other organisms, and whole ecosystems by this nutrient surplus gave the reason to define European Directives for nitrate (91/676/EEC; Nitrate Directive, 1991), water management (2000/60/EC; Water Framework Directive (WFD), 2000), and drinking water (98/83/EC; Drinking Water Directive, 1998) to implement strategies for cross-border, sustainable, and ecological water resource management into national legislation. Several laws and regulations were revised regarding the application of N fertilizers in agriculture and the protection of water resources in Germany such as the Fertilizer Act (DüG, 2009; replaced the 1977 Act and was revised in 2015), the accompanied Fertilizer Ordinance (DüV, 2007; replaced the 1996 Act and was revised in 2012) with recommendations for the ‘code of best practice’, the Water Resources Law (WHG, 2009; revised in 2016), and the Drinking Water Ordinance (TrinkwV, 2001; revised version in 2016).

So far, the success of restrictions regarding further N pollution of ecosystems is evident in reduced numbers of highly eutrophic water bodies because of an efficient wastewater treatment for industry and municipalities (BMU, 2001). However, still existing elevated nitrogen amounts especially in agricultural ecosystems show room for improvements (Bodirsky et al., 2014). In Germany, approx. 48% of natural and semi-natural terrestrial ecosystems showed indications of eutrophication; 8% of those were acidified, *e.g.*, showed low pH values, because of alkali leaching (SRU, 2015). Current results demonstrated that the ambitious goals stated by the WFD in 2000 were not achieved until 2015. Intermediate results from 2011 proved ‘good’ (< 50 mg L^{-1} of NO_3^- or < 11.3 mg L^{-1} of NO_3-N according to the Nitrate Directive (1991)) ecological conditions for 75% and 100% of evaluated groundwater and surface-water bodies, respectively (SRU, 2015). The actual target amount of 2.5 mg L^{-1} of NO_3-N according to quality class II for watercourses defined by the LAWA (1998) and the Federal Environmental Agency (UBA) to ensure demands of the WFD (2000) were exceeded by 85% of examined watercourses. Data evaluation also identified negative impacts of agricultural activities on the chemical quality of water bodies resulting in significantly elevated NO_3-N concentrations in regions with high proportion of arable land. Present situation shows several reasons for inadequate target achievement to reduce N pollution by agriculture: measures implementation on voluntary basis (particular activities and guidance for farmers), privileged status of agricultural laws, *e.g.*, Fertilizer Act and Ordinance, against environmental laws (WHG, 2009; BBodSchG, 1998), and low frequency of control and evaluation of measures (SRU, 2015). As result of this non-compliance with the European Directive for nitrate (Nitrate Directive, 1991), the European Commission has taken steps to initiate infringement proceedings against Germany since July 2014 (Press release of the European Commission on April 28, 2016; Sundermann et al., 2016).

As is known that the risk of excessive N losses from agriculture increases with the applied amount of N fertilizer, it would be at best to implement management actions to reduce all emissions at source. Any surplus of N remaining at the end of the vegetation period is likely to increase N losses from fall to early spring. It is necessary to assess the amount of applied N fertilizer dependent on the available mineral-N content in soil to meet the predicted plant demand at various stages of development. Beside adequate strategies for N fertilization, low-loss techniques, and blocking periods for the disposal of organic fertilizers, meaningful and unbiased nutrient accounting on the basis of provable operating data must be determined as minimum standard for agricultural companies, *i.e.*, as so-called gross nutrient balance according to the WFD (2000) and the Nitrate Directive (1991) (Bach et al., 2016; Taube, 2014). Key measures are predominantly further reduction of nutrient surplus in agricultural practice, improved guidance for farmers, and the limiting of uncertainties based on scientific evaluations (UBA, 2009). Following practices are qualified to achieve the aim of reduced N losses that may go in part beyond the currently accepted minimum requirements according to the ‘code of best practice’ (in its current version from 2009): i) further reduction of recommended amounts of N fertilizers, ii) increased cultivation of undersown/catch crops, iii) all-season canopy cover and conserving soil tillage, iv) low-loss application of organic fertilizers, v) establishment of riparian strips, vi) promotion of extensive agriculture such as ecological farming, and vii) improved agricultural guidance (SRU, 2015). Although, the structural shift in agriculture is present in Germany and may support some of these recommended measures, significant conflicts of aims have appeared particularly with regard to the production of biogas and the corresponding expansion of silage maize cultivation (Destatis, 2015; UBA, 2013). The noticeable competition for land between conventional food production and high-yield energy production is likely to continue in the future accompanied by cautious acceptance regarding demands for reduced nutrient losses in conventional intensive agriculture (SRU, 2015).

Versatile and expanded crop rotations with undersown and catch crops such as sole grass or clover-grass in silage maize cultivation are recommended in arable farming as well as sustainable use of permanent grassland as pasture or mown meadow. Despite divergent results regarding the efficiency of catch crops, potential benefits of bi-cropping are evident for reduced soil erosion and increased soil organic matter (UBA, 2011) but show also increased variability regarding nitrogen losses highly dependent on site-specific climate, soil, and management conditions (Bakhsh and Kanwar, 2011; Büchter et al., 2003; Justes et al., 2012; Peratoner et al., 2013; Tauchnitz et al., 2015). As a consequence of plowing and N fertilization, processes such as decomposition and mineralization are usually accelerated. High soil mineral-N contents (NO_3-N and ammonium (NH_4-N)) induce higher N uptake by plants at best, *e.g.*, when the N demand is at maximum. But elevated NO_3-N mobilization can occur periodically at worst, for instance, in times with above-average precipitation, associated elevated seepage-water amount, and low soil temperatures (Hatch et al., 2002). Although nutrient transformations increase with higher temperatures, the risk of NO_3-N leaching in soil is usually low during the vegetation period due to sufficient plant-N demand and in case of adjusted N fertilization. The potential risk for NO_3-N leaching is often elevated from late fall to early spring in Northern Germany because of mild, wet Atlantic climate conditions, especially for bare soil without immobilized N in soil organic matter or hibernating catch crops (Büchter et al., 2003; Loges et al., 2008; Wachendorf et al., 2006a). Therefore, all-season fodder production may support both the formation of soil organic matter in humus and the reduction of NO_3-N leaching as long as short-term yield maximization is not a priority matter and supplied N fertilizer is thus balanced (Jarvis, 2011).

In comparison to that, little attention was paid to measures limiting NO_3-N leaching by drainage systems despite their high relevance in the Northern lowland (Pfannerstill et al., 2012). Main concerns of drainage systems are usually reduced water and nutrient retention in soil, increasing flooding events, and an accelerated transport of NO_3-N in the seepage water from unsaturated soil into surface water or rather groundwater later on. Furthermore, mineralization processes such as nitrification can be, thus, increased compared with limited denitrification potential because of increased ventilation and limited water-filled pore space of subsoils. Compared with efficient drainage, poor or controlled drainage systems may limit the NO_3-N leaching in well-drained soil but can pose a risk of elevated N_2O amounts because of enhanced and incomplete denitrification (Pomowski et al., 2011; Stevenson et al., 2011; Easton and Lassiter, 2013) especially in presence of efficient electron acceptors like NO_3^- ions to prevent the reduction of N_2O to N_2 (Eickenscheidt et al., 2014; Matschullat et al., 2013). Significant relationship between nitrate concentrations and runoff was also stated at small-scale level, *e.g.*, in sub-surface drainage pipes and open trenches (LUMV, 2012).

1.2 Quantification of NO_3-N leaching considering sources of uncertainty

The quantitative determination of N losses by leaching beside denitrification is still difficult because of complex soil processes regarding the N cycling (Butterbach-Bahl and Gundersen, 2011). This quantification is often implemented on the basis of estimations and extrapolations considering site-specific factors as observed mineral-N contents and calculated seepage-water amounts in soil (Hatch et al., 2002). Results obtained usually correspond to the potential NO_3-N leaching that is often modestly comparable with highly variable NO_3-N leaching under field conditions because transformation of organically bound N in soil organic matter is considered inadequately (Jarvis, 2011). As a result of complex N dynamics in agricultural systems, the demand for quantification tools focused on N processes in soil has increased and resulted in numerous balancing and modeling approaches. In the course of comprehensive consideration of relevant factors regarding climate, soil, crop, and management including important below- and above-ground processes, the problem of increasing uncertainty arises necessarily.

Both differentiation and relationship between variability (heterogeneity) and true uncertainty (lack of precise knowledge) in measured data and modeling is needed as well as the relationship between both sources of variation in data and modeling has to be evaluated. Measurement uncertainties caused by natural variability and measurement errors were not discussed in this thesis in detail but observed mean values were often shown within their standard deviation when discussed in particular chapters. One source of model uncertainty is usually the estimation of input-parameter values beside general problems regarding formulating and implementing appropriate algorithms, *i.e.*, the structural uncertainty, as well as the calculation and interpretation of model results. The first mentioned uncertainty of input parameters can be quantified with variance propagation techniques. Beside simple 'rule-of-thumb' approaches, complex stochastic models were determined by the precision of input variables and the accuracy, in which the model algorithms were able to describe the relevant natural processes (WHO, 1995). Based on the Bayesian theorem of conditional likelihoods and assuming that model parameterization was the only source of uncertainty, a simple rule was followed to update the prior likelihood of a particular hypothesis when new data became available. In statistics, the Marcov-Chain-Monte-Carlo (MCMC) method is often applied to obtain a sequence of random samples from a multi-dimensional likelihood distribution, especially when the number of dimensions or input parameters in case of model applications is high. The result of sampling from the posterior likelihood after a number of steps is the so-called Marcov chain containing the desired stationary distribution computed using the likelihood and the prior distribution. The convergence time of the Marcov chain to reach the stationary distribution is highly dependent on the starting point also defining running time of the algorithm (Mossel and Vigoda, 2006). To avoid problems as parameter insensitivity and local minima from single starting point optimization in the parameter space, the development of population-based search algorithms was stimulated to locate the global optimum using different starting points concurrently. Regarding optimization methods to quantify parameter uncertainties based on Beven and Binley (1992), consideration of individual error sources in input data and model structure led to advocate informal statistical approaches using the Generalized Likelihood Uncertainty Estimation (GLUE) by Beven and Binley (1992) (Beven, 2006, 2009; Beven and Freer, 2001; Beven et al., 2008). The inability to reproduce how natural processes work exactly in a mathematical model was the underlying motivation of the GLUE resulting in several equally acceptable or behavioral models that represented observations in a satisfactory way. The GLUE approach originated from the idea of an informal likelihood measure avoiding the elimination of parameter space to find a set of behavioral representations being acceptable consistent with the non-error-free observations (Marmy et al., 2016; Sadegh and Vrugt, 2013). Until now, the philosophy of the GLUE approach is still discussed because of rejecting the formal Bayesian paradigm, lacking appropriate mathematical basis and being subjective. Hence, the GLUE has been applied widespread for uncertainty assessment in hydrology (Wu et al., 2016) and soil sciences, *e.g.*, crop yields, soil organic carbon (Wang et al., 2005), and greenhouse gas emissions (Gärdenäs et al., 2011; Metzger et al., 2015). Blasone et al. (2008) noted that the GLUE can predict the uncertainty within the context of Monte Carlo analysis in combination with Bayesian estimation and uncertainty propagation despite existing problems for high-dimensional parameter estimations and the corresponding computational time. Altogether, GLUE applications are still popular because of several reasons: conceptual simplicity, ease of implementation and use as well as the handling of different error structures without major changes to the method itself (Blasone et al., 2008; Sadegh and Vrugt, 2013).

The complex soil-vegetation-atmosphere-transfer (SVAT) model CoupModel (Jansson and Karlberg, 2010) is applicable to simulate coupled heat, water, carbon, and nitrogen dynamics in unsaturated soil and vegetation. A brief, conceptual overview of the model is shown in *Fig. 1.1*. The parameterization of multi-species cropping systems is possible within the CoupModel structure to investigate concepts of competition and above- and below-ground interactions between crop/weed and crop/crop. Furthermore, validity and robustness of CoupModel have been already evaluated by stochastic optimization approaches, *e.g.*, Bayesian calibration and GLUE, for different sites and data sets (Conrad and Fohrer, 2009b,c; He, 2015; Khoshkhoo et al., 2015; Klemedtsson et al., 2008; Marmy et al., 2016; Nylinder et al., 2011; Wu et al., 2016; Yang et al., 2016).

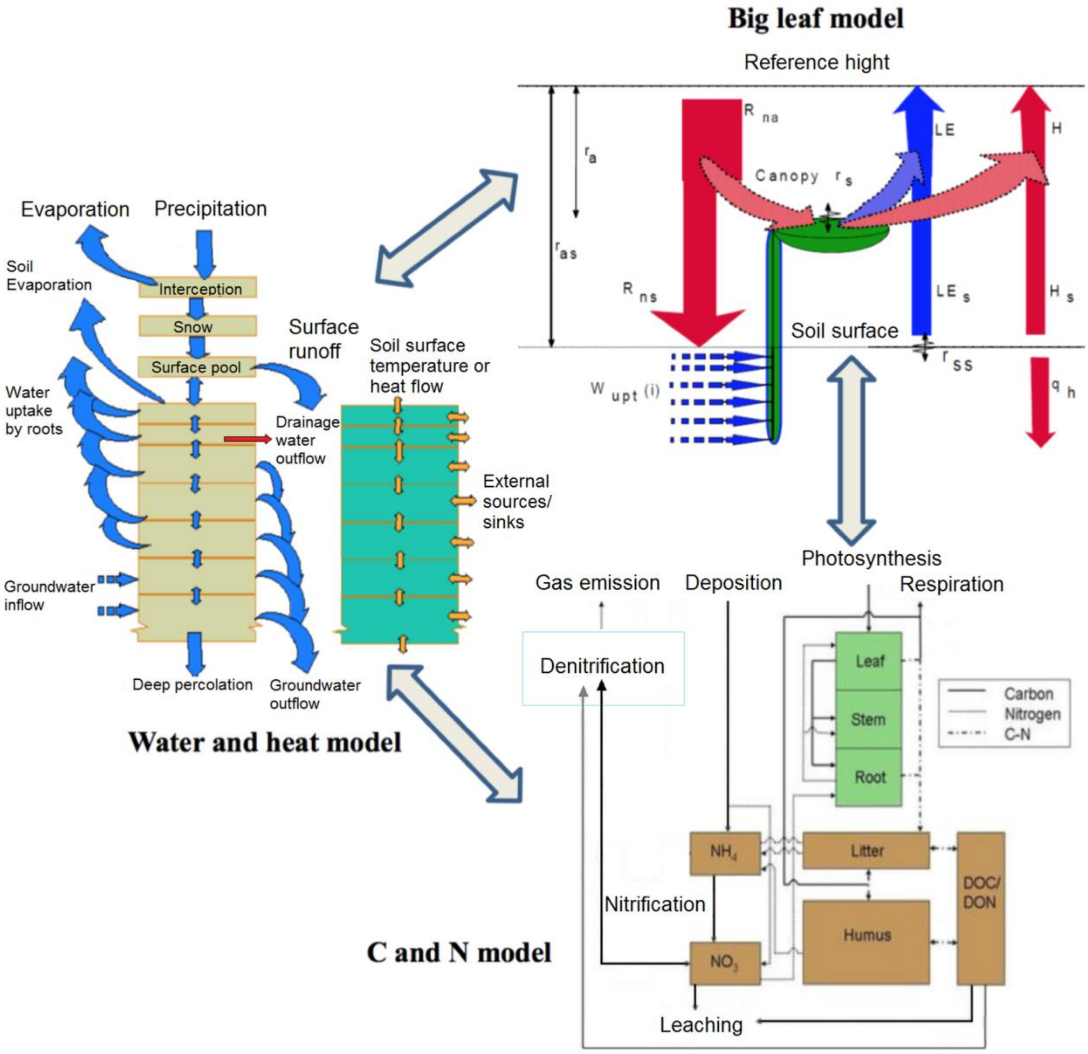

Fig. 1.1: Brief conceptual representation of the CoupModel (adjusted from He (2015)).

1.3 Site descriptions and the review of existing data

The natural region of Northern Germany in the particular case of Schleswig-Holstein located between North Sea and Baltic Sea is characterized by the last ice age (Pleistocene from 2.59 million to 10,000 years B.C.) resulting in different geographic sub-regions. Main features are the relatively flat terrain interrupted by slightly hills in the Eastern sub-region and shallow groundwater levels caused by less permeable subsoils and sufficient precipitation between 800 mm year^{-1} (East part) and 1000 mm year^{-1} (West part). Therefore, artificial subsurface drainage is needed to avoid long-term flooding of agricultural area especially for grassland that is usually located in land depressions. Arable land is predominantly found in the Eastern sub-region where small-scale subsurface drainage is often used on demand in the hilly landscape.

1.3.1 Lindhof

The experimental farm ‘Lindhof’ of the Kiel University is located in the northern part of the peninsula ‘Dänischer Wohld’ at the south coast of the Bay of Eckernförde. The investigation area is part of the young moraine landscape of Schleswig-Holstein characterized by slopes and knolls, land depressions with bogs and colluvia, coastal plains, and cliffed headlands. Subglacial meltwater deposits accompanied by partially small-scale substrate changes from fine, middle, and coarse sands to clay bands but also gravels formed various landforms in the ‘Lindhof’ area: hills, terraces, and plates (Russok and Bork, 2006). Therefore, upper soils at the ‘Lindhof’ area can be described as sandy loam and loamy sand (Ad-hoc-Boden, 2005; Ziogas, 1995) resulting in ideal growing conditions for crops because of evenly distributed annual precipitation of approx. 800 mm and mean daily temperature of 8.7 °C. Farm management is focused on organic crops and extensive beef, pig, and chicken/egg production on approx. 150 ha of arable land. The conversion from conventional to organic farming was initialized in 1994 where an area of 50 ha was cultivated according to guidelines of BIOLAND and NATURLAND as two important German organic growers’ organizations. The second step of conversion started in 1997 and was finished completely in 2001. Important crops beside cereals (oat, winter spelt, and wheat) and potatoes are N fixing species such as red clover and grain legumes (*e.g.*, narrowleaf lupin) cultivated partially in grass mixtures as temporary grassland or catch crops to avoid soil erosion and nutrient losses during winter until following spring crops were sown (Loges et al., 2006).

During conversion from conventional to organic farming (1994–2001) different crop rotations were implemented at particular fields focused on the evaluation of productivity, N balance, and NO_3-N leaching (project ‘CONBALE’). Beside the conventional crop rotation consisting of oilseed rape, winter wheat, and sugar beet with an average fertilizer-N input of 186 kg N ha^{-1}, two organic crop rotations with 50% and 33% legumes in a rotation consisting of oat, grain legumes, grass/clover, and winter rye were investigated. The NO_3-N leaching was also determined by the product of seepage-water amount and observed NO_3-N concentrations in the soil leachate collected by 300 ceramic suction cups on the whole farm area. The sampling took place on fields with different crop rotations from 2001 to 2004 and showed variable effects of bi-cropping white clover and winter wheat as well as different catch crops on reduced N leaching below the rooting zone (Neumann, 2005; Loges et al., 2008). The volume of seepage water was calculated according to the climatic water balance. Comparison between conventional and organic farming showed that NO_3-N leaching below the rooting zone did not differ significantly with N losses between 20.1 kg N ha^{-1} (33% legumes) and 23.6 kg N ha^{-1} (conventional) in spite of significantly higher N input and N surplus in conventional systems (Loges et al., 2006). The relatively high NO_3-N leaching in organic crop rotations possibly originated predominantly from mineralized grass/clover mulch independent on the portion of legumes. Therefore, harvest of grass/clover herbage to feed animals is often applied to reduce NO_3-N leaching by almost 40% from grass/clover mixtures. In contrast, intercropping winter cereals with fall-sown catch crops, *e.g.*, oat or forage rape, seemed to be more efficient to reduce the NO_3-N leaching despite its increased risk in winter mild climate (Loges et al., 2008).

Nutrient losses by artificial drainage on demand were monitored at two fields from 1998 to 2004, and drainage pipes were rerouted through measuring stations to gauge discharge and analyze several parameters at a daily time step such as pH value, E.C., NO_3-N, and SO_4^{2-} concentrations. Results obtained from these observations confirmed that NO_3-N leaching was close connected to N supply and crop growth. Perennial plants, undersown, and catch crops such as grass/clover leys can reduce the N load considerably compared with bare soil when biomass was removed for harvest before winter. Otherwise, mulching of grass/clover leys usually leads to elevated NO_3-N concentrations and leaching especially during wet periods in fall and early spring (Deunert and Fohrer, 2006).

1.3.2 Karkendamm

The experimental farm ‘Karkendamm’ of the Kiel University is located in central Schleswig-Holstein near the receiving water ‘Osterau’ of the tributary ‘Bramau’ in the river ‘Stör’ basin that drains in southwestern direction into the river ‘Elbe’. The investigation area is part of the so-called ‘Geest’ area and represents a glacial geomorphological landscape unit in Northern Germany, the Netherlands, and Denmark formed during the glacial melting behind the moraine ridge. The ‘Geest’ area is a plateau-shaped region between young moraine and lower ‘Marsch’ land characterized by sandy and mostly nutrient-poor soils, *e.g.*, podzolic soil (or Podzol). The investigated area is relatively flat and influenced by near-surface groundwater usually in winter because of the nearby, small river ‘Osterau’. Upper soil horizons in such land depressions are often humus rich because of reduced mineralization but are also very sandy (> 90%) resulting in long-term use as grassland. A period of agricultural intensification started in the 1950s resulting in large-scale melioration of previously unfavorable agricultural land. One measure of this land improvement was the deep-plowing of grassland to enhance both hydraulic conductivity and distribution of organic matter in the whole soil profile. Plowed Podzols show slanted soil layers to the maximum depth of plowing (here 80 cm; variation of 60–250 cm).

The experimental farm ‘Karkendamm’ is focused on conventional milk and forage production at permanent grassland and arable land. Between 1997 and 2003 research at the farm was focused on nitrogen use efficiency in dairy farms on well-drained sandy soils with special attention to NO_3-N leaching under permanent grassland and silage maize cultivations (‘N-project Karkendamm’).

As already mentioned for the 'Lindhof' site, NO_3-N leaching was determined by observed NO_3-N concentrations collected by ceramic suction cups (Mullit, length of 50 mm, Ø 20 mm, maximum pore size of 1 µm, maximum permanent negative pressure of 400 hPa) installed in 50–60 cm of depth during five seepage-water periods from November 1997 to March 2002 (Büchter et al., 2002). According to recommendations of UMS (2008), ceramic suction cups installed in textured soil such as coarse and medium sand often collect soil water only partially because of sudden change of pore size at the interface between sand particles and ceramic cup. The defined permanent negative pressure determines the accessibility of defined soil pores, and the applied pressure of −400 hPa might be applicable for sandy soils to collect only free-draining soil water. Otherwise the applied permanent water tension can affect partially weakly bound retained soil water in narrow coarse pores, and a maximum pressure of −60 hPa is thus recommended (UMS, 2008). The volume of drainage water was also calculated according to the climatic water balance (Büchter, 2003). Experiments were established on permanent grassland consisting of white clover and grass species to compare different grassland management systems regarding yield, quality, and N losses via leaching and denitrification (Wachendorf et al., 2004) as well as under different silage maize cultivations (Wachendorf et al., 2006a,b). The following important grassland management systems were tested: cutting (repeated harvest and removal of herbage), grazing, and two mixed treatments of cutting and grazing. All systems included various levels of mineral-N fertilizer (100, 200, 300, and 400 kg N ha^{-1}) and slurry applications (0 and 20 m^3 ha^{-1}, 2.4 kg N m^{-3}). Basically, applied N fertilizer and defoliation type showed the highest influence on the NO_3-N leaching with minimum NO_3-N concentrations equivalent to 23 kg N ha^{-1} $year^{-1}$ in cutting treatments and maximum NO_3-N concentrations equivalent to 114 kg N ha^{-1} $year^{-1}$ for grazed-only grassland (average drainage amount of 205 mm). Leaching losses, *i.e.*, NO_3-N and dissolved organic-N, occurred under all investigated grassland systems especially from fall to early spring; even though negative N surpluses were calculated possibly caused by an underestimated symbiotic-N fixation of white clover (Rotz et al., 2005). Measured total N_2O emissions varied between 1.7 and 4.9 kg N ha^{-1} at soil surface for an 11-month period (April 2001 to March 2002) with lowest amounts for grassland fertilized with 100 kg N ha^{-1} of mineral-N. Maximum N_2O emissions occurred in treatments with combined mineral-N (100 kg N ha^{-1}) and slurry-N application (74 kg N ha^{-1}). Differences between investigated cutting treatments regarding emitted N_2O amounts were not significant over the whole period, but significantly elevated emissions were found in fertilized grassland systems from April to July 2001 (Lampe, 2005). The contribution of N_2O emitted during freezing and thawing in winter was also not negligible because of possibly increased microbial activity during snowmelt and enhanced C availability from microorganisms killed during freezing (Rotz et al., 2005). Second important crop cultivation at the 'Karkendamm' site from 1997 to 2003 was silage maize fertilized with different N applications (mineral-N: 0, 50, 100, and 150 kg N ha^{-1}; slurry-N: 0, 20, and 40 m^3 ha^{-1}; combined mineral-N and slurry-N) and grown in monoculture and undersown with annual ryegrass (Wachendorf et al., 2006a,b). Similarly to grassland, positive correlation between N input and NO_3-N leaching was also found for silage maize with maximum N losses for monocultures at the highest N level with combined mineral/slurry-N application. However, NO_3-N leaching of maize was often lower than below grassland because of reduced total N fertilization and omitted grazing (Büchter et al., 2003; Wachendorf et al., 2006a,b).

Additional studies addressed simulation analyses of grassland and maize farming at the ‘Karkendamm’ site to evaluate the long-term performance of farming systems depending on various influencing factors such as climate, soil, and farm management (Herrmann et al., 2005a,b; Rotz et al., 2005, Bleken et al., 2009). Rotz et al. (2005) applied the Integrated Farm System Model (IFSM) on data from the ‘Karkendamm’ projects comprising 40 grassland scenarios with different defoliation methods and N-fertilization levels, and 24 treatments for silage maize including monoculture and bi-cropping from 1997 to 2000. The model predictions regarding NO_3-N leaching for all scenarios were reasonably accurate considering both measurement errors and model deficits, even though predicted trends were more consistent across the scenarios in the simulations than those determined by observed NO_3-N concentrations. Especially for investigated silage maize treatments, modeled NO_3-N leaching was higher than observed over a wide range of fertilization and crop conditions. Unfortunately, particular annual NO_3-N leaching could not be distinguished between monoculture and bi-cropping systems on the basis of Rotz et al. (2005). However, determination of leached N based on NO_3-N concentrations and an estimated seepage-water amount for well-drained soil showed that undersown grass used as catch crop after maize harvest can reduce NO_3-N leaching during winter significantly (Büchter, 2003; Büchter et al., 2003) despite high variability and dependence on climate conditions of particular periods.

1.4 Research questions and objectives

The reliability of modeling results was often criticized, even though simulations may indicate the high variability of complex natural processes rather than problems arising from inadequate parameterization. This still requires the realistic description of investigated systems with the model. Given the fact that multiple observations can also show considerable variation already at plot scale because of spatial heterogeneity beside temporal fluctuations, the consideration of uncertainties arising from model parameterization can be as useful as taking particular descriptive statistics of observations into account. Therefore, process-based modeling might improve the understanding of important soil-related processes that are subject to considerable variations.

The model-based determination of NO_3-N leaching depends highly on the model structure, *i.e.*, implemented algorithms and particular response functions, and associated parameters, especially in complex soil-vegetation-atmosphere-transfer (SVAT) models. Dependent on the site characteristics, it is, thus, necessary to identify sensitive input parameters controlling soil water and N dynamics at first. SVAT models usually show considerable complexity associated with a high number of input parameters that may hinder clear identification of most important parameters and their particular values. Therefore, this PhD thesis was focused on following research questions regarding the quantification of NO_3-N leaching in agriculture:

(I) Is the process-based model CoupModel able to reproduce temporal dynamics of discharge and NO_3-N leaching by drainage?

To answer this question, the general applicability of the CoupModel must be ensured to reproduce water drainage and associated NO_3-N leaching for specific crops realistically at plot scale. For this, model parameterization can be made by means of manual calibration based on site-specific observations as well as defined conditions, *e.g.*, for drainage systems and crop species, and literature values without consideration of model uncertainties. The outcome of comprehensive sensitivity analyses can also help to identify dominant input parameters that must be adjusted to determine the NO_3-N leaching, *e.g.*, in an artificial drainage system, plausibly.

Main disadvantage of manual calibration is usually the focus on the best agreement between measured and modeled means without consideration of natural variabilities and model uncertainties. Consequently, universal usability of parameterized models is often limited because of high variations of site-specific conditions. Furthermore, available data from different sites can also differ in terms of type as well as quality and quantity, and impacts from site conditions might not be negligible. The question is whether or not the adaptation of an existing model structure including adjusted parameter values on new conditions can be made more efficiently by assuming uncertainties of particular input parameters. The basic idea was that a number of parameter combination can result in plausible outcome, *e.g.*, for the NO_3-N leaching, describing the problem of equifinality. In this context, the second research question emerged regarding the most appropriate optimization procedure of the CoupModel to identify the most plausible combinations of input-parameter values:

(II) Can stochastic optimization methods such as the Bayesian calibration and the GLUE approach be used for parameter estimations to achieve reliable results for the NO_3-N leaching?

To answer this question, different optimization methods must be tested comprehensively, not only for the same site and data but also for different crops at different plots. An important issue raised by stochastic optimization in this respect concerns appropriate sampling procedures, mostly realized by MCMC methods. Both methodologies for inverse uncertainty quantification estimate the value of unknown model parameters and the deviation between measured and simulated results. The consideration of several input parameters and validation variables present a particular challenge in this context.

With the identification of both important input parameters and the most appropriate optimization method, it is possible to apply the preferred approach on different conditions to investigate water and nitrogen dynamics in detail. Against the background of increasing complexity of sustainable agricultural production and required compliance with actual environmental standards, the extensive cultivation of silage maize in Northern Germany was chosen exemplarily to investigate effects of bi-cropping on water and nitrogen dynamics in soil. A prerequisite for reliable results of NO_3-N leaching and associated N dynamics is the realistic representation of soil hydrology, especially the soil water balance. For this reason, the final task focused on detailed measures to reduce the NO_3-N leaching under winter mild, humid climate influenced by subsurface drainage comprised two linked research questions:

(III) Does undersown annual grass affect the soil water balance under silage maize negatively?

(IV) Can the NO_3-N leaching be reduced by bi-cropping of silage maize and annual grass considering sources of uncertainty?

These questions can be answered by parameterization of different scenarios for silage maize in monoculture and bi-cropping dependent on different N fertilizers as well as levels of N fertilization. Furthermore, impacts of parameter uncertainties on modeled outcome for soil water and N dynamics have to be considered by means of the GLUE approach. Reason for that is the high spatial and temporal variability of natural processes that cannot be described completely by models also because of computational limitations. Even in case of highly variable observations, the consideration of variations in modeled outcome has to be accepted consequently.

Finally, the sequence of the presented research questions was in line with the development of the CoupModel during the last decade. It shows that state of the art methods regarding optimization/calibration of models can also be applied to models focused on small-scale soil-related issues. However, long time series of data are often not available for particular sites compared with hydrologic observations of water bodies. The overarching question of this thesis addressed the following problem in soil sciences:

Does the consideration of both multiple observations and parameter uncertainties improve the process-based modeling at plot scale resulting in reliable quantification of NO_3-N leaching in agriculture?

Possible use of the presented model structures can be the identification of problematic periods regarding NO_3-N leaching for arable crops in general. The improved understanding of significant leaching paths can also give indications for necessary adjustments of the soil management, *e.g.*, amount and timing of N fertilization, and particular crop rotations. Furthermore, it may support the implementation of future-oriented farming systems if current legal rules will be enforced and examined at last. An overview of the thesis structure is given in *Fig. 1.2*.

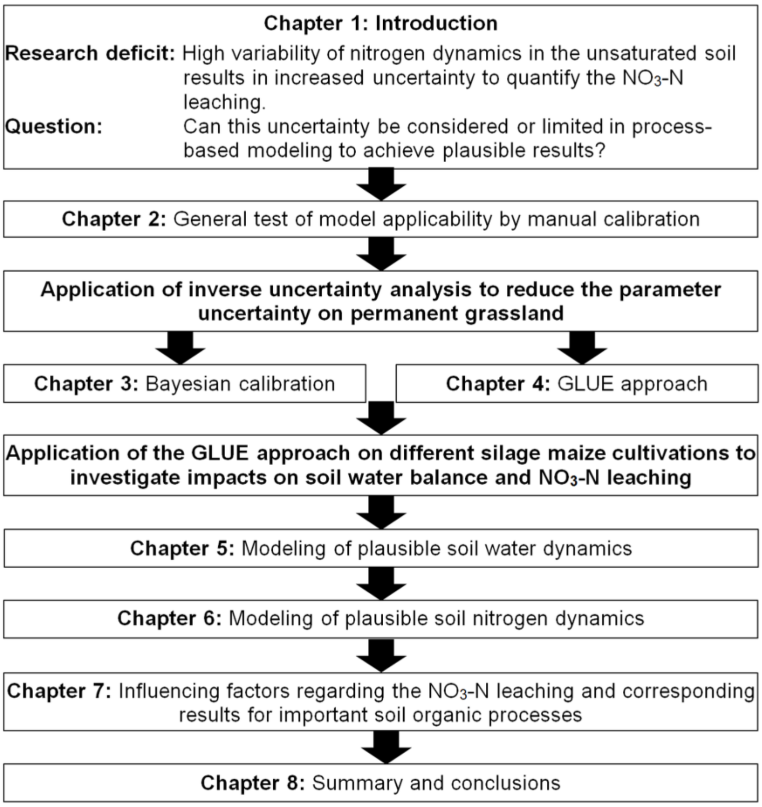

Fig. 1.2: Structure of this thesis.

Chapter 2
Modeling of nitrogen leaching under a complex winter wheat and red clover crop rotation in a drained agricultural field

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Abstract

The European Water Framework Directive requires conformity of water management structures all over Europe to pursue a good water quality for all water bodies. The highest nitrate concentrations in the water were measured in regions with well-drained soils, plowed pastures, and high nitrogen inputs. The objective of this study was to calculate the nitrate-nitrogen (nitrate-N) leaching out of a subsurface drainage system under organic farming conditions, especially for the seepage-water period in winter. Water and nitrogen fluxes between soil and vegetation were simulated with the soil-vegetation-atmosphere-transfer model CoupModel using data from an 8 years lasting monitoring program on a field in Northern Germany. Modeling was focused on a crop rotation sequence consisting of winter wheat with undersown red clover followed by two years of red clover used as temporary grassland.

Measured soil temperature in a depth of 15 cm was reproduced very well (Nash–Sutcliffe-efficiency *NSE* = 0.95; R^2 = 0.98). Results also indicated that CoupModel accurately simulated drainage discharge and nitrate-N loss under winter wheat from 2001 to 2002 with a *NSE* of 0.73 for the drainage discharge and a *NSE* of 0.49 for the nitrate-N leaching. For the following red clover period the accordance between simulated and measured drainage discharge (*NSE* = 0.01) and nitrate-N loads in the drainage (*NSE* = 0.31) was much lower. The inaccuracy in the modeling results in November 2002 seems to origin from an inadequate description of soil covering and thus the interception of the hibernating red clover. Secondly, the high nitrogen leaching in February 2004 could not be matched due to poorly adapted nitrogen dynamics in the model. The reason could be that common single parameter values in the mineralization part of the model were not suitable to reproduce an abrupt, short-term N leaching. In general, the results demonstrate the potential of CoupModel to predict water and nitrate-N fluxes under complex crop rotations including bi-cropping and legumes.

Keywords: Water quality, Tile drainage, CoupModel, Nitrate leaching, Crop rotation, Legumes

2.1 Introduction

Agricultural land use is often related to a risk for surface and subsurface water quality because of an inadequate nitrogen management. Investigation results document as well that generalized statements regarding the extent of N leaching cannot be made for certain management systems. There is a need for more appropriate N management strategies (*e.g.*, 'Good Farming Practice' (EC, 2003)) that are adjusted to regional characteristics according to the European Water Framework Directive (WFD, 2000).

Especially in north-western Germany, the nitrate-nitrogen (NO_3-N) leaching is significantly higher during fall and winter because of an above-average precipitation in combination with well-drained soils (Hatch et al., 2002). Investigations on sandy soils and in combination with green manure have shown highest NO_3-N leaching losses with increasing N input in conventional management systems (Kelm et al., 2007; Bobe, 2004; Trott et al., 2003; Büchter, 2003). A considerable N leaching was also found under plowed pastures (Di and Cameron, 2002; Webster et al., 1999). Organic farming is one management strategy to reduce environmental problems related to N leaching up to 66% (Goulding et al., 1999). Results from farm comparisons showed a significantly lower nitrate N leaching in organic farming compared to conventional farming systems in several studies (Gruber et al., 2003a; Haas et al, 2002; Stolze et al., 2000). But differences between conventional and N-reduced organic farming systems become smaller for loamy soils (Loges et al., 2005; Blume et al., 1993). In comparison, increased N leaching was measured for traditional crop rotations of winter cereal after grain legumes or clover-grass without catch crops in organic farming practice in sandy soils (Gruber et al., 2003b).

Applications of winter-grown crops or catch crops suggest a reduction of N losses during the seepage-water period (Neumann, 2005; Dreymann, 2005). Early sown winter catch crops are most effective in reducing NO_3-N leaching (Macdonald et al., 2005; Shepherd, 1999; Lewan, 1994; Sorensen and Thorup-Kristensen, 1993). Consequently, these crops could preserve N into their biomass and offer a soil covering during winter. Soil frost, however, can promote decomposition of organic-N compounds (*e.g.*, root residues) in the topsoil, leading to higher inorganic-N contents. Although the application of catch crops may reduce NO_3-N leaching (Aronsson, 2000; Böhm et al., 1999; Sattell et al., 1999), crop rotations with plowing or mulching of catch crops may increase the N-mineralization potential over few years (Lewan, 1994; Francis et al., 1992). High mineralization rates combined with high precipitation and warm temperatures may result in considerable N losses (Burtin et al., 1998), especially if the soil is left bare (Macdonald et al., 2005).

The main objective of this study was to apply the physically based soil-vegetation-atmosphere-transfer (SVAT) model CoupModel (Jansson and Karlberg, 2004) on a site-specific data set to determine the NO_3-N leaching in an organic arable forage crop rotation. The output in daily resolution could help to mark short-term mineralization events over time in N-reduced management systems.

2.2 Study site and measurements

2.2.1 The field site

The field site is situated at the experimental station 'Lindhof' in Northern Germany (lat. 54°28'N, long. 10°0'E, average alt. 23 m). The climate conditions can be described as maritime with an average annual precipitation of 750 mm and an annual average air temperature of 8.4 °C (Kiel-Holtenau, 1961–1990). Site-specific climate data were available between 1998 and 2002 (Deunert, 2005). From 2003 to 2004, meteorological data were taken from the agri-meteorological measurement station 'Birkenmoor' (Agrarwetter Schleswig-Holstein, 2006) at a distance of 8 km from the study site.

The climatic water balance for precipitation, actual evapotranspiration, and the accumulated average air temperature sum above 5 °C between fall 2001 and spring 2004 is shown in *Table 2.1*. The threshold of 5 °C was chosen because many cultivated plants in the temperate zone in Europe start to grow above this air temperature (Keller, 1997). The hydrological year 2001/2002 was characterized by high precipitation over the year and an early warming up period after the winter. The following year 2002/2003 was drier than 2001/2002 (only 65% of the precipitation) with an exceptionally dry summer.

Table 2.1: Climatic water balance for the hydrological years between fall 2001 and spring 2004.

Hydrological year	**2001/2002**		**2002/2003**		**2003/2004**
Period	**Oct. 2001– March 2002**	**April 2002– Sept. 2002**	**Oct. 2002– March 2003**	**April 2003– Sept. 2003**	**Oct. 2003– March 2004**
Precipitation P[a]	456	556	379	281	**369**
Total (mm)	**1012**		**660**		
Drainage discharge	328	124	148	7	**133**
Total (mm)	**452**		**155**		
Actual evapotrans-piration ETa[b]	36	234	34	207	**34**
Total (mm)	**270**		**241**		
Air temperature sum	366	1825	170	1757	**175**
Total (≥ 5 °C)	**2191**		**1927**		

[a] Measured with correction because of measurement errors (*e.g.*, wind, evaporation, snow).
[b] Calculated from potential evapotranspiration according to Haude (1955) and Sponagel (1981).

According to soil investigations from Ziogas (1995), the soil at the 'Lindhof' station shows a high heterogeneity with high percentages of loamy sand and sandy loam according to the German soil texture classification (Ad-hoc-AG Boden, 2005), covering thick layers of glacial loam and till up to a depth between 2 and 5 m. For consideration of the natural soil heterogeneity, two soil profiles were analyzed on the observed field. These soils in the drainage area were mainly classified as loamy sand with varying organic matter content (profile A: Humic Gleysol; profile B: Anthrosol; FAO, 2006). Detailed soil information is shown in *Table 2.2* and *Fig. 2.1*. The field declines towards a small depression area with the gauging station. A frequently high groundwater level is responsible for reduced mineralization in this waterlogged part of the field site. This depression had shown no natural drainage; therefore an artificial drainage system was required to allow agricultural crop production. The tile drain system consists of four sub-drains towards the hill peak, routing all into a main drain to the drainage station.

Table 2.2: Grain size distribution, organic matter content and soil classification for profiles A and B.

	Profile A			Profile B		
mbs	**0–0.30**	**0.31–0.60**	**0.61–0.90**	**0–0.30**	**0.31–0.60**	**0.61–0.90**
%						
Sand	57	53	29	73	74	70
Silt	29	33	53	20	19	23
Clay	14	14	18	7	7	7
Organic matter	13.1	10.6	13.2	5.6	3.2	1.3
Carbon content	7.6	6.2	7.7	3.3	1.9	0.8
Bulk density ($g\ cm^{-3}$)	1.13	1.24	1.15	1.39	1.47	1.68
German soil classification	Sl4 very loamy sand	Sl4 very loamy sand	Lu silty loam	Sl2 loamy sand	Sl2 loamy sand	Sl2 loamy sand

The drainage area measures approx. 1.0 ha. According to the existing drainage map, the distance between the sub-drains is approx. 16 m. The depth of the tile drains varies between 0.35 and 0.70 m below surface (mbs) (Deunert and Fohrer, 2006). Profile A is located in the depression, and measurements have shown high contents of organic matter between 10.6% and 13.2% up to a depth of 0.90 m. Profile B is set up in the upper level of the drainage catchment, characterized by higher sand and lower organic matter contents in comparison to profile A. According to spatial oriented results from Ziogas (1995), 80% of the catchment area is characterized by loamy sand in top- and subsoil but with varying horizontal thickness. In *Fig. 2.1* the spatial distribution of soil types according to Ziogas (1995), the location of both soil profiles for the investigated area, the drainage network and the measurement station are shown.

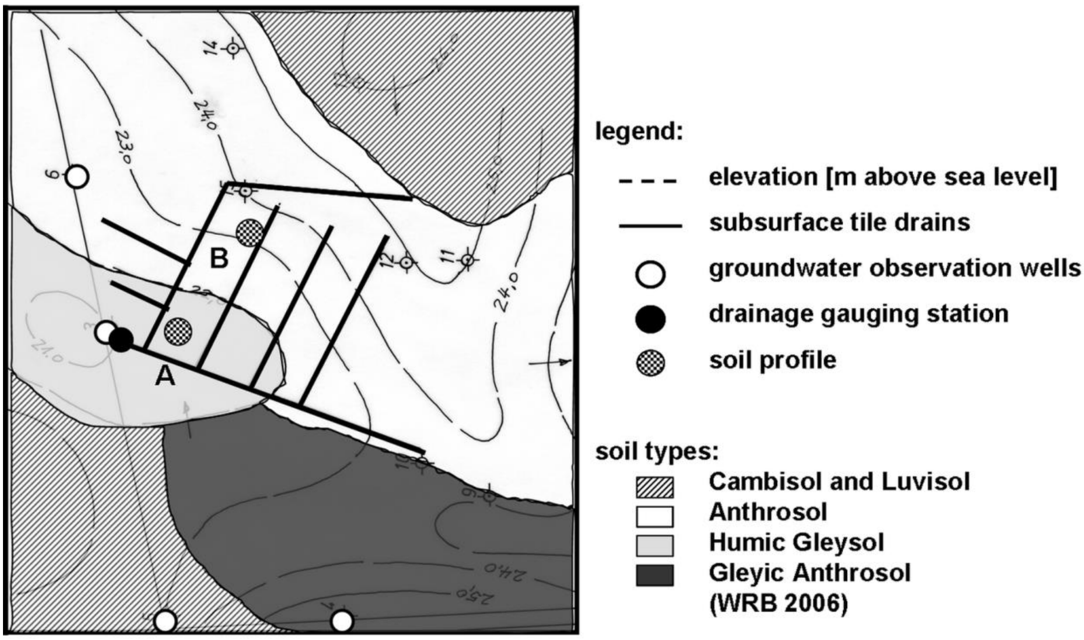

Fig. 2.1: Distribution of soil types and drainage system in the investigated area.

2.2.2 Crop rotation and field management

The drainage area is located in the western part of a slightly sloped (mean value < 2% towards southwest) agricultural field converted to organic farming in 2001. Crop rotation and important soil management activities between 2001 and 2004 are shown in *Table 2.3*.

Before conversion to organic farming, conventional crop rotation consisted of winter wheat, corn, sugar beet, and winter canola. The last input of mineral-N (100 kg ha^{-1}) was given in March 2000 (Loges, 2006). After the conversion to organic farming, only organic fertilizers, *i.e.*, cattle manure, were possible N inputs beside atmospheric sources and biological-N fixation by legumes. No manure was applied between 2001 and 2003. Possible high soil-N contents could therefore be reduced. Winter wheat was sown shortly after plowing in November 2001. Red clover was spread directly into the growing wheat in April 2002. Mulching of this undersown clover was done after the wheat harvest in August 2002. In the following year 2003, red clover was used as temporary grassland with two cuts for silage and seed production in July and August. Between both cuts a partial mulching of weed and white clover was carried out. The plowing of the clover took place in April 2004 before the following oat was sown. Cattle manure (46 t ha^{-1}) was incorporated into soil after the harvest of oat in August 2004 (Loges, 2006).

Table 2.3: Crop rotation and soil management between 2001 and 2004.

Year	Crop	Sowing	Harvest	Yield	Soil management
2001	Potatoes	May 11th	October 15th	17.5 t ha^{-1}	Surface cultivation (October 26th) Plowing (November 3rd)
2001/ 2002	Winter wheat with undersown red clover	November 3rd, 2001 April 23rd, 2002	August 17th 2002 none	4 t ha^{-1} of grain	Mulching (August 20th, 2002)
2003	Red clover (cut)	None	June 1st (1st cut, silage) August 16th (2nd cut, seeds production)	19.8 t ha^{-1} of DW 0.33 t ha^{-1} of seeds	Mulching of weed and white clover spots (July 1st)
2004	Oats	April 2nd	August 17th	5.6 t ha^{-1} of grain	Surface cultivation (March 26th); plowing of red clover (April 1st); application of cattle manure (August 25th, 100 kg N ha^{-1})

DW – dry weight

2.2.3 Field Measurements

2.2.3.1 Discharge drainage

The drainage station was established in fall 1998 for measuring discharge and water quality parameters during the conversion from conventional to organic farming. Automatic gauging of discharge and analyses on NO_3-N concentration has been carried out. The drainage flow was measured with a ventury flume by continuously logging the water level. Discharge values were calculated from the water level-discharge calibration curve for the used flume (Deunert and Fohrer, 2006; Deunert, 2005).

2.2.3.2 Measurements of NO_3-N in the drainage water

Water samples were taken every ten minutes and were pooled to 14-hour samples stored at a constant temperature of 4 °C until the weekly data collection. The samples were then analyzed for nitrate-N concentrations

(NO_3-N) by ion chromatography according to the standard ISO 10304-1-DEV D19 and converted into nitrate concentrations (in mg NO_3^- L^{-1}). Nitrate-N loads were obtained by multiplying daily discharge from the drainage area by the corresponding NO_3-N concentration (Deunert and Fohrer, 2006).

2.2.3.3 Groundwater level observations

The monitoring of the groundwater level was carried out from 2000 until 2005 once a week at four different locations surrounding the drained area (*Fig. 2.1*). One observation well was installed directly next to the gauging station. This information was used for a general definition of the drainage area and groundwater flow direction. The measurements were limited to the near-surface groundwater aquifer. The mean distance from groundwater to soil surface varies from 0.17 m in the depression to 1.0 m at the starting point of the sub-pipes towards the hill according to data from Ziogas (1995) for the mean groundwater levels in this area.

2.2.3.4 Soil temperature

Measurements of soil temperature in 15 cm depth were taken from local measurements between 1998 and 2004 (Deunert, 2005; Krüger, 2006). Missing values were completed with data from 20 cm depth measured at the weather station ‘Birkenmoor’ (Agrarwetter Schleswig-Holstein, 2006). Soil properties are assumed to be comparable to the ‘Lindhof’ characteristics, but no information about vegetation was available at the time of measurement.

2.3 Model structure

2.3.1 General description

CoupModel is a physically based, ecosystem modeling package (Jansson and Moon, 2001), which can be used to design thermal and hydrologic processes and corresponding biological processes such as carbon (C) and nitrogen (N) fluxes in soil-plant-atmosphere systems. Fluxes of heat, water, and nutrients are calculated for a one-dimensional, vertical layered soil column. Above the soil surface, one or several vegetation layers can be defined (Karlberg et al., 2006). Water flows in the soil are required to be laminar and described for unsaturated soil water conditions by the Richards’ equation (Jansson and Halldin, 1979). Groundwater flow, *i.e.*, drainage, is described as a sink term in the model (Jansson and Karlberg, 2004). The physically based drainage equation by Hooghoudt (1940) can be used to calculate flows above and below parallel drain pipes. The depth of the horizontal drainage influences the simulated groundwater table. The abiotic part of the model provides a number of simulated daily driving variables, *i.e.*, soil water content and soil temperatures, for the nutrient fluxes in soil and plant. C and N turnover in the soil may be simulated (Johnsson et al., 1987; Eckersten et al., 1998) as well as plant growth for multiple plant covers. Detailed information about CoupModel can be found in Jansson and Karlberg (2004).

2.3.2 Model application and parameterization

2.3.2.1 Soil characteristics

The basic structure in CoupModel is the one-dimensional soil column. To consider the spatial variability of the observed soil conditions, the drainage discharge and NO_3-N leaching were simulated in two soil profiles for the crop rotation. Two sets of data from soil texture *(Table 2.2*) were used. The topsoil of each profile was divided into three layers (0–0.1, 0.1–0.2, 0.2–0.3 m), the subsoil down to 2 m into 6 horizons (0.3–0.45, 0.45–0.6, 0.6–0.9, 0.9–1.5, 1.5–2.0 m).

2.3.2.2 Parameterization of vegetation

Crop rotation between fall 2001 and spring 2004 has already been described in ch. 2.2.2. Calculations of actual evapotranspiration (ETa) were based on the Penman–Monteith equation (Penman, 1953; Monteith, 1965). In this study two canopies existed at the same time. An eventual shadowing must be considered for the estimation depending on the actual leaf area index (LAI). Due to the fact that carbon and nitrogen flows were simulated in the model, the plant cover was assumed to produce biomass. Important plant characteristics, *i.e.*, canopy height, LAI, and root development, were derived from the crop growth module. For each plant accumulated air temperature sums for sowing, emergence, and maturing had to be defined to mark the growth stages. The plant was divided into five compartments for carbon and nitrogen respectively for grain crops, *i.e.*, leaf, stem, root, grain, and mobile pools, and in addition three compartments for perennial vegetation. Allocation of C and N was governed by the growth stage index and different environmental responses for water, temperature, and nitrogen stress. Harvests were specified at fixed dates (Jansson and Karlberg, 2004).

2.3.2.3 Soil carbon and nitrogen dynamics

Measured data for the initial nitrogen content of both litter and humus pools in the soil were not available for this site. Averaged nitrogen amounts of crop residues for loamy soil were derived by Köhnlein and Vetter (1953). The selected litter pools L1 and L2 differed in initial values of total organic nitrogen content and C:N ratio assuming fast and slowly decomposing organic residues, but reflecting also a medium C:N ratio for decomposition. The litter pool L1 was defined according to published values to contain 1.5 g m^{-2} of organic nitrogen (Köhnlein and Vetter, 1953) and a C:N ratio of 20 (Kathan and Püschel, 2007). The slower decomposing litter pool L2 was estimated to be 1 g m^{-2} total organic nitrogen, assuming a C:N ratio of 25. Chosen parameter values, used in the first time period, reflected conditions without high organic input from harvest residues compared with nitrogen amounts over 10 g m^{-2} in residues from red clover/grass-, pure grass- or pure red clover-covers, used as green manure on the investigated site (Dreymann, 2005). The nitrogen content of the humus pool was defined to be 500 g m^{-2} based on model setups in Blombäck et al. (2003) and Lewan (1994) on sandy loam with an organic matter content of about 5% and humus-N content of 700 g m^{-2} with a C:N ratio of 16.4 in the topsoil. Scheller (2002) reported also total organic-N contents between 400 and 600 g m^{-2} in arable loamy soils. The lower amount of humus-N in this study was set under consideration of the long conventional cultivation history without continuously applied farmyard manure as described in Blombäck et al (2003). A C:N ratio of 10 was derived from Capriel (2006) representing an average value for sandy loam under conventional management. Initial concentrations of NO_3-N and ammonium-N (NH_4-N) were set to 10 mg N L^{-1} decreasing with depth. Corresponding nitrate concentration of 44 mg L^{-1} in the upper soil was also measured after plowing of mulched clover-grass in organic farming (Dreymann, 2005).

The atmospheric-N deposition was set to 1.9 mg L^{-1} in the wet fraction (Lehmhaus et al., 1998) and 1.5 g m^{-2} $year^{-1}$ in the dry deposition (LANU, 2007), which is relatively low compared to the mineralization rates. A simple approach for nitrogen fixation by micro-organisms was used to consider symbiotic fixation by legume plants if plant demand for nitrogen is still higher than the uptake (Jansson and Karlberg, 2004). No additional fixation was assumed for the first simulation period with winter wheat and the undersown crop.

2.3.2.4 Calibration procedure

Single simulations with fixed parameter values were achieved in two steps caused by the changes in crop and management parameters in summer 2002. The first simulation period included the plowing of the precedent crop residues in November 2001, drilling and harvesting of winter wheat, and drilling and mulching of the undersown red clover in August 2002. A pre-simulation period of five years was chosen to minimize the influence of assumed initial values in the first period. A sensitivity analysis was carried out for approx. 25% of all parameters in this period. The selection of the most sensitive parameters for drainage discharge and NO_3-N leaching is shown in *Table 2.4*. These parameters were identified manually by changing start values to ±25% and were used for a calibration in the single runs. Profile A was used for this calibration and the examination of sensitive parameters. The validation of the first crop sequence was conducted on profile B. Thus new soil characteristics from the database for water retention and hydraulic conductivity and new slope values were applied. In this way the reaction of drainage and NO_3-N leaching could be evaluated in a well-drained soil compared to profile A.

The red clover period was performed from August 2002 to March 2004 with the same pre-simulation period to prevent implausible phenomena in plant growth at the beginning of the second period. This may occur if initial values derived from the previous simulation instead of a pre-simulation period are used. The parameter set for the manual calibration from the first simulation period for each profile was adopted. Changes related to physical attributes of the plant, *e.g.*, specific leaf area, maximum height, and root depth, were necessary to parameterize the red clover as shown in *Table 2.4*. Additional parameter values characterizing the ecosystems had to be derived from literature.

Table 2.4: Important parameter values characterizing both simulation periods.

Property, *symbol*	**Unit**	**Value (1st period)**		**Source (1)**	**Value (2nd period)**	**Source (2)**
		Wheat	**Undersown**		**Red clover**	
Soil hydraulics						
Empirical factor for pores geometry, a_{scale}	–	0.001		Calibrated against discharge	0.001	Same as source (1)
Empirical factor for $k_{mat} = f(k_{sat})$, h_{sens}	mm d^{-1}	0.5 / 0.8		Calibrated against discharge	0.5 / 0.8	Same as source (1)
Plant						
Stomatal half–light response, g_{ris}	J m^{-2} d^{-1}	5e+6	13e+6	Heidmann et al. (2000)	13e+6	Same as source (1)
Maximum leaf conductance, g_{max}	m s^{-1}	0.012	0.009	Jensen et al. (1993)	0.009	Same as source (1)
Resistance to vapor pressure deficits, g_{vpd}	Pa	1300	1100	Heidmann et al. (2000)	1100	Same as source (1)
Temp SumCrit, t_{crit}	°C	3		Keller (1997)	1	Assumed
Temp SumStart, t_{start}	°C days	30		Assumed (default value)	30	Assumed (default)
Specific leaf area, $p_{l,sp}$	g C m^{-2}	10	3	Calibrated against yield, discharge	4	Same as source (1)
Maximal height, H_p / root depth, z_{root}	m	0.85 / −0.8	0.45 / −0.8	Kutschera and Lichtenegger (1982)	0.45 / −0.8	Same as source (1)
External N–Input						
Dry deposition (N rate), p_{dry}	g N m^{-2} d^{-1}	0.004		LANU (2007), Lehmhaus et al. (1998)	0.004	Same as source (1)
Wet deposition (N concentration), p_{cwet}	mg N L^{-1}	1.9		Lehmhaus et al. (1998)	1.9	Same as source (1)
Empirical factor for N Fixation, n_{fix}		–		Not assumed	0.3	Calibrated against N leaching
Plant growth						
Radiation use efficiency, ε_L	g DW MJ^{-1}	3	2	Calibrated against yield, discharge	2	Same as source (1)
Optimum temperature interval, $p_{o1} - p_{o2}$	°C	15–25		Assumed	15–25	Same as source (1)
Min/max temperature (leaf), $p_{mn} - p_{mx}$	°C	5–35		Assumed	5–35	Same as source (1)
Mineralization and immobilization						
Nitrification rate, n_{rate}	–	0.4		Calibrated against N leaching	0.2	Assumed (default)
Nitrate:Ammonium ratio, $r_{nitr,amm}$	–	10		Calibrated against N leaching	5	Same as source (1)
Fraction of available mineral nitrogen, f_{Nupt}	d^{-1}	0.05		Calibrated against N leaching	0.08	Assumed (default)
Potential denitrification rate, d_{pot}	g N m^{-2} d^{-1}	0.04		Jansson and Karlberg (2004)	0.04	Same as source (1)
Physical drainage equation		**Profile A**		**Profile B**	**Source**	
DLayer, z_D	m	0.6		0.9	Assumed; Ziogas (1995)	
DrainLevel, z_p	m	−0.6		−0.55	Deunert and Fohrer (2006)	
DrainSpacing, d_p	m	16		16	Deunert and Fohrer (2006)	
RadiusPipe, r_p	m	0.033		0.033	Deunert and Fohrer (2006)	
Initial groundwater level	m	−0.6		−0.8	Assumed Deunert (2005)	

2.3.2.5 Comparison between simulations and measurements

The model was tested against measured soil temperature at 15 cm depth, drainage discharge, NO_3-N load in the drainage, and groundwater dynamics. Measurements for drainage discharge and NO_3-N leaching corresponded to a heterogeneous drainage area with two main soil types. Because CoupModel describes processes in a one-dimensional soil column without spatial variation, weighted average values of the simulated drainage discharge and NO_3-N load from both soil profiles were compared to measured data. Weighting was not applied to the simulated soil temperature and the groundwater level.

Qualitative measures of agreement between measured and observed results, used in this study and shown in *Table 2.6*, were based on the Nash-Sutcliffe model efficiency (*NSE*) (Nash and Sutcliffe, 1970), the coefficient of determination (R^2), and the root mean squared error (*RMSE*). *NSE* is better suited to evaluate the model goodness-of-fit than the R^2, because R^2 is insensitive to additive and proportional differences between model results and measurements (Harmel and Smith, 2007). These statistical indicators represent the result of a special parameter combination. Reasons for a mismatch between observation and model results, however, cannot be explained.

2.4 Results

2.4.1 Water balance

In *Table 2.5*, the differences (in%) between observed and simulated water balance components are shown for each vegetation and seepage-water period between 2001 and 2004. Measurements were set to 100%. As stated in the footnote of *Table 2.5*, there was no discrepancy in precipitation because of its status as driving variable. The model overestimated the drainage discharge in most of the years with a maximum deviation of 100% in the dormancy period of the red clover (2002/2003). A deficit in the drainage discharge was calculated for the dry summer 2003. Especially in the vegetation period, the actual evapotranspiration (ETa) from the soil surface is the competing factor for the runoff. In most periods the model calculated a higher ETa compared to the calculations according to Haude (1955) and Sponagel (1981) for the selected crops. Because no specific factors for red clover were available by Haude and Sponagel, values for grassland were used. Differences in the seepage periods (winter term) were much lower than for the vegetation periods or negative. Possible reasons were found in different approaches to calculate the actual evapotranspiration. The CoupModel is based on the Penman-Monteith approach (Penman, 1953; Monteith, 1965) and the interception loss is already included in the results. Both the potential evapotranspiration according to Haude (ETp) and the following calculation of the actual evapotranspiration according to Sponagel (1981) are based on empirical, crop-specific factors, which are not influenced by phenological plant characteristics or surface covering. In addition, both simple approaches do not take into account the interception loss from the plant surface. Consequently, evapotranspiration will be underestimated. But as no related measurements were done, only standard values for ETa and phenological data could be used to calibrate the model.

Table 2.5: Differences between observed and simulated water balance.

Hydrological year	2001/2002		2002/2003		2003/2004
Period	**Oct. 2001– March 2002**	**April 2002– Sept. 2002**	**Oct. 2002– March 2003**	**April 2003– Sept. 2003**	**Oct. 2003– March 2004**
Precipitation *P* (%)[a]	0	0	0	0	**0**
Total (%)		**0**		**0**	
Drainage discharge *D* (%)	+14	+29	+100	−29	**+35**
Total (%)		**+18**		**+90**	
Actual evapotrans-piration *Eta* (%)[b]	+19	+66	−20	+51	**−35**
Total (%)		**+60**		**+41**	
Other components *R* (%)[c]	−58	−97	−73	−153	**−10**
Total (%)		**−84**		**−93**	

[a] No difference because precipitation is a driving variable in CoupModel.
[b] Observed values are calculations acc. to Haude (1955) and Sponagel (1981) without interception loss.
[c] Other components *R* (= *P−D−ETa*) could be: interception, soil water storage, and surface runoff.

This general approach may imply a high uncertainty because of standardization. Reference values for the ETa are given in Sponagel (1981). For winter wheat, the ETa value can reach 480 mm year^{-1}, for grassland an ETa value of 500 mm year^{-1} is stated. CoupModel simulated an ETa of 390 mm for winter wheat in summer 2002 and 313 mm for red clover in summer 2003. During the seepage-water period in winter, ETa values showed variations between 22 mm (red clover) and 43 mm (wheat). As shown in *Table 2.1*, calculated ETa according to Haude and Sponagel were only 234 mm (winter wheat) or 207 mm (red clover) in the summer periods. Since the model has calculated higher values for both drainage discharge and actual evapotranspiration, the resulting term *R* in the water balance equation (*R = P–D–ETa*) showed negative differences (over 80%) related to the observations or calculations (*Table 2.5*). The term *R* in *Table 2.5* includes the other hydrological components in this soil-plant-atmosphere system (*e.g.*, surface runoff, interception (if still not included), soil water storage) which could not be measured individually.

2.4.2 Soil temperature

As shown in *Fig. 2.2*, the model performed well throughout the range of measured data for the soil temperature in a depth of 15 cm for both soil profiles. The measurement was carried out on a nearby field plot with similar soil characteristics. No information about the soil covering was available. Consequently, the influence of the soil covering on the heat flows in the soil profile can hardly be explained.

Only minor deviations in soil temperature between the different soil profiles were pointed out because no parameter changes were made for the soil temperature dynamics in the model. Between November 2001 and March 2002, simulated values showed an average overestimation of 2.2 °C (profile A) and 2.0 °C (profile B) compared to the observations. From May to September 2003, simulated soil temperature was 1.6 °C (profile A) and 1.5 °C (profile B) less than the actual measurements.

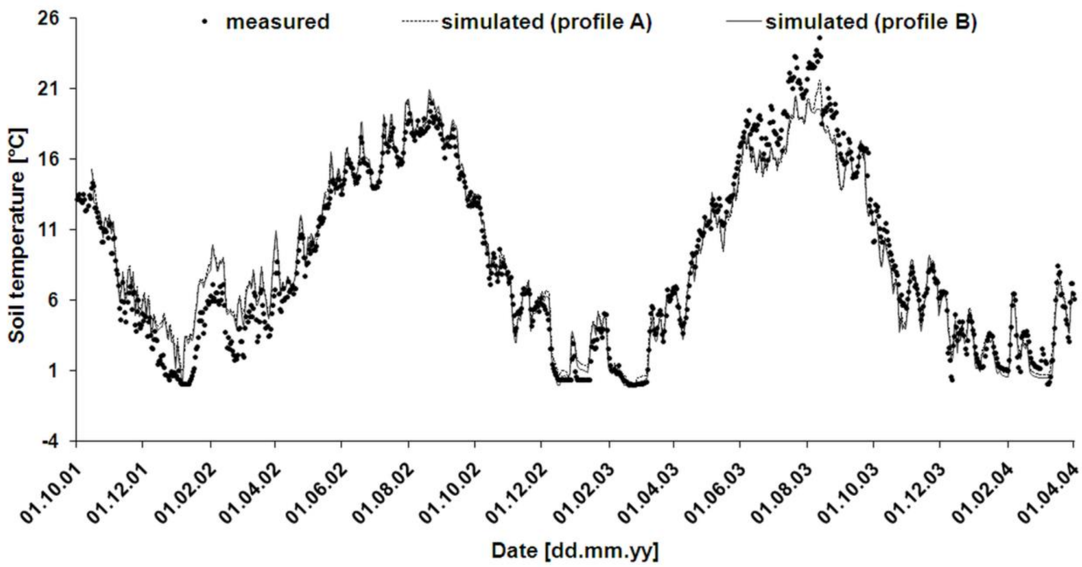

Fig. 2.2: Measured and simulated soil temperature in a depth of 15 cm.

These non-systematic deviations in different periods could be caused by differences in soil covering between observed and simulated area or by the general parameterization of the thermal fluxes in the model. Better results could be obtained with a more physically based approach. The iterative solution of the surface energy balance includes both water and corresponding heat flows at the soil surface. Values for *NSE* of 0.92 for the first and 0.97 for the second time period, and R^2 = 0.98, demonstrated a very good model efficiency related to modeling of soil heat fluxes in both soil profiles (*Table 2.6*).

Table 2.6: Statistical measures of calibration and validation depending on crop.

Parameter	Statistical measure[a]	Profile A		Profile B	
		Wheat + undersown	Red clover	Wheat + undersown	Red clover
Soil temperature	*NSE*	0.92	0.97	0.92	0.97
	RMSE	1.67	1.21	1.55	1.21
	R^2	0.98	0.98	0.98	0.98
Ground-water level	*NSE*	0.51	0.58	0.12	0.48
	RMSE	0.12	0.11	0.17	0.12
	R^2	0.63	0.80	0.61	0.81
		Simulated and weighted results from profile A and B			
		Winter wheat + undersown		Red clover	
Drainage discharge	*NSE*	0.73		0.01	
	RMSE	0.80		0.97	
	R^2	0.81		0.52	
NO_3-N load	*NSE*	0.49		0.31	
	RMSE	0.07		0.07	
	R^2	0.56		0.31	

[a] *NSE*: Nash–Sutcliffe efficiency; *RMSE*: root mean squared error; R^2: squared Pearson's correlation coefficient.

2.4.3 Groundwater level

As shown in *Fig. 2.3*, modeling results for the groundwater level below soil surface also suggested that CoupModel was able to reproduce the measured data over the whole simulated time period in a satisfying way. Simulated groundwater levels could not exactly match measured data because the applied drainage function according to Hooghoudt (1940) is based on the assumption that the groundwater level is modeled between two drainage pipes. The groundwater observation well, however, was located outside of the drainage area next to the gauging station on the boundary ridge. Therefore, the measurements probably did not reflect the exact situation in the drainage area. In addition, the vegetation on the field and on the boundary ridge close to the well was different.

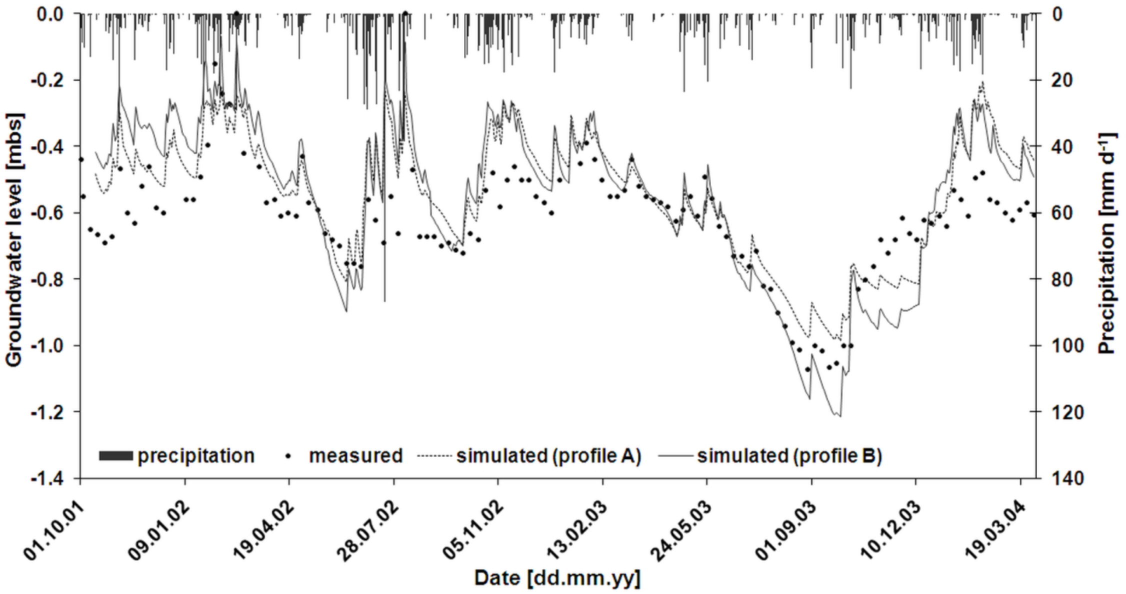

Fig. 2.3: Measured and simulated groundwater level.

For this reason the water uptake from near-surface groundwater can differ, especially if temporary arable crops are compared with perennial grassland. It is likely that due to the drainage depth the distance between well and each profile is important for the comparison. Profile A was located closer to the drainage station and the observation well. Therefore, the simulated groundwater level of profile A has shown a better agreement with observed data (mean *NSE* = 0.55, mean R^2 = 0.72) than profile B (mean *NSE* = 0.30, mean R^2 = 0.71). The model tended to overestimate the groundwater level especially for profile B of the first observation period between October and December 2001. In contrast to the daily resolution of simulated groundwater level, measurements were taken only once a week. The statistical indicators *NSE*, *RMSE* and R^2 were computed for the weekly resolution. *NSE* decreased for the first time period from 0.51 (profile A) to 0.12 (profile B), while R^2 showed stable values of 0.63 (profile A) and 0.61 (profile B), according to its low sensitivity for extreme values. As shown above, the groundwater levels in the second simulation period showed higher correlation to the measurements (profile A: *NSE* = 0.58, R^2 = 0.80; profile B: *NSE* = 0.48, R^2 = 0.81; *Table 2.6*) than in the first time period. The physical approach in the model indicated the situation between the drainage pipes and, consequently, does not necessarily match the situation outside of the drainage area with a specified parameter set for the drainage function. Profile A was set in a distance of 25 m with an altitude difference of 0.5 m and the same soil characteristics. Compared to these similarities, profile B was located in a distance of 50 m and 2 m above the observation well.

2.4.4 Drainage discharge

As shown in *Fig. 2.4*, the best agreement between simulated and measured drainage discharge was found for the winter wheat in the first period, since it was the first calibration step. The *NSE* values were derived from weighted simulation results according to the relative proportions of both soil profiles in the drainage area. Between the crops, the first period matched best for the simulated drainage discharge (*NSE* = 0.73, R^2 = 0.81) compared to the very low agreement in the red clover treatment (*NSE* = 0.01, R^2 = 0.52) respectively. Sandy conditions as in profile B resulted in faster drainage discharge dynamics. Accumulated drainage discharge showed 18% higher values in the simulations (541 mm) than in the measurements (451 mm) for the first simulation period. Because of short-term deviations for the discharge in the seepage-water periods, higher differences occurred in the second time period (red clover crop) with overestimated drainage values of 62% in the model.

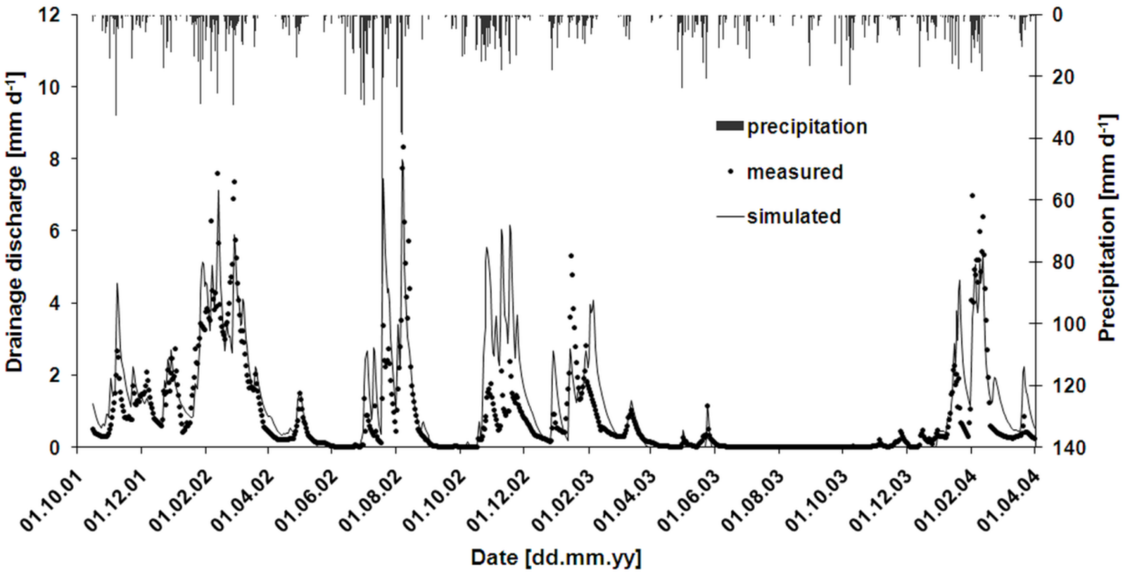

Fig. 2.4: Measured and simulated drainage discharge.

The transfer and adaptation of the parameters from the first crop (see *Table 2.4*) did not fit in the second crop period for the single simulations. An overestimation between October and November 2002 caused a decreasing correlation between model and measurements with *NSE* of 0.01 (*Table 2.6*). The reason for this low reproducibility of the observed results may lie in the plant parameterization of the second period with single fixed values. The plant development, *i.e.*, leaf surface for interception, and the water uptake by perennial plants were seen as major influences on drainage water flows in fall. A missing leaf area or plant covering after the vegetation period has led to decreasing evapotranspiration rates including interception loss in the model, causing a higher infiltration. Consequently, the plant growth in fall was still too low and the water uptake from the soil layers was not high enough to reduce the drainage rates.

2.4.5 NO_3-N leaching in the drainage discharge

As shown in *Fig. 2.5*, simulated and measured NO_3-N leaching in the drainage agreed well for the first simulation period until August 2002. The simulated values again represent a weighted NO_3-N leaching from the simulations for both profiles, because the measured signal is a combination of both single results. Especially simulated NO_3-N leaching between February and September 2002 matched the observed data well. A slight overestimation occurred from October to November 2001 and caused the higher accumulated NO_3-N leaching of 10% in the model (24 kg ha^{-1}) compared with 22 kg ha^{-1} in the observations (*Table 2.7*).

The best match was achieved for the calibration of the winter wheat period. Statistical measures for the corresponding adaptation of the red clover vegetation showed satisfying results for the NO_3-N leaching. As shown in *Table 2.6*, the simulated and measured NO_3-N load differed more with NSE = 0.31 and R^2 = 0.31 from the first simulation period. The latter result can be explained by a high overestimation from October to November 2002. Big differences in discharge between model and actual measurement led to differences in the N load, because it is the product of the drainage and NO_3-N concentration. In winter 2004, the model showed an underestimation of NO_3-N leaching.

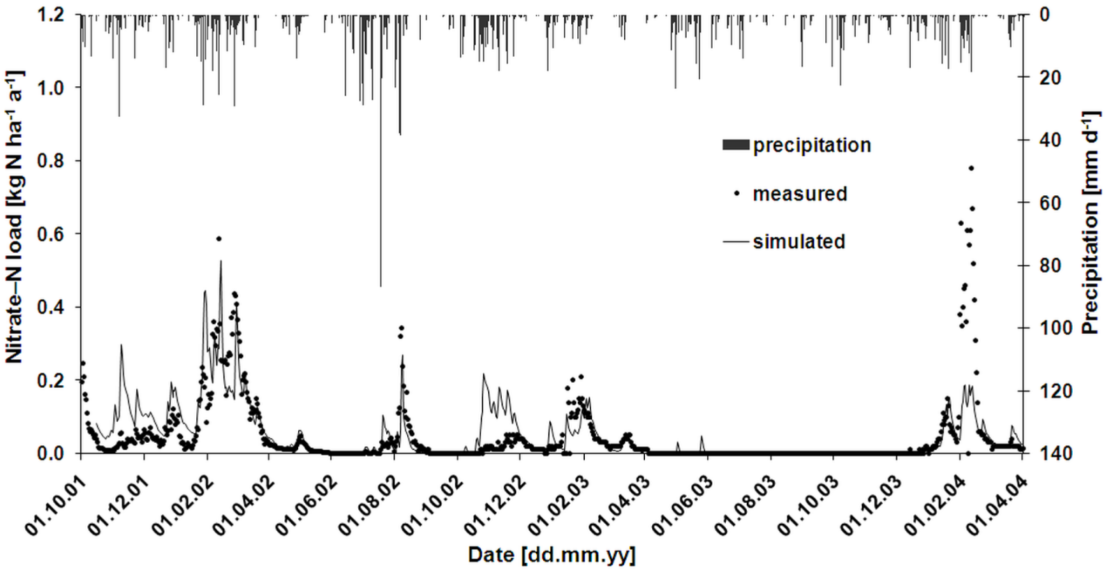

Fig. 2.5: Measured and simulated NO_3-N load in the drainage discharge.

Table 2.7: Accumulated NO_3-N load in the drainage discharge for each hydrological period.

Hydrological year NO_3-N leaching (kg ha^{-1} $period^{-1}$ or $year^{-1}$)	**2001/2002 Oct. 2001– March 2002**	**April 2002– Sept. 2002**	**2002/2003 Oct. 2002– March 2003**	**April 2003– Sept. 2003**	**2003/2004 Oct. 2003– March 2004**
Measured	18	3.7	5.9	0.0	**10.9**
Total		**21.7**		**5.9**	
Simulated	20.9	3	10.1	0.2	**5.9**
Total		**23.9**		**10.3**	

As shown in *Table 2.7*, the accumulated NO_3-N leaching between October 2002 and March 2004 was almost the same in the model (16 kg ha^{-1}) and the observations (17 kg ha^{-1}). There are, however, still problems in timing of the NO_3-N leaching in the model. Observations have shown the maximum leaching during a few days in February 2004, but the simulation could not match the increased NO_3-N leaching in this period.

The observed increased NO_3-N leaching loss under red clover (*Trifolium pratense L.*) monocultures was also reported by Scherer-Lorenzen et al. (2003) with maximum NO_3^- values of up to 350 mg L^{-1} under similar conditions. Sampling occurred in stagnic gleysols indicating a former agricultural tillage. The soil texture varied between loamy sand and sandy clay with temporary groundwater influences up to 0.1 m below the surface. The observed year 1998 was characterized by a precipitation of 816 mm $year^{-1}$ with a remarkably dry summer and a wet fall (Scherer-Lorenzen et al., 2003), which is comparable to the observations in this study. Intercropping experiments showed an increase of available soil NO_3-N under legumes due to the root and litter decomposition and thus to the release of symbiotically fixed nitrogen by N mineralization (Ledgard and Giller, 1995). Increased mineralization rates and NO_3-N leaching caused by decaying plant residues and higher temperatures in winter were also found by Gruber et al. (2003a, 2003b) under organic farming practices. The NO_3-N leaching under pure white clover cultivations can increase up to 140 kg ha^{-1} $year^{-1}$ if the accompanying grasses are suppressed (Loiseau et al., 2001).

2.5 Concluding remarks

CoupModel showed a high potential to describe complex interactions under different crops with defined sowing and harvest dates. An intensive adjustment of parameter values, however, was necessary. The model was applied to describe water and N fluxes in a drained agricultural field under an organic arable forage crop rotation in Northern Germany. Both the calculated water balance for the modeled system and the simulated daily values showed plausible results compared to the measurements, even though short-term events in the seepage-water period indicated discrepancies in drainage and NO_3-N leaching. The first simulation period with winter wheat and later undersown red clover was used for the first calibration step and showed a good agreement with measured drainage and NO_3-N leaching. For the second crop period with the regrowing red clover, simulation results were less consistent and problems occurred with the correct timing of drainage and NO_3-N leaching.

Consequently, the calibration method with single fixed values for a defined crop has to be modified. Because of the complex N dynamics in the soil-plant system not only one fixed parameter value can be considered. A range of parameter values would probably be more suitable for this purpose. In addition, discrepancies in deviation between observed and simulated results could be caused not only by the spatial variability of NO_3-N leaching in the soil but also by possible measurement errors and by the uncertainty in the model parameterization. These factors cannot be clearly separated from each other. The understanding of transformations between organic and inorganic components in soil and plant, including the plant growth, must still be improved. On the other hand, the soil structure in the model is changing only with depth but not with time. Most agricultural soils, however, are subject to structural changes from seeding to harvest time with decreasing saturated hydraulic conductivities, especially for soils without mulch and increasing runoff rates (Hanks and Gardon, 2003). To take into consideration the uncertainty both in observation and modeling, a statistically based automatic calibration method can be applied (Klemedtsson et al., 2008).

Since artificial drainage systems are widely used in Northern Germany, reflecting also potential risks for water quality under agricultural land, the N management in agricultural areas with connections to surface water bodies should be carried out according to the 'Good Farming Practice' (EC, 2003). It is important to ensure a minimum soil covering during periods with higher rainfall, mainly the seepage-water period from late fall to early spring, in order to preserve nitrogen into the biomass. Similarly, the soil management, including the crop rotation, must be modified to prevent longer periods without any soil covering and N uptake. One example is the plowing of temporary pure clover or clover-grass which can lead to relevant nitrate N leaching especially for well-drained soils (Dreymann, 2005). Plowing in late fall has a higher N mineralization potential than hibernating clover-grass and following plowing in spring. Finally, the most important factor to reduce NO_3-N leaching in agriculture is to calculate the N supply according to the plant demand and available mineral-N in the soil. For the practical application this means that mineral-N should be measured to evaluate the potential N leaching before a new crop is sown. Undersown crops can be used to prevent problematic periods in the crop rotation, while competition to the main crop could reduce the main yield in stressful periods.

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Chapter 3
Application of the Bayesian calibration methodology for the parameter estimation in CoupModel

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Abstract

This study provides results for the optimization strategy of highly parameterized models, especially with a high number of unknown input parameters and joint problems in terms of sufficient parameter space. Consequently, the uncertainty in model parameterization and measurements must be considered when highly variable nitrogen losses, *e.g.*, N leaching, are to be predicted. The Bayesian calibration methodology was used to investigate the parameter uncertainty of the process-based CoupModel. Bayesian methods link prior probability distributions of input parameters to likelihood estimates of the simulation results by comparison with measured values. The uncertainty in the updated posterior parameters can be used to conduct an uncertainty analysis of the model output. A number of 24 model variables were optimized during 20,000 simulations to find the 'optimum' value for each parameter. The likelihood was computed by comparing simulation results with observed values of 23 output variables including soil water contents, soil temperatures, groundwater level, soil mineral-N, nitrate concentrations below the root zone, denitrification, and harvested carbon from grassland plots in Northern Germany for the period 1997−2002. The posterior parameter space was sampled with the Markov-Chain-Monte-Carlo approach to obtain plot-specific posterior parameter distributions for each system. Posterior distributions of the parameters narrowed down in the accepted runs, thus uncertainty decreased. Results from the single-plot optimization showed a plausible reproduction of soil temperatures, soil water contents and water tensions in different soil depths for both systems. The model performed better for these abiotic system properties compared to the results for harvested carbon and soil mineral-N dynamics. The high variability in modeled nitrogen-N leaching showed that the soil nitrogen conditions are highly uncertain associated with low modeling efficiencies. Simulated nitrate-N leaching was compared to more general, site-specific estimations, indicating a higher leaching during the seepage-water periods for both simulated grassland systems.

3.1 Introduction

The prediction of nutrient losses under agricultural land use is an important factor for the economic and ecologic evaluation of specific farming systems. The movement of nutrients and pollutants, which can be identical, namely nitrogen (N), but different in their load/concentration, has been concerned with various environmental effects (Lewis et al., 2003). Especially for intensive grassland systems, nitrogen leaching can produce unfavorable risks for surface water and near-surface groundwater. Various methods to quantify the complex interactions between components of the nitrogen balance have been developed, where extensive measurements would be too expensive and difficult (Jovanovic et al., 2008). General estimations of nitrogen losses are mostly based on simple mass balances at field or farm-gate scale. These N budgets measure or estimate the inputs and outputs of nutrients without detailed measurements of losses such as leaching, denitrification and volatilization (OECD, 2001). Such pure behavior imitation of 'black box' approaches is necessary for the operational application of models at catchment scale, even if extrapolation purposes in space and time are limited (Casper, 2002).

Simulation models represent a modern alternative to observations. Greater understanding of nitrogen dynamics in soils at field scale can potentially improve agricultural practices regarding N use efficiency and minimizing pollution. Detailed process knowledge is necessary to evaluate model results. But point measurements or process observations are less useful for optimization and evaluation of models with increasing degree of model abstraction or higher spatial scale (Casper, 2002). Only robust parameterization techniques allow for plausible explanations of system behavior in physically based models. Due to complex transformations of soil N and carbon, many models express this complexity by a high number of input parameters, which implicates the need for a careful model optimization (Pappenberger and Beven, 2006). Until recently, calibration of highly parameterized models was performed by an intensive sensitivity analysis and fitting modeling results to measurements by 'trial and error' procedure until observed values were reproduced well. Several procedures such as single, multiple or sequential parameter calibration procedures to optimize process-based models were tested, but the uncertainty in model input parameters and observations were not taken into account (Reinds et al., 2008). Consequently, only that parameter setting resulting in the best agreement between model and observations was accepted. But several combinations of input parameters may give the same model result, which makes it difficult to define a unique set of input parameters. Optimization methods that include uncertainties in model and measurements are thus to be preferred over 'single best fit' methods without uncertainty assessment.

The Bayesian calibration methods have been used for optimization of forest ecosystems (Van Oijen et al., 2005; Klemedtsson et al., 2008) or watershed models (Vrugt et al., 2006). Bayesian approaches include probability distributions of model input parameters, based on prior assumptions about their magnitude and uncertainty, combined with likelihood estimates of the model results by comparison with observations for model output variables. Consequently, parameter uncertainty can be quantified by this combined information. The updated parameter uncertainty can be used to analyze model output uncertainty. Reinds et al. (2008) defined the Bayesian calibration as a twofold extension of Maximum Likelihood estimation including prior information about input parameters and identifying a single parameter vector with maximum probability and its uncertainty estimate. The Bayesian calibration technique was applied in this study to optimize the CoupModel (Jansson and Karlberg, 2004) on two different grassland systems in Northern Germany. Data on soil temperatures, soil water contents, groundwater (= saturation) level, nitrate-nitrogen (NO_3-N) concentration, soil nitrogen contents, denitrification and harvested carbon were available (Wachendorf et al., 2004; Herrmann, 2005a; Lampe, 2005). Single-plot optimizations were carried out for 24 input parameters to investigate effect of parameter space and start value for each grassland system. The aim of this study was to test the applicability and usefulness of the Bayesian optimization technique for the parameterization of grassland systems. Obtained results could be helpful for parameterization of CoupModel in terms of the complex and uncertain soil N fluxes.

3.2 Materials and methods

3.2.1 Site description and measurements

Measured data were provided by the integrated project 'The nitrogen project: A system approach to optimize nitrogen use efficiency on the dairy farm' located at the experimental farm 'Karkendamm' in Northern Germany and carried out between 1997 and 2003 (Taube and Wachendorf, 2001). Multi-factorial field experiments were conducted to investigate crop quality, soil nitrogen balance, and groundwater quality. The climate at 'Karkendamm' is maritime temperate with a mean annual temperature of 8.6 °C and a mean precipitation of 865 mm year^{-1} (Herrmann et al., 2005a). Investigated grassland plots were dominated by perennial ryegrass (*Lolium perenne* L.) with up to four harvests per year. Two fertilization levels were considered: non-fertilized (N0) and highly fertilized (N300; 300 kg ha^{-1} year^{-1} of mineral-N). Dominating soil types are Podzols (FAO, 2006) with low nutrient storage capacity and high leaching potential. The original soil profile was deep-plowed in 1981 to improve the hydraulic conductivity leading to slanted soil layers between 0.27 and 0.80 m (Scholz, 1999). Sand contents varied between 85.7% and 93.0% up to a depth of one meter. Total organic carbon was highest in the upper soil profile with 3.8–5.6%, just as the total N with 0.21–0.27%. Available measurements are listed in *Table 3.1* and were used to assess the CoupModel performance by comparing these observations with corresponding model results. In addition to measured soil water contents observed with TDR sensors and gravimetric technique, averaged soil water tensions in 30, 50, and 70 cm depth of the mown grassland were used to validate soil water conditions. Measurements were taken with puncture tensiometers with a rubber septum at the top during summer 1998 and 1999. Further information about data acquisition can be derived from Conrad and Fohrer (2009c). Observed soil solution concentrations can vary considerably, and measurement uncertainty is affected most likely by the spatial variability within the plot (Reinds et al., 2008). De Vries et al. (1999) reported a spatial variability of measured soil solution concentrations between 20–60% depending on depth and type of ion in forest soils from the Netherlands. In Reinds et al. (2008), an uncertainty of 30% was used for major ions at 40–60 cm depth for the Dutch forest plots. For low concentrations that are often measured for NO_3-N or aluminum, the measurement uncertainty is probably higher than 30%. Harmel et al. (2006) presented literature data about the uncertainty in sampling, preservation and analysis of solved nitrogen species in water samples. The error of solved NO_3-N varied between −47% and −14%, when samples were refrigerated and analyzed within 54 h. The uncertainty in the laboratory analysis can range from ±75% to 400% for NO_3-N, while the colorimetric technique showed error ranges from −4% to 9%. In this study, we assumed a relative error of ±20% for the measured variables except for the NO_3-N concentration in the non-fertilized grassland (relative error: ±50%). An absolute error was assumed for the soil temperatures with ±1 °C according to manufacturer's information on the temperature sensors and for the groundwater level with ±0.05 m.

Table 3.1: Available measurements at the 'Karkendamm' site (Wachendorf et al., 2004), used for stochastic optimization.

Variable	**Depth (m)**	**Measuring period**	**Numbers of samples**
Soil temperature (°C)	0.05, 0.10, 0.15	1997−2002	1648
Soil water content (Vol.%)	0.10, 0.30, 0.40, 0.50, 0.60, 0.70, 0.80	1998−2002	20−198
Groundwater level (m)		1997−2002	146
NO_3-N concentration (mg N L^{-1})	0.60	1997−2002	995 (N0), 952 (N300)
Harvested carbon (g C m^{-2})	above ground	1997−1999	3 (N0), 0 (N300)[a]
Soil mineral-N (SMN) (g N m^{-2})	0−0.30, 0−0.60, 0−0.90	1999−2002	11−16
Soil NO_3-N (g N m^{-2})	0−0.30, 0−0.60, 0−0.90	1999−2002	11−17
Soil NH_4-N (g N m^{-2})	0−0.30, 0−0.60, 0−0.90	1997−2002	19−24
Denitrification (g N m^{-2})	non-fertilized plot	Apr.−Jul. 2001	32

[a] N0: additional estimates for 2000 and 2001; N300: estimated from harvested clover-grass (highly fertilized).

The NO_3-N leaching below the rooting zone (> 60 cm) in the experimental data set from 'Karkendamm' was not measured directly but calculated as a product of the averaged NO_3-N concentration and an estimated seepage-water amount according to the climatic water balance equation (DVWK, 1996). This approach presented by Büchter (2003) is simple but best practice when water balance conditions can only be estimated and was called further model 'Büchter'. In our study, results of CoupModel and model 'Büchter' were compared regarding the calculations for seepage-water amount and NO_3-N leaching.

3.2.2 CoupModel setup

CoupModel (Jansson and Karlberg, 2004) is an ecosystem process model used to calculate coupled heat, water, carbon, and nitrogen fluxes under one-dimensional, unsaturated soil conditions. Several plant covers can be defined above the horizontal layered soil profile, where the Richards' equation is solved for water flow and the Fourier's law of diffusion is used for heat fluxes. Lower boundary condition can be defined as free drainage or saturated. Potential transpiration was calculated from Penman's combination equation in the form given by Monteith (1965). The surface and aerodynamic resistance values were dependent on indices for the plant and leaf area, where these vegetation properties were calculated from the dynamic above ground biomass development. Compensatory water uptake by plant roots determined actual transpiration, where effects of soil temperature and salt on water uptake were ignored. Carbon and nitrogen dynamics were regulated by several plant and soil compartments linked by transfer and decay coefficients such as for biomass, litter or soil organic pools. Further information on nitrogen dynamics in soil and plant can be obtained in Jansson and Karlberg (2004). The CoupModel has been applied since 2002 for roadsides (Lundmark, 2008), forests (Norman et al., 2008), and arable ecosystems (Karlberg et al., 2007; Zhang et al., 2007; Conrad and Fohrer, 2009a,c) at the plot scale. Major changes in the model structure associated with parameter uncertainty have happened since 2007, where the Bayesian (Klemedtsson et al., 2008) and the GLUE approach (Lundmark, 2008) were introduced and tested. Following the results of sensitivity analysis in Conrad and Fohrer (2009a,c), the majority of input parameters was fixed at pre-defined values in this model setup. The remaining 24 parameters were selected for the stochastic optimization (*Table 3.2*). The first parameter in *Table 3.2*, *i.e.*, *ThScaleLog(1)*, regulates soil heat flow from the uppermost soil layer. The other parameters are responsible for biotic system properties such as plant development, nutrient uptake, mineralization, nitrification, and denitrification. The parameter space was defined by minimum (Min) and maximum (Max) values based on plausible reasoning. We have chosen mainly soil biotic parameters because they were highly uncertain due to small and site-specific data sets. These parameters were most sensitive on the NO_3-N leaching below the rooting zone.

3.2.3 Calibration method

The CoupModel was optimized using the Bayesian calibration applied by Van Oijen et al. (2005). The posterior probability distribution $p(\theta/D)$ for the parameter vector θ was derived by the likelihood function $p(D/\theta)$ and the prior distribution $p(\theta)$ of the parameter vector according to:

$$p(\theta|D) = c * p(D|\theta) * p(\theta) \tag{3.1}$$

where the value of *c (=1/p(D))* was independent. The likelihood $p(D/\theta)$ was computed assuming measurement errors were Gaussian and uncorrelated:

$$\log p(D|\theta) = \sum_{i-1}^{n} \left(-0.5 \left(\frac{O_i - S_i}{M_i} \right)^2 - 0.5 \log(2\pi) - \log M_i \right) \tag{3.2}$$

where the S_i are model results and O_i observations, n is the number of observations and M_i is the standard deviation or error of measured values. The logarithm of the data likelihood (log $p(D/\theta)$= '*LogLi*') was used to avoid rounding errors when likelihood values were decreasing with increasing number of data points (Klemedtsson et al., 2008). We assumed that structural errors were ignored and thus estimates of model output uncertainty showed only the contribution from parameter uncertainty (Reinds et al., 2008). A numerical solution of Eq. 3.2 was often carried out in the form of a Markov-Chain-Monte-Carlo (MCMC) approach with a large number of simulations.

The Metropolis-Hastings random walk, a simple MCMC algorithm, was used to calculate posterior probabilities for an appropriate number of parameter combinations by randomly stepping through the parameter space. An adequate sampling during MCMC was achieved by combination of the number of steps and the step size. If for a new candidate point the product of the prior probability and the likelihood was higher than for the current point, the new point was accepted. The total '*LogLi*' was derived from the sum of all '*LogLi*' values of the validation variables in *Table 3.1*. This procedure resulted in a chain of points in the multi-dimensional parameter space, where the first 10% of the runs were ignored. The remaining chain includes all accepted parameter points, which were used to calculate the posterior distribution of each parameter and correlation and covariance matrices.

In practical application, each grassland system was optimized separately in a 'single-plot' calibration. The posterior distribution with its mean value and variability were derived for each optimized parameter depending on the selected output variables. A number of 20,000 simulation runs were carried out within the same parameter space for the tested systems according to *Table 3.2*.

Table 3.2: Parameters selected for the stochastic optimization in CoupModel and their initial value and uncertainty ranges.

Property	**Description**	**Start value**	**Ranges**		**Unit**
			Min	**Max**	
Soil thermal properties:					
ThScaleLog(1), $x_{hf(1)}$	Scaling coefficient for the thermal conductivity in soil layer 1	0.5	−0.5	1	–
Plant specific properties:					
Specific LeafArea, $p_{l,sp}$	Leaf mass per unit leaf area	6	4	8	g C m^{-2}
RadEfficiency, ε_L	Radiation use efficiency	3.5	2	4	g DW MJ^{-1}
NUptFlexibilityDeg, $n_{Uptflex}$	Compensatory N uptake from soil	0.3	0.1	0.5	–
NUptMaxAvailFrac, f_{Nupt}	Fraction of mineral-N for uptake	0.04	0.01	0.1	d^{-1}
Decomposition and mineralization:					
CN ratio microbes, cn_m	C:N ratio in microbes	10	9	11	–
Eff Litter1, $f_{e,l1}$	Efficiency of decay of litter 1	0.15	0.1	0.3	d^{-1}
Eff Litter2, $f_{e,l2}$	Efficiency of decay of litter 2	0.15	0.1	0.3	d^{-1}
Eff Humus, $f_{e,h}$	Efficiency of decay of humus	0.6	0.4	0.8	d^{-1}
HumFracLitter1, $f_{h,l1}$	Fraction of C and N from litter 1 to humus	0.2	0.1	0.4	d^{-1}
HumFracLitter2, $f_{h,l2}$	Fraction of C and N from litter 2 to humus	0.2	0.1	0.4	d^{-1}
Init H N Tot, $i_{h,N}$	Initial total N in humus	500	400	600	g N m^{-2}
Init L1 N Tot, $i_{l1,N}$	Initial total N in litter 1	5	4	6	g N m^{-2}
Init L2 N Tot, $i_{l1,N}$	Initial total N in litter 2	1	0.5	2	g N m^{-2}
RateCoefHumus, k_h	Coefficient for the decay of humus	5e−5	1e−5	1e−4	d^{-1}
RateCoefLitter1, k_{l1}	Coefficient for the decay of litter 1	0.1	0.01	0.5	d^{-1}
RateCoefLitter2, k_{l2}	Coefficient for the decay of litter 2	0.1	0.01	0.5	d^{-1}
RateCoefSurf L1, l_{l1}	Fraction of above ground residues to litter 1	1	0.05	1	d^{-1}
RateCoefSurf L2, l_{l2}	Fraction of above ground residues to litter 2	1	0.05	1	d^{-1}
Nitrification process:					
NitrateAmmRatio, $r_{nitr,amm}$	NO_3:NH_4 ratio for nitrification	1	0.1	1.5	–
NitrificSpecificRate, n_{rate}	Specific nitrification rate	0.1	0.08	0.15	d^{-1}
Denitrification process:					
DenitDepth, d_z	Depth where the denitrification capacity ceases	−1.5	−1.6	−1.2	m
DenitNitrateHalfSat, $d_{NhalfSat}$	Effect of NO_3-N concentration on denitrification	10	8	12	mg N L^{-1}
DenitPotentialRate, d_{pot}	Potential denitrification rate	0.1	0.05	0.2	g N m^{-2} d^{-1}

DW — dry weight

3.3 Results

3.3.1 Posterior parameter distributions

The Bayesian calibration provided the joint posterior distribution, which contained also correlations between parameters. In this study, we focused on the marginal distributions expressed as posterior mean and coefficient of variation (*CV*) for the individual parameters. The variability or dispersion of a parameter was expressed as *CV* (= standard deviation *SD* divided by the mean *M*), which was low in case of CV < 1 (100 %). Broad prior distributions should narrow down with low *CV* values leading to reduced parameter uncertainty when measurements were conclusive. For most parameters, differences between the posterior mean occurred for both systems forced by the observations according to Eq. 3.2, even though same prior mean values were assumed (*Table 3.3*).

Table 3.3: Prior mean, posterior mean and coefficient of variation (CV) of the optimized parameters for both grassland plots at the 'Karkendamm' site.

Property	**Prior mean**	**Non-fertilized plot (N0)**		**Highly fertilized plot (N300)**	
		Post mean	***CV* (%)**	**Post mean**	***CV* (%)**
Soil thermal properties:					
ThScaleLog(1), $x_{hf(1)}$	0.25	−0.50	0.9	0.66	1.5
Plant specific properties:					
Specific LeafArea, $p_{l,sp}$	6	6.8	0.6	4.0	0.6
RadEfficiency, ε_L	3	3.7	0.3	3.9	0.3
NUptFlexibilityDeg, $n_{Uptflex}$	0.3	0.32	1.0	0.38	2.0
NUptMaxAvailFrac, f_{Nupt}	0.055	0.006	1.4	0.02	3.5
Decomposition and mineralization:					
CN ratio microbes, cn_m	10	10.6	0.1	10.3	0.2
Eff Litter1, $f_{e,l1}$	0.20	0.23	1.1	0.10	2.7
Eff Litter2, $f_{e,l2}$	0.20	0.15	1.4	0.11	1.1
Eff Humus, $f_{e,h}$	0.60	0.55	1.0	0.78	1.1
HumFracLitter1, $f_{h,l1}$	0.25	0.19	0.9	0.21	1.9
HumFracLitter2, $f_{h,l2}$	0.25	0.23	1.5	0.20	3.1
Init H N Tot, $i_{h,N}$	500	505	0.4	481	0.7
Init L1 N Tot, $i_{l1,N}$	5	5.2	0.2	4.6	0.3
Init L2 N Tot, $i_{l1,N}$	1.25	0.63	0.1	0.59	3.3
RateCoefHumus, k_h	5.5e−5	5.9e−5	0.6	6.6e−5	1.3
RateCoefLitter1, k_{l1}	0.255	0.18	2.0	0.154	5.9
RateCoefLitter2, k_{l2}	0.255	0.303	2.4	0.119	3.1
RateCoefSurf L1, l_{l1}	0.525	0.85	1.0	0.920	0.6
RateCoefSurf L2, l_{l2}	0.525	0.59	3.0	0.930	1.0
Nitrification process:					
NitrateAmmRatio, $r_{nitr,amm}$	0.80	1.38	0.5	1.07	1.9
NitrificSpecificRate, n_{rate}	0.115	0.087	0.5	0.100	0.5
Denitrification process:					
DenitDepth, d_z	−1.40	−1.49	0.4	−1.54	0.4
DenitNitrateHalfSat, $d_{NhalfSat}$	10	9.8	0.2	10.7	0.2
DenitPotentialRate, d_{pot}	0.125	0.051	3.6	0.136	1.8

Parameters with similar posterior mean values indicated a low sensitivity on individual parameters from the data behind for each system. This was found, *e.g.*, for the factor of the compensatory N uptake from different soil layers (*NUptFlexibilityDeg*), the C:N ratio of the microbes (*CN ratio microbes*), the decay efficiency of litter pool 2 (*Eff Litter2*), the carbon (C), and N fractions transferred from litter pools 1 and 2 to the humus pool (*HumFracLitter1*, *HumFracLitter2*), and the initial N content in litter pool 2 (*Init L2 N Tot*). In this study, the *CV* varied between 0.1% and 3.6% emphasizing a low variability of selected parameter values that were robust during optimization. The highest difference between the two grassland systems was found for the scaling factor of the thermal conductivity *ThScaleLog(1)*, but with minor influence on the model efficiency (*RMSE*, R^2) for soil temperatures (*Table 3.4*). Remaining parameters differed in their posterior mean values between both systems, especially for plant specific parameters that were linked to the biomass production (*RadEfficiency*, *Specific LeafArea*), and for the denitrification (*DenitPotentialRate*). In general, the dispersion of the parameters (*CV*) was higher for the N300 than for the N0 plot.

3.3.2 Comparison with measurements

The total '*LogLi*' according to Eq. 3.2 was used as objective function to find the accepted simulations among 20,000 runs. *Table 3.4* shows the resulting modeling efficiency of the 23 validation variables for both systems. The root mean squared error (*RMSE*) and the coefficient of determination (R^2) were used to compare simulated mean values with the mean value of the measurements.

Table 3.4: R^2 and RMSE values for the comparison between simulated mean of the accepted runs and the observed values.

Efficiency measure	***RMSE***		***R^2***	
System	**N0**	**N300**	**N0**	**N300**
Soil temperature (°C days)				
0.05 m	1.64	1.46	0.93	0.94
0.10 m	1.38	1.26	0.95	0.95
0.15 m	1.25	1.11	0.95	0.96
Soil water content (Vol.%)				
0.10 m	6.45	5.52	0.60	0.59
0.30 m	6.73	5.05	0.34	0.51
0.40 m	3.04	3.83	0.85	0.91
0.50 m	10.66	4.77	0.35	0.55
0.60 m	6.85	2.23	0.95	0.94
0.70 m	12.6	7.58	0.41	0.57
0.80 m	7.56	5.18	0.43	0.72
Soil water tension (hPa)[a]				
0.30 m	94	448	0.44	0.43
0.50 m	21	349	0.30	0.19
0.70 m	20	156	0.25	0.10
Groundwater level (m)				
Nearest point	0.15	0.21	0.41	0.39
Soil mineral-N (g N m^{-2})				
0–0.3 m	1.12	8.89	0.12	0.06
0–0.6 m	2.29	10.37	0.28	0.01
0–0.9 m	2.66	7.69	0.0005	0.03
NO_3-N (g N m^{-2})				
0–0.3 m	0.54	6.69	0.01	0.04
0–0.6 m	0.52	6.21	0.006	0.0005
0–0.9 m	0.54	8.45	0.03	0.14
NH_4-N (g N m^{-2})				
0–0.3 m	1.37	2.79	0.24	0.03
0–0.6 m	2.43	1.80	0.31	0.01
0–0.9 m	2.83	1.93	0.20	0.04
NO_3-N concentration (mg N L^{-1})				
Seepage-water period	3.37	22.1	0.02	0.14
Denitrification (g N m^{-2})				
(total)	0.0004	0.002	0.19	0.21
Harvested carbon (g C m^{-2})				
(cumulative)	71	730	0.27	0.008

[a] Not optimized during the Bayesian calibration; posterior comparison to validate soil water conditions.
R^2: coefficient of determination (1 or −1 [0; 1 or −1]; *RMSE*: root mean square error (0 [−∞; +∞]).

Soil temperatures were simulated well for all depths with $R^2 > 0.93$. The *RMSE* varied between 1.11 and 1.64 with lowest deviations for the depth of 0.15 m in both systems, but with better values for N300 than N0. The agreement between modeled and observed soil water contents differed inside soil with R^2 values from 0.43 (depth of 0.30 m) to 0.95 (depth of 0.60 m). The *RMSE* value was lowest in the depth of 0.40 m, and higher *RMSE* > 10 were found for the N0 system in depths of 0.50 and 0.70 m. The groundwater level agreed satisfactorily with measurements from the nearest observation point with R^2 values between 0.41 (N0) and 0.39 (N300). However, the model could not match the observed dynamic for both systems. But a lower *RMSE* value was achieved for the N0 than the N300 plot. Soil water tensions, which represented mean values for the mown grassland plot during summer 1998 and 1999, were compared with model results for both fertilization levels in 30, 50, and 70 cm depth (*Fig. 3.1*).

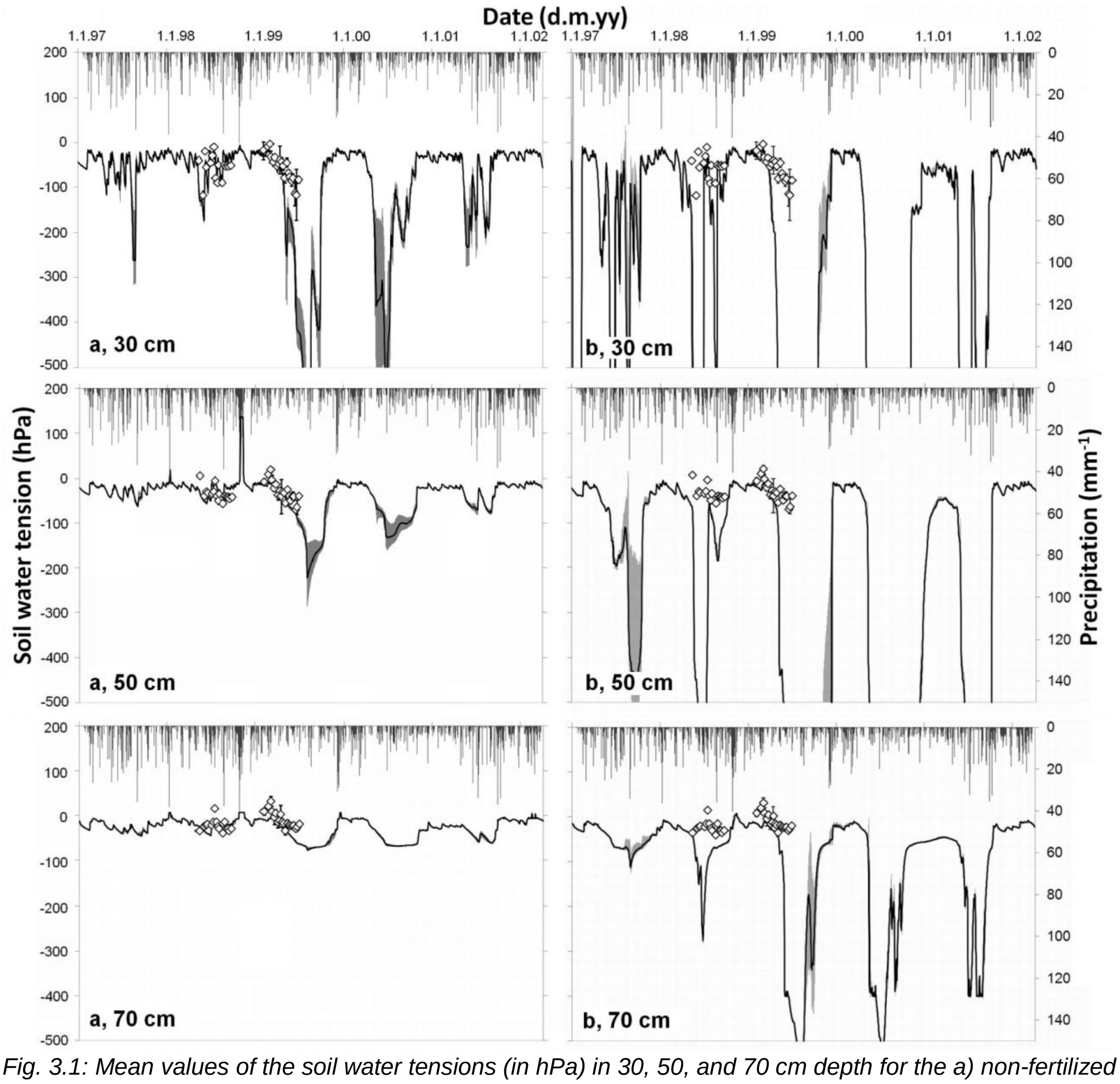

Fig. 3.1: Mean values of the soil water tensions (in hPa) in 30, 50, and 70 cm depth for the a) non-fertilized and b) highly fertilized mown grassland. Simulated results (solid line) are shown within the 5th and 95th percentiles and observations (◇) of the mown grassland with their standard deviations.

Model results were highly variable with soil water tensions between +146 hPa (saturated) and −2000 hPa (≈ pF 3.3 in 30 cm depth). Contrary to the model outcome, measured soil water tension was lowest with −117 hPa (≈ pF 2.1) at a depth of 30 cm, where also the best agreement between observation and model was achieved regarding R^2 values of 0.44 (N0) and 0.43 (N300) (see *Table 3.4*). *RMSE* values decreased with increasing depth, which indicated lower variability in the modeled results for deeper soil layers. Uncertainty was higher during summer than spring in both model and observation. Differences between CoupModel and field data were based on model limitations regarding slanted soil layers and the used water retention curve from the laboratory investigation. Fixed parameter values for each soil layer were possibly not representing heterogeneous field conditions with highly variable water contents within the field replicates (Karrasch, 2005). Secondly, measurements taken with a puncture tensiometer were biased; the technique had to be installed carefully to prevent pressure changes in the tube during needle injection. The accuracy of the device was not as high as in systems with an in-site manometer or pressure sensor (Smith and Mullins, 2001). Systematic underestimation of actual tensions by up to 23 hPa was found for single-puncture tensiometer readings with a maximum error of approx. 10% (Greenwood and Daniel, 1996).

The comparison of daily simulated mean values for the soil mineral-N (SMN) with the measurements showed only low coefficients of determination $R^2 < 0.31$ (*Table 3.4*), which did not suggest some evidence for an under- or overestimation. SMN contents between 0–0.90 m are shown in *Fig. 3.2* indicating an overestimation of both the NH_4-N in the N0 plot and the NO_3-N content in the N300 system, respectively. In general, *RMSE* values were lower for the non-fertilized plot than for the N300 (*Table 3.4*) due to overestimations in CoupModel associated with the NO_3-N content in the highly fertilized system. Modeled peaks in the right charts of *Fig. 3.2* can identify the applied mineral fertilizer in the N300 plot. The few observations indicated only that the SMN content in spring was higher than in autumn. Deviations between modeled and measured results were possibly caused by an inadequate plant-N uptake and soil nitrogen transformation (*e.g.*, denitrification; see below) in CoupModel during summer. Consequently, the total SMN was also overestimated by CoupModel indicating much more uncertainty in the prediction of soil N dynamics of highly fertilized systems due to the input of mineral nitrogen. CoupModel considered mineral fertilizer input on the soil surface, where the fraction of NH_4-nitrogen (the rest was NO_3-N) and specific dissolution rate of the applied commercial fertilizer were defined. In our study, fixed values for fractioning and dissolution rate were used in CoupModel, which was maybe not representative for the applied $Ca(NH_4NO_3)$ fertilizer. Further reason for the overestimation of modeled NO_3-N, which was not observed for NH_4-N, could be the uptake of mineral-N by the grass vegetation that prefers ammonium (Maci et al., 2007). The denitrification process is also a possible sink for soil NO_3-N. This gaseous nitrogen loss was very likely underestimated in the N300 system by CoupModel. The NO_3-N content was reproduced better in the N0 plot than the NH_4-N content, which was possibly caused by an underestimated nitrification rate. Reason for that could be found in the soil NO_3-N concentrations that were seen as very uncertain with highly variable observations (*Fig. 3.3*).

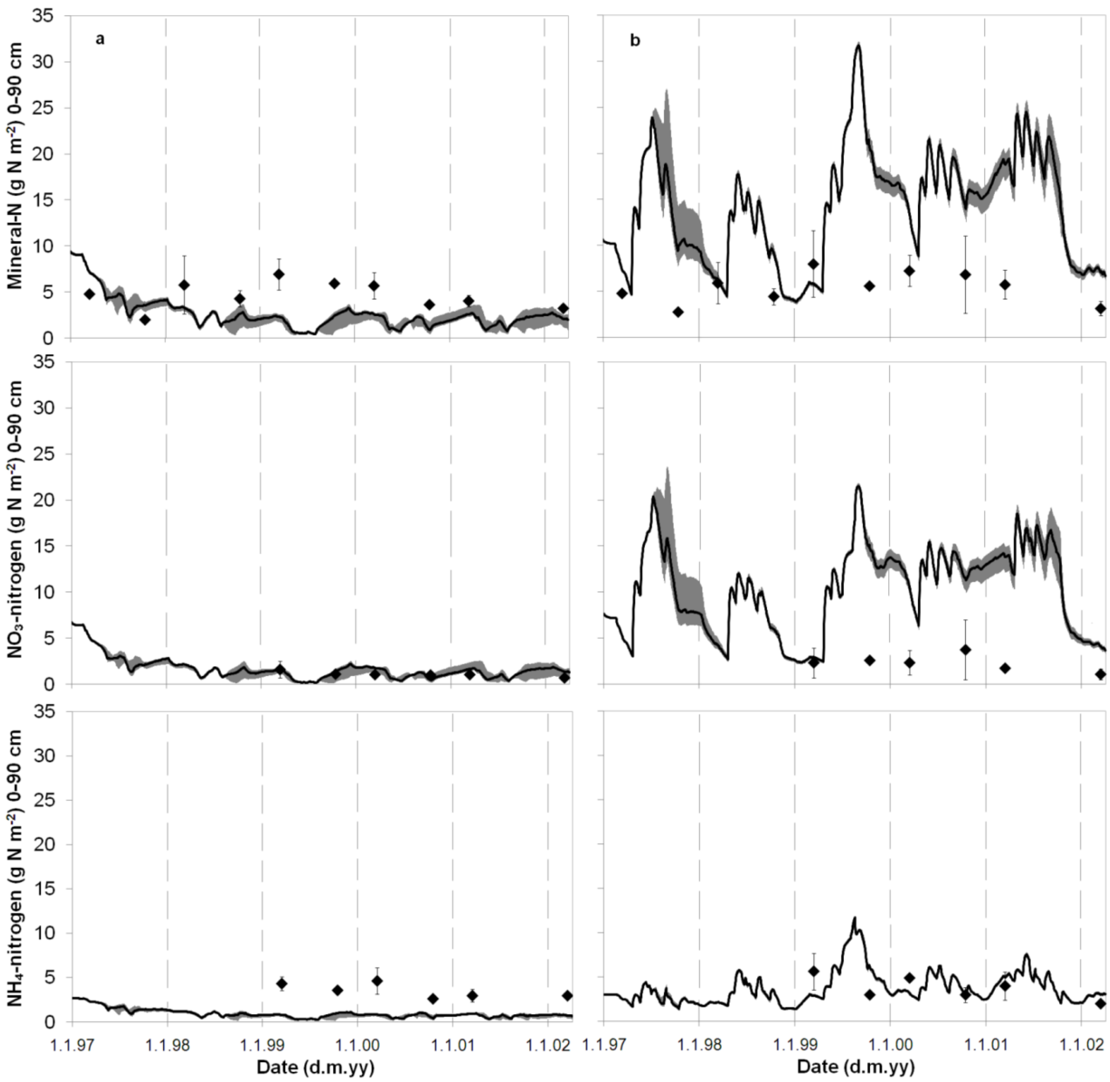

Fig. 3.2: Mean values of the total Mineral-N (SMN), NO_3-nitrogen and NH_4-nitrogen in the a) non-fertilized and b) highly fertilized grassland plots. Simulated results (solid line) are shown within the 5th and 95th percentiles and observations (◆) with their standard deviations.

Concerning this, the simulated mean of the NO_3-N concentration was forced to be within the standard deviation of the measurements during modeling. For the N0 system the simulated mean was only 94% (4.6 mg NO_3-N L^{-1}) of the measured mean (4.9 mg NO_3-N L^{-1}) indicating that too much NH_4-N remained in the soil profile. The R^2 value of the averaged NO_3-N concentrations was higher for the N300 (0.14) than for the N0 plot (0.02), which was maybe caused by less variable observations from day to day in the highly fertilized system. It can be discussed if the R^2 value is an adequate performance measure for soil solution concentrations without considering data variability in model and measurements. The difference between modeled (24 mg NO_3-N L^{-1}) and observed mean (11 mg NO_3-N L^{-1}) of the N300 plot amounted to 125% demonstrating an overestimation of simulated soil NO_3-N. The *RMSE* value was six times lower in the N0 plot, indicating also a good agreement for the non-fertilized system. One important process to reduce soil NO_3-N in CoupModel is the denitrification process, which was compared with measurements from a temporary cutting period of a non-fertilized grassland plot (*Fig. 3.4*).

The *RMSE* from the N0 system was lower than for N300, while the R^2 values were similar for this short period. In *Fig. 3.3*, the N300 plot shows a highly variable denitrification amount according to the input of mineral-N and humid winter conditions. The denitrification decreased during summer due to lower soil water contents and significant N uptake for biomass production. Modeled annual harvested C was compared with calculated values derived from observed pure grass biomass between 1997 and 1999 and estimations for 2000 and 2001 for the N0 plot (Ingwersen, 2002; see *Table 3.1*).

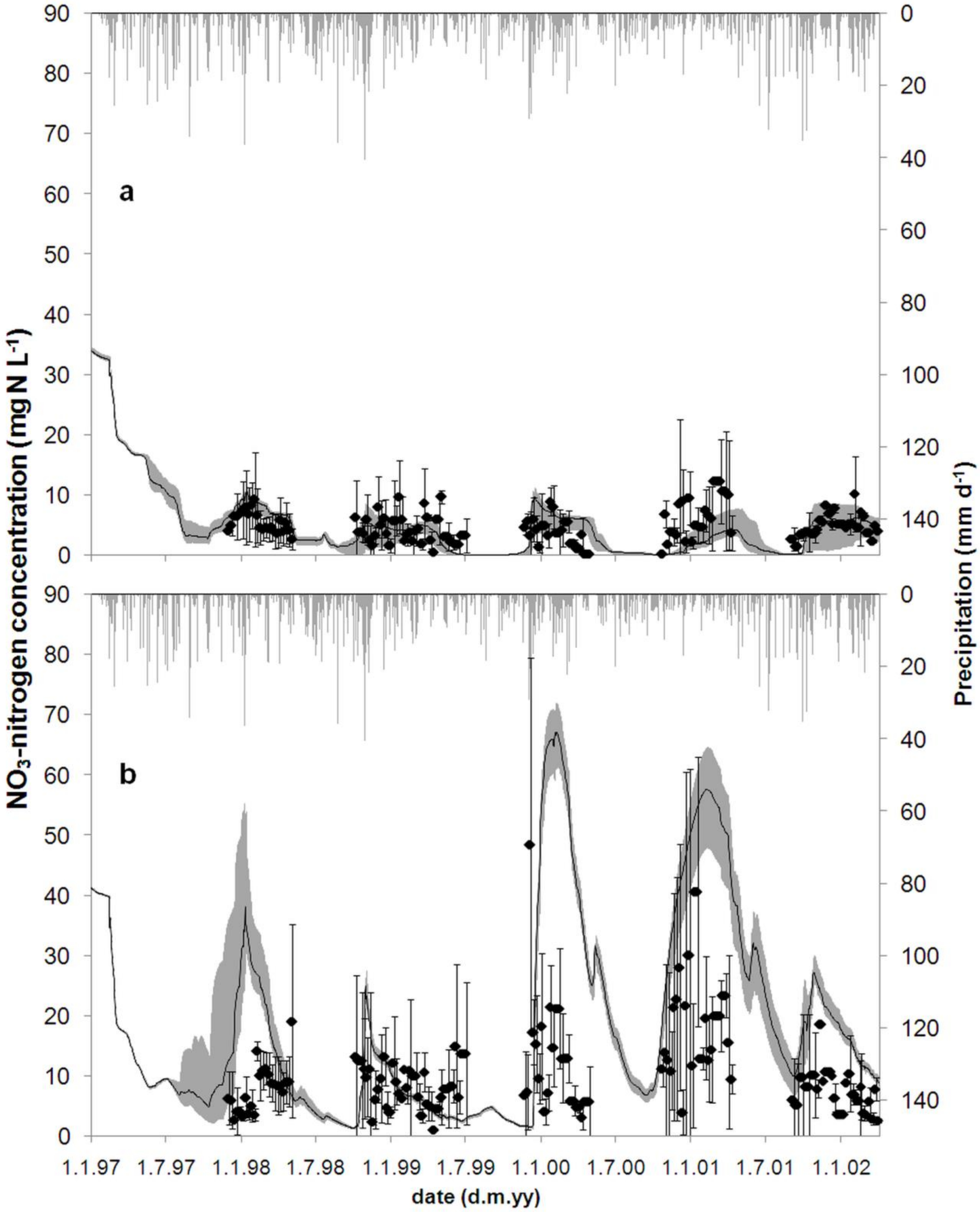

Fig. 3.3: Mean values of the soil NO_3-N concentration in 60 cm depth for the a) non-fertilized and b) highly fertilized grassland plots. Simulated results (solid line) are shown within the 5th and 95th percentiles and observations (♦) with their standard deviations.

The comparisons between harvested C for the N300 plot was based on estimations from harvested clover-grass biomass fertilized with 30 kg N ha^{-1} year^{-1} (Trott, 2003). The agreement was better for the N0 plot (R^2 = 0.27) than for the N300 plot (R^2 = 0.008) indicating that the model was not able to reproduce realistic annual harvest amounts in both cases (*Table 3.4*). Biomass production was overestimated because the N uptake by plants was much less important than a good reproduction of measured SMN contents. The comparison with estimates from harvested clover-grass, which showed unstable harvest yields with increasing N fertilization due to the decline of clover (Herrmann et al., 2005a), could be a second reason for the low agreement regarding the harvested C in the N300 system.

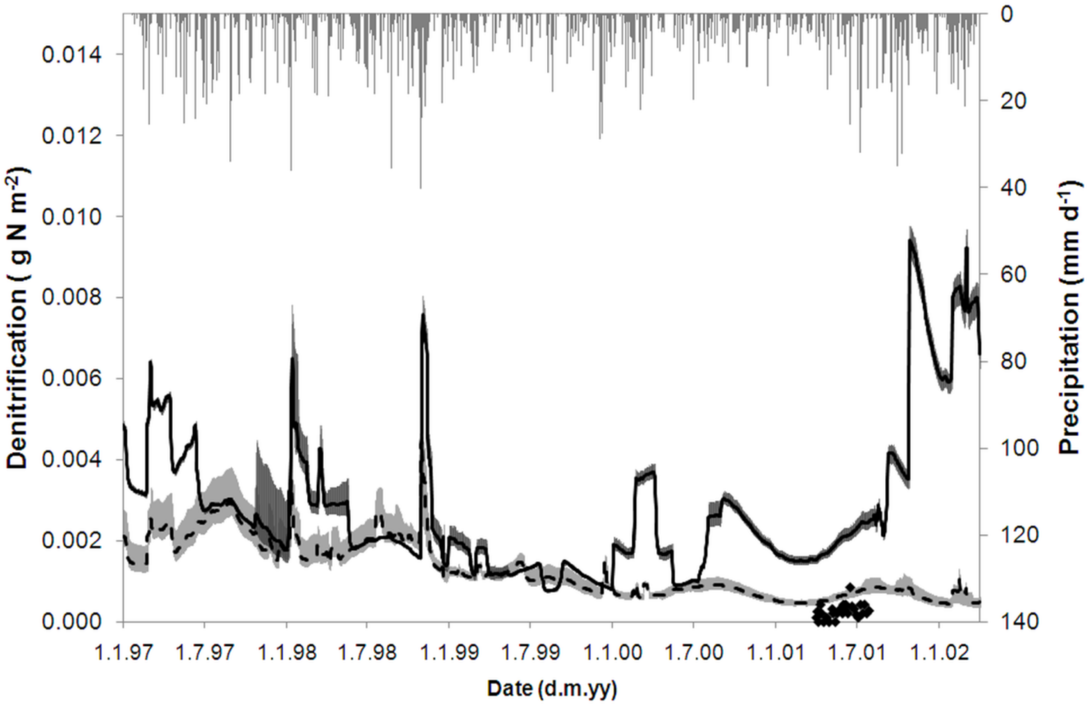

Fig. 3.4: Total denitrification in the non-fertilized (dashed line) and highly fertilized (solid line) grassland plots. Simulated results are shown within the 5th and 95th percentile and observations (♦) of a non-fertilized system.

In *Fig. 3.5*, simulated NO_3-N leaching below the rooting zone located between 60 and 65 cm depth was compared to the model 'Büchter' (Büchter, 2003) for the seepage-water periods. For the non-fertilized plot N0, CoupModel calculated an averaged leaching amount of 18 kg NO_3-N ha^{-1} compared to 10 kg NO_3-N ha^{-1} by the model 'Büchter'. Averaged NO_3-N leaching for the highly fertilized system in CoupModel added up to 49 kg N ha^{-1}, which was 63% higher than the leaching of 30 kg N ha^{-1} in the model 'Büchter'. Major differences were found in the dynamic of the leaching, which showed more peaks in the CoupModel realizations and in the drainage water amount. CoupModel accounted a 65% higher drainage water amount for the N0 plot and 16% lower for the N300 system, compared to a standard value of 180 mm by the model 'Büchter'. An additional reason for an underestimation by the model 'Büchter' is the failure of the suction cups methodology to capture the whole NO_3-N leachate in available soil pores. This sampling method for soil water solutions is widely used in unstructured soils, but it showed a tendency to underestimate N concentrations on an average of 8% compared to free drainage experiments (Erhart et al., 2007).

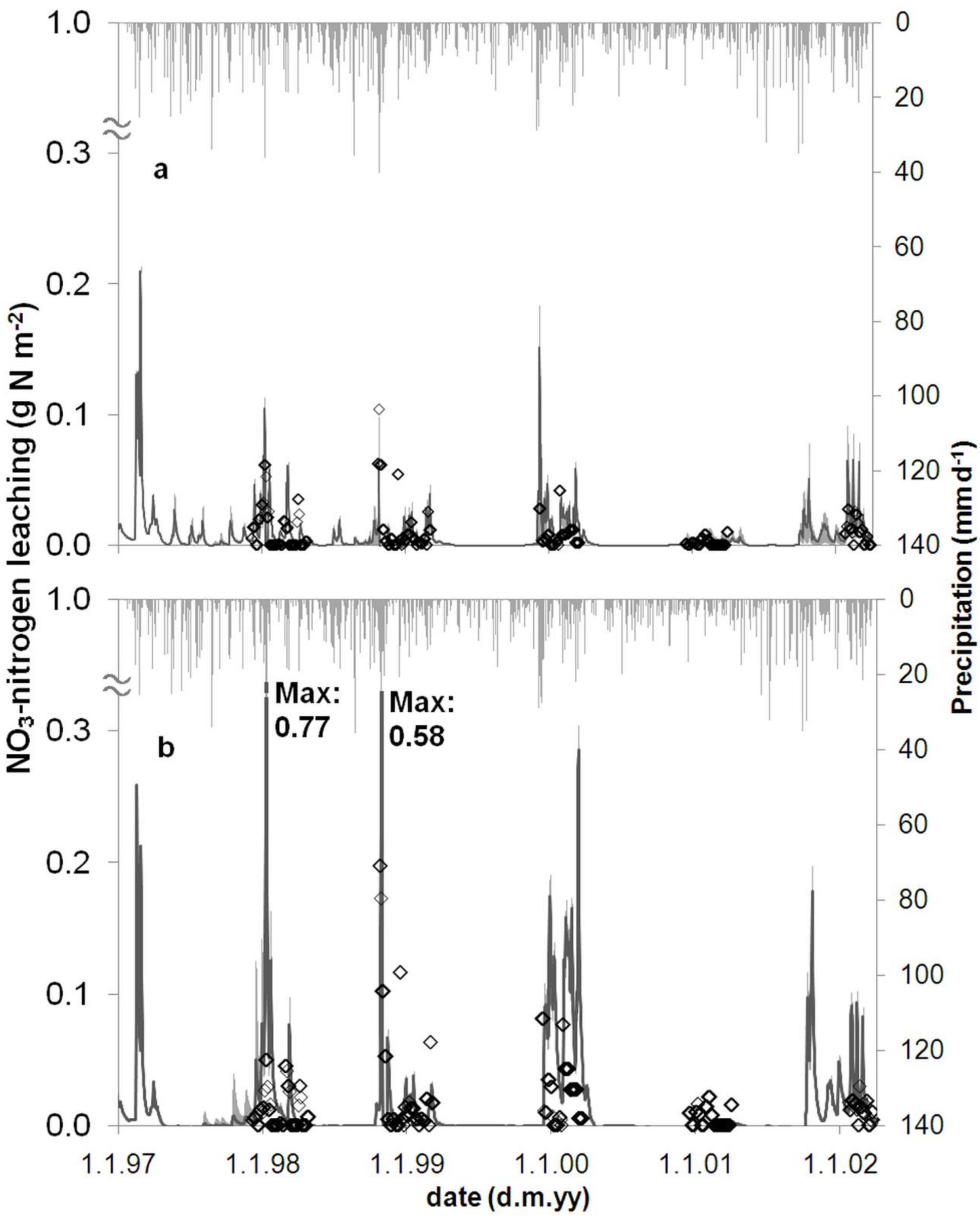

Fig. 3.5: NO_3-N leaching below the rooting zone (60−65 cm) in the a) non-fertilized and b) highly fertilized grassland plots. CoupModel results (solid line) are shown within the 5th and 95th percentiles compared to the model 'Büchter' (Büchter, 2003) (◇).

Reasons for this deviation are possible anion absorption and the small cross-sectional area of the ceramic cups, which is maybe not representing spatial soil variability. An error of ±30% or more should be expected in field studies, literature values must be handled with care, unless a representative number of ceramic suction cups are installed. Accordingly, NO_3-N leaching has to be interpreted carefully, if obtained with this sampling method. Korsaeth et al. (2003) modeled the NO_3-N leaching for grassland in Norway indicating that 5–23% of the N input can be leached out depending on soil, 98% of this amount was NO_3-N. In our study, where an additional atmospheric-N deposition of 20 kg N ha^{-1} $year^{-1}$ was assumed, the NO_3-N leaching of the non-fertilized plot amounted to 90% of the N input and approx. 15% for the N300 system. Changes in the SMN storage were not considered in this simple N balance.

3.4 Conclusions

The understanding of ecosystem processes involves an increasing model complexity with non-linear structural equations and useful methods for automated parameter estimation. Uncertainties in model parameterization and measurement have to be considered, but in practice rigorous uncertainty analysis is still rare (Stow et al., 2007). Model applications often fail to do an uncertainty assessment because many ‘competing methods’ make it difficult to choose the most appropriate method and interpret the results (Pappenberger and Beven, 2006). Stochastic optimization can help to diminish the difficulties in terms of parameter estimation. In this paper, the applicability of the Bayesian calibration technique was demonstrated for the parameter optimization in the CoupModel. Efficient estimates of the most-likely parameter set and its underlying frequency distribution were provided during optimization runs. We performed two case studies demonstrating effects of multiple validation data on the parameter uncertainty. In spite of considerable differences between model and measurements, the prediction uncertainty associated with the parameter estimates was low, indicating that the main part of the uncertainty originated from the residuals between measurements and model predictions. Satisfying results were found for modeled abiotic properties, *i.e.*, soil temperature, water content, water tension, and groundwater level. On the whole, CoupModel results agreed better with observations for non-fertilized than highly fertilized conditions regarding soil N dynamics and harvested C. Uncertainty was highest for modeled soil NO_3-N concentrations in both systems; plausible results were also found for leached NO_3-N. One reason for the mismatch between model and measurements could be that simulated results were based on one soil profile, whereas observations were taken over a larger area ranging from few centimeters (*e.g.*, installed equipment for soil temperature and water content) to several meters (*e.g.,* mean values for harvested C and SMN). Further work must be done to understand the limitation of this approach because of its subjective choice of the probability distribution and likelihood measure.

Acknowledgments

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Chapter 4
A test of CoupModel for assessing the nitrogen leaching in grassland systems with two different fertilization levels

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Abstract

Land-use and crop-biomass development influence water and nutrient dynamics in soils. Nitrate-N leaching rises with increasing mineral-N input during seepage-water periods in sandy soils. Leaching of N was simulated for two grassland treatments (N0: unfertilized; N300: highly fertilized: 300 kg mineral-N ha^{-1} year^{-1}) with CoupModel. Parameter uncertainty was considered by an automated calibration based on the General Likelihood Uncertainty Estimation (GLUE) approach. The results of this optimization approach showed a realistic reproduction of abiotic and biotic patterns of the system. Modeled abiotic parameters, *i.e.*, soil temperatures and water contents in different soil depths, led to plausible results with minor differences between fertilization levels and some respect for discrepancies due to heterogeneous soil conditions. Groundwater levels were slightly underestimated by CoupModel with a smoother dynamic than measured in both treatments. CoupModel provided plausible results for nitrate-N concentrations below the rooting zone at 60 cm depth with higher uncertainty ranges than standard deviations of the measurements. Simulated nitrate-N concentrations of the unfertilized grassland confirmed the measurements, and no potential environmental risk for water bodies existed according to the standards of the European Drinking Water Directive. The model reproduced satisfactorily the observations for the N300 system with a slightly overestimation in 40% of the simulated seepage-water periods. Higher uncertainties were found for the simulated N300 than for the N0 plot. Modeled N flows below the rooting zone of 11 kg nitrate-N ha^{-1} per seepage-water period were comparable to calculations of the model 'Büchter' with a mean of 10 kg nitrate-N ha^{-1}. For the N300 plot, a more than twice as high N-leaching amount of 74 kg nitrate-N ha^{-1} was modeled compared with a calculated average of 30 kg nitrate-N ha^{-1}. Finally, small-scale modeling can provide plausible results for nitrate-N leaching on plot-scale when uncertainties in soil water, N flows, and biomass growth were considered.

Keywords: Nitrate leaching, Soil water content, Grassland, Northern Germany, CoupModel, GLUE

4.1 Introduction

Nitrogen (N) losses from agricultural areas cause economic but also environmental risks. The large-area use of permanent grassland in N Germany can lead to potential diffuse pollutions of surface and subsurface water bodies. Especially nitrate-N (NO_3-N) leaching is increased during seepage periods between September and April where the nutrient uptake by plants is low. The N surplus rises with increasing grazing intensity and N-fertilizer rate for pastures, whereas mown swards tend to have a lower N surplus (Trott et al., 2004). In Northern Germany, mixed systems with one or two cuts per season followed by short grazing cycles are prevalent management strategies, but exclusively mown or grazed grassland is also important (Lampe, 2005). NO_3-N leaching is the dominant fraction of total N losses from grassland soil, while ammonium (NH_4^+) leaching is negligible due to its preferred adsorption to soil particles. Wachendorf et al. (2004) stated that leached NO_3-N amounts are mainly dependent on the total N fraction in the soil and the amount of seepage water in arable and grassland systems. Generally, sandy soils show a higher N-leaching potential than loamy or clay soils (Jarvis, 1992). Several measurements on dairy farms on sandy soils in Northern Germany and Denmark have demonstrated large and variable NO_3-N-leaching losses (Büchter, 2003; Eriksen and Vinther, 2002; Eriksen and Søegaard, 2001). Quantification of N losses under varying management systems is required to assess potential environmental risks and moreover to reduce N losses from grassland. In fact, the N leaching differs considerably due to local climate regime, soil conditions, N management, and measurement technique like lysimeter experiments or ceramic suction cups. Additionally, N transformations in soils are very complex and the governing processes are ammonification, nitrification, and denitrification.

The main objectives of the present study were (1) to investigate the uncertainty of water and nitrogen dynamics for different grassland systems with an uncertainty-assessment approach using the process-based CoupModel (Jansson and Karlberg, 2004), (2) to quantify the NO_3-N-leaching loss below the rooting zone for different grassland systems.

4.2 Methods

4.2.1 Data acquisition

All experimental data sets were provided by the integrated research project ‘The nitrogen project: A system approach to optimize nitrogen use efficiency on the dairy farm’ carried out between 1997 and 2003 (Taube and Wachendorf, 2001). The project was located at the experimental farm ‘Karkendamm’ belonging to the Faculty of Agriculture and Nutrition Sciences of the University of Kiel (Northern Germany). Different management strategies were tested in a multifactorial field experiment, through investigations of crop yield, forage quality, soil N balance, and groundwater quality (Ingwersen, 2002; Trott, 2003; Büchter, 2003; Wachendorf et al., 2004; Bobe, 2005; Lampe, 2005, Karrasch, 2005).

According to the Köppen classification, the climate at ‘Karkendamm’ is maritime temperate (Peel et al., 2007) with a 30-years mean annual temperature of 8.6 °C and mean annual precipitation of 865 mm (Ingwersen, 2002). Most important management systems were grassland and maize for forage production. Grassland was divided into pure-grass plots dominated by ryegrass (*Lolium perenne* L.) and mixed swards with white clover (*Trifolium repens* L.) in different variations. Our study was limited to pure-grass swards, which were fertilized with mineral-N and harvested four times per year for silage production. Dominating soil types at the site were Podzols, and Endogleyic Podzols (FAO, 2006) in case of shallow groundwater. To improve the soil hydraulic conductivity, the Podzol under the grassland site was deep-plowed in 1981 up to a depth of 0.80 m. Consequently, buried and slanted soil layers with varying soil properties can be found under recent topsoil (*Table 4.1*; Scholz, 1999). Productivity of this Spodic Endogleyic Anthrosol (FAO, 2006) was specified with 18–25 from 100 points (Ingwersen, 2002) indicating a relative low expected yield of approx. 20% of the optimal yield.

Site-specific measurements had been carried out between 1997 and 2002 (*Table 4.2*). Soil temperature was measured daily without replicates during the whole period (Herrmann, 2006). Water contents were recorded weekly or biweekly with time-domain-reflectometry (TDR) sensors and presented mean values for the mown grassland plots over all N treatments (Klees, 1999; Scholz, 1999; Karrasch, 2005). More frequent measurements were obtained with the gravimetric technique between 0 and 15 cm depth (mean of 10 cm) by Lampe (2005), whereas only few observations were available for the lower depths in 1999. Groundwater levels were measured from weekly to monthly (summer 1997) under selected treatment plots with an acoustic plummet (Bobe, 2005). Averaged values from the four nearest observation points varied between 0.35 and 1.80 m below surface depending on location and seasonal water input from 1997 to 2002 (Klees, 1999).

Table 4.1: Soil properties of the Spodic Endogleyic Anthrosol (FAO, 2006) at the experimental site.

Horizon[a]	**Depth** (m)	**Soil bulk density** (g cm^{-3})	**Sand** (%)	**Total pore volume** (Vol.%)	**Plant available water content** (Vol.%)	**pH value** ($CaCl_2$) (–)	**Total organic C** (%)	**Total N** (%)	**C:N ratio** (–)
Ah	0–0.06	1.30	88.7	49.3	28.3	4.9	4.1	0.23	18
Ap	0.06–0.27	1.16	86.6	51.3	32.6	4.6	3.8	0.21	18
R/Ap[b]	0.27–0.80	1.22	86.4	54.3	22.3	4.2	5.6	0.27	21
R/Bsh		1.22	86.7	54.3	20.3	4.1	3.9	0.17	23
R/Bhs		1.20	85.7	54.3	25.0	4.4	1.2	0.11	11
R/Gro		n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
Gro	0.80–1.09	1.45	93.0	47.4	10.2	4.6	0.3	0.06	6

[a] According to *Ad-hoc-AG Boden* (2005)
[b] R: deeply plowed (0.80 m) horizon with a tilt angle of approx. 45° referred to soil surface.

Nitrate concentrations below the rooting depth, which was assumed to be 60 cm, were measured with up to six porous ceramic suction cups for one treatment (Büchter, 2003; Bobe, 2005; Herrmann, 2006). A vacuum pump was used to maintain a stable vacuum controlled by soil tensiometers located at 50 cm soil depth, and it was switched on when soil water tension fell below −300 hPa (Bobe, 2005). For detailed information on sample preparation and analysis, see Wachendorf et al. (2004). Since seepage water was reduced by plant water uptake in summer, no sampling could be achieved during the vegetation periods. Dry-matter yields for pure-grass and mixed swards were derived from cutting the aboveground biomass up to 5 cm above field surface and drying at 65 °C for 18 h (Ingwersen, 2002; Trott, 2003; Karrasch, 2005). The C content in the harvested dry matter (DW) of grassland species was assumed to be 46% to convert DW ha^{-1} into g C m^{-2}, but variations between 40% and over 50% were observed (Nikolaisen, 1998; Spitzer et al., 1996).

Büchter (2003) calculated the NO_3-N-leaching loss below the rooting zone (0–60 cm soil depth) for different grassland treatments at the 'Karkendamm' site during the seepage-water periods. Since no measurements of seepage-water amount had been conducted, the NO_3-N leaching was calculated as a product of averaged NO_3-N concentrations and an estimated seepage-water amount according to the climatic water-balance equation (DVWK, 1996), whereas the soil water storage was not considered in this approach (Büchter, 2003). Time periods with measured nitrate concentrations but without calculated seepage water indicated that the NO_3-N leaching was likely underestimated in the model 'Büchter'. Further disadvantage of this approach is the neglects of potential seepage water outside of the seepage-water periods. Consequently, the uncertainty of N leaching of the model 'Büchter' was defined by both, the variability of soil nitrate concentrations and estimated seepage-water amount.

Table 4.2: Observed variables used to optimize the model at 'Karkendamm' for scenario modeling.

Variable	**Measuring period**	**Number of samples over time**	**Repli-cate**	**Source**
Soil temperature (°C)				
0.05 m	1997–2002	1648	1	Herrmann, 2006
0.10 m	1997–2002	1648	1	
0.15 m	1997–2002	1648	1	
Soil water content (Vol.%)				
0.10 m	1999	77	11	Klees,1999;
	1998–2001	20	2	Karrasch, 2005;
	2001–2002	67	1	Lampe, 2005
0.30 m	1998	198	11	Scholz, 1999;
	1999	179	11	Klees, 1999
0.40 m	1999	179	11	Klees, 1999
0.50 m	1998	198	11	Scholz, 1999;
	1999	173	11	Klees, 1999
0.60 m	1999	166	11	Klees, 1999
0.70 m	1998	198	11	Scholz, 1999;
	1999	148	11	Klees, 1999
0.80 m	1999	96	11	Klees, 1999
Groundwater level (m)				
Nearest observation point	1997–2002	146	1	Bobe, 2005
Averaged value	1997–2002	1314	1	
NO_3-N concentration at 60 cm depth (mg N L^{-1})				
N0	1997–2002	426	1–6	Büchter, 2003
N300	1997–2002	484		
Soil mineral-N (NO_3-N + NH_4-N); NO_3-N; NH_4-N (g N m^{-2}) (N0 and N300)				
0–0.3 m	1997–2002	11	1–2	Herrmann, 2006
0–0.6 m	1997–2002	11	1–2	
0–0.9 m	1997–2002	19	1–2	
Harvested C content (g C m^{-2}) (annual values)				
N0 (measured: 1997–1999; linear regression: 2000–2001)	1997–1999	3 (+2 estimates)	1	Ingwersen, 2002
N300 (estimated from clover-grass yield)	1997–2001	5 estimates	1	Trott, 2003

A modified empirical equation of Turc/Wendling (Wendling et al., 1991) was used to estimate the actual evapotranspiration (Büchter, 2003; Wachendorf et al., 2004). Daily data on air temperature, precipitation, relative humidity, wind speed, and global radiation were obtained from measurements at the farm site.

Observations from a nearby weather station of the German Meteorological Service (DWD) were used in case of gaps during on-site data acquisition.

4.2.2 Modeling approach

The ecosystem process model CoupModel (Jansson and Karlberg, 2004; former model names: SOIL+SOILN, WinSOIL) was used to calculate (one) 1-dimensional, coupled fluxes of heat, water, C, and N in a soil-plant-atmosphere-transfer system. A layered soil profile with horizontal dimensions was defined covered by one or several plant layers above. The Richards' equation was solved numerically for water flows and the Fourier's law of diffusion for heat including convective flows (Jansson and Halldin, 1979). Energy-balance equations were used to quantify soil evapotranspiration, soil-surface temperature, and snow melt. Water contents were modeled according to the water-retention curve and hydraulic conductivity based on pedotransfer functions as proposed by Rawls and Brakensiek (1989), which can be adapted to laboratory measurements. Plant water uptake was realized by a soil-plant-atmosphere-continuum approach, using the Penman-Monteith equation (Penman, 1953; Monteith, 1965). Carbon and N turnover was calculated in several soil and plant compartments. Biomass was produced according to the radiation-use-efficiency (RUE) approach (Monteith, 1977) and was partitioned into above- and below-ground C and N pools. Regulating factors were plant water uptake, leaf temperature, and plant N stress. Carbon and N were allocated to leaf, stem, coarse and fine roots, and fruiting body according to pre-defined allocation factors and C:N ratios. Litter was produced as fraction of above- and below-ground plant residues and entered the soil organic pool. Two litter pools were considered with different turnover rates beside one humus pool. Inorganic-N dynamics were simulated based on water flows between soil layers, N turnover, and mineral-N contents in each soil compartment. Leaching of NO_3-N below the root zone was assumed as vertical NO_3-N flow at 65 cm soil depth to compare simulated results with calculations of the model 'Büchter'.

4.2.3 Uncertainty analysis with the GLUE approach

The model-uncertainty analysis aimed at quantifying joint probability distributions of different model input factors (*e.g.*, model structures/parameter sets) representing acceptable conditions of a natural system (Arhonditsis et al., 2008; Pappenberger and Beven, 2006; Reichert and Omlin, 1997). The widely used Generalized Likelihood Uncertainty Estimation (GLUE) framework was proposed by Beven and Binley (1992) and applied high numbers of Monte Carlo simulations to find 'equally good' parameters sets according to their modeling performance. The whole parameter space was investigated assuming uniform probabilities for selected input variables in the GLUE and rejecting the concept of an optimal parameter set. The modeled parameter combinations were weighted according to 'likelihood' or modeling performance measures and divided into acceptable and unacceptable sets (Henderson and Bui, 2005; Beven and Freer, 2001). In this study, statistical measures (R^2, Bias, and *RMSE*) were used as objective functions to describe the goodness of model fit for the respective parameter set (*cf.,* ch. 4.2.5). The uncertainty boundaries included simulated mean values within the 5th and 95th percentiles of all model runs above a subjectively defined threshold value (*cf.,* ch. 4.3). The GLUE approach usually required a large number of multiple simulations if random parameter sampling was performed. A number of 10,000 runs was recommended by Uhlenbrook and Sieber (2005). McIntyre et al. (2002) concluded that the GLUE approach was robust and multifunctional to analyze parameter uncertainties when uncertainties in the model structure cannot be clearly identified. The GLUE approach was possibly limited by the subjective nature of the likelihood, chosen threshold values (Henderson and Bui, 2005), and the data quantity, but more advantages over the Bayesian approach by van Oijen et al. (2005) were found by Conrad and Fohrer (2009b).

4.2.4 Model parameterization

Soil water and N dynamics in a pure-grass sward, which was harvested four times per year, were simulated with daily resolution on sandy soil between 1997 and 2002 for two fertilization levels, unfertilized (N0) and highly fertilized (N300). Fertilization was realized by mineral-N in four applications (130/70/50/50 = 300 kg N ha^{-1} $year^{-1}$) as Ca-ammonium-nitrate ($Ca(NH_4NO_3)$). Most parameters in the model were chosen as fixed values based on previous experiences with the model (Conrad and Fohrer, 2009a) or were default values due to their minor sensitivity on the investigated output. The hydraulic properties such as water-retention curves were estimated from soil texture for each soil layer. Additionally, values were adapted to measurements for site-specific soil water-retention characteristics (Scholz, 1999) at five soil water tensions (pF values of 0, 0.6, 2.3, 2.5, and 4.2). The saturated hydraulic conductivity in each soil layer was also adapted to site-specific measurements (Klees, 1999). The choice of the model parameters for the automated optimization was complex because soil-vegetation-atmosphere-transfer models are often overparameterized relative to their calibration data. At first, a number of 350 input parameters was selected for a simple sensitivity analysis according to Lenhart et al. (2002) to investigate influences on abiotic (*e.g.*, water content, soil temperature, evapotranspiration) and biotic (*e.g.*, soil mineral-N content, nitrate concentration, harvested C) output variables. Parameters were changed ±25% of the initial value, and the effect on 29 output variables focused on soil temperature, soil water, soil N dynamics, and harvested C was evaluated. First of all, parameters with high/moderate sensitivities to each of the selected output were considered. Because of complex interactions between input and output variables, some input parameters without or with low sensitivities were additionally chosen for this optimization to test if the GLUE results were comparable with results of the previously used sensitivity analysis. A number of 30 input parameters was defined within their ranges and general sensitivity on 29 output variables (*Table 4.3*). Wu et al. (1998) reported biomass-allocation parameters as most sensitive on N leaching and harvested N in the combined SOIL+SOILN model (Wu and McGechan, 1998a).

4.2.5 Model-performance indicators

The following model-efficiency measures were used as objective functions (OF) to identify the best performing parameter sets. Therefore, subjective ranges for the coefficient of determination (R^2) and the mean error (*ME* or bias) were applied on the abiotic output, *i.e.*, soil temperature, water and groundwater dynamics, for the 10,000 runs (*Table 4.4*). The model-performance indicators for the soil N dynamics, which are not shown in this study, as well as the root mean square error (*RMSE*) of the accepted runs were results of this limitation strategy. The R^2 is sensitive to the simulated and observed relative increase/decrease of variables such as concentrations, even if the absolute values do not fit well (Uhlenbrook and Sieber, 2005). Consequently, parameter sets and their corresponding output with objective functions not exceeding a certain threshold value were excluded in the GLUE approach.

4.3 Results and Discussion

4.3.1 Soil water dynamics

Soil water contents in different depths and the groundwater level were used to evaluate the model performance for soil water dynamics in the unfertilized (A) and highly fertilized (B) plot. Only those simulated soil water contents with $R^2 > 0.4$ and *ME* values between −4.5 and 21 were accepted in this study. Higher differences between both systems were found for the upper soil layers. The model efficiency measures (*Table 4.4*) indicated an overestimation of modeled water contents with positive *ME* values for both plots.

When site-specific field measurements were compared to results from soil dewatering/drying tests, the on-site TDR sensors measured 15–25% lower water contents due to hysteresis effects during wetting (Scholz, 1999). These effects were considered in CoupModel with five general input parameters that showed no sensitivity on the water contents when changed ±25% of the initial value (*Table 4.3*). In the deeper soil layers, the uncertainty of the corresponding modeled soil water contents were increased due to temporal conflicts to match the observed groundwater level. The simulation of the groundwater level was optimized with data from the nearest groundwater observation point. A number of five parameters with medium sensitivity for groundwater outflow were selected for the automated optimization (*Table 4.3*).

For comparison between model and observations, the mean of all observation points of the mown grassland was also considered. Correlation between simulated and observed groundwater level under the unfertilized (A) and highly fertilized (B) system (*Fig. 4.1*) indicated lower simulated levels than at the nearest observation points with higher deviations for the N300 system. A better agreement was found for both systems when model results were compared to averaged groundwater levels (*cf.,* ch. 4.2.1), with the best match for the N0 grassland. The comparison with averaged observed water levels still indicated an underestimation by the model (*Fig. 4.1*). However, modeled levels showed lower amplitudes than measured data indicating that this automated optimization against fluctuating values was not very satisfactory. Consequently, only moderate R^2 values between 0.27 (N300) and 0.33 (N0) were achieved (*Table 4.4*). The altitude of the grassland plots was 0.17 m deeper than for the other trials, and the influence by shallow groundwater had to be therefore considered. Interactions with the small river ‘Osterau’ located nearby caused also changes in the shallow groundwater level. The modeled groundwater level was calculated by both the vertical water percolation including an empirical drainage equation and a constant groundwater-inflow rate. In natural systems, changes in horizontal groundwater flows according to the recharge rate were more typical.

Table 4.3: List of parameters chosen for the GLUE optimization approach (additional info see page 55).

Parameter	Description	Minimum	Maximum	Unit	Sensitivity[a]
a) Drainage and deep percolation:					
DrainLevelLowerB, z_{p2}	Drainage depth for calculation of deep percolation	−5	0	m	medium
DrainSpacingLowerB, d_{p2}	Distance between the drainage system for calculation of deep percolation	0	200	m	medium
EmpGFLevBase, z_2	Base and peak levels for groundwater flow to diffuse sink	−5	0	m	medium
EmpGFLevPeak, z_1		−2	0	m	medium
EmpGFlowBase, q_2	Base and peak values for the maximal rates of groundwater flow to diffuse sink	0	10	mm d^{-1}	medium
EmpGFlowPeak, q_1		0	20	mm d^{-1}	medium
GWSourceFlow, q_{sof}	Constant rate of groundwater source flow	0	5	mm d^{-1}	medium
b) Soil water flows:					
InitialGroundWater	Initial groundwater level	−2.0	−0.1	m	no
c) Soil hydraulic properties:					
MinimumCondValue, $k_{min\ uc}$	Minimum hydraulic conductivity	1.0e−6	0.1	mm d^{-1}	medium
d) Soil thermal properties:					
ThScaleLog(1), $x_{hf(1)}$	Scaling coefficient for the thermal conductivity of layer 1 and 2	−1	1	–	yes[b]
ThScaleLog(2), $x_{hf(2)}$		−1	1	–	yes[b]
e) Potential transpiration:					
CondVPD, g_{vpd}	Vapour pressure deficit that corresponds to a 50% reduction of stomata conductance	50	2000	Pa	medium
CondMax, g_{max}	Maximum conductance of fully open stomata	0.001	0.05	m s^{-1}	medium
f) Plant water uptake:					
CritThresholdDry, Ψ_c	Critical pressure head for reduction of potential water uptake	100	1000	cm water	low
AirMinContent, θ_{Amin}	Minimum amount of air that prevents any reduced water uptake	0	20	Vol.%	no
AirCoefRed, p_{ox}	Rate coefficient governing increase of plant resistance when oxygen level is decreasing	0	20	–	no
g) Plant development and carbon allocation:					
Specific LeafArea, $p_{l,sp}$	Leaf mass per unit leaf area	1	50	g C m^{-2}	low
Leaf c1, l_{c1}	Fraction of the mobile C allocated to the new shoots	0	1	–	medium
Root Mass c1, r_{Mc1}	Fraction of mobile C allocated to the roots	0	1	–	medium
RadEfficiency, ε_L	Radiation use efficiency	0	4	g DW MJ^{-1}	no
h) Decomposition process:					
Eff Litter1, $f_{e,l1}$	Efficiency of decay of litter 1	0.1	0.8	d^{-1}	high
Eff Litter2, $f_{e,l2}$	Efficiency of decay of litter 2	0.1	0.8	d^{-1}	medium
Eff Humus, $f_{e,h}$	Efficiency of decay of humus	0.1	0.8	d^{-1}	medium
RateCoef Humus, k_h	Coefficient for the decay of humus	1.0e−6	0.001	d^{-1}	no
RateCoef Litter1, k_{l1}	Coefficient for the decay of litter 1	1.0e−5	1	d^{-1}	medium
RateCoef Litter2, k_{l2}	Coefficient for the decay of litter 2	1.0e−5	1	d^{-1}	medium
i) Nitrification process:					
NUptFlexibilityDeg, $n_{Uptflex}$	Compensatory N uptake from soil	0	1	–	high
NUptMaxAvailFrac, f_{Nupt}	Fraction of mineral-N for plant uptake	0.01	0.2	d^{-1}	low
NitrateAmmRatio, $r_{nitr,amm}$	NO_3-N:NH_4-N ratio for nitrification	0.1	5	–	no
NitrificSpecificRate, n_{rate}	Specific nitrification rate	0.01	0.5	d^{-1}	medium

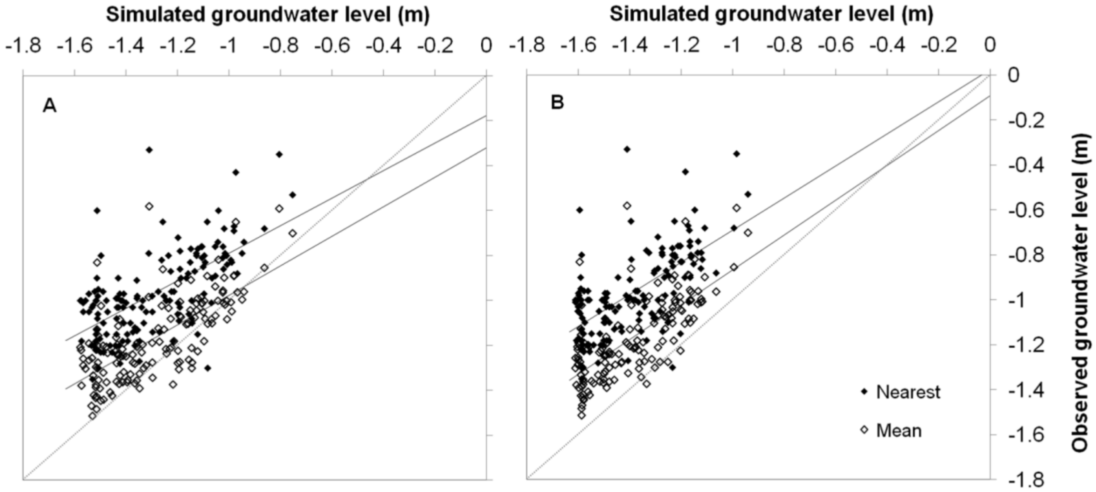

Fig. 4.1: Linear regression between averaged simulated and observed groundwater levels for system N0 (A) and N300 (B).

Obvious interactions between shallow groundwater and surface-water bodies that can affect inflow rates were observed in the Northern Lowland of Germany (Schmalz and Fohrer, 2009). However, standard deviations (*SD*) between 0.025 and 0.24 indicated higher variable shallow groundwater levels for the four nearest observation points than for the whole grassland site (minimum *SD* = 0.11, maximum *SD* = 0.22) considering also the topography of the grassland.

The seepage-water amount is most important for the vertical NO_3-N leaching in the unsaturated soil, but it was not directly measured during the experiments (Büchter, 2003). Model results of the vertical water flow at a depth of 65 cm were based on the hydrologic winter half-year and compared with calculated seepage-water amounts according to Büchter (2003) for each seepage-water period (*Fig. 4.2* A and *Table 4.5*).

CoupModel showed higher vertical water flows in the seepage periods 1999/2000, 2000/2001, and 2001/2002. A mean of 272 (±125) mm per seepage-water period (*i.e.*, 17–45% of annual precipitation of 865 mm or 55% of winter-term precipitation of 500 mm) was modeled compared to 180 (±119) mm (*i.e.*, 7–35% of annual precipitation or 36% of winter-term precipitation) by Büchter (2003). The accuracy of the calculated seepage water by Büchter (2003) cannot be evaluated due to the lack of measured data. Changes in soil water storage were not assumed in this approach, and time periods with calculated seepage water were independent of the hydrologic half-year. Maybe, a potentially too low seepage-water amount (approx. −25%) resulted. Differences in simulated vertical water flows of the two treatments were small with 10 mm per hydrologic winter half-year (*Table 4.5*), which was also reported by Korsaeth et al. (2003) in a lysimeter study from southern Norway. In our study, the water balance showed an actual evapotranspiration of approx. 481 (±35) mm year^{-1}, *i.e.*, 56% of annual precipitation.

[1] Additional declarations for *Table 4.3*:

[a] Sensitivity analysis according to Lenhart et al. (2002); high (sensitivity Index I > 0.9), medium (0.1 < I < 0.9), low (0.01 < I < 0.1), no (I < 0.01)

[b] No index I available; remark about absolute changes compared to the initial value of 0; DW – dry weight.

Table 4.4: *Model efficiency for comparison between means of simulated and observed/calculated values.*

Efficiency measure	**OF**[a]		***ME***		***RMSE***		***R***^{2}	
System	R^2	*ME*	N0	N300	N0	N300	N0	N300
Soil temperature (°C)	> 0.9	$-1 < x < 0$						
0.05 m			−0.68	−0.68	2.19	1.94	0.92	0.93
0.10 m			−0.58	−0.55	1.69	1.59	0.95	0.95
0.15 m			−0.44	−0.41	1.54	1.45	0.95	0.96
Soil water content (Vol.%)	> 0.4	$-4.5 < x < 21$						
0.10 m			0.36	1.68	6.66	7.19	0.46	0.42
0.30 m			0.62	2.32	6.03	6.17	0.44	0.44
0.40 m			−0.59	0.79	4.18	3.67	0.86	0.84
0.50 m			5.85	8.22	8.68	9.84	0.42	0.46
0.60 m			5.49	6.45	6.73	8.01	0.91	0.90
0.70 m			9.67	10.38	12.02	12.48	0.45	0.48
0.80 m			4.00	2.33	9.54	8.56	0.55	0.43
Groundwater level (m)	–	$-0.7 < x < 0.7$						
Nearest point			−0.32	−0.42	0.40	0.49	0.33	0.27
NO_3-N concentration (mg N L^{-1})	–	−5 / +10; −5 / +70	−1.25	11.55	5.16	28.93	0.04	0.05
Harvested carbon (g C m^{-2}) (cumulative)	> 0.9	±100; ±1000	−10.58	−227.37	68.87	664.92	0.99	0.98

[a] Used objective functions (OF) to identify acceptable simulations; differences between treatments were made for nitrate concentration and harvested carbon,
ME: Mean Error, Bias (best fit: 0; range: [−∞; +∞]); *RMSE*: root mean square error (0; [−∞; +∞]); R^2: coefficient of determination (1 or −1; [0; 1] or [0; −1]).

Differences in the accumulated annual flows were explained by possible small-scale soil heterogeneities of different plots by Erhart et al. (2007). Better agreement between simulated (SOIL model) and observed drainage-water amounts was achieved when water flow was recorded directly in artificial drainage systems or lysimeters (McGechan et al., 1997).

Finally, discrepancies can be caused by model limitations regarding the soil profile. The water flows in CoupModel were calculated between horizontal soil layers compared to tilted soil horizons between 0.27 and 0.80 m below surface in the investigated profile. Possible influences on water flow by tilted layers were excluded in the model because of model limitations and minor differences in bulk density, sand content, and total pore size for the deep-plowed layers (*Table 4.1*).

4.3.2 Nitrate-N leaching below the rooting zone

The vertical NO_3-N leaching was not optimized in the GLUE to match calculated NO_3-N leaching of the model 'Büchter' due to the assumed uncertainty of this approach (*cf.*, ch. 4.2.1). Cumulative values of modeled NO_3-N leaching were compared with the model 'Büchter' for each seepage period (*Table 4.5*). Data before November 1997 and during the summers were excluded from comparison.

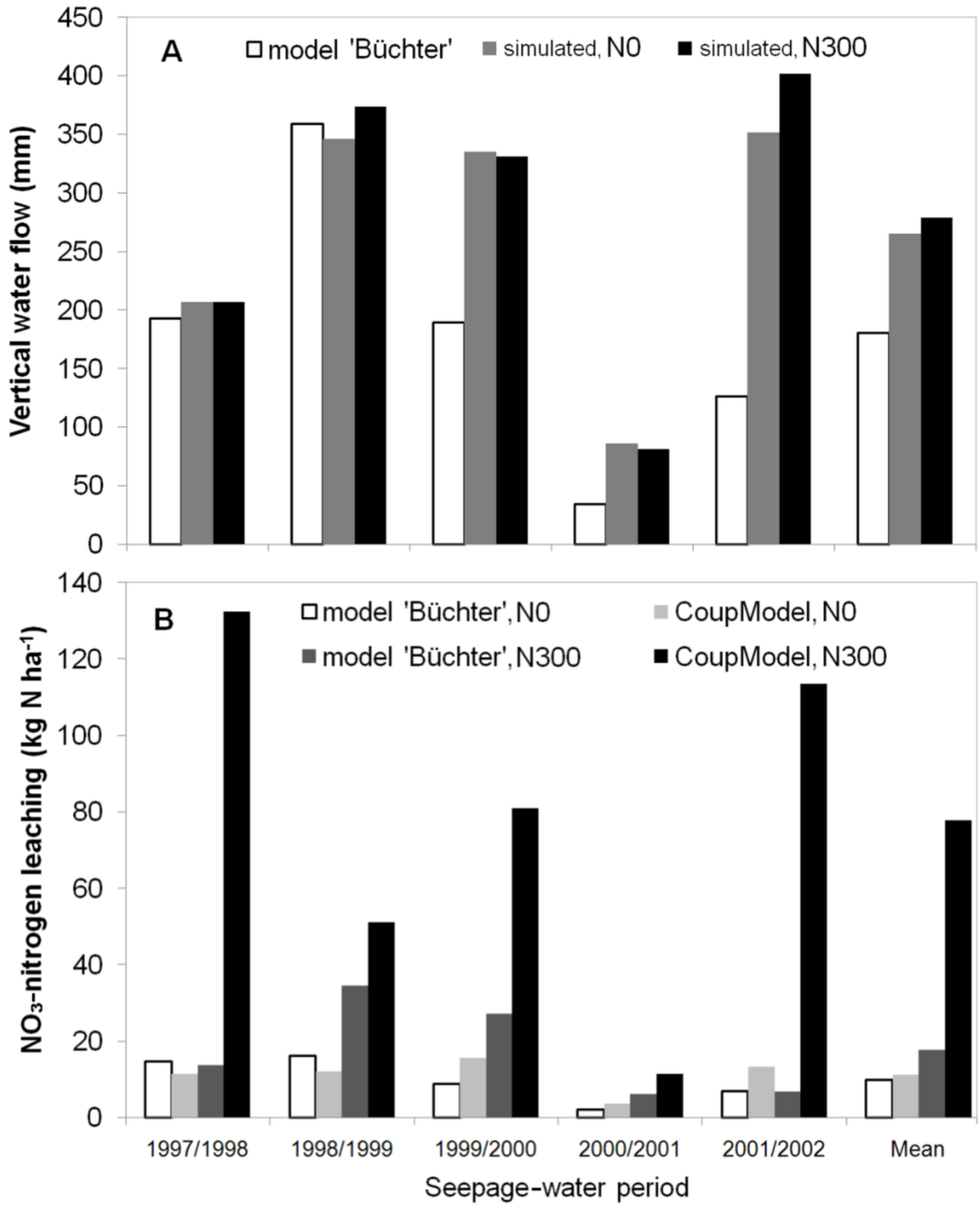

Fig. 4.2: Mean simulated vertical water flows at 65 cm depth compared to calculated seepage-water amount according to Büchter (2003) (A) and comparison between mean simulated and calculated NO_3-N leaching (Büchter, 2003) (B) for each seepage period and in both systems.

CoupModel calculated an averaged NO_3-N leaching of 11 (±5) kg N ha^{-1} and seepage-water period for the unfertilized plot, which was comparable with 10 (±6) kg N ha^{-1} of the model 'Büchter'. Erhart et al. (2007) also stated NO_3-N leaching losses up to 10 kg N ha^{-1} for unfertilized plots under arable land use. A NO_3-N leaching of averaged 74 (±48) kg N ha^{-1} was found for the highly fertilized grassland by CoupModel and the model 'Büchter' calculated 30 kg N ha^{-1}. Korsaeth et al. (2003) demonstrated nitrate leaching for grassland systems under different fertilizer regimes with a combined CoupModel and SoilN_NO (Vold et al., 1999) approach and found that 5–23% of imported N (with 98% as NO_3-N) can be leached out highly dependent on soil type. Lewis et al. (2003) reported differences in simulated NO_3-N leaching between 30 and 80 kg N ha^{-1} for an artificially drained sandy soil under grassland in Scotland and Ireland depending on climate, soil type, and N-fertilizer input (mineral-N + slurry-N = 490 kg N ha^{-1}). The variability of the CoupModel results indicated a higher uncertainty of NO_3-N leaching in highly fertilized grassland systems. Deviations in NO_3-N leaching between CoupModel and model 'Büchter' were mainly caused by different quantification methods with specific complexity (*cf*., ch. 4.2.1 and 4.2.2) in addition to possible reasons for the underestimation in the model 'Büchter' (*cf*., ch. 4.2.1).

Table 4.5: Comparison between modeled vertical water flow, averaged cumulative NO_3-N leaching and harvested C, N and calculations by Büchter (2003) for both grassland systems. Standard deviations (SDs) were shown in brackets.

System	**Unfertilized grassland, N0**		**Fertilized grassland, N300**	
	calculated	simulated	calculated	simulated
Seepage water amount (vertical water flow) (mm)	180 (±119)[a]	265 (±117)	180 (±119)[a]	279 (±133)
NO_3-N leaching (kg N ha^{-1})	10 (±6)[a]	11 (±5) 14 (±4)[b]	30 (–)[a, f]	74 (±48) 29 (±15)[b]
Harvested C (g C m^{-2} year^{-1})	158 (±35)[c]	149 (±28)	472 (±51)[d]	432 (±109)
Harvested N (g N m^{-2} year^{-1})	7 (±1.5)[e]	4.3 (±1.6)	30 (±2.4)[d]	21 (±5.1)

[a] Mean values from the 'Karkendamm' project per seepage period (Büchter, 2003).
[b] Product of mean simulated vertical flow and measured NO_3-N concentrations to evaluate the error of the N submodel.
[c] Calculated from measurements (1997–1999) (Ingwersen, 2002), linear regression for 2000 and 2001.
[d] Estimated from measurements of a clover-grass plot with 61% *Lolium Perenne* L. and 5% *Trifolium repens* L. of DW, mineral-N fertilizer rate of 300 kg N ha^{-1} year^{-1} (Trott, 2003).
[e] Measurements (1997–1999) (Ingwersen, 2002).
[f] Published value (Büchter, 2003) without information about *SD*.

The error of the N submodel in CoupModel was assessed regarding the NO_3-N leaching by comparing simulated results with the product of simulated vertical water flow and measured NO_3-N concentration. The averaged result of this assessment showed 27% (14 kg N ha^{-1}) higher NO_3-N leaching than originally simulated (11 kg N ha^{-1}) with CoupModel for the unfertilized plot (*Table 4.5*). This outcome was also confirmed by higher measured NO_3-N concentrations than modeled (see negative *ME* values in *Table 4.4*). The NO_3-N leaching of the N300 plot showed a mean of 29 kg N ha^{-1} per seepage-water period for the error assessment of the N submodel in CoupModel. This result was 61% lower than the modeled mean NO_3-N flow at 65 cm soil depth, but it was within the standard deviation of the originally modeled NO_3-N leaching of 74 (±48) kg N ha^{-1}. Positive *ME* values for the NO_3-N concentrations of the N300 plot confirmed this outcome.

Therefore, differences between the NO_3-N leaching of CoupModel and model 'Büchter' were caused mainly by the soil N dynamics in CoupModel. Due to the fact that soil mineral-N contents do not represent the actual dissolved-N amount, the NO_3-N concentration below the rooting zone was used as an indicator for the N leaching. Modeled and observed NO_3-N concentrations were compared as a function of time at a depth of 60 cm for the unfertilized (A) and the highly fertilized (B) mown grassland (*Fig. 4.3*). Measurements represented averaged values within standard deviations (*SD*) over each sampling interval (between 5 and 14 d) of the suction cups. Simulated values were shown within the 5th and 95th percentiles of the accepted runs describing the model uncertainty. Modeling results agreed well with the measurements within *SD* for the unfertilized system. High initial values caused higher concentrations in 1997, whereas a potential risk by exceeding concentrations above the European threshold for nitrate of 50 mg NO_3^- L^{-1} (= 11.3 mg NO_3-N L^{-1}) in drinking water could not be stated.

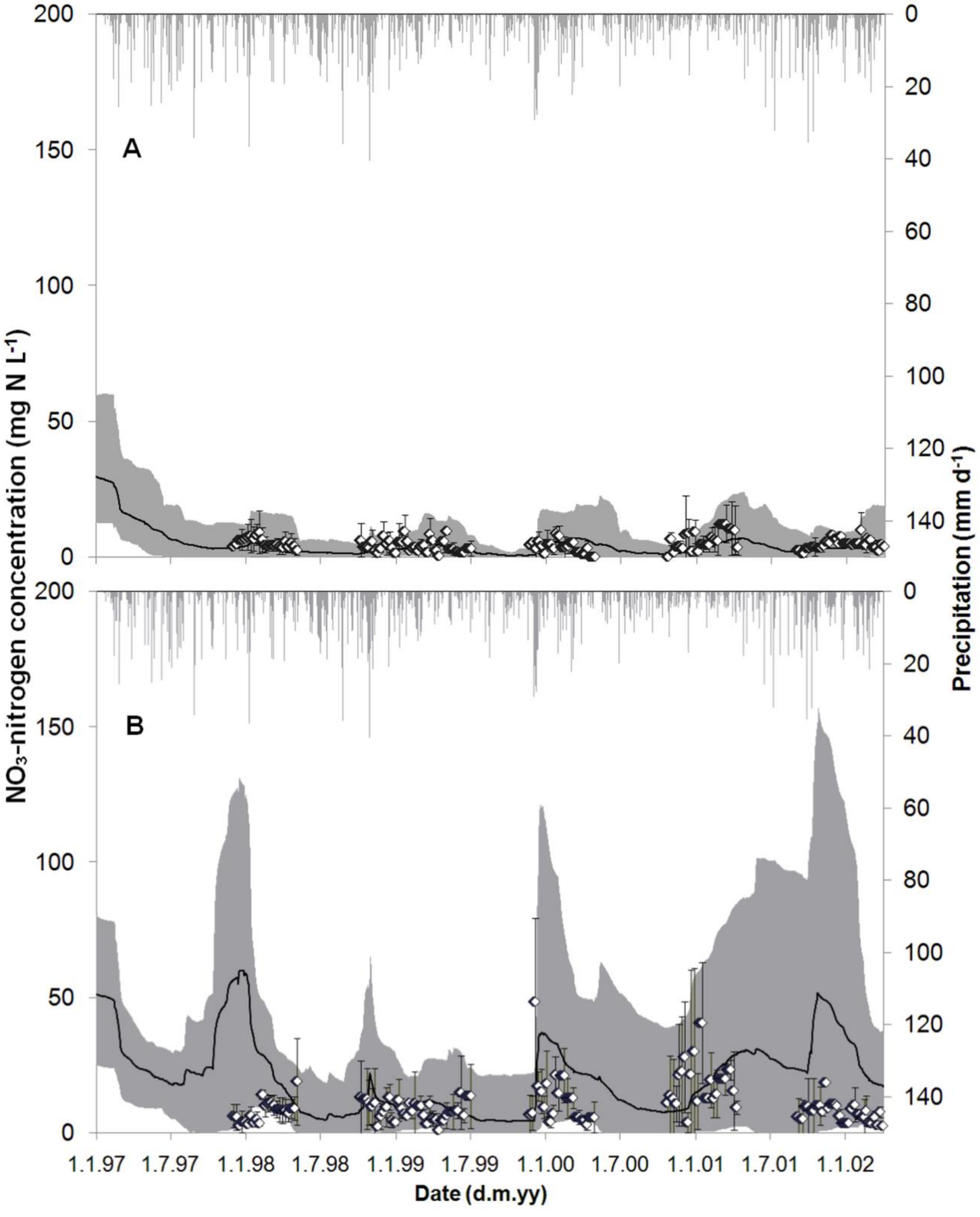

Fig. 4.3: Mean simulated NO_3-N concentration at 60 cm depth (solid line) compared to mean observed values (◇ ± standard deviation SD) for system N0 (A) and N300 (B). The 5th and 95th percentiles (gray area) represented the uncertainty boundaries of the model.

Compared to this result, the highly fertilized system showed highly variable concentrations in modeling and measurement, and, therefore, a potential risk for shallow groundwater bodies can be stated. Uncertainty was higher in the N300 system than in the unfertilized plot, and observed *SD* values confirmed this result. CoupModel tended to overestimate the concentration in the seepage-water periods 1997/98 and 2001/02, resulting in lower model efficiencies than for the N0 system (see *Table 4.4*). Suction cups were installed in fall 1997 (Büchter, 2003), and information about a successful conditioning was missing. Therefore, these measurements could be highly uncertain because of an imbalance of NO_3^- ions in the ceramic cups and a tendency to underestimate N concentrations on an average of 8% compared with free drainage systems (Erhart et al., 2007). Additionally, the composition of these soil water samples is highly dependent on applied vacuum, connected soil pores, and preferential flows around the ceramic suction cups (Grossmann et al., 1987). Finally, comparison between highly variable observations (up to ±30%; Erhart et al., 2007) from one soil depth and modeling results was difficult due to gaps of knowledge about the whole soil nitrate profile. Low R^2 values (0.05, see *Table 4.4*) and high uncertainties in field and modeling resulted from this lack of data.

Results from our study indicated that calculations based on measured soil nitrate concentrations maybe underestimate the NO_3-N leaching and may not represent the high variability of the NO_3-N leaching. The CoupModel approach can be applied to simulate complex systems combined with an uncertainty assessment. Otherwise, the model 'Büchter' can be used as a practical tool to estimate the NO_3-N leaching when only few system details were available or needed. In case of high external N inputs, N transformation and flows in a soil profile are very uncertain depending on interactions between many environmental factors, *e.g.*, climate, other nutrients, plant-specific N uptake, and competition.

4.3.3 Harvested carbon and nitrogen contents

Soil N dynamics can be influenced by the biomass development due to carbon assimilation and N uptake controlled by the C:N ratio. Modeled and measured/estimated harvested C yields per year (*cf.*, *Table 4.2*) were compared as annual mean values (*Table 4.5*). The agreement with measured/estimated values from the 'Karkendamm' project was fitted according to limitations of the used objective functions (cf., *Table 4.4*) leading to high $R^2 \geq 0.98$ for the harvested C. On average, the model slightly underestimated the biomass and corresponding C yield in both systems with higher variability for the highly fertilized plot. Mean errors of both systems were negative confirming the underestimation by CoupModel. But results agreed better for the unfertilized (N0) than for the fertilized (N300) grassland (*Table 4.5*). The modeled uncertainty ranges confirmed the higher yield variability of pure-grass swards with increasing N fertilization (Herrmann et al., 2005a). Due to general differences between model and measurements regarding biological processes, the discrepancy for the cumulative averaged harvested C over five years was approx. 5.7% (N0) and 8.5% (N300). These deviations were acceptable compared to an error of 5% of mown biomass reported by Wu and McGechan (1998a) for modeled grasslands (SOILN + grass growth submodel).

In this study, the annual average of modeled harvested N was compared with corresponding site-specific measurements (Ingwersen, 2002) and estimations based on Trott (2003). Less plant-N uptake was modeled than measured or estimated for both simulated systems (mean values; N0: −38%; N300: −30%) but within plausible ranges (*Table 4.5*). Wu and McGechan (1998a) confirmed these modeling results of an underestimated plant-N uptake of averaged −16% derived from the 'SOILN + grass growth model'. Results of both model applications, *i.e.*, CoupModel and 'SOILN+grass growth model', were assumed to be comparable due to general similarities in the nitrogen submodels. A low NO_3-N leaching is primarily attributed to a high plant-N uptake (Korsaeth et al., 2003). The modeled N balance of pure grassland in Scotland (UK) from 1994 to 1996 confirmed these interactions between N uptake and N leaching with over 20 g N m^{-2} harvested N compared to leached N < 5 g N m^{-2} (Wu and McGechan, 1998b). The opposite effect was found in our study, where a low plant-N uptake was associated with differing modeled NO_3-N leaching (*Table 4.5*). The plant-N uptake is very variable and the N-uptake efficiency (% available N) can differ significantly between growth periods within years due to complex interactions between climate, nutrient availability, and diseases. This can lead to consequences for the accumulated and leached N (Eckersten et al., 2007). In the same study, N uptake and N leaching of a grass ley in Sweden were modeled with a CoupModel+SOILN approach. The simulated N uptake was 20–30% of the observed N uptake linked to an overestimation of modeled N leaching by 40%. Another reason for the underestimated harvested N in our study can be found in the estimations by Trott (2003) that were based on C and N contents of clover-grass, which contained usually more N due to the atmospheric-N fixation by the clover.

4.4 Conclusions

Process-based models have been an essential tool for addressing environmental issues, *e.g.*, understanding complex interactions between soil, vegetation, and atmosphere. Realistic predictive links between management actions and nutrient response can be only attained through probabilistic approaches comprising uncertainty analysis of various error sources, such as measurement errors, parameter uncertainty, and general discrepancies between model and reality (Arhonditsis et al., 2008). Overparameterization of models and parameter correlations were further sources of uncertainty leading to an equifinality problem with equally good simulation results for different model parameter sets.

In our study, the structural and parametric uncertainty was considered in the automated calibration based on the General Likelihood Uncertainty Estimation (GLUE) approach. The second objective was to investigate the capability of CoupModel (Jansson and Karlberg, 2004) to perform on grassland sites aiming at quantification of NO_3-N leaching under pure-grass swards for two fertilizer levels (N0: no additional N; N300: 300 kg mineral-N ha^{-1}). Optimization aimed at matching abiotic (*e.g.*, soil temperature and water contents) and biotic (*e.g.*, NO_3-N concentrations and harvested C) output variables simultaneously. The model was tested to achieve the most plausible results for all output variables used in GLUE.

CoupModel reproduced well soil temperatures and provided plausible results for soil water contents and groundwater level over five years. However, CoupModel was able to simulate NO_3-N concentrations at 60 cm depth within the observed standard deviation in the unfertilized grassland. Variations in the measured NO_3-N concentrations of the highly fertilized treatment were reproduced satisfactorily by the model mean within higher uncertainty ranges. Simulated NO_3-N leaching was comparable with the calculated value by Büchter (2003) for the unfertilized system, and 2.5 times higher losses were assessed for the N300 plot. Differences between the NO_3-N leaching of CoupModel and model 'Büchter' resulted mainly from the N submodel in CoupModel, because the uncertainty of the vertical water amount was smaller than for the modeled NO_3-N flows. Simulated averaged vertical water flow of both systems was 50% higher than calculated according to the mean value by Büchter (2003), which was only 36% of the averaged winter-term precipitation of 500 mm. Crop growth was simulated dynamically for each year, and model results of harvested C reproduced the observations well compared to an underestimated N uptake in both plots.

Further work is required to test whether or not significant improvements can be made to prediction of nitrate leaching in combination with realistic accounts for decomposition, nitrification, and denitrification and the N uptake by grassland plants. Additional optimization will be required for microbial activity due to its sensitivity to temperature and moisture conditions.

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Chapter 5

Simulating impacts of silage maize (*Zea mays*) in monoculture and undersown with annual grass (*Lolium perenne* L.) on the soil water balance in a sandy-humic soil in Northwest Germany

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Abstract

This study was focused on modeling soil water, carbon (C), and nitrogen (N) dynamics in soil and crop emphasizing uncertainties in model parameterization and the evaluation of potential water stress for silage maize cultivations on a drained field. The CoupModel was applied on different management systems for silage maize (*Zea mays*) in monoculture and undersown with grass (*Lolium perenne* L.) on a sandy-humic soil. Four different fertilization levels with 0, 150 kg of mineral-N, 40 m^3 of cattle slurry (72–148 kg N ha^{-1} $year^{-1}$), and combined slurry/mineral-N (222–298 kg N ha^{-1} $year^{-1}$) were simulated over five years. Results were based on most plausible parameter combinations regarding simulated biomass obtained from 10,000 runs by the Generalized Likelihood Uncertainty Estimation (GLUE) approach. The uncertainty in model parameterization was reduced significantly by limiting the number of simulations for each treatment sequentially resulting in quartile coefficients of variation (CV^*) < 25% for 26% and 36% of selected input parameters in bi-cropping and monoculture systems, respectively. Average soil temperatures in upper soil depths, the groundwater level, water potentials, and water contents between 10 and 80 cm of depth were reproduced plausibly with the model as well as plant C and N contents. The CV^* values of evapotranspiration and total runoff ranged between 0 and 26% and 8–21%, respectively, on half-yearly basis. Significant differences between the cropping systems were found, even though the soil water balance was positive for all systems, and the potential water stress was only minor in bi-cropping systems.

Keywords: Silage maize, Bi-cropping, Catch crop, Water balance, CoupModel, Uncertainty analysis

5.1 Introduction

The cultivation of **silage maize** is economically worthwhile in Germany according to the revised Renewable Energy Sources Act (EEG, 2014) resulting in a significantly increased cultivation area during the last decade (Destatis, 2015). Taking into account that maize usually leaves the ground almost bare after harvest, **undersown crops** (here synonymous with **catch crops**) such as hardy ryegrass species potentially store residual soil N left over from previous and main crops in autumn and during winter (Malézieux et al., 2009; Malone et al., 2014; Schiermann, 2004). In case of mixed cropping, negative effects of undersown crops on water and nitrogen supply of maize plants especially during the early growth period cannot be excluded (Justes et al., 2012; Kuo et al., 2001; Volkers, 2005; Whitmore and Schröder, 2007). For example, general stability of maize yields undersown with perennial grass species cannot be assumed. Negative, positive, and insignificant effects on maize biomass were reported by Volkers (2005) as well as Whitmore and Schröder (2007) because of variable competitiveness of undersown grass for soil water and nitrogen. Basically, climatic and site-specific factors are as important for the high variability of crop yields as the N input by fertilization (Malone et al., 2014; Schiermann, 2004).

Artificial drainage systems are frequently used in Northern Germany to control water and nutrient flows below agricultural land (Pfannerstill et al., 2012) with various influences on soil infiltration and surface runoff (Maalim and Melesse, 2013). However, tile drains are also known causes of enhanced nitrate-nitrogen (NO_3-N) leaching because of faster water transport through soil pores directly into deeper layers and surface-water resources as well as of lowering the groundwater level (Conrad and Fohrer, 2009a; Pfannerstill et al., 2012; Wesström et al., 2014).

Crop-simulation techniques combined with water and nutrient flow models are already integrated in soil-vegetation-atmosphere-transfer models to analyze effects of climate and soil management on plant growth at plot scale (Bleken et al., 2009; Conrad and Fohrer, 2009a; Herrmann et al., 2005b; Knörzer et al., 2011; Malézieux et al., 2009; Wallach et al., 2006). The need for models representing multi-species cropping systems is still evident to investigate concepts of competition and above- and below-ground interactions between crop/weed and crop/crop. These include models such as CropSys (Caldwell and Hansen, 1993), STICS (Malézieux et al., 2009), CoupModel (Jansson and Karlberg, 2010), and CERES-wheat or CERES-maize (Knörzer et al., 2011). Otherwise, a number of complex processes in soil and plant vary with season and site and have a constitutional variability that has to be also considered in modeling. Observed system properties imply therefore a source of uncertainty because of indirect measurements, estimations from other variables (Bert et al., 2007), and the unknown degree of homogenization of these data sets (Smith et al., 2007). For all these reasons, both the natural variability in observations and uncertainties in modeling are reasons for accepting more than one model realization as most plausible outcome. This fundamental idea is called the problem of equifinality suggesting the existence of multiple parameter combinations that result in acceptable representation of the system behavior (Beven, 2006). The uncertainty of the structural model error can be investigated within the Generalized Likelihood Uncertainty Estimation (GLUE) framework presented first by Beven and Binley (1992). The validity and robustness of models for different sites and data sets were already evaluated by the GLUE approach (Bert et al., 2007; Conrad and Fohrer, 2009c; Klemedtsson et al., 2008).

The objective of this study was to apply the CoupModel to silage maize in monoculture and bi-cropping with annual hardy ryegrass in Northern Germany during five consecutive years to investigate effects of uncertainties in model parameterization on water-related output. In this context, the question of potential water stress in bi-cropping systems on sandy-humic soil influenced by subsurface drainage was examined.

5.2 Methodology

5.2.1 The study area

This study was based on data from plot experiments carried out in Northwest Germany at the experimental farm ‘Karkendamm’ (53°55’N, 9°55’E, alt. 14 m) of the university of Kiel to investigate effects of farm management on N-use efficiency and N flows in soil-plant-animal systems on specialized dairy farms (1997–2003). Detailed and concluding results of the interdisciplinary research project ‘Karkendamm’ regarding climatic conditions, soil characteristics, crop yield, N losses, and groundwater quality under maize cultivation were published in, *e.g.*, Bleken et al. (2009), Bobe (2005), Büchter et al. (2003), Herrmann et al. (2005b), Volkers (2005), and Wachendorf et al. (2006a,b). The climate at the experimental site is maritime temperate with a 30-year average annual temperature of 8.6 °C and mean annual precipitation of 865 mm resulting in a positive climatic water balance of 312 mm $year^{-1}$. The dominating soil type was classified as Gleyic Podzol (FAO 2006) with less than 5% of clay, high contents of organic matter between 4.2 and 7.5% in 0–30 cm of depth, and an iron B-horizon between 95 and 98 cm of depth (Karrasch, 2005). Selected physical properties for the investigated soil profile are given in *Table 5.1*. Detailed information about water-retention characteristics based on the ceramic pressure-plate method and undisturbed soil samples, preparation of soil samples in addition to measured water contents, soil temperatures, and groundwater level can be found in Bleken et al. (2009), Bobe (2005), and Herrmann et al. (2005b).

Table 5.1: Characteristics of the soil profile (Gleyic Podzol) according to Ad-hoc-AG Boden (2005) (Herrmann et al., 2005b).

Horizon[a]	**Depth** (m)	**Soil bulk density** ($g\,cm^{-3}$)	**Sand content** (%)	**Total pore volume** (Vol.%)	**Plant available water content** (Vol.%)	**pH value** ($CaCl_2$) (–)	**Total organic C** (%)	**Total N** (%)	**C:N ratio** (–)
Ap	0–0.28	1.06	90.4	54.0	27.0	5.3	7.47	0.30	24.9
Ae + Bh	0.28–0.57	1.43	91.6	42.3	22.3	4.5	1.49	0.07	21.3
GoBh	0.57–0.79	1.62	91.8	34.3	16.1	4.1	0.89	0.04	22.3
Gor	0.79–0.94	1.65	93.6	37.4	17.1	4.2	0.40	0.02	20.0
IIFw1	0.94–0.98	1.67	94.4	37.8	28.8	4.3	1.22	0.06	20.3
fFw2	0.98–1.03	1.56	92.0	49.1	31.8	4.3	0.65	0.04	16.3
IIIGr	> 1.03	1.59	94.0	39.7	21.0	5.4	0.31	0.04	7.8

[a] According to Ad-hoc-AG Boden (2005) described as: Ap – plowing zone; Ae + Bh – toothed eluvial (Ae) and illuvial zone (Bh); GoBh and Gor – groundwater influenced mineral zone with changing oxygen conditions; IIFw1, fFw2 – different substrate (II) of lake deposits (f means fossil); IIIGr – different substrate (III) of groundwater influenced soil.

The total field plot that consisted of 48 sub-plots with a total area of 254x60 m was influenced by near-surface groundwater fluctuating between 18 and 180 cm below soil surface. High groundwater levels frequently led to temporary waterlogged conditions to the soil surface during winter, even though the area was integrated in an artificial drainage system (Karrasch, 2005). Field trials at 'Karkendamm' were focused on forage crop production dominated by silage maize and grassland between spring 1997 and spring 2002. All treatments based on 12 different N-fertilization levels and two cropping systems (maize monoculture and bi-cropping) were performed as a split-plot design with four replicates. The investigated field was grown with maize monoculture until 1996 and was fertilized with cattle manure (30 t ha^{-1} in 1995) or slurry (30–40 m^3 ha^{-1} in 1993, 1994 and 1996) combined with 50 kg ha^{-1} of mineral-N each year between 1993 and 1996. From 1997–2001, the early maize hybrid 'Naxos' was planted between late April and early May with a row width of 75 cm resulting in a final plant density of 10–11 plants m^{-2} (Herrmann et al., 2005b). Sampling of above-ground biomass varied from bi-weekly to once per year during the vegetation period resulting in different sampling dates from 1997 to 2001 for particular treatments (see ch. 5.2.2.3). More details about the preparation of crop samples can be obtained in Bleken et al. (2009). The grass species *Lolium perenne* L. was sown between the maize rows with a row width of 12.5 cm when maize plants reached the three to four-leaf stage in the bi-cropping systems (Volkers, 2005). The total biomass of undersown grass was sampled in late fall, up to six weeks after the maize harvest, and in spring, before killing with Glyphosate and used as green manure before plowing. Average N-fertilization input on each plot varied between 0 and 262 kg N ha^{-1} $year^{-1}$ depending on the defined N level: unfertilized, mineral-N (50, 100, and 150 kg N ha^{-1}), organic-N (20 and 40 m^3 ha^{-1} cattle slurry), and combined slurry/mineral-N (Büchter, 2003).

5.2.2 CoupModel – modeling approach

5.2.2.1 General information about soil water and plant growth dynamics

The complex ecosystem-process model CoupModel (Jansson and Karlberg, 2010) is applicable to simulate coupled heat, water, carbon, and nitrogen dynamics in unsaturated soil and vegetation. Sub-modules for water and nutrient flows, carbon (C) and nitrogen (N) transformations, and crop growth can be selected individually depending on the desired model complexity. Important driving variables were daily weather and soil management data in this study. The soil profile was divided into user-specified soil layers with variable depth increments determined by soil texture and water-retention characteristics. The Richards' equation was solved numerically for water dynamics and the Fourier's law of diffusion for heat including convective flows between horizontal soil layers. Soil water contents were calculated according to water-retention characteristics and hydraulic properties based on pedotransfer functions as proposed by Rawls and Brakensiek (1989). This grain size-based calculation was adjusted for each modeled soil layer with the help of data from laboratory determination of water-retention characteristics of particular soil layers. A constant groundwater-inflow rate was defined as driving parameter because the fluctuating shallow groundwater level limited the unsaturated soil zone. To prevent oversaturation of the whole soil profile by groundwater, horizontal drainage discharge (Drain) was also considered in the soil layer above the uppermost fully saturated layer. Therefore, an empirical drainage equation was selected to reproduce site-specific artificial drainage (details see ch. 5.2.2.3). No horizontal drainage was taken into account for the saturated soil layers. A vertical water flow from the lowest soil layer defined as deep percolation (Deep) was calculated with the seepage equation considering the saturated conductivity of the lowest compartment (see ch. 5.2.2.3). Soil evaporation was calculated with the iterative solution of the soil-surface energy-balance equation. The Penman-Monteith combination equation (Monteith, 1965; Penman, 1953) was used to determine potential transpiration that was necessary to estimate actual transpiration rate and plant water uptake. Both processes were calculated in consideration of possible compensatory water uptake by roots in soil horizons without water stress when the simulated root depth reached these soil depths and other layers were exposed to water stress.

Vegetation was simulated dynamically by means of C accumulation as a function of growth-stage indices (GSI, see below) regulated by several functions for air temperature, $f(T_l)$, water, $f(E_{ta}/E_{tp})$, and nitrogen, $f(CN_l)$, status in soil. Estimates of potential plant growth were based on the radiation use efficiency (RUE) approach by Monteith (1977). The total growth rate, $C_{Atm\rightarrow a}$, of different plant storages, *i.e.*, leaf, shoot, root, and grain, was derived from atmospheric-C assimilation that was proportional to global radiation absorbed by the canopy, $R_{s,pl}$:

$$C_{Atm\rightarrow a} = \varepsilon_L \eta f(T_l) f(CN_l) f(E_{ta}/E_{tp}) R_{s,pl} \tag{5.1}$$

where ε_L is the radiation use efficiency and η is a factor to convert biomass into C contents. Multiple plants cover the same area and were simulated by defining different properties for each plant (*Table A.2*); and thus, competition for light, water, and nitrogen within a plant community was considered. Allocation of C to particular plant storages was determined by plant development stages, synonymous for the GSI, and different environmental response functions. Threshold temperatures and temperature sums were specified according to the GSI for sowing, emergence, grain development, maturing, and harvest (*Table A.2*). In this study, harvest dates were fixed by measured data because of indications that harvest had occurred before the optimum temperature sum was reached (Herrmann et al., 2005). Although plant-N dynamics follow mostly the patterns of C allocation, the plant-N demand was governed by the C contents acting as driving force for the N uptake from soil. Soil-N contents were not only influenced by N uptake, decomposition, mineralization, and other below-ground processes but also by the land-surface management. The latter requirement was determined by dates for plowing, sowing, and harvesting including date and amount of applied N fertilizers. Beside atmospheric-N deposition, mineral-N and organic-N fertilizers were two external-N sources applied to a certain soil layer. Manure was defined as mixture of organic matter distributed into soil-N litter, soil ammonium-N (NH_4-N), and feces-N pool after application. Switches for soil management such as 'deep plowing' and 'surface cultivation' allowed the mixing of manure and litter into particular soil depths on the date of application. Ammonia volatilization (NH_3) from soil surface was not considered in the model setup. Below-ground C and N dynamics were considered by processes of decomposition and mineralization in corresponding organic pools, *i.e.*, humus, soil litter, and feces, in addition to inorganic soil pools, *e.g.*, NH_4-N and NO_3-N. Important input-parameters values different from default setting were specified in *Table A.1* and *Table A.2*. For more details see also previous model applications focused on different natural and agricultural systems: (i) forest (Klemedtsson et al., 2008; Norman et al., 2008) and (ii) agricultural systems such as arable farming (Conrad and Fohrer, 2009a; Zhang et al., 2007) and grassland (Conrad and Fohrer, 2009b,c).

5.2.2.2 Model parameterization with the GLUE approach

The description of management systems with CoupModel depends on the complexity of soil-plant-atmosphere interactions and the associated number of input parameters. The importance of each input parameter can differ in its relative importance for a specific model result, *i.e.*, the corresponding validation variable. General agreement between model and reality regarding particular system variables can be improved with multi-objective calibration that might be better qualified for un-calibrated conditions. To obtain acceptable model realizations, a number of 10,000 runs with random combinations of defined input parameters according to the Monte-Carlo sampling technique were simulated for each treatment in this study. Those input parameters that were assumed as uncertain according to their sensitivity on above-ground biomass and soil water were considered to vary within predefined ranges (*Table 5.2*). In general, four main groups separating abiotic from biotic conditions and above-ground from below-ground processes were specified for multiple simulations: (i) water-related parameters, (ii): plant properties governing evapotranspiration, (iii) soil nitrogen, and (iv) plant-growth dynamics. Large parameter ranges required a great number of simulations and resulted in many unrealistic parameter sets. Therefore, parameter ranges were limited to avoid inefficient and prohibitively expensive GLUE analysis (Arabi et al., 2007).

Main difference between the input parameter sets of particular treatments (MMx: maize monoculture; MUx: maize with an undersown grass; x represents particular N levels; see ch. 5.2.2.3) was the number of selected uncertain or so called ‘flexible’ input parameters. A number of 16 parameters were specified for multiple runs describing maize monocultures. In addition, eight parameters were selected to consider undersown grass in multiple runs resulting in a total number of 24 input parameters for bi-cropping systems. Remaining input parameters were fixed at defined values, and input parameters with values different from the default values are shown in *Table A.1* and *Table A.2*. The agreement between defined model output, *i.e.*, specific validation variables, and measurements (*Table 5.3*) was determined for each parameter combination using the ‘LogLikelihood’ (*LogLi*) measure as objective function for each validation variable.

Table 5.2: Input parameters used for the GLUE optimization.

Management system		**Input-parameter ranges**		
Parameter name	**Description**	Minimum	Maximum	Unit
(I) Properties of groundwater dynamics				
GWSourceFlow, q_{sof}	Constant rate of groundwater inflow	0.5	0.8	mm d^{-1}
(II) Vegetation characteristics for evapotranspiration				
Specific LeafArea (Plant 1), $p_{l,sp(1)}$	Parameter to estimate the leaf area index of plant 1 and plant 2 from C content in leaf	1	20	g C m^{-2}
Specific LeafArea (Plant 2), $p_{l,sp(2)}$		1	20	g C m^{-2}
(III) Below-ground nitrogen processes				
NitrificSpecificRate, n_{rate}	Nitrification rate in the response function for soil NO_3-N and NH_4-N content	0.05	0.4	d^{-1}
Eff Litter1, $f_{e,l1}$	Efficiency of the decay of litter pool 1	0.3	0.5	d^{-1}
Eff Litter2, $f_{e,l2}$	Efficiency of the decay of litter pool 2	0.3	0.5	d^{-1}
Eff Humus, $f_{e,h}$	Efficiency of the decay of humus pool	0.2	0.4	d^{-1}
RateCoef Litter1, k_{l1}	Rate coefficient for the decay of litter pool 1	0.01	0.1	d^{-1}
RateCoef Litter2, k_{l2}	Rate coefficient for the decay of litter pool 2	0.05	0.5	d^{-1}
NitrateAmmRatio, $f_{nitr,amm}$	NO_3-N : NH_4-N ratio in the nitrification function	3	10	–
(IV) Plant growth				
Root Water c1 (Plant 1), $r_{Wc1(1)}$	Fraction of the mobile carbon assimilates allocated to the roots of plant 1 and 2 in the response function for water stress when 'Root Allocation Water is independent'	0.2	0.5	–
Root Water c1 (Plant 2), $r_{Wc1(2)}$		0.2	0.5	
Root CN c1 (Plant 1), $r_{CNc1(1)}$	The constant part of the linear function for the allocation of mobile carbon assimilates to the roots of plant 1 and 2 in the response function for nitrogen concentration in leaves when 'Root allocation N Leaf is a linear function'	0.2	0.5	–
Root CN c1 (Plant 2), $r_{CNc1(2)}$		0.2	0.5	
Root Mass c1 (Plant 1), $r_{Mc1(1)}$	Fraction of the mobile carbon assimilates allocated to the roots in the response function for nitrogen concentration in leaves when 'Root Allocation Mass is independent'	0.2	0.5	–
Root Mass c1 (Plant 2), $r_{Mc1(2)}$		0.2	0.5	
Leaf c1 (Plant 1), $l_{c1(1)}$	Fraction of the mobile carbon assimilates is allocated to the new shoots of plant 1 and 2 when 'Leaf Allocation Shoot is independent'	0.2	0.5	–
Leaf c1 (Plant 2), $l_{c1(2)}$		0.2	0.5	
CN Ratio Min Roots (Plant 1), $cn_{MinRoot(1)}$	Minimum C:N ratio for roots of plant 1 and 2 to control N allocation to the roots from the mobile pool	20	28	–
CN Ratio Min Roots (Plant 2), $cn_{MinRoot(2)}$		10	25	–
Radiation use efficiency (Plant 1), $\varepsilon_{L(1)}$	Conversion factor for photosynthesis at optimum temperature, moisture and C:N ratio	2	4	g DW MJ^{-1}
Radiation use efficiency (Plant 2), $\varepsilon_{L(2)}$		2	4	g DW MJ^{-1}
C Seed (1), $c_{Seed(1)}$	Initial C content of plant 1 and 2 at sowing day without effects on plant C pool, respiration or photosynthesis	1	10	g
C Seed (2), $c_{Seed(2)}$		1	10	g

DW – dry weight

Table 5.3: Validation variables and additional measurements used for evaluation of the model performance.

Treatment	**MM1**	**MU1**	**MM2**	**MU2**	**MM3**	**MU3**	**MM4**	**MU4**
Validation variables (used for selection); sampling dates for MM (1997–2001) and MU (1998–2002)								
Above-ground C in maize (g C m^{-2})[a]	48+4	40+4	48+4	40+4	29+4	21+4	29+4	21+4
Total-C in undersown grass (g C m^{-2})	–	8	–	8	–	8	–	8
Above-ground N in maize (g N m^{-2})	45+4	40+4	45+4	37+4	29+4	21+4	26+4	21+4
Total-N in undersown grass (g N m^{-2})	–	8	–	8	–	8	–	8
Soil mineral-N content (0–90 cm) (g N m^{-2})	11	8	10	8	11	8	10	8
Number of records for additional validation variables (not used for selection)								
Soil temperature in 5, 10, and 20 cm of depth (°C)[b]	1648							
Soil water contents in 7 depths (Vol.%)[c]	13–31							
Soil water potential in 30, 50, and 70 cm depth (hPa)	33							
Groundwater level (m below surface)	110							
NO_3-N concentration in 60 cm of depth (mg N L^{-1})	802	690	808	690	783	629	799	665

[a] Two data sets were available (Set 1 + Set 2).
[b] Data from two grassland sites.
[c] Observed depths with 10 cm increments: 10 (13 records), 30, 40, 50, 60, 70, and 80 cm.

The *LogLi* measure introduced by Van Oijen et al. (2005) in the Bayesian calibration approach was calculated as the likelihood $p(D/\theta)$ assuming measurement errors were Gaussian and uncorrelated:

$$\text{Log}\ p(D/\theta) = \sum_{i=1}^{n} [-0.5\ ((O_i - S_i)/M_i))^2 - 0.5\ \text{Log}(2\pi) - \text{Log}M_i] \qquad (5.2)$$

where the S_i are model results, the O_i are observations, n is the number of observations, and M_i is the standard deviation or error of measured values (Klemedtsson et al. 2008). In the GLUE procedure, the number of acceptable behavioral simulations was directly defined by the value of the user-defined threshold criteria of an objective function with more flexibility in the selection than in the Bayesian approach. Selection of accepted simulations was conducted stepwise in this study, at first for above-ground C contents in maize and followed by total-C amounts in the undersown grass of the bi-cropping treatments (details see ch. 5.3.1.1). This was done to investigate effects of variations in biomass on soil water dynamics. The *LogLi* value was hardly comparable with other performance measures because of the consideration of measurement errors (*cf.,* Eq. 5.2), and therefore well-known measures such as the coefficient of determination R^2, the *NSE* (Nash and Sutcliffe, 1970), and the average magnitude of the error (*RMSE*) were used to evaluate the accuracy of simulated biomass (see ch. 5.3.1.2).

5.2.2.3 Input data for CoupModel

Total simulation period was specified from January 1996 to March 2002 including a pre-run period from January to October 1996 that was excluded from data evaluation to minimize impacts from initial values. Furthermore, this pre-run period was not extended because of unknown information on soil-related and management issues, except for the amount of N fertilizer, as well as maize yields before 1997. Corresponding daily weather information including average air temperature, precipitation, humidity, wind speed, and global radiation was derived from data of two local climate stations. Additionally, measured daily precipitation was corrected by +10% in the model setup according to Richter (1995) as a result of measurement errors for wind and evapotranspiration loss.

Simulations were based on information on observed soil layers (*cf.*, *Table 5.1*), but modeled soil increments varied from 5 cm in the two uppermost layers to 50 cm below 135 cm of depth. According to Karrasch (2005), an artificial drainage system was located next to the field plot, however, details on dimension and depth of drain pipes were not available. Therefore, an empirical drainage equation was selected in the model setup to reproduce site-specific horizontal drainage conditions. The net drainage amount was based on two flow components, the base flow and the more rapid peak flow, calculated as net horizontal flows from the soil layer where the simulated groundwater level was located, *i.e.*, the matrix potential was zero there. Following input parameters were adjusted to match the groundwater level: level, z_1, and flow, q_1, of the peak flow in addition to level, z_2, and flow, q_2, of the base flow component (*Table A.1*). Deep percolation was calculated with the seepage equation considering saturated conductivity of the lowest compartment, modeled groundwater level, and two adjusted input parameters characterizing the geometry of deep percolation: spacing distance, d_{p2}, and depth, z_{p2}, of the drainage level (*Table A.1*).

A number of eight treatments of silage maize in monoculture (MM) and bi-cropping (MU) with variable N-fertilization rates were considered in the simulations. In addition to unfertilized treatments (MM1 and MU1), three different N-fertilization levels with mineral-N (150 kg N ha^{-1}; MM2 and MU2), organic-N (40 m^3 ha^{-1} cattle slurry with different N contents for 1997, 1998, 1999, 2000, and 2001: 2.4, 1.8, 3.4, 3.7, and 3.3 kg N m^{-3}; MM3 and MU3) and combined slurry/mineral-N input (MM4 and MU4) were selected for modeling (*Table 5.4*).

Table 5.4: Crop characteristics and N-input management of the modeled treatments (Herrmann et al., 2005b).

Treatment	**MM1**	**MU1**	**MM2**	**MU2**	**MM3**	**MU3**	**MM4**	**MU4**
Maize monoculture (MM)	Yes	No	Yes	No	Yes	No	Yes	No
Undersown grass (MU)	No	Yes	No	Yes	No	Yes	No	Yes
Annual-N input:								
Atmospheric deposition (kg N ha^{-1})	20	20	20	20	20	20	20	20
Mineral-N (kg N ha^{-1})	0	0	150	150	0	0	150	150
Cattle slurry (m^3 ha^{-1})	0	0	0	0	40	40	40	40
Total-N input (kg N ha^{-1} year^{-1})								
1996[a]	20	20	70	70	140	140	190	190
1997	20	20	170	170	116	116	266	266
1998	20	20	170	170	92	92	242	242
1999	20	20	170	170	156	156	306	306
2000	20	20	170	170	168	168	318	318
2001	20	20	170	170	152	152	302	302
Mean-N input (without pre-run period):	**20**	**20**	**170**	**170**	**137**	**142**	**287**	**292**

[a] Pre-run period (data from January 1st to October 31st was excluded from evaluation).

Apart from the excluded pre-run-period from data assessment, the applied N-fertilizer rate in 1996 was also simulated different from information given in ch. 5.2.2.1. In this way, uncertain effects of the initial period and impacts from changing N inputs in 1997, especially for unfertilized treatments, on the results were excluded. In this context and as additional deviation from field tests, bi-cropping was also simulated in 1997 because of model requirements and to allow comparison of model results between monoculture and bi-cropping systems for five vegetation periods (see ch. 5.2.3).

The conversion of measured dry matter into C contents was necessary before modeling and was based on an estimated C amount in biomass of 45%. *Table 5.3* shows that the number of crop samples differed considerably between monoculture and bi-cropping systems, *e.g.*, with maximum records for unfertilized and mineral-N fertilized monocultures, compared with only two sampling dates per year for undersown grass. Moreover, only annual records at harvest date of maize were taken by Volkers (2005) in both bi-cropping systems and corresponding monocultures between 1998 and March 2002. To improve comparison between model and observations in the GLUE, particular C and N yields for maize in bi-cropping systems were estimated based on detailed results from monocultures (Herrmann et al., 2005) and annual reduction factors calculated by Volkers (2005). Therefore, two data sets were used for selection: detailed C and N contents including observed (monoculture) and estimated values (bi-cropping) in data set 1, and annual records for maize in addition to half-yearly records for undersown grass in data set 2.

5.2.3 Data evaluation and Statistical analysis

Limitation of the original input-parameter range according to applied thresholds of acceptance was based on the range ratio R (in%) that is described as:

$$R = (X_{p95} - X_5) / (X_{max,set} - X_{min,set}) * 100 \qquad (5.3)$$

where X_{p95} and X_5 are the 95th and 5th percentiles, respectively, for the accepted values of an input parameter, and $X_{max,set}$ and $X_{min,set}$ are the highest and lowest parameter value, respectively, in the GLUE setup for particular treatments. Actual range reductions R^* were presented as percentage $(1 - R)$ of the original parameter space (= 100%) for all selected input parameters.

The quartile coefficient of variation (CV^*) shows the extent of variability and was calculated to evaluate the dispersion of both accepted input parameters and particular model results with:

$$CV^* = (Q_3 - Q_1)/Q_2 \qquad (5.4)$$

where Q_1, Q_2, and Q_3 are the 25th, 50th, and 75th percentile, respectively, of a ranked data set. The second quartile Q_2 is also called median, and the term $(Q_3 - Q_1)$ determines the interquartile range. The calculated CV^* is a more robust measure, *i.e.*, it is not affected by outliers of the ranked data, than the coefficient of variation (CV) that is defined as ratio of the standard deviation (SD) to the mean (M). In general, the greater the CV value is, the higher the dispersion of the variable can be assumed, and distributions with CVs > 1 (100%) represent significant variation in the data set.

Data evaluation of simulated runoff components, evapotranspiration, and soil water storage to 30 and 90 cm of depth was done from November 1996 to March 2002 divided into six seepage-water and five vegetation periods. Mean values were aggregated for hydrological years (November to October), seepage-water periods (SWP; November to April), and vegetation periods (VP; May to October) separately. Analysis of significant differences between monoculture and corresponding bi-cropping treatment were applied on that using statistics tools of R (Version: 3.1.2 (2014-10-31); R Development Core

Team, 2013) with the R Commander GUI (Version: 2.0-x; Fox, 2005). Preliminary tests on normal distribution (Shapiro-Wilk test; level of significance $\alpha = 5\%$) and homogeneity of variances (Levene test; level of significance $\alpha = 5\%$) were carried out for simulated total runoff, evapotranspiration, water balance, and soil water storage. Obtained test results were used to apply conclusive tests for significant deviations between maize monocultures and bi-cropping treatments dependent on the period of aggregation. Depending on results of preliminary tests, either comparison of arithmetic means (single factor analysis of variance (ANOVA); level of significance $\alpha = 5\%$) or median values (non-parametric tests: Wilcoxon-Rank sum test; two-sided, level of significance $\alpha = 2.5\%$) was used. Results were significantly different between treatments in case of $p \leq 0.05$ (ANOVA) or $p \leq 0.025$ (Wilcoxon-Rank sum test) labeled with defined letters (a < b for comparing correspondent cropping systems).

5.3 Results and Discussion

5.3.1 Assessment of model performance and parameter uncertainty

5.3.1.1 Selection procedure for the most plausible simulations

Stepwise reduction of model runs to achieve those that were most plausible regarding biomass yields was based on the limitation of individual *LogLi* measures for selected validation variables (*Table 5.5*). The basic assumption of this selection procedure was a multi-objective (decision) model to balance multiple output variables with possibly different sensitivity to particular input parameters.

Table 5.5: Order of adjustment and selection thresholds of the 'LogLikelihood' function for the used validation variables and resulting number of accepted simulations.

Treatment	**Order**		**MM1**	**MU1**	**MM2**	**MU2**	**MM3**	**MU3**	**MM4**	**MU4**
Objective function	MM	MU	LogLikelihood (*LogLi*)							
Above-ground C in maize; Set 1	1	1	−2e+5	−3e+5	−5e+5	−3e+5	−5e+4	−1e+5	−1.3e+5	−8e+4
Above-ground C in maize; Set 2	2	2	−2e+4	−5e+4	−6e+4	−1e+5	–	−5e+4	–	−8e+4
Total-C in undersown grass		3		−4e+4		−1e+5		−5e+4		−8e+4
Above-ground N in maize; Set 1	3	4	–	–	–	–	−300	−200	−200	−300
Above-ground N in maize; Set 2	4	5	–	–	–	–	–	–	–	−100
Total-N in undersown grass		6		–		–		–		−200
Soil mineral-N content (0–90 cm)		7	–	–	–	–	–	–	–	−500
To achieve a number of accepted runs of: (total number of runs = 10,000)			73	62	78	73	56	43	32	33

Evidently, the definition of individual *LogLi* measures by trial and error was not really impartial, but in case of several considered output variables there was always the risk of poor agreements between model and observation. Optimum solution to compare model results from different treatments was certainly a common set of threshold criteria that was used for all scenarios. According to that, common criteria set led to a highly variable sample size of accepted simulations applied to all treatments. The reason for this inconsistency was found in differences between the treatments regarding particular validation variables, *i.e.*, the variance between used data sets, especially for those with only few observations (*cf., Table 5.3*). An automatic selection procedure considering all validation variables equally was not practical, and therefore the *LogLi* value of a selected validation variable was adjusted individually to a threshold value in the same order as shown in *Table 5.5*. As a result of limiting the *LogLi* threshold value of the C content in above-ground maize biomass to more positive numbers, the *LogLi* ranges of all the rest of selected validation variables as shown in the upper part of *Table 5.3* were also adjusted to new values. Finally, the limitation to a particular *LogLi* threshold value was done with the objective to reduce the number of simulations considerably under the condition that well-known performance measures remained as high as possible, *e.g.*, for R^2 and *NSE*, or rather remained low in case of the sample standard deviation *(RMSE)*. In the process, the number of measurements usually influences the explanatory power of the model performance significantly. In this study, the number of samples was not only very different (*cf., Table 5.3*) between the treatments but also between the investigated years. To minimize negative effects from this heterogeneity on the comparison between measured and simulated results of maize in bi-cropping systems, two data sets for the above-ground C and N content in maize were used to select the most plausible model realizations in two steps. Therefore, the *LogLi* value based on the comparison between data set 1, which contained the complete number of available above-ground C contents in maize from 1997 to 2001, and corresponding modeling results was limited at first for each treatment. In case of bi-cropping systems, the same comparison was done with data set 1 that included extrapolated C contents in maize from 1998 to 2001 according to comments in ch. 5.2.2.3. Data set 2 containing annual records at harvest for the above-ground C content of maize was used for further reduction of model realizations in a second step. After that, the *LogLi* value of total-C in undersown grass was limited in bi-cropping systems. This selection procedure was then applied to the N contents in maize and grass in the same way as described for the C contents. As a result of considering several validation variables in the order specified, the selection of most plausible runs was more or less predefined. The chosen sequence of considered validation variables implied consequently a potentially subjective decision on which validation variables were more important than the rest of them. Finally, the maximum number of accepted simulations was fixed at 80 of 10,000 parameter combinations to limit time and effort of posterior data analysis.

5.3.1.2 Evaluation of the agreement between model and measurement

5.3.1.2.1 Plant growth and nitrogen uptake

Resultant comparison between observed and modeled results showed variable performance measures for several validation variables (*Table 5.6*). Modeled C and N amounts predominantly used for selection of the most plausible simulations matched measurements better when more data were available for comparison. The R^2s were mostly greater than 0.5 for maize and even less for undersown grass, whereas corresponding *NSE*s were mainly less than zero, except for the above-ground C in maize, as a result of their sensitivity to peak values including the small number of samples.

Table 5.6: Maximum and minimum model performance measures (R^2 − coefficient of determination (0–1; best = 1), RMSE – Root mean squared error (−∞ to ∞; best = 0), and NSE − Nash-Sutcliffe efficiency (−∞–1; best = 1)) for validation variables used for selection (upper part) and additional comparison.

Validation variable	**Performance measure**	**Minimum value in treatment:**		**Maximum value in treatment:**	
Above-ground C in maize; Set 1	*R^2*	0.59	MU1	0.96	MM3
(g C m^{-2}, n = 21–48)	*RMSE*	65	MU4	135	MM2
	NSE	0.30	MM3	0.94	MU4
Above-ground C in maize; Set 2	*R^2*	0.005	MM4	0.81	MM1
(g C m^{-2}, n = 4)	*RMSE*	91	MM1	339	MM4
	NSE	−171	MM3	−0.9	MU1
Total-C in undersown grass;	*R^2*	0.16	MU4	0.28	MU2
(g C m^{-2}, n = 8)	*RMSE*	94	MU1	99	MU2
	NSE	−2.0	MU2	−0.08	MU3
Above-ground N in maize; Set 1	*R^2*	0.48	MU1	0.93	MU4
(g N m^{-2}, n = 21–43)	*RMSE*	2.2	MM1	5.3	MU2
	NSE	−0.20	MM3	0.77	MM4
Above-ground N in maize; Set 2	*R^2*	0.02	MM4	0.82	MU2
(g N m^{-2}, n = 4)	*RMSE*	1.9	MM1	9.4	MM4
	NSE	−39	MM4	−1.4	MM2
Total-N in undersown grass;	*R^2*	0.05	MU2	0.20	MU4
(g N m^{-2}, n = 8)	*RMSE*	2.2	MU1	4.7	MU4
	NSE	−6.8	MU2	−0.9	MU3
Soil mineral-N content (0–90 cm)	*R^2*	0.01	MU1	0.17	MU2
(g N m^{-2}, n = 8–11)	*RMSE*	2.2	MU1	8.8	MM4
	NSE	−13.5	MM4	−1.3	MM3
Soil temperature in 5 cm of depth	*R^2*	0.88		0.89	
(°C, n = 1648)	*RMSE*	2.4	MU1	2.7	MM2, MM3
	NSE	0.77	MM2, MM3	0.82	MU1, MU2
Soil temperature in 10 cm of depth	*R^2*	0.90		0.91	
(°C, n = 1648)	*RMSE*	2.05	MU1	2.3	MM2
	NSE	0.83	MM2, MM3	0.86	MU1-4
Soil temperature in 15 cm of depth	*R^2*	0.91		0.92	
(°C, n = 1648)	*RMSE*	1.8	MU1	2.0	MM2, MM3
	NSE	0.85	MM2-4	0.88	MU1-3
Water content in 30 cm of depth	*R^2*	0.60	MU2	0.66	MM1
(Vol.%, n = 31)	*RMSE*	5.6	MM1	7.0	MU2
	NSE	0.33	MU2	0.57	MM1
Water content in 50 cm of depth	*R^2*	0.72	MU2	0.81	MM4
(Vol.%, n = 31)	*RMSE*	6.5	MM1	7.4	MU1
	NSE	−0.1	MU1	0.17	MM1
Water content in 70 cm of depth	*R^2*	0.25	MU2	0.33	MM4
(Vol.%, n = 31)	*RMSE*	7.5	MM1	8.1	MU1
	NSE	−0.21	MU1	−0.03	MM1
Soil water potential in 30 cm of	*R^2*	0.001	MM4	0.05	MU1
depth (hPa, n = 33)	*RMSE*	572	MM1	995	MU2
	NSE	−792	MU2	−332	MM1
Soil water tension in 50 cm of	*R^2*	0.005		0.08	MU1
depth (hPa, n = 33)	*RMSE*	313	MM1	607	MU2
	NSE	−570	MU2	−209	MM1
Soil water potential in 70 cm of	*R^2*	0.10	MU2, MU4	0.21	MM1, MU1
depth (hPa, n = 33)	*RMSE*	45	MM1	115	MU1
	NSE	−81	MU1	−5.5	MM4
Groundwater level	*R^2*	0.18	MU3	0.40	MM1
(m, n = 110)	*RMSE*	0.28	MM1	0.37	MU3, MU4
	NSE	−0.57	MU3	0.04	MM1
NO_3-N concentration in 60 cm of	*R^2*	0.09	MU1	0.41	MM2
depth (mg N L^{-1}, n = 629–808)	*RMSE*	6.0	MU1	42	MU4
	NSE	−30.5	MU4	−0.5	MU1

In general, presented performance measures confirmed not only plausibly simulated biomass by limiting their *LogLi* values but also major differences between measured and modeled soil mineral-N contents. Reasons for weak statistics in the latter case were possibly found in both the small number of observations and the variability of measured and modeled results indicated by standard deviations (*SD*s) even as high as arithmetic means implying increased uncertainty (detailed data not shown).

Comparison between observed and modeled C (*Fig. 5.1*) and N contents (*Fig. 5.2*) in maize and undersown grass showed good agreements for maize biomass but also highly variable C and N contents in grass from 1996 to 2002. The modeled overall average C content in maize was only slightly greater than observed in monoculture (MMm) by +3% and bi-cropping (MUm) by +7% caused by the compensation of under- and overestimation in the corresponding treatments. The same effect was found for the total-C amount in grass that was both under- and overestimated ranging between −19% (MU1) and +28% (MU4). In the majority of all treatments, modeled N contents of above-ground maize biomass were also greater than observed with overestimations between +21% (MM2) and +88% (MU3) at harvest date. Similar plausible simulation results regarding dry matter and plant-N yields in maize monocultures were stated in Herrmann et al. (2005b) for the same treatments. In contrast, the CoupModel considered two plants in parallel with the ability to reproduce bi-cropping cultivations. A significant decrease of C amounts in undersown grass was found for mineral-N fertilized treatments as also reported by Volkers (2005). Indications for increased competition pressure regarding simulated above-ground C and N contents in maize were most evident in fertilized bi-cropping treatments. However, considerable variability in both observed and modeled results showed that mean total-C contents in undersown grass were not significantly different, neither between fall and spring nor between model and observations. Model description of multiple plant covers was therefore associated with an increased uncertainty in the model for the undersown grass.

5.3.1.2.2 Soil temperature, soil water content, and groundwater level

The model performance of abiotic system variables such as soil temperature, water content, water potential, and groundwater level were also compared to measurements to evaluate model plausibility in general. As shown in *Table 5.6*, simulated soil temperatures to 15 cm of depth agreed well with non-site-specific data measured at a nearby grassland site (Herrmann, 2006) indicated by R^2s > 0.88, *NSE*s > 0.72, and *RMSE*s of 1.8–2.7 °C. Modeled results showed higher variability for maize monocultures than for bi-cropping systems because of increased RMSE, whereas NSE indicated better model performance for monocultures. The predicted uncertainty of simulated soil temperatures expressed as standard deviation value of all accepted runs on daily resolution was significantly lower than the difference between model results and single measurements from the grassland plot (*Fig. 5.3*).

Especially in early spring when young maize plants had already emerged, modeled soil temperatures to 15 cm of depth increased significantly as a result of elevated air temperatures and rapid warming-up of partially covered soil. Model results were consequently greater than observed under grassland resulting in maximum negative differences in periods without complete ground covering.

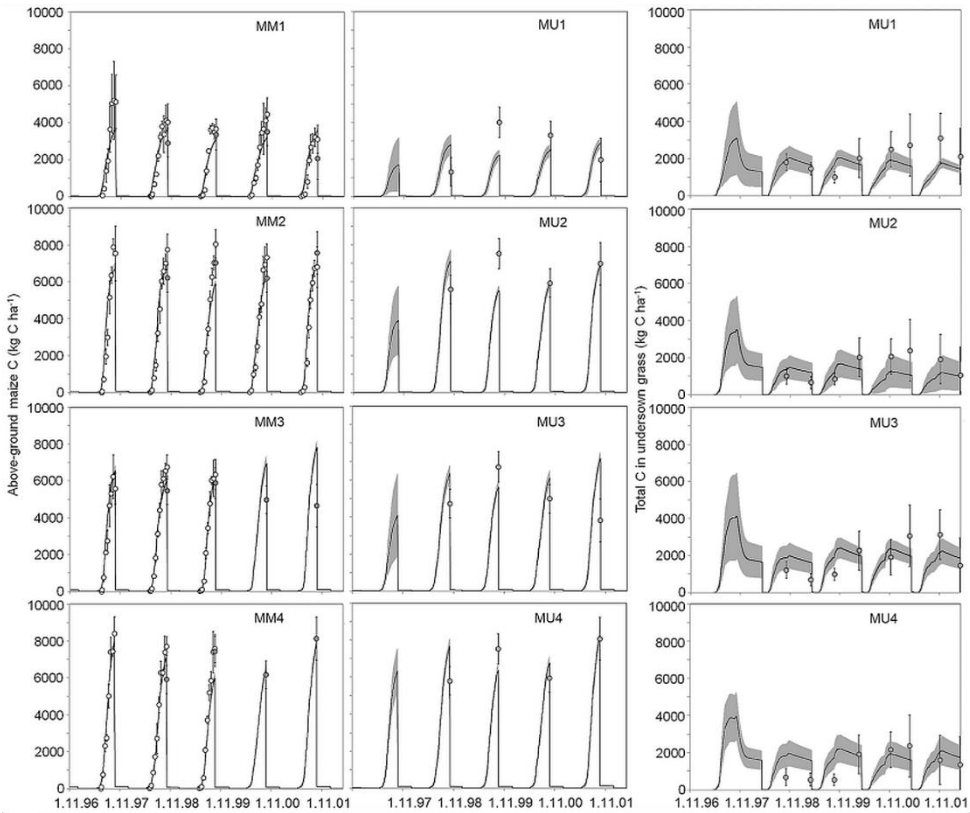

Fig. 5.1: Comparison between measured (circle) and simulated (line) above-ground C in maize and total-C contents in undersown grass for each treatment. Results are shown as daily mean values within SD.

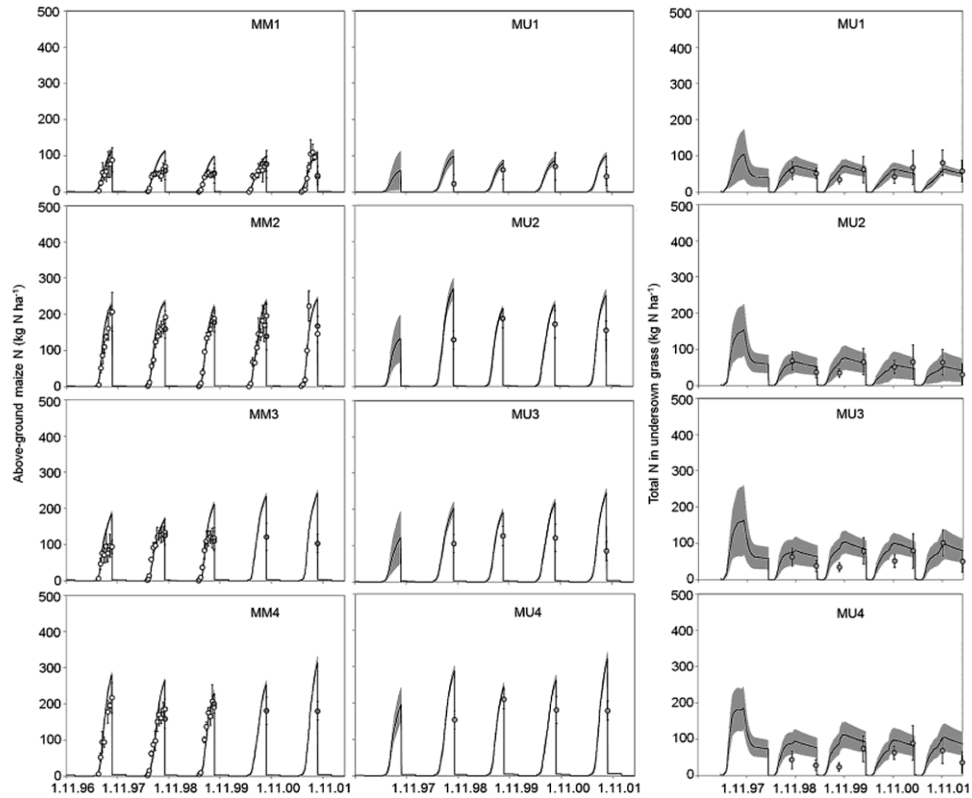

Fig. 5.2: Comparison between measured (circle) and simulated (line) above-ground N in maize and total-N contents in undersown grass for each treatment. Results are shown as daily mean values within SD.

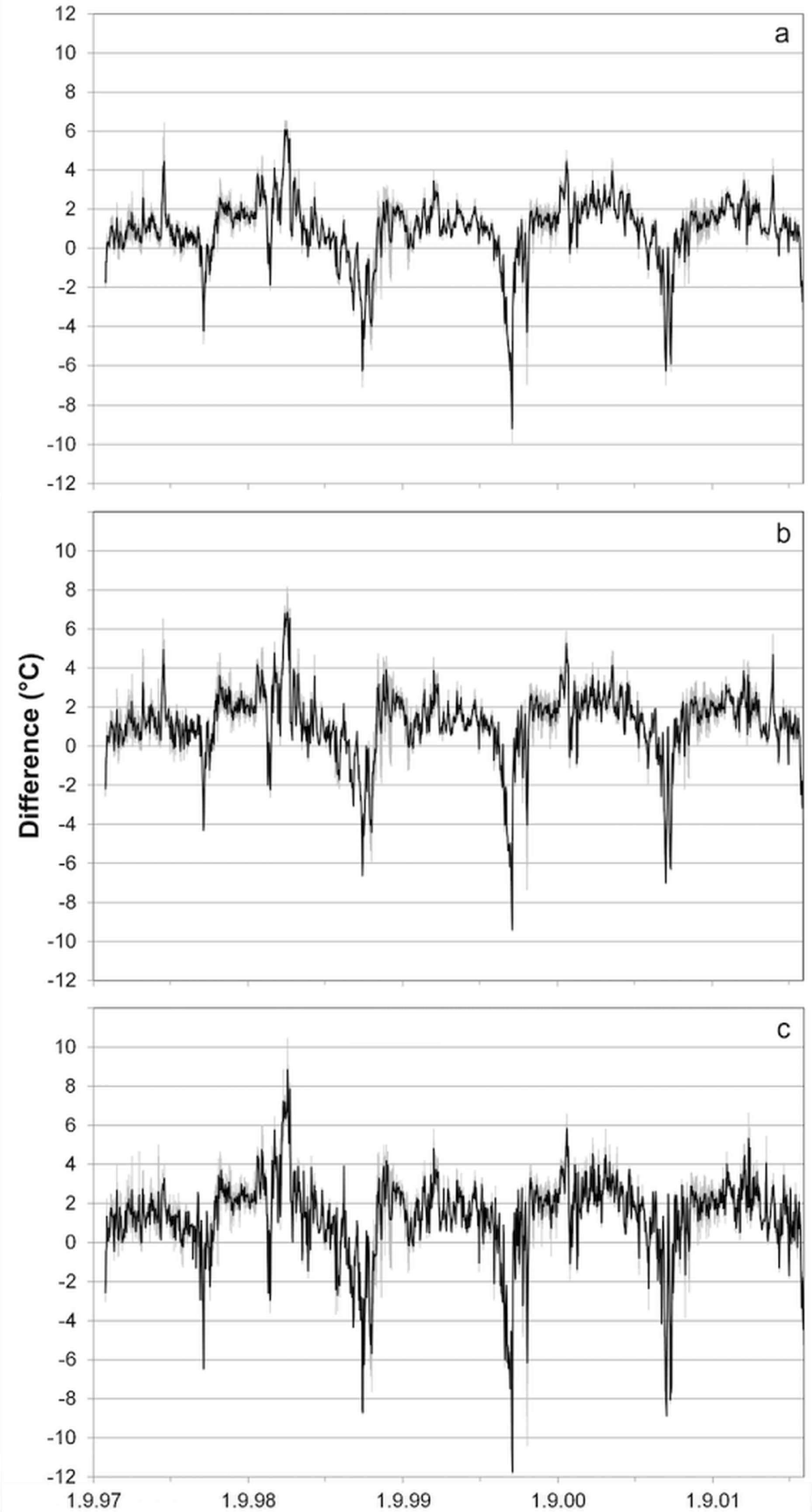

Fig. 5.3: Difference between measured and mean simulated soil temperatures in 5 cm (a), 10 cm (b), and 15 cm (c) of depth. Results are shown within SD (gray area) of the modeled results from 1997 to 2002.

Differences between observation and model were predominantly positive within average error ranges of approx. 3 °C indicating that measurements from grassland sites represented conditions of covered soil with slightly increased soil temperatures even in winter.

Comparison between particular cropping systems showed higher variability, *i.e.*, greater *RMSE*, of both water content and water potential for bi-cropping systems than for monocultures, their R^2 and *NSE* were slightly increased on the other hand (*cf., Table 5.6*). Soil water contents were simulated plausibly and agreed well with measured data to 50 cm of depth, but best matches were found in 40 cm of depth confirmed by maximum R^2 of 0.70–0.80 and *NSE* of 0.50–0.70 (data not shown in *Table 5.6*). The uncertainty of modeled water contents varied significantly over the whole simulation period but less than observed variability (*SD* not shown). Corresponding soil water potentials were modeled with even higher uncertainty, especially for dry periods, but also showed lower model performance. Apparent discrepancy between water content and corresponding water potential below 50 cm of depth may obviously be caused by spatial heterogeneity, small number of samples, field conditions deviating from determined water-retention characteristics, and overestimation of the modeled groundwater level (*Fig. 5.4*).

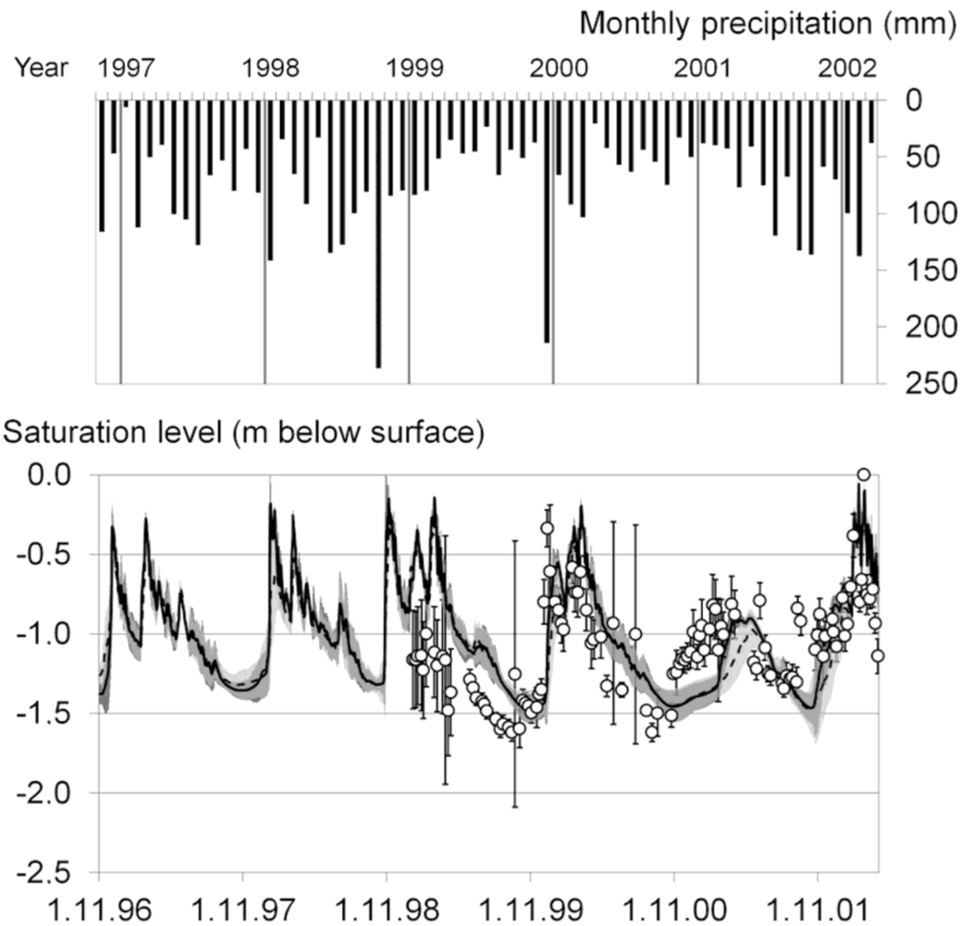

Fig. 5.4: Simulated mean of monoculture (MMm: —) and bi-cropping (MUm: - - -) systems compared to measured (o) groundwater levels with information on monthly precipitation (bar). Results are shown as means within SD (MMm: dark gray, MUm: light gray) from 1997 to 2002.

However, simulations reproduced annual dynamics of measured groundwater level plausibly. Overall comparison between measurements and modeling results confirmed significant deviations with undistinguished R^2 and *NSE* accompanied by relatively high *RMSE* (*cf., Table 5.6*). The maximum *RMSE* of 0.37 cm was calculated for the highly fertilized treatment. Simulated groundwater level varied according to the monthly-based precipitation pattern to distinguish between wet, *e.g.*, fall 1998, winter 1999/2000 or winter 2001/2002, and dry periods, *e.g.*, winter 1999/2000. Modeled groundwater levels also showed slightly less variability, *i.e.*, average *SD* of 0.10 cm, than observations, *i.e.*, average *SD* of 0.16 cm. Reason for modeled overestimations in particular periods especially from spring to fall 1999 could be the steady groundwater-inflow rate specified to match the average saturation level. In contrast, simulations underestimated the observed groundwater level from winter 2000/2001 to spring 2001 when precipitation was below-average.

5.3.1.3 Evaluation of the input-parameter uncertainty

Limitation of parameter ranges by means of adjusting *LogLi* values of defined output variables showed rather divergent results for each input parameter (*Table 5.7*). Selection of the most plausible simulations limited the parameter space by 10–25% for the most input parameters.

Reductions of more than 50% were found for the radiation use efficiency (RUE) in five of six fertilized treatments indicating that RUE values between 2.5 and 4.0 g DW MJ^{-1} matched corresponding above-ground C contents of maize. The RUE value varied between 2.0 and 4.0 g DW MJ^{-1} for unfertilized plots. Reason for only minor limitations in general might be the defined input-parameters ranges, *e.g.*, for the groundwater inflow, however, pre-analysis showed implausible modeled groundwater levels in case of higher or lower inflow rates.

Another cause of deviations without uniform pattern was predominantly found in differences in the calculated *LogLi* values based on particular measured and simulated output variables in each treatment. Therefore, multiple and stepwise applied thresholds of acceptance were most effective for first validation variable(s) but with potentially adverse effects on following variables because of complex interactions between plant growth and soil water.

The quartile coefficient of variation (*CV**) was calculated for ‘flexible’ input parameters to assess particular dispersion of parameter values among the accepted runs on a statistical basis. As shown in *Table 5.7*, *CV**s < 25% were found for a number of input parameters such as groundwater inflow, efficiency of decomposition, radiation use efficiency, and specific C-allocation parameters for plant growth. Only few input parameters showed variations greater than 100% up to 172% indicating that some soil and plant-related parameters were highly uncertain in treatments exclusively fertilized with mineral-N or slurry-N. Site-specific parameter values were difficult to determine; indeed *CV**s < 25% were found for all treatments with variable proportions from 21% (MU2) to 44% (MM1) on the total number of ‘flexible’ input parameters.

5.3.1.4 Variability of simulated water balance components

Consequently, quartile coefficients of variation (*CV**) were also calculated for selected output variables, *i.e.*, evapotranspiration, total runoff, and soil water storage to 30 and 90 cm of depth within their minimum and maximum ranges and for particular periods (*Table 5.8*). Data dispersion of selected output variables was not only highest in bi-cropping treatments with maximum *CV** values of 22–26% for evapotranspiration, but also total runoff showed similar increased variability in bi-cropping. By comparison, *CV** values of water storage to 30 and 90 cm of depth were much less ranging between 0 and 10%, and an increased data dispersion was also found in the vegetation period (VP). The implementation of an undersown crop in modeling to ensure continuous ground cover can potentially increase the uncertainty of particular water-related components especially during growth. Comparison between *CV** values of ‘flexible’ input parameters and half-yearly water-related output variables also suggested that the smaller percentage of parameters with low dispersion (*CV** < 25%) in bi-cropping systems, *i.e.*, averaged 26% compared with 36% in monocultures, resulted in an elevated dispersion of examined water-related output.

5.3.2 Comparison between modeled treatments regarding soil water balance and water storage

The soil water balance was positive for all treatments varying between +18 mm year^{-1} (MU3) and +35 mm year^{-1} (MM1) without significant differences between monoculture and corresponding bi-cropping treatment or between all treatments, except for the unfertilized monoculture (MM1) because less groundwater inflow of approx. 10 mm year^{-1} was simulated there (*Table 5.9*).

This water surplus increased slightly with both applied-N amount and existing undersown grass and was highest during the SWP with maximum values for the high-fertilized bi-cropping system because of reduced total runoff (*cf., Fig. 5.5*). The reverse effect was found from May to October with varying water deficit between −13 mm (MM1) and −94 mm (MU4) as a result of dominant evapotranspiration losses.

Deviations in the water balance between monoculture and corresponding bi-cropping system were significant during plant growth, although calculated water deficits provided indications of only minor water stress in the VP especially for fertilized bi-cropping systems.

Total runoff and evapotranspiration (ETI) as basic components of the water balance were aggregated to half-yearly amounts (*Fig. 5.5*). Following major elements were distinguished: horizontal drainage (Drain), deep percolation (Deep), surface runoff (SurfOutflow), evaporation (Evap), transpiration (Transp), and interception (Intercep). First of all, plausible significantly increased total runoff was found from November to April, unlike the vegetation period between May and October, because of reduced ETI amounts during the SWP in all treatments. Absolute difference between maximum (MM1) and minimum (MU3) total runoff was approx. 74 mm during the SWP compared with a mean *SD* of 120 mm reflecting the high variability of modeled results on half-yearly basis.

Table 5.7: Reduction of the parameter space (R) and the quartile coefficient of variation (CV*) for the GLUE input parameters of the accepted simulations.*

	Reduction of the parameter space *R (%)[a]**								**Quartile coefficient of variation *CV** (%)[b]**							
Treatment	**MM1**	**MU1**	**MM2**	**MU2**	**MM3**	**MU3**	**MM4**	**MU4**	**MM1**	**MU1**	**MM2**	**MU2**	**MM3**	**MU3**	**MM4**	**MU4**
Selected input parameters																
GWSourceFlow, q_{sof}	12	8	12	17	10	13	10	13	20	20	16	20	22	15	17	15
Specific LeafArea (Plant 1), $p_{l,sp(1)}$	60	24	14	7	18	13	41	13	19	48	87	97	66	15	15	29
Specific LeafArea (Plant 2), $p_{l,sp(2)}$		17		11		22		22		59		57		84		56
NitrificSpecificRate, n_{rate}	13	5	5	7	16	6	25	6	83	81	86	79	54	64	97	72
Eff Litter1, $f_{e,l1}$	5	4	5	17	8	10	9	10	30	27	24	24	22	19	18	15
Eff Litter2, $f_{e,l2}$	12	12	13	8	16	8	14	8	17	20	23	21	20	27	26	21
Eff Humus, $f_{e,h}$	17	8	7	7	12	5	6	5	21	29	29	33	29	38	33	31
RateCoef Litter1, k_{l1}	20	9	6	7	6	10	1	10	71	64	109	111	172	74	97	90
RateCoef Litter2, k_{l2}	16	11	10	7	7	11	11	11	71	71	86	79	94	104	72	74
NitrateAmmRatio, $f_{nitr,amm}$	10	11	14	6	11	8	14	8	48	51	59	50	49	49	35	26
Root Water c1 (Plant 1), $r_{Wc1(1)}$	27	10	23	11	8	16	3	16	40	40	34	35	41	41	51	38
Root Water c1 (Plant 2), $r_{Wc1(2)}$		3		8		3		3		41		50		35		45
Root CN c1 (Plant 1), $r_{CNc1(1)}$	29	13	13	5	12	16	9	16	29	53	32	43	49	31	50	35
Root CN c1 (Plant 2), $r_{CNc1(2)}$		8		7		24		24		33		35		34		25
Root Mass c1 (Plant 1), $r_{Mc1(1)}$	32	13	26	10	15	8	36	8	31	48	36	37	38	21	31	45
Root Mass c1 (Plant 2), $r_{Mc1(2)}$		2		10		9		9		34		38		39		33
Leaf c1 (Plant 1), $l_{c1(1)}$	56	26	23	25	15	33	39	33	14	23	33	28	34	25	20	28
Leaf c1 (Plant 2), $l_{c1(2)}$		27		12		10		10		24		42		36		36
CN Ratio Min Roots (Plant 1), $cn_{MinRoot(1)}$	23	12	12	18	20	9	2	9	9	18	15	11	14	14	17	18
CN Ratio Min Roots (Plant 2), $cn_{MinRoot(2)}$		17		9		3		3		28		40		32		27
Radiation use efficiency (Plant 1), $\varepsilon_{L(1)}$	24	12	54	53	57	57	35	57	22	35	11	13	11	20	17	10
Radiation use efficiency (Plant 2), $\varepsilon_{L(2)}$		18		10		13		13		18		43		29		32
C Seed (1), $c_{Seed(1)}$	43	38	8	6	8	5	41	5	42	33	103	105	66	24	45	54
C Seed (2), $c_{Seed(2)}$		35		16		13		13		33		71		76		76

(Different from the layout of the published article, following markers are used to highlight important findings:
[a] Gray-shaded areas represented reductions of the parameter space *R** > 30%.
[b] Gray-shaded areas represented input parameter variability *CV** < 25% of the selected simulations.)

Table 5.8: Maximum and minimum quartile coefficient of variation (CV) for selected output variables influencing the soil water balance.*

Output variable		**Evapotranspiration**			**Runoff**			**Water storage (0–30 cm of depth)**			**Water storage (0–90 cm of depth)**		
Period		Nov.–April **(SWP)**	May–Oct. (**VP)**	**Year**	Nov.–April **(SWP)**	May–Oct. (**VP)**	**Year**	Nov.–April **(SWP)**	May–Oct. (**VP)**	**Year**	Nov.–April **(SWP)**	May–Oct. (**VP)**	**Year**
***CV** (%) for**	**MM:**	0	4–8	3–6	8–10	11–17	9–12	0	3–4	1–2	1	4–6	2–3
	MU:	13–26	4–22	5–12	14–16	13–21	14–18	2–5	5–8	3–7	3–5	6–10	4–6

Table 5.9: Simulated annual and semi-annual water input and resulting soil water balance for all treatments.

Treatment	**MM1**	**MU1**	**MM2**	**MU2**	**MM3**	**MU3**	**MM4**	**MU4**	**Mean MMm**	**Mean MUm**
Total water input (Win; precipitation = 897 mm year^{-1} and mean groundwater inflow = 246 mm year^{-1}; (mm, *SD* within parentheses), 11/1996–03/2002)									1141 (40)	1146 (41)
Nov.–April									532 (38)	534 (37)
May–Oct.									608 (32)	610 (33)
Water balance (delta = Win - (R + ETI); (mm)[a]										
Nov.–April	+74 a	+62 a	+95 a	+100 a	+105 a	+112 a	+106 a	+119 a	+95 a	+98 a
May–Oct.	−13 b	−30 a	−63 b	−80 a	−69 b	−88 a	−72 b	−94 a	−54 b	−73 a
Mean (*year*$^{-1}$)	+35 b	+23 a	+26 a	+25 a	+20 a	+18 a	+21 a	+22 a	+27 a	+20 a

[a] Letters a and b (with a < b) were indicators of significant differences between monoculture and corresponding bi-cropping treatment based on ANOVA (α = 5%) or non-parametrical test (Wilcoxon-Rank sum test; two-sided, α = 2.5%).

In the majority of all treatments, total runoff was slightly greater in maize monocultures (MMm: M = 151 mm, SD = 32 mm) than in bi-cropping systems (MUm: M = 148 mm, SD = 28 mm) during the VP. In contrast, total runoff differed significantly between monoculture (MMm: M = 319 mm, SD = 117 mm) and bi-cropping treatments (MUm: M = 283 mm, SD = 125 mm) in the SWP. Reason for this difference was the decreased drainage amount of 22 mm year^{-1} in bi-cropping. Simulation results with the soil-crop model STICS confirmed that catch crops reduced the annual drainage-water amount on an average of less than 10% with at most 25% in dry winter periods (Justes et al., 2012). The same study stated that the absolute decrease in drainage water of average 30 mm and variations between 0 and 80 mm verified missing negative effects of catch crops on water consumption of the succeeding crop. To sum up, the main discharge period ranged from November to April with horizontal drainage proportions between 33% (MUm) and 37% (MMm) of half-yearly precipitation. Tiemeyer et al. (2009) specified tile drainage proportions higher than 50% of precipitation during winter; although site-specific characteristics were different to this study, *i.e.*, less precipitation of 665 mm year^{-1} and different soil types were stated. Reason for reduced drainage portions in this study was possibly the excessive vertical water transport because of high sand contents at the 'Karkendamm' site.

Plausible evaporation loss of 120 mm was calculated for bare soil in monocultures; and moreover, approx. 38% less soil evaporation was found for catch crops during the SWP confirmed by Bodner et al. (2007). Compared with reduced evapotranspiration during the SWP, total ETI amounted to 682 mm year^{-1} (MMm) and 696 mm year^{-1} (MUm), respectively, in monoculture and bi-cropping for the whole hydrologic year (November 1st to October 31st). Differences regarding the ETI were significant between SWP and VP or rather between monoculture and corresponding bi-cropping system during SWP and VP. The ETI in bi-cropping systems was determined slightly higher (+20–+50 mm SWP^{-1}) because of significant transpiration by hardy grass. In comparison with real ETI data from maize on groundwater-influenced sandy soil in East Germany (Müller et al., 2005), total evapotranspiration was up to 45% greater during summer in this study. Reasons for elevated ETI amounts might be the intermediate water storage in the total pore volume of the 0–28 cm layer because of strongly humic conditions (*cf., Table 5.1*), and twice as much precipitation in Northwest Germany. The interception loss as part of the ETI was generally increased in bi-cropping systems because of almost permanent soil covering. The interception can amount up to 24% of precipitation for grassland canopy in Northwest Europe (Sutanto et al., 2012) that was comparable to findings in this study of maximum 21% for undersown grass during the SWP (MU1).

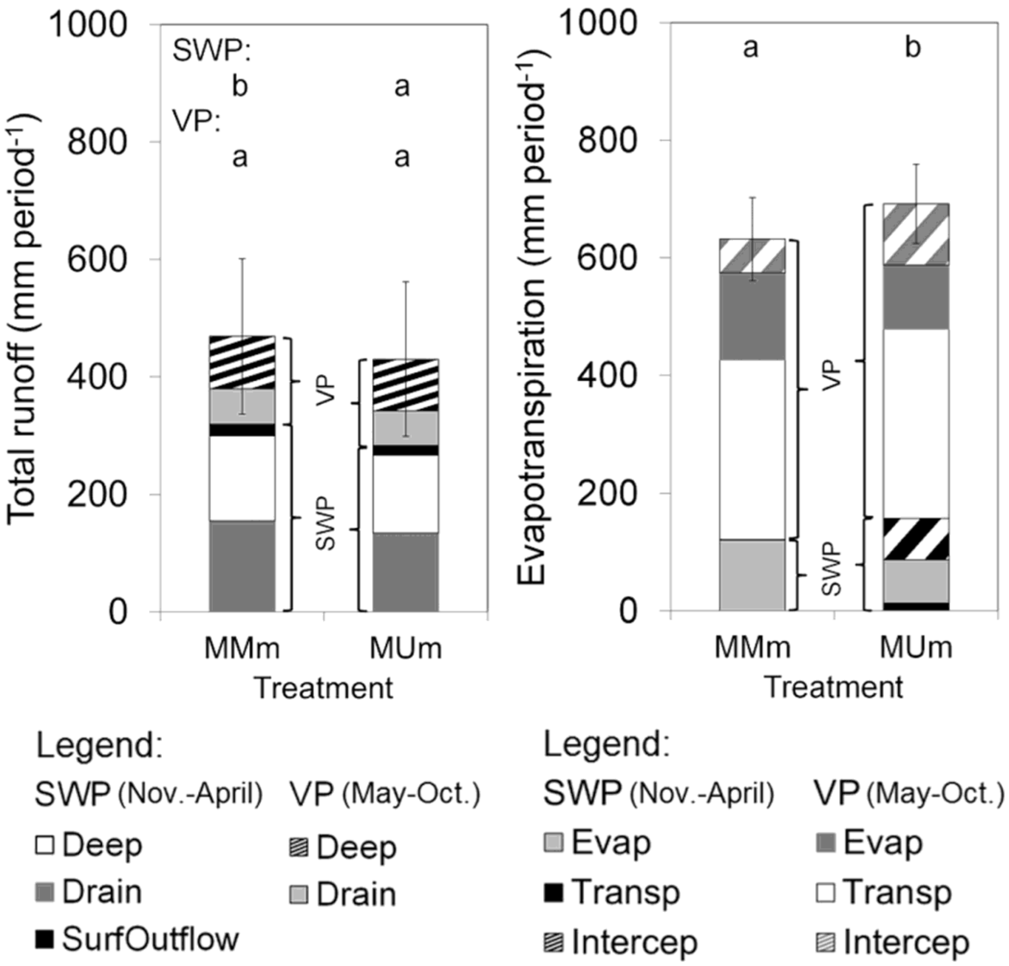

Fig. 5.5: Simulated total runoff (left) and evapotranspiration (right) for means of monoculture (MMm) and bi-cropping (MUm) systems. Total bar size corresponds to annual amounts within SD. (Letters a and b are indicators of significant differences between monoculture and corresponding bi-cropping treatment based on ANOVA (α = 5%)).

More suitable to assess the soil water status under different management systems is possibly the modeled soil water storage. Differences between SWP and VP were significant with approx. 40% higher soil water storage from November to April for both cropping systems (*Fig. 5.6*). The soil water storage to 30 and 90 cm of depth was 5–6 mm (corresponding to 3–6%) lower in bi-cropping than in monoculture systems. Differences between N-fertilization levels were only minor, even though slightly more stored soil water was calculated for unfertilized treatments in the upper soil. Bodner et al. (2007) stated for more arid conditions that the considerable water loss to the atmosphere resulted from compensatory water uptake of catch crops with up to 10% reduction in soil water storage. Simulated maximum water amounts to 30 and 90 cm of depth were plausibly close to the maximum capacity according to the total porosity of 160 and 390 mm, respectively (*cf., Fig. 5.6*). Furthermore, minimum soil water storage in the upper soil horizon varied considerably between 32 mm (MU1) and 48 mm (MM4) indicating minor but significant differences between monoculture and bi-cropping systems during five years of investigation. Finally, these results showed that bi-cropping was not necessarily connected with increased water deficit during the VP when near-surface groundwater input was also considered in the water balance.

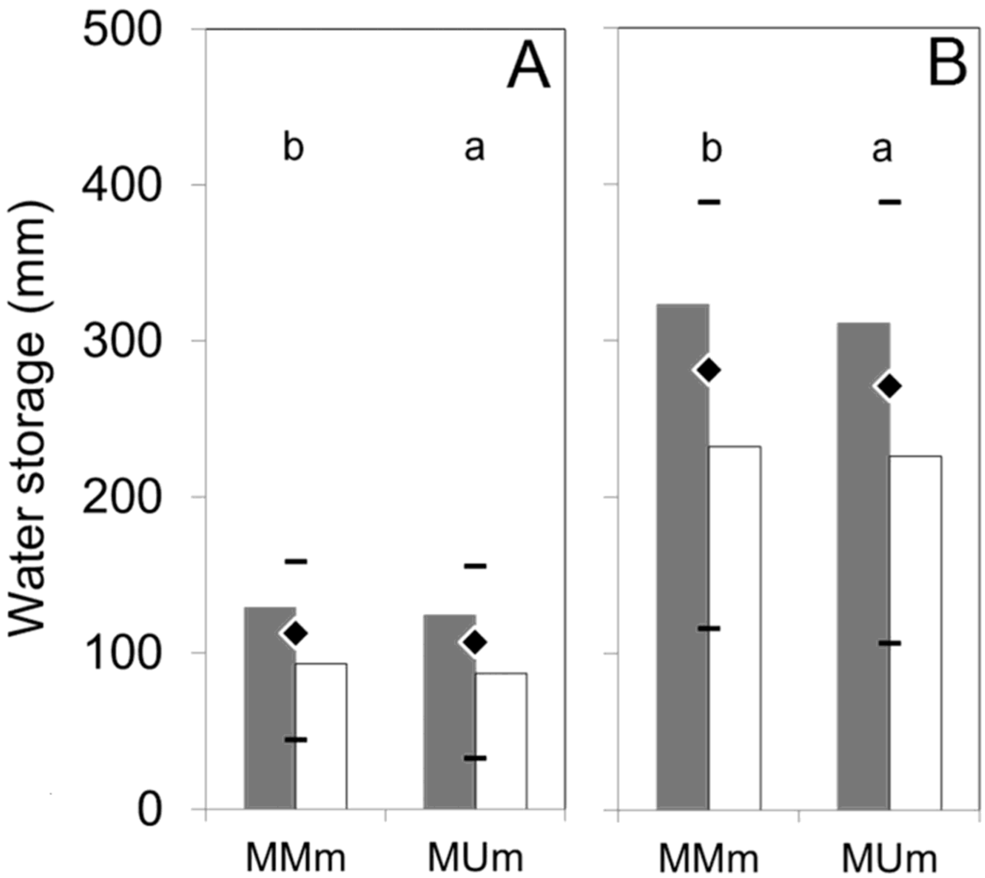

Fig. 5.6: Simulated water storage between 0–30 cm (A) and 0–90 cm of depth (B) for means of monoculture (MMm) and bi-cropping (MUm) systems separated into vegetation period (white bar) and seepage-water period (gray bar). Mean values (♦) are shown within maximum and minimum amounts (▬). (Letters a and b are indicators of significant differences between monoculture and corresponding bi-cropping treatment based on ANOVA (α = 5%).

5.4 Conclusions

In response to the issues of this study, following concluding remarks were given:
Stepwise adjustment of particular acceptance criteria on defined validation variables reduced the number of accepted simulations considerably but resulted in different model performance measures for the selected output. Reduced parameter space was found for only few input parameters, and generalized patterns were not identified. Among the accepted simulations, the uncertainty of selected input-parameters values was still high, and reduced dispersion (CV* < 25%) was found only partially. These results confirmed that both the question of how to select meaningful results and the problem of equifinality in modeling must be balanced against each other. Increased data dispersion of selected input parameters and water-related output was mainly found in bi-cropping systems indicating that parameterization of multiple plants can increase the variability of model results considerably. Consequently, the extent of limiting the input-parameter uncertainty by range reduction on particular output variables seemed to be dependent on their process-based relationships in the model structure. However, impacts from precipitation input on soil water dynamics must be dominant and can also mask influences from parameterization in this context.

Significant effects regarding soil water dynamics were detected for all treatments and soil depths on half-yearly basis. Most significant water stress was found in the upper 10 cm of depth with 8% less soil moisture in bi-cropping systems. The influence of undersown grass on the water storage reached up to 90 cm of depth, especially under fertilized cultivation. However, climate conditions, *i.e.*, seasonal temperature and precipitation patterns, seemed to be more important for changes in soil water storage than the vegetation. Evapotranspiration was significantly increased by undersown grass with apparent effects on the water balance, and higher water surplus was found in maize monocultures. Finally, bi-cropping maize and annual grass seemed to be tolerable in Northern Germany because of balanced conditions regarding precipitation and temperature resulting in missing negative impacts on the soil water status.

Overall, various plausible results indicated that this modeling approach demonstrates the high potential of uncertainty estimation in soil-vegetation-atmosphere models. Nevertheless, discussions about the most conclusive objective functions accompanied by the need for reproducibility are ongoing against the background that both models and observations contain uncertainties that should be considered.

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Chapter 6
Modeling the temporal dynamics of nitrate-nitrogen leaching under silage maize (Zea mays) in monoculture and bi-cropping with annual grass on a drained field considering model uncertainties

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Abstract

This study was focused on modeling carbon (C) and nitrogen (N) dynamics in soil and crop between 1997 and 2002 emphasizing the reduction potential of undersown grass regarding the nitrate-nitrogen (NO_3-N) leaching under silage maize on a drained field. The CoupModel was applied on different systems for silage maize (*Zea mays*) in monoculture and bi-cropping with annual hardy ryegrass (*Lolium perenne L.*) on sandy-humic soil in Northern Germany. Four different N-fertilization levels were simulated: unfertilized, 150 kg N ha^{-1} year^{-1} of mineral-N, 40 m^3 ha^{-1} year^{-1} of cattle slurry (72–148 kg N ha^{-1} year^{-1}), and combined slurry/mineral-N fertilizer (222–298 kg N ha^{-1} year^{-1}). The Generalized Likelihood Uncertainty Estimation (GLUE) approach was used to identify the most plausible parameter combinations obtained from 10,000 runs to match observed C and N contents of crops primarily. The coefficient of determination (R^2) used to determine the predictable variance between total NO_3-N leaching and the set of accepted input-parameter values showed maximum values of 0.35–0.56 in maize monocultures for parameters governing the decomposition of litter. In contrast, additional input parameters predominantly determining plant growth were found for bi-cropping systems with maximum R^2 = 0.38 in fertilized treatments. The NO_3-N leaching showed highly variable data dispersion or quartile coefficients of variation (CV^*) of 11–80% with increased CV^*s in bi-cropping systems. In general, total NO_3-N leaching was modeled with significant differences between the leaching by horizontal drainage and by deep percolation. Maximum N losses were found in highly fertilized maize monoculture during the seepage-water period (SWP) (MM4: M = 45 kg N ha^{-1}, SD = 23 kg N ha^{-1}), whereas annual N losses ranged on average from 17 to 66 kg N ha^{-1} year^{-1} (SD = 7–27 kg N ha^{-1} year^{-1}). A general significant reduction of NO_3-N leaching under maize undersown with grass was not demonstrable during the SWP (MMm: M = 19.6 kg N ha^{-1}, SD = 15 kg N ha^{-1}; MUm: M = 19.5 kg N ha^{-1}, SD = 13 kg N ha^{-1}) and was only stated for the highly fertilized bi-cropping treatment (MU4: M = 34 kg N ha^{-1}, SD = 20 kg N ha^{-1}). Problematic months with increased N losses under maize monoculture and undersown with grass ranged predominantly from February to May, the period with increasing soil temperatures and high mineralization potential. In contrast, significantly decreased NO_3-N leaching was found in and after periods with below-average precipitation and from September to January for undersown grass with reductions of 0–33%. Consequently, NO_3-N leaching was highly influenced by weather conditions, and significant differences were mostly identified in case of changing amount of precipitation.

Keywords: Nitrogen-nitrogen leaching, Silage maize, Bi-cropping, Undersown grass, Artificial drainage, CoupModel

6.1 Introduction

Since July 2014, in which the European Commission has aimed to file first a claim against Germany for failing to limit nitrate (NO_3) concentrations in groundwater below 50 mg NO_3^- L^{-1} (= 11.3 mg NO_3-N L^{-1}), discussion about further strengthening of regulations regarding the application of fertilizers in agriculture has been ongoing in Germany (Sundermann et al., 2016). Increasing proportion (50–60%) of affected surface-near groundwater with nitrate-nitrogen (NO_3-N) concentrations above the limit value is present in regions with intensive dairy and meat production as well as cultivation of energy crops, *e.g.*, **silage maize**, in Northern Germany (SRU, 2105). Because of both proven impacts from nitrogen status of seepage water in soils below agricultural land on near-surface groundwater and strong interactions between the latter one and surface water, mobile NO_3-N from agriculture constitutes a main cause for present nitrogen pollution of water bodies.

Understanding the temporal dynamics of NO_3-N leaching on drained soils can improve the development of strategies for its effective mitigation in particular farming systems. Extensive artificial subsurface drainage is commonly used throughout Northwest Germany in order to improve water and nutrient flows of poorly-drained soils (Maalim and Melesse, 2013; Pfannerstill et al., 2012). However, an efficient drainage system can bypass the N utilization of crops leading to increased NO_3-N contents in deeper soil layers and surface-near water bodies (Conrad and Fohrer, 2009a; Wesström et al., 2014). High NO_3-N loads can be found in tile drainage water, *e.g.*, in sandy soils influenced by elevated groundwater levels, in response to N fertilization, soil tillage, and crop fertility (Randall and Goss, 2008; Carlson et al., 2013). Fuller et al. (2010) stated that decreasing NO_3-N loads were more frequently observed below permanent forage crops because of increased evapotranspiration and N uptake than in maize rotations. Despite this difference, the same study also concluded that the extent of NO_3-N leaching was not significantly different between investigated crops. Perennial vegetation such as **undersown or catch crops** in row crop agricultural systems can extend the N uptake during periods with elevated mineralization potential resulting in decreased NO_3-N in soil and drainage water (Perego et al., 2012; Randall and Goss, 2008; Zavatarro et al., 2012; Zhou et al., 2000). Malone et al. (2014) and Strock et al. (2004) reported that fall-planted catch crops reduced both drainage discharge, because of lower tile and surface peak flow, and NO_3-N leaching compared with bare soil during winter under continental climate. In contrast, a general recommendation for undersown grass to reduce NO_3-N leaching under silage maize was not stated for temperate, humid climate (Büchter, 2003; Büchter et al., 2003; Justes et al., 2012) despite of significantly decreased NO_3-N concentrations in seepage water below the rooting zone during the seepage-water period (Constantin et al., 2010; Martinez and Guiraud, 1990; Svoboda et al., 2015).

Seasonality in climate conditions, *e.g.*, air temperature and precipitation amount, is one major factor controlling NO_3-N flows in soil because of associated processes such as N uptake by plants, decomposition, and mineralization. For instance, less NO_3-N is usually assimilated by crops during poor vegetation periods characterized by below-average precipitation or air temperatures. Increased NO_3-N contents can be found thus in upper soil depths indicating not only sufficient N storage for plant growth but also potentially increased NO_3-N leaching in subsequent years in case of sufficient rainfall

(Randall and Goss, 2008). The change from dry to wet periods can then result in considerable NO_3-N exports (Bakhsh and Kanwar, 2011; Peratoner et al., 2013; Tauchnitz et al., 2015). Therefore, seasonal effects of precipitation on tile drainage flow and subsequent NO_3-N leaching are most evident. Bakhsh et al. (2007) reported that about 60% of artificial drainage amount and NO_3-N leaching occurred between March to May under continental climate.

Soil-vegetation-atmosphere-transfer (SVAT) models such as STICS (Malézieux et al., 2009), CoupModel (Jansson and Karlberg, 2010), and CERES-wheat or CERES-maize (Knörzer et al., 2011) are extensively used to simulate complex interactions between atmosphere, soil, and plant at plot scale (Bleken et al., 2009; Conrad and Fohrer, 2009a, 2016) considering also multi-species cropping to investigate particular plants' interactions (Constantin et al., 2012). However, the variability of natural processes in soil and plant is usually high and often dependent on season and site, and this constitutional uncertainty has to be also considered in modeling. The so-called observed variability has to be distinguished from structural uncertainties in modeling because of algorithms and parameter values that are often not representative for natural processes (Tian et al., 2014). More systematic calibration procedures have been applied recently to dynamic models such as the Generalized Likelihood Uncertainty Estimation (GLUE) approach (Beven and Binley, 1992; Efstratiadis and Koutsoyiannis, 2010; Sadegh and Vrugt, 2013) considering the assumed variation of input-parameter values and dealing with the problem of equifinality (Beven, 2006). Therefore, the acceptance of more than one model realization as most plausible result is necessary to consider various sources of uncertainties.

The present study addressed the quantification of NO_3-N leaching under different silage maize cultivations in sandy-humic soil influenced by subsurface drainage in Northwest Germany with the CoupModel (Jansson and Karlberg, 2010). Key issues involved not only the influence of selected input parameters on modeled N losses but also temporal dynamics and the reduction potential of NO_3-N leaching by undersown grass.

6.2 Methodology

6.2.1 The study site

This modeling study was based on data from field experiments focused on silage maize carried out at the experimental farm 'Karkendamm' (53°55'N, 9°55'E, alt. 14 m) in Northwest Germany during 1997 and 2003. Concluding results of the interdisciplinary research project 'Karkendamm' can be obtained from, *e.g.*, Büchter et al. (2003), Bobe (2005), Herrmann et al. (2005a,b), Volkers (2005), and Wachendorf et al. (2006a, 2006b). The maritime temperate climate at the study site is characterized by moderate seasonal temperature variation, long-term annual temperature of 8.6 °C, and mean annual precipitation of 865 mm. The dominating soil type was classified as Gleyic Podzol (FAO, 2006) with pronounced organic matter contents of 4.2−7.5% in the plow layer (0−30 cm of depth), less than 5% of clay, and a distinct iron B-horizon from 95 to 98 cm of depth (Karrasch 2005). Several soil physical properties for the investigated soil profile are shown in *Table 6.1*, and more detailed information about test setup, sample preparation, and applied water retention characteristics based on the ceramic pressure-plate method and undisturbed soil samples can be found in Bleken et al. (2009) as well as

Herrmann et al. (2005b). The near-surface groundwater level varied from 18 to 180 cm below the soil surface between 1999 and 2002, and temporary waterlogged conditions occurred during winter (Bobe, 2005). The investigated field was surrounded by an artificial drainage system (Karrasch, 2005).

The total field plot had an area of 254x60 m and consisted of 48 sub-plots focused on different silage maize cultivations. All treatments were performed as two-factor split-plot design with four randomized blocks as replicates and were based on 12 N-fertilization levels between 1997 and 2002. Previous fodder production at the investigated field was maize monoculture with different N fertilizers: cattle manure (30 t ha^{-1} in 1995) or slurry (30 to 40 m^3 ha^{-1} in 1993, 1994, and 1996) in addition to 50 kg N ha^{-1} $year^{-1}$ of mineral-N fertilizer. The cultivation of the early maize hybrid 'Naxos' started between late April and early May with a row spacing of 75 cm resulting in a final plant density of 10 to 11 plants m^{-2}, whereas ryegrass was sown in six seed rows between two adjacent maize rows when maize plants reached the three- to four-leaf stage. The average fertilization per plot differed between 0 and 262 kg N ha^{-1} $year^{-1}$ dependent on the particular N level: unfertilized, mineral-N (50, 100, and 150 kg N ha^{-1}), organic-N (20, 40 m^3 ha^{-1} of cattle slurry), and combined slurry/mineral-N (Büchter, 2003). The sampling interval of above-ground biomass ranged from bi-weekly to once per year during the vegetation period in monocultures resulting in different data records from 1997 to 2001 (see ch. 6.2.2.3). In contrast, above-ground maize yields were reported only at harvest in bi-cropping systems, and total grass biomass including roots was sampled twice a year: in late fall, up to six weeks after maize harvest, and in spring before using as green manure and plowing.

Table 6.1: Main characteristics of the soil profile (Gleyic Podzol) according to Ad-hoc-AG Boden (2005) (Herrmann et al., 2005b).

Horizon[a]	**Depth** (m)	**Soil bulk density** (g cm^{-3})	**Sand content** (%)	**Total pore volume** (Vol.%)	**Plant available water content** (Vol.%)	**pH value** ($CaCl_2$) (–)	**Total organic C** (%)	**Total N** (%)	**C:N ratio** (–)
Ap	0–0.28	1.06	90.4	54.0	27.0	5.3	7.47	0.30	24.9
Ae + Bh	0.28–0.57	1.43	91.6	42.3	22.3	4.5	1.49	0.07	21.3
GoBh	0.57–0.79	1.62	91.8	34.3	16.1	4.1	0.89	0.04	22.3
Gor	0.79–0.94	1.65	93.6	37.4	17.1	4.2	0.40	0.02	20.0
IIFw1	0.94–0.98	1.67	94.4	37.8	28.8	4.3	1.22	0.06	20.3
fFw2	0.98–1.03	1.56	92.0	49.1	31.8	4.3	0.65	0.04	16.3
IIIGr	> 1.03	1.59	94.0	39.7	21.0	5.4	0.31	0.04	7.8

[a] According to Ad-hoc-AG Boden (2005), detailed description see Conrad and Fohrer (2016).

6.2.2 CoupModel – modeling approach

6.2.2.1 General information about soil water and plant-growth dynamics

The process-based CoupModel (Jansson and Karlberg, 2010) is applicable to coupled heat, water, carbon (C), and nitrogen (N) dynamics in the unsaturated soil combined with plant growth at plot scale. Depending on the particular complexity of the simulated system, sub-modules for water and nutrient flows, C and N transformations in soil and vegetation can be selected individually. Daily weather and soil management data mainly served as input data, and the soil profile was defined in layers with variable thickness including particular soil texture and water-retention characteristics. The numerical solution of water and heat flows including convective flows between horizontal soil layers was provided in compliance with the Richards' equation and the Fourier's law of diffusion, respectively.

Soil water-retention characteristics and hydraulic properties based on pedotransfer functions by Rawls and Brakensiek (1989) were used to calculate soil water contents of each soil layer. This calculation approach needs data from grain size distribution and laboratory determination of water-retention characteristics to adjust retention parameters of particular modeled soil layers. Given the fact that the study site was influenced by near-surface groundwater, especially during winter, a constant groundwater-inflow rate was defined as additional driving parameter. In this case, horizontal outflow was considered as drainage discharge (Drain) in the soil layer above the uppermost fully saturated layer to prevent oversaturation of the whole soil profile with groundwater. Therefore, an empirical drainage equation was selected in the model setup to reproduce site-specific drainage conditions; even though both dimensions and depths of drain pipes were not specified. No horizontal drainage was taken into account for saturated soil layers, but a vertical water flow from the lowest soil layer, the so-called deep percolation (Deep), was calculated with the seepage equation (see ch. 6.2.2.3; Conrad and Fohrer, 2016).

The iterative solution of the soil-surface energy-balance equation was used to determine soil evaporation. The Penman-Monteith equation (Penman, 1953; Monteith, 1965) was chosen to calculate potential transpiration rates for estimating both water uptake and actual transpiration rate of each plant. Compensatory water uptake by roots in soil layers without water stress was also considered in case that the root depth was sufficient and water shortage occurred in other soil horizons. Biomass development was simulated dynamically, *i.e.*, C and N amounts of different plant storages such as leaf, shoot, root, and grain were calculated as functions of growth-stage indices (GSI) regulated by several functions for air temperature, water, and nitrogen status in soil. When different plants covered the same area, particular properties especially for growth were parameterized for each plant, *e.g.*, threshold temperatures and temperature sums according to the GSI for sowing, emergence, grain development, maturing, and harvest (*cf.*, Conrad and Fohrer, 2016). In case of perennial plants determined C and N amounts were transferred from leaf, stem, and root compartments to corresponding 'old' pools at the turn of the year, unless plants were less than 180 days old. When roots already existed at emergence as defined for perennial plants, no seed was planted but the C amount of roots was used for the allocation process. The N demand of each plant was governed by the C contents in particular compartments acting as driving force for the N uptake. Soil management was determined by dates for plowing, sowing, date and amount of N fertilization, and harvest. Because of indications that the harvest of silage maize occurred before optimum temperature sum was reached (Herrmann et al., 2005b), the harvest dates were set to observed data in this study. Mineral-N and organic-N fertilizers were main external-N sources applied to a certain soil layer beside atmospheric-N deposition. Ammonia volatilization (NH_3) from soil surface was not taken into account.

Below-ground processes regarding C and N transformations were controlled by several organic and inorganic pools with defined properties, *e.g.*, particular transformation rates. In addition to three mandatory organic-C pools in soil (SOC), *i.e.*, humus, litter, and feces, secondary litter pool with an increased decay rate was introduced. Litter formation at the soil surface from above-ground biomass and in soil produced by root residues was also governed by temperature sums. The initial amount of total SOC was defined for the whole soil profile assuming an exponential decline with depth according to observations (*cf., Table 6.1*). Initial values used in this modeling study were based on detailed information stated in Karrasch (2005). The vertical transport of dissolved SOC was neglected. Decomposition was defined as a first-order rate process with specific decomposition rates for each organic pool, and products of C decomposition were humus, carbon dioxide (CO_2), and microbial biomass. The latter component was subject to an internal cycling in litter and feces pool because microbial biomass was not explicitly simulated as separate storage for nitrification. Soil-N flows were associated with C dynamics from litter and feces to the humus pool determined by the microbial C:N ratio, cn_m, that was given as 10 in this study. N mineralization and immobilization were dependent on the C:N ratio in particular source pools, *i.e.*, humus, litter, and feces, when microbes were implicitly simulated. Nitrification of ammonium-N (NH_4-N) into NO_3-N was affected by temperature, soil moisture, and the corresponding NO_3-N and NH_4-N contents. Furthermore, the mobility of NH_4-N was neglected resulting in full adsorption in soil. Other gaseous N losses, *e.g.*, N oxides such as NO_2, NO, and N_2O, were only calculated as total-N amounts in a simple denitrification approach.

The simulated total NO_3-N leaching was determined as sum of the NO_3-N flows at the bottom of the profile (vertical downward flow, q_{NO3dp}) and by drainage (horizontal flow, q_{NO3dr}) from layers above the groundwater level as:

$$q_{NO3dp} = q_{dp}\frac{N_{NO3}}{\theta(z)\Delta z} \quad (6.1) \quad \text{and} \quad q_{NO3dr} = q_{dr}\frac{N_{NO3}}{\theta(z)\Delta z} \quad (6.2)$$

where q_{dp} and q_{dr} are the total water amounts of deep percolation (Deep) and horizontal drainage (Drain), respectively, N_{NO3} is the amount of NO_3-N, and $\theta(z)$ is the soil moisture content in the particular depth of soil layer Δz.

6.2.2.2 Model parameterization with the GLUE approach

At this point it should be noted that the detailed procedure to select the most plausible simulations regarding plant biomass was presented first in Conrad and Fohrer (2016) but results were focused on the water balance. The basic idea of the GLUE approach is the acceptance of a number of model realizations with differences in parameterization but comparable model performance. Complex soil-plant-atmosphere interactions required an adequate parameterization with several input parameters in the CoupModel (Conrad and Fohrer, 2009b,c; Nylinder et al., 2011). The list of so-called 'uncertain' input parameters (*Table 6.2*) resulted from previous sensitivity analyses and was not representative for un-calibrated conditions because of the limited parameter ranges to avoid an inefficient GLUE analysis (Arabi et al., 2007). Differences in the number of selected input parameters between monoculture (total number = 16) and bi-cropping (total number = 24) systems resulted from the consideration of a second plant, the undersown grass, in bi-cropping. Therefore, a number of 10,000 simulations were run for each treatment with random combinations of defined input parameters according to the Monte-Carlo sampling technique.

The second key question arising from this approach was to define particular validation variables for the selection procedure by comparing model results to measurements. Given the fact that a comprehensive description of differences between particular cropping systems was of interest, biomass data were chosen as main validation variables to select the most plausible simulations (*Table 6.3*). The adjustment on the basis of available abiotic validation variables was not meaningful because of two reasons: non-site and non-treatment specific data in case of soil temperatures and groundwater level, respectively, as well as irregular measured water contents and water potentials during few months.

However, the number of records for above-ground C and N contents in maize varied considerably and two data sets were used for the stepwise selection procedure in the order as specified (*Table 6.3*). Consequently, the match between modeled results and data set 1 with the highest number of records, *i.e.*, detailed above-ground C contents in maize during the vegetation periods from 1997 to 2001, was adjusted first by limiting particular performance measures to satisfying threshold values (*cf.,* ch. 6.2.2.3). Several performance measures such as the coefficient of determination R^2, the Nash-Sutcliffe-efficiency (*NSE*) (Nash and Sutcliffe, 1970), and the average magnitude of the error (*RMSE*) were calculated in CoupModel. In this study the **'LogLikelihood' (*LogLi*)** measure (Van Oijen et al., 2005) was used as objective function to evaluate the match between model and observation. The *LogLi* was determined as the likelihood $p(D/\theta)$ assuming measurement errors are Gaussian and uncorrelated:

$$\text{Log } p(D/\theta) = \sum_{i=1}^{n} [-0.5\ ((O_i - S_i)/M_i))^2 - 0.5\ \text{Log}(2\pi) - \text{Log}M_i] \qquad (6.3)$$

where O_i are observations, S_i are the corresponding model results, M_i is the observed standard deviation, and n is the number of measurements (Klemedtsson et al. 2008). The number of most plausible simulations in the GLUE was directly defined by the user-defined *LogLi* threshold criteria with consequences for the performance measures of all the other selected validation variables. It means that after limiting the *LogLi* of above-ground C contents in data set 1, all performance measures were recalculated as well as the number of accepted runs was reduced. This procedure was done next with C contents of maize at harvest contained in data set 2, followed by the total-C content in ryegrass in case of bi-cropping, and so on as listed (*Table 6.3*).

Standard criteria set applied to all treatments led to a highly variable sample size of accepted simulations because of the existing variance between used data sets of validation variables with only few observations. Therefore, it was necessary to include up to four additional validation variables in the selection procedure to reduce the maximum number of accepted simulations to less than 80 of 10,000 parameter combinations. However, Juston et al. (2009) noted that the consideration of many output variables implied the risk of poor agreements between simulation and measurements, even if the comparison between various treatments was only dependent on the number of accepted solutions. Further results for the selection of most plausible parameter combinations regarding plant biomass can be found in Conrad and Fohrer (2016).

Table 6.2: Input parameters used for the GLUE optimization.

Management system		**Input-parameter ranges**			
Parameter name	**Description**	Minimum	Maximum	Unit	#
(I) Properties of groundwater dynamics					
GWSourceFlow, q_{sof}	Constant rate of groundwater inflow	0.5	0.8	mm d^{-1}	1
(II) Vegetation characteristics for evapotranspiration					
Specific LeafArea (Plant 1), $p_{l,sp(1)}$	Parameter to estimate the leaf area index of plant 1 and plant 2 from C	1	20	g C m^{-2}	2
Specific LeafArea (Plant 2), $p_{l,sp(2)}$	content in leaf	1	20		3
(III) Below-ground nitrogen processes					
NitrificSpecificRate, n_{rate}	Nitrification rate in the response function for soil NO_3-N and NH_4-N content	0.05	0.4	d^{-1}	4
Efficiency Litter1, $f_{e,l1}$	Efficiency of the decay of litter pool 1	0.3	0.5	d^{-1}	5
Efficiency Litter2, $f_{e,l2}$	Efficiency of the decay of litter pool 2	0.3	0.5	d^{-1}	6
Efficiency Humus, $f_{e,h}$	Efficiency of the decay of humus pool	0.2	0.4	d^{-1}	7
RateCoef Litter1, k_{l1}	Rate coefficient for the decay of litter pool 1	0.01	0.1	d^{-1}	8
RateCoef Litter2, k_{l2}	Rate coefficient for the decay of litter pool 2	0.05	0.5	d^{-1}	9
NitrateAmmRatio, $f_{nitr,amm}$	NO_3-N : NH_4-N ratio in the nitrification function	3	10	–	10
(IV) Plant growth					
Root Water c1 (Plant 1), $r_{Wc1(1)}$	Fraction of the mobile carbon assimilates allocated to the roots of plant 1	0.2	0.5	–	11
Root Water c1 (Plant 2), $r_{Wc1(2)}$	and 2 in the response function for water stress when 'Root Allocation Water is independent'	0.2	0.5		12
Root CN c1 (Plant 1), $r_{CNc1(1)}$	The constant part of the linear function for the allocation of mobile carbon	0.2	0.5	–	13
Root CN c1 (Plant 2), $r_{CNc1(2)}$	assimilates to the roots of plant 1 and 2 in the response function for nitrogen concentration in leaves when 'Root allocation N Leaf is a linear function'	0.2	0.5		14
Root Mass c1 (Plant 1), $r_{Mc1(1)}$	Fraction of the mobile carbon assimilates allocated to the roots in the	0.2	0.5	–	15
Root Mass c1 (Plant 2), $r_{Mc1(2)}$	response function for nitrogen concentration in leaves when 'Root Allocation Mass is independent'	0.2	0.5		16
Leaf c1 (Plant 1), $l_{c1(1)}$	Fraction of the mobile carbon assimilates is allocated to the new shoots of	0.2	0.5	–	17
Leaf c1 (Plant 2), $l_{c1(2)}$	plant 1 and 2 when 'Leaf Allocation Shoot is independent'	0.2	0.5		18
CN Ratio Min Roots (Plant 1), $cn_{MinRoot(1)}$	Minimum C:N ratio for roots of plant 1 and 2 to control N allocation to the	20	28	–	19
CN Ratio Min Roots (Plant 2), $cn_{MinRoot(2)}$	roots from the mobile pool	10	25		20
Radiation use efficiency (Plant 1), $\varepsilon_{L(1)}$	Radiation use efficiency: conversion factor for photosynthesis at optimum	2	4	g DW	21
Radiation use efficiency (Plant 2), $\varepsilon_{L(2)}$	temperature, moisture and C:N ratio	2	4	MJ^{-1}	22
C Seed (1), $c_{Seed(1)}$	Initial C content of plant 1 and 2 at sowing day without effects on plant C	1	10	g	23
C Seed (2), $c_{Seed(2)}$	pool, respiration or photosynthesis	1	10		24

DW – dry weight.

Table 6.3: Validation variables used to identify the most plausible simulations and the order of their selection as well as additional measurements to evaluate the model performance.

Treatment	MM1	MU1	MM2	MU2	MM3	MU3	MM4	MU4	Order of selection	
Validation variables (used for selection); sampling dates for MM (1997–2001) and MU (1998–2002)									MM	MU
Above-ground C in maize – Set 1 ($g\,C\,m^{-2}$)[a]	48	40	48	40	29	21	29	21	1	1
Above-ground C in maize – Set 2 ($g\,C\,m^{-2}$)[b]	4	4	4	4	4	4	4	4	2	2
Total-C in undersown grass ($g\,C\,m^{-2}$)[b]	–	8	–	8	–	8	–	8		3
Above-ground N in maize – Set 1 ($g\,N\,m^{-2}$)[a]	45	40	45	37	29	21	26	21	3	4
Above-ground N in maize – Set 2 ($g\,C\,m^{-2}$)[b]	4	4	4	4	4	4	4	4	4	5
Total-N in undersown grass ($g\,N\,m^{-2}$)[b]	–	8	–	8	–	8	–	8		6
Soil mineral-N content (0–90 cm) ($g\,N\,m^{-2}$)	11	8	10	8	11	8	10	8		7
Number of records for additional validation variables (not used for selection)										
Soil temperature in 5, 10, and 20 cm depth (°C)[c]	1648									
Soil water contents in 7 depths (Vol.%)[d]	13–31									
Soil water potential in 30, 50, and 70 cm depth (hPa)	33									
Groundwater level (m)	110									
NO_3-N concentration in 60 cm of depth ($mg\,N\,L^{-1}$)	802	690	808	690	783	629	799	665		

[a] Data from Herrmann et al. (2005b): observed for monocultures and extrapolated for bi-cropping treatments based on Volkers (2005).
[b] Data from Volkers (2005).
[c] Data from two grassland sites.
[d] Observed depths: 10 (13 records), 30, 40, 50, 60, 70, and 80 cm.

6.2.2.3 Input data for CoupModel simulations

Simulations were conducted from January 1996 to March 2002 including a pre-run period from January to October 1996 and were focused on four different N-fertilization levels for maize monoculture (MM) and the corresponding bi-cropping (MU) treatment. Applied N amounts included in each case two unfertilized (0 $kg\,N\,ha^{-1}\,year^{-1}$; MM1, MU1), mineral-N (150 $kg\,N\,ha^{-1}\,year^{-1}$ as calcium ammonium nitrate (CAN); MM2, MU2), organic-N (40 $m^3\,ha^{-1}\,year^{-1}$ cattle slurry with different N contents for 1997, 1998, 1999, 2000, and 2001: 2.4, 1.8, 3.4, 3.7, and 3.3 $kg\,N\,m^{-3}$; MM3, MU3), and combined slurry/mineral-N fertilized treatments (150 $kg\,N\,ha^{-1}\,year^{-1}$ CAN and 40 $m^3\,ha^{-1}\,year^{-1}$ cattle slurry; MM4, MU4) leading to a number of eight simulation scenarios (*Table 6.4*).

The bi-cropping treatments were simulated during the same period as maize monocultures to compare modeled outcome over the same period from November 1996 to March 2002. Confirming model requirements, the conversion of observed dry matter into C amounts was necessary based on an estimated C content in dry biomass of 45%. The number of biomass samples differed considerably between the treatments (*cf.,* ch. 6.2.2.1 and *Table 6.3*) especially between maize monoculture and corresponding bi-cropping system. Therefore, it was necessary to generate additional data for maize in bi-cropping during growth based on particular yields of maize in monoculture from 1997 to 1999 (*cf.*, Herrmann et al., 2005b) and annual reduction factors determined by Volkers (2005) between 1998 and 2002. Consequently, two different data sets for maize in monoculture and bi-cropping were applied with (i) detailed above-ground C and N contents as measured in monoculture and estimated in bi-cropping in data set 1, and (ii) annual observed records for silage maize at harvest as well as half-yearly records for undersown grass in data set 2.

Table 6.4: Crop characteristics and N-input management of the modeled treatments.

Treatment	**MM1**	**MU1**	**MM2**	**MU2**	**MM3**	**MU3**	**MM4**	**MU4**
Maize monoculture (MM)	Yes	No	Yes	No	Yes	No	Yes	No
Undersown grass (MU)	No	Yes	No	Yes	No	Yes	No	Yes
Annual-N input:								
Atmospheric deposition (kg N ha^{-1})	20	20	20	20	20	20	20	20
Mineral-N (kg N ha^{-1})	0	0	150	150	0	0	150	150
Cattle slurry (m^3 ha^{-1})	0	0	0	0	40	40	40	40
Total-N input *(kg N ha^{-1} $year^{-1}$)*								
1996[a]	20	20	70	70	140	140	190	190
1997	20	20	170	170	116	116	266	266
1998	20	20	170	170	92	92	242	242
1999	20	20	170	170	156	156	306	306
2000	20	20	170	170	168	168	318	318
2001	20	20	170	170	152	152	302	302
Mean-N input (without pre-run period):	**20**	**20**	**170**	**170**	**137**	**142**	**287**	**292**

[a] Pre-run period (data from January 1st to October 31st was excluded from evaluation).

Daily weather data such as air temperature, precipitation, humidity, wind speed, and global radiation were obtained from two local climate stations. The simulated soil profile was based on observed soil information (*Table 6.1*), but particular layers were defined differently with variable increments of 5 cm (0–5 cm of depth), 10 cm (5–95 cm of depth), 20 cm (95–135 cm of depth), and 50 cm (135–185 cm of depth). Details on the parameterization of the artificial drainage system and particular values of fixed input parameters were reported in Conrad and Fohrer (2016). However, the empirical determination of horizontal drainage above the uppermost fully saturated soil layer was chosen because of the unknown dimension and depth of drains. Vertical outflow of water from the lowest soil layer as so-called deep percolation was calculated with the seepage equation considering the saturated conductivity of the lowest compartment, modeled groundwater level, and the geometry of deep percolation. Both horizontal drainage and deep percolation were necessary to determine the particular NO_3-N fractions but simulated N loss by deep percolation according to Eq. 6.1 was not available in the model output, and the vertical NO_3-N flow in a depth of 135 cm was used instead.

6.2.3 Data evaluation and Statistical analysis

Total NO_3-N leaching was calculated as the sum of vertical and horizontal N losses and was aggregated separately for different periods: annual (November to October), half-yearly for the seepage-water period (SWP; November to April) and the vegetation period (VP; May to October), and monthly. The agreement between measured and simulated validation variables was determined first to evaluate the model performance by means of performance measures such as the coefficient of determination R^2, the *NSE*, and the *RMSE* (see ch. 6.3.1). In addition, correlation between accepted input parameters and corresponding half-yearly leaching amounts was calculated to identify influences from parameterization on the NO_3-N leaching for particular treatments (see ch. 6.3.2).

The quartile coefficient of variation (CV^*) represents the extent of variability within ranked data set and was determined for the NO_3-N leaching of all accepted simulations:

$$CV^* = (Q_3 - Q_1)/Q_2 \qquad (6.4)$$

where Q_1, Q_2, and Q_3 are the 25th, 50th, and 75th percentile of the data set, and ($Q_3 - Q_1$) determines the interquartile range. The greater the CV^* value of a particular variable is, the more the data set of this variable is scattered, and distributions with $CV^* > 1$ (100 %) represent increased dispersion.

Analyses of significant differences between maize monoculture and corresponding bi-cropping treatment as well as between all treatments were carried out with the statistics tools of R (Version: 3.1.2 (2014-10-31), R Development Core Team, 2013) and the R Commander GUI (Version: 2.0-x, Fox, 2005). Specific preliminary tests such as on normal distribution (Shapiro-Wilk test, level of significance $\alpha = 5\%$) and homogeneity of variances (Levene test, level of significance $\alpha = 5\%$) were applied on modeled NO_3-N leaching for the above-mentioned periods. This was done to identify significant patterns in NO_3-N leaching of maize monoculture and bi-cropping by differentiation between comparing arithmetic means (single factor analysis of variance (ANOVA); level of significance $\alpha = 5\%$) or median values (non-parametric Wilcoxon-Rank sum test, two-sided; level of significance $\alpha = 2.5\%$) on the basis of preliminary tests. Results were significantly different between the treatments when $p \leq 0.05$ (ANOVA) or $p \leq 0.025$ (Wilcoxon-Rank sum test) labeled with defined letters (a < b for comparison between two corresponding treatments). Subgroups without significant differences between arithmetic means of all treatments were also identified by a single factor ANOVA with subsequent Tukey test (level of significance $\alpha = 5\%$; A to F with A < B < C < D < E < F for subgroup comparison between all treatments).

6.3 Results and Discussion

6.3.1 Evaluation of the model performance regarding plant growth and nitrogen dynamics in soil

Plausible agreement between observed and simulated above-ground C and N contents in maize was shown by satisfying model performance for particular treatments (*cf.,* Conrad and Fohrer, 2016) despite certain data dispersion regarding presented mean values of the accepted simulations (*Fig. 6.1*a,b). Considering the apparent variability of total-C and total-N contents in grass for particular bi-cropping treatments (*Fig. 6.1*c,d) as shown by high standard deviations (*SD*s), significant uncertainty in both simulated and measured outcome was detected.

Reported variability possibly increased with decreasing number of observed data in the model validation. However, the propagation of uncertainties may also rise with increasing number of species because of their parameterization with significant impacts on other site-specific system variables. Reasonable accuracy of modeled dry matter is often stated, although deviations between model and measurements were greater than 15% in many cases, especially for multi-species simulations confirmed by Constantin et al. (2012) as well as by Corson et al. (2007). Furthermore, observations clearly showed that undersown grass influenced silage maize yields with negative, positive, and insignificant effects in particular years (Justes et al., 2012; Kuo et al., 2001; Martinez and Guiraud, 1990; Volkers, 2005; Whitmore and Schröder, 2007; Zhou et al., 2000) because of the competition for light, water, and nutrients between different species.

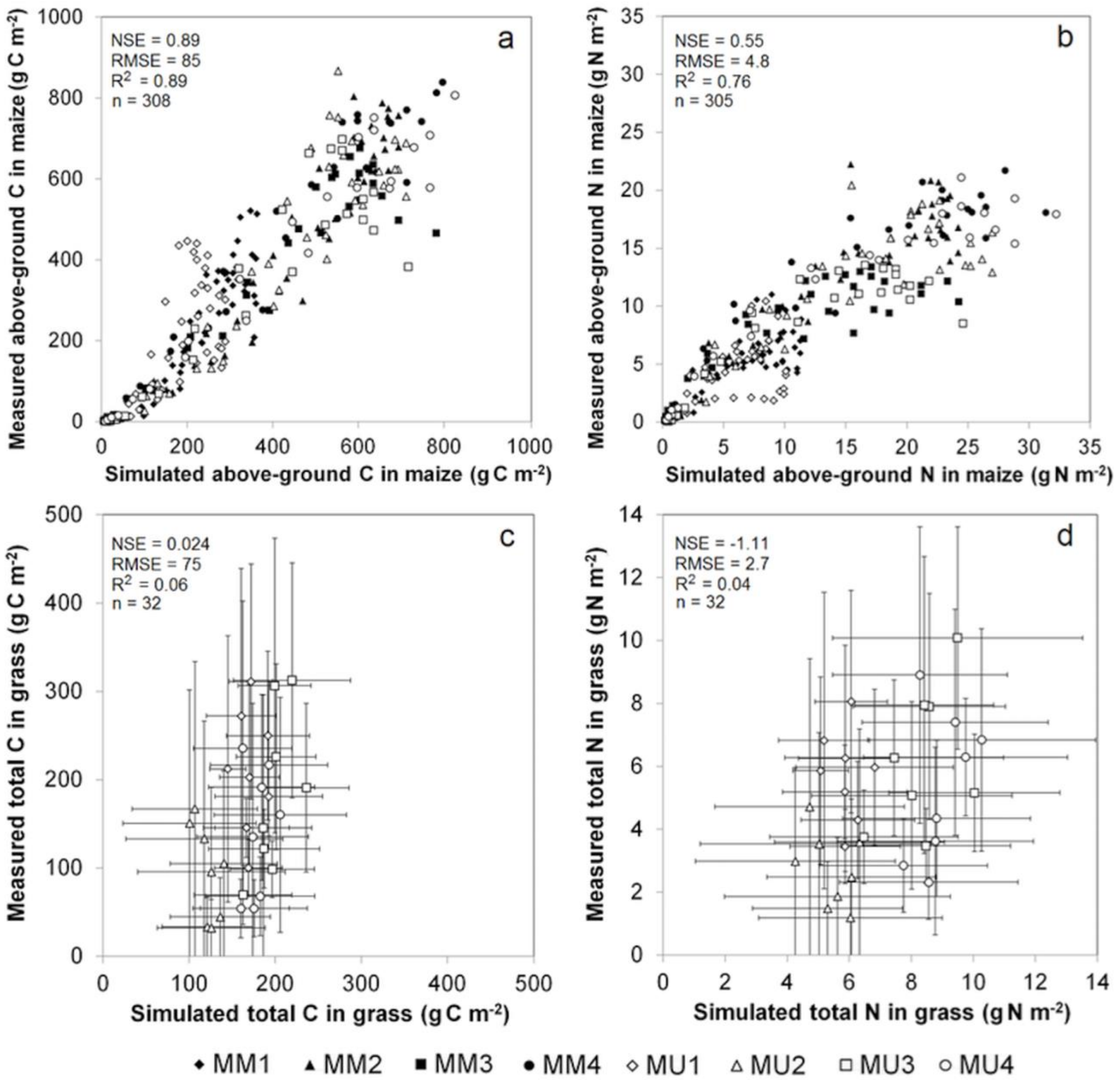

Fig. 6.1: Agreement between detailed measured/estimated and modeled above-ground C (a) and above-ground N (b) contents in maize as well as measured total-C (c) and total-N (d) contents in undersown grass for all treatments. Results are shown as mean values within SD unless otherwise omitted for reasons of clarity (a and b).

The SMN content is an indicator for the potentially soluble-N fraction to a defined soil depth, whereas the NO_3-N concentration represents the effective amount of dissolved NO_3-N for a specific water volume and depth. Satisfactory agreement between modeled and measured SMN contents to 90 cm of depth indicated slightly underestimated SMN amounts for the most treatments except for the highest N fertilization level (*Fig. 6.2*). In this case, overestimation amounted to more than 50%, even though the variability or rather the *SD* of measured SMN contents was mostly higher than simulated. Reason for underestimated SMN contents, as well as reduced simulated NO_3-N concentrations below the rooting zone in 60–65 cm of depth (*Fig. 6.3*), especially in monoculture treatments without or exclusive mineral-N fertilization might be found in reduced litter formation and mineralization. In contrast, presented overestimation of simulated above-ground N contents at harvest in corresponding bi-cropping treatments (*cf.,* Conrad and Fohrer, 2016) was not accompanied by reduced SMN contents between 0–90 cm of depth and underestimated NO_3-N concentrations below the rooting zone, but both were rather overestimated temporarily in highly fertilized treatments (*cf., Fig. 6.2* and *Fig. 6.3*).

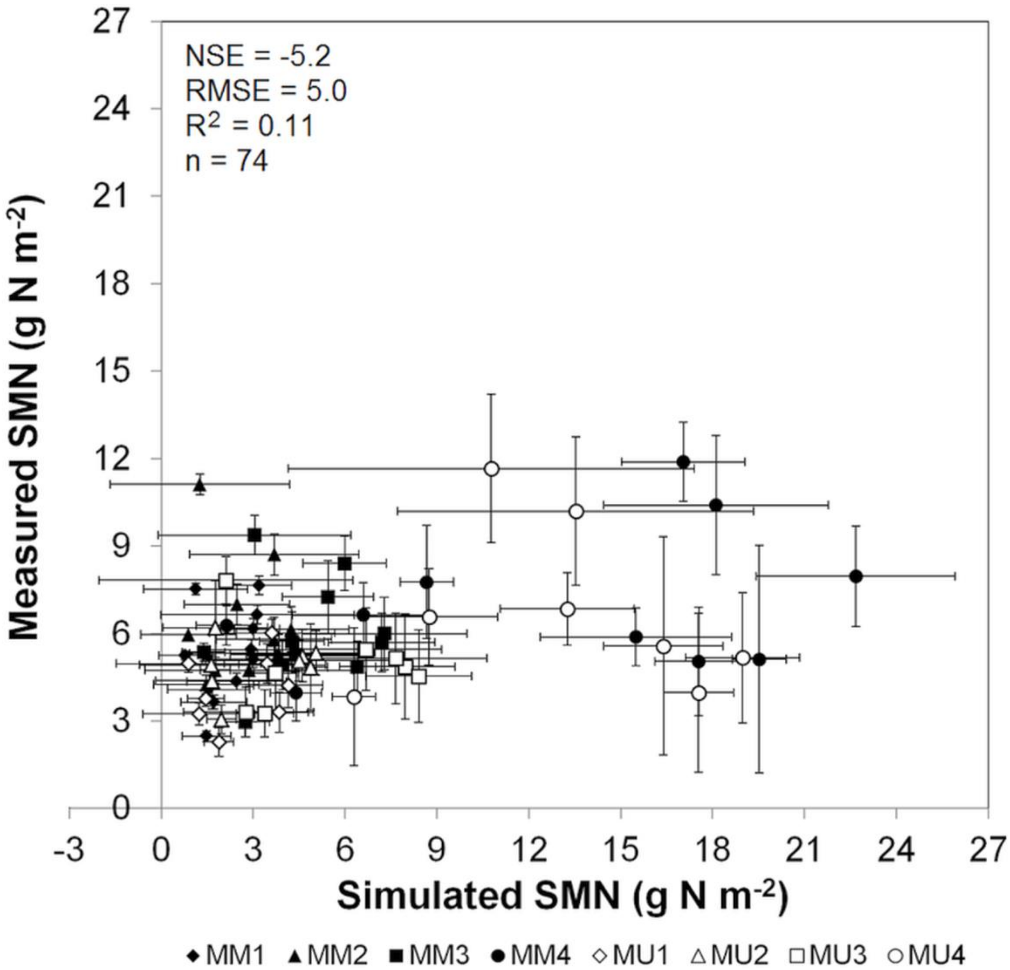

Fig. 6.2: Agreement between measured and modeled soil mineral-N (SMN) contents between 0–90 cm of depth for all treatments. Results are shown as mean values within SD.

The SMN contents are usually highly variable in sandy soils with poor sorption capacity and higher aeration potential compared with clay soils with lower aeration and, to some extent, reduced microbial activity (NLWKN, 2012; Schiermann, 2004). Elevated SMN amounts often indicate a high risk of NO_3-N leaching and usually remain stable during winter in case of soil freezing and reduced mineralization. In consequence of these highly variable results, significant differences between measured and simulated SMN amounts were not provable, even though the opposite can be assumed because of low model performances on an average. However, Herrmann et al. (2005b) stated systematic deviations between modeled and observed SMN contents with increasing N input for monocultures and soil depth confirmed by Bleken et al. (2009) in a further modeling study at this site. Explanations for this discrepancy might be the underestimated mineralization and denitrification potential in the model as well as unconsidered ammonia volatilization during the vegetation period, but its importance was not evaluated in this study. Furthermore, the efficiency of undersown grass to reduce SMN contents in fall and spring was also not evident for average results. Obviously, reduced SMN amounts in both seasons were found in observed bi-cropping systems except for the highest fertilization level (Wachendorf et al., 2006b). This relationship was not found for bi-cropping systems in this study, especially for SMN contents in spring. In contrast, Van Dijk et al. (1997) proposed reduced SMN amounts in fall because of an additional N uptake of 40 kg N ha^{-1} by grass species. Renius et al. (1992) reported increased SMN contents after maize harvest in case of a late plowing date of previous grass species (*Lolium perenne L.*) that referred to slowed mineralization of plant residues in the vegetation period.

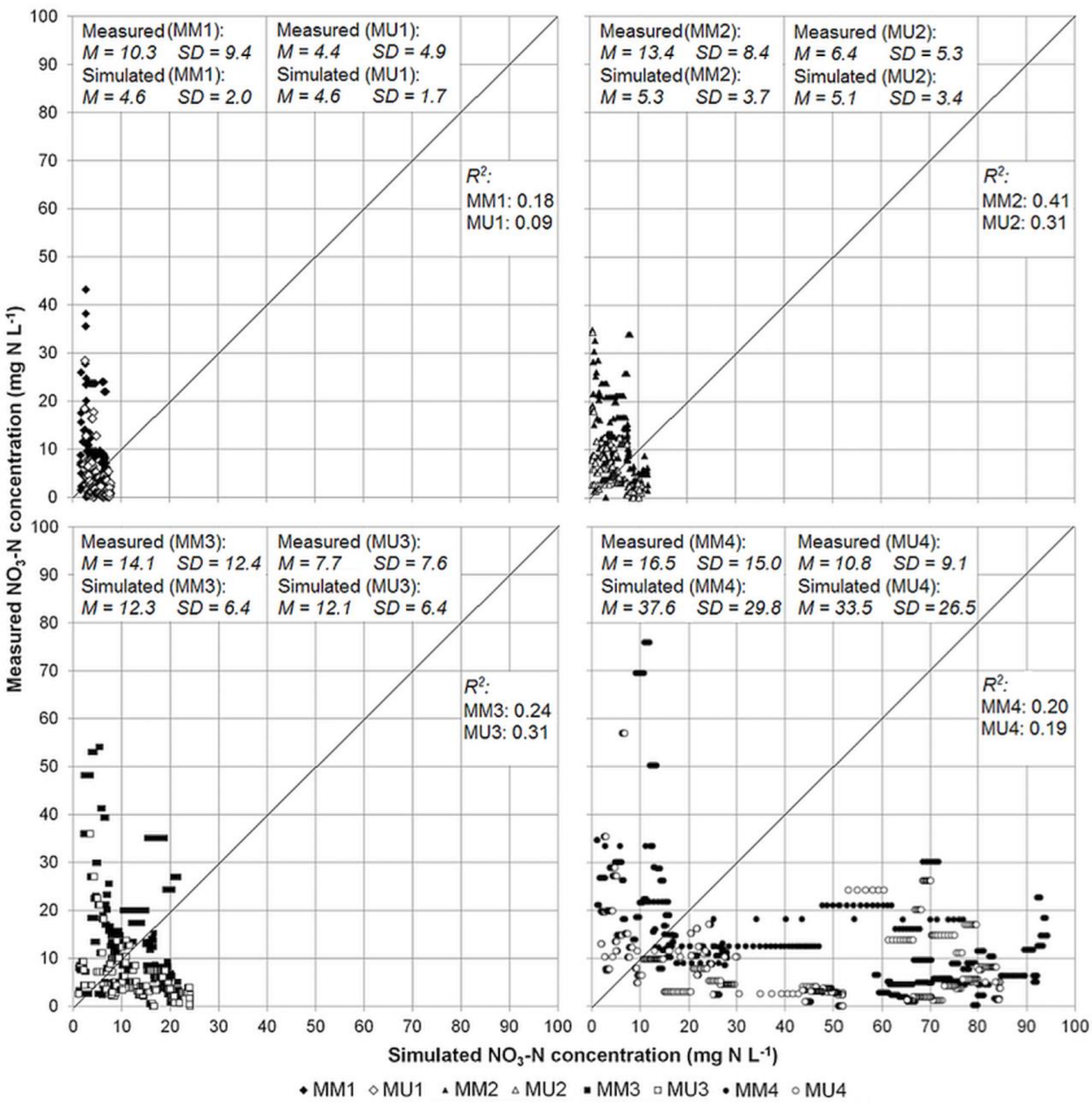

Fig. 6.3: Agreement between measured and modeled NO_3-N concentrations in 60–65 cm of depth for particular monoculture and bi-cropping systems during the SWP. Results are shown as mean values accompanied by the coefficient of determination (R^2) for comparison between model and measurement.

The dependence between catch crop efficiency and SMN level was proved by Justes et al. (2012) with limitations on moderate SMN contents, shallow and permeable soils, high precipitation, and certain catch crops. Similar pattern of SMN contents and NO_3-N concentrations below rooting zone for particular treatments demonstrated the impact of mineral-N amounts on dissolved-N in soil, even though weak correlation between both were stated because of stronger influences from soil moisture on NO_3-N concentrations. In general, high variability of SMN contents and NO_3-N concentrations in defined soil depths caused limitations regarding conclusions about significant differences between observation and model. Simulated surplus of N in plant and soil was possibly caused by fixed percentages of harvest residues that were at maximum after maize harvest in highly fertilized treatments resulting in an overestimated litter-N amount. There were also indications of delayed vertical water flows in periods with below-average precipitation, *e.g.*, SWP00/01, leading to significant deviations between modeled and measured NO_3-N concentrations. However, influences of soil organic matter on SMN turnover might be considered in the further model applications. Surprisingly, observed NO_3-N concentrations presented in Bleken et al. (2009) as time series and compared with the simulated outcome were different from those shown in this study (*cf.*, *Fig. 6.3*) because a number of records were different or missing, especially in SWP00/01 indicating the influence of preceding data evaluation and homogenization.

6.3.2 Correlation analysis between accepted 'flexible' input parameters and total NO_3-N leaching

In general, R^2s < 0.2 were detected for the majority of all selected input parameters indicating that impacts from single input-parameter uncertainty on total NO_3-N leaching were only minor in both the VP and SWP (*Fig. 6.4*). Maximum R^2s of 0.38–0.56 were found in maize monocultures for input parameters governing litter decomposition, *i.e.*, Efficiency Litter 1 and RateCoef Litter 1, with minor differences between SWP and VP. In contrast, additional input parameters with R^2s > 0.3 were found in bi-cropping systems. These include plant-growth parameters such as the specific leaf area of grass (Specific LeafArea (Plant 2)), the minimum C:N ratio of roots for N allocation (CN Ratio Min Roots (Plant 1) and (Plant 2)), and particular allocation factors. Furthermore, impacts from the above-named parameters differed slightly between VP and SWP in bi-cropping, however maximum number of most influencing input parameters was found in the highly fertilized bi-cropping treatment. Finally, these results showed that none of the selected and adjusted input parameters influenced the total NO_3-N leaching clearly, but reasons for that can be various, *e.g.*, direct effects of parameterization and the temporal aggregation of the NO_3-N leaching.

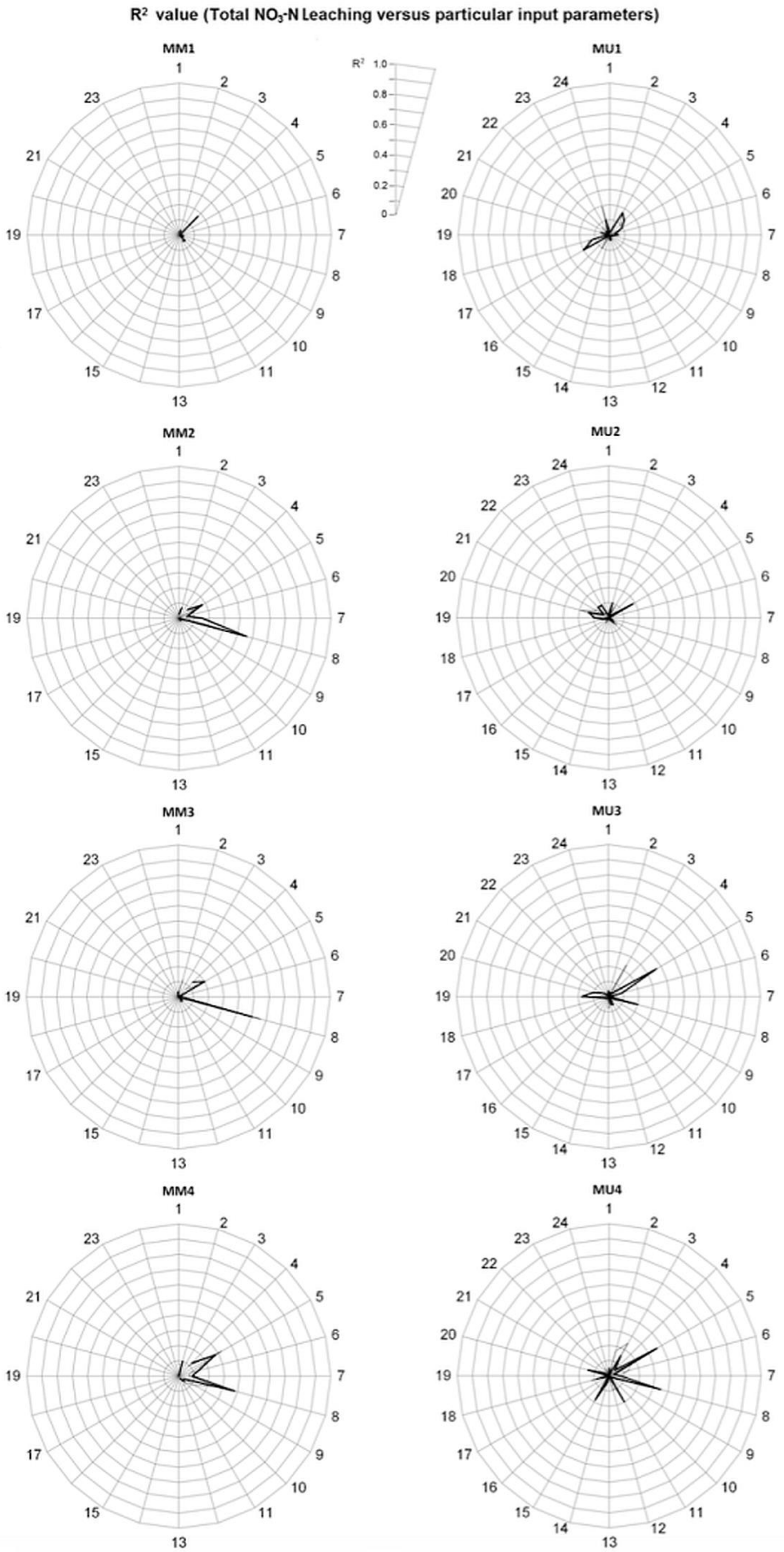

Fig. 6.4: Coefficient of determination (R^2) of total NO_3-N leaching and selected 'flexible' input parameters for particular monoculture (MM) and bi-cropping (MU) systems. The numbering of particular input parameters corresponds to the numbers in column # of Table 2.

6.3.3 Variability and temporal dynamics of the modeled NO_3-N leaching

Horizontal (I), vertical (II), and total (III) NO_3-N leaching to 135 cm of depth were aggregated for average periods such as VP, SWP and the hydrological year (*Fig. 6.5*). Dependent on results of tests on significant differences between monoculture and corresponding bi-cropping treatment, arithmetic mean or median (marked with #) values were compared but only means within total *SD*s were presented.

Proportions of NO_3-N lost through horizontal drainage varied between 60% (MM1) and 87% (MU3) in the VP and the SWP, respectively. The proportion between SWP and VP for horizontal-N flows was approx. 2 : 1, which was relatively similar to results of vertical-N losses. Comparison between monoculture and corresponding bi-cropping treatment identified higher N losses by drainage in bi-cropping treatments with dependence on the N level and the type of fertilizer regardless of the period. A universal significant reduction of NO_3-N leaching was stated exclusively for bi-cropped maize at the highest fertilization level (MU4), which was also reported by Kaluli et al. (1999) as well as by Büchter et al. (2003). In contrast, vertical NO_3-N leaching of bi-cropping systems was significantly lower than or rather similar to monocultures, even though dispersion of vertical-N flows, *i.e.* their particular *CV**s, were significantly higher than horizontal-N losses for all treatments and periods of aggregation (*Table 6.5*). Data dispersion of horizontal and total NO_3-N leaching was very similar because of high percentages of horizontal drainage, and increased variability was generally found in bi-cropping systems especially for the unfertilized treatment (MU1). The *CV**s of all NO_3-N fractions were elevated from May to October indicating that processes associated with plant growth, N uptake, and N transformations in soil during summer and fall may influence the NO_3-N leaching considerably.

Conversely, differences regarding the variability of total NO_3-N leaching between means of monoculture (MMm) and bi-cropping (MUm) systems were minor for the VP as well as the hydrological year. It should be noted that minimum variability was stated for the highly fertilized maize monoculture (MM4), even though uniform pattern was not found regarding the modeled uncertainty in particular treatments. Unfortunately, differentiation between vertical-N and horizontal-N flows was not validated by observations but Kaluli et al. (1999) reported an increased NO_3-N leaching with dropping drainage level in tile drainage systems. Potentially high vertical transport of dissolved NO_3-N can also occur in shallow drainage systems (Wirth et al., 2008; Pfannerstill et al., 2012) possibly increasing the N export from soil horizons by free drainage. Thus, considerable NO_3-N leaching was also plausible during periods with deeper groundwater level that can be often observed during the vegetation period.

According to the outcome for SMN contents and confirmed by Perego et al. (2012), total NO_3-N leaching increased, the more N fertilizer was applied. Annual NO_3-N leaching of 18–21 kg N ha^{-1} $year^{-1}$ in treatments fertilized exclusively with mineral-N (MM2, MU2) was on a level with unfertilized treatments (MM1, MU1; 17–20 kg N ha^{-1} $year^{-1}$). Minor differences between these treatments can be explained by both underestimated as well as similar SMN contents in monocultures (MM1, MM2) from fall to spring and insignificant deviations between corresponding monoculture and bi-cropping treatments regarding simulated NO_3-N concentrations after 1998 (data not shown).

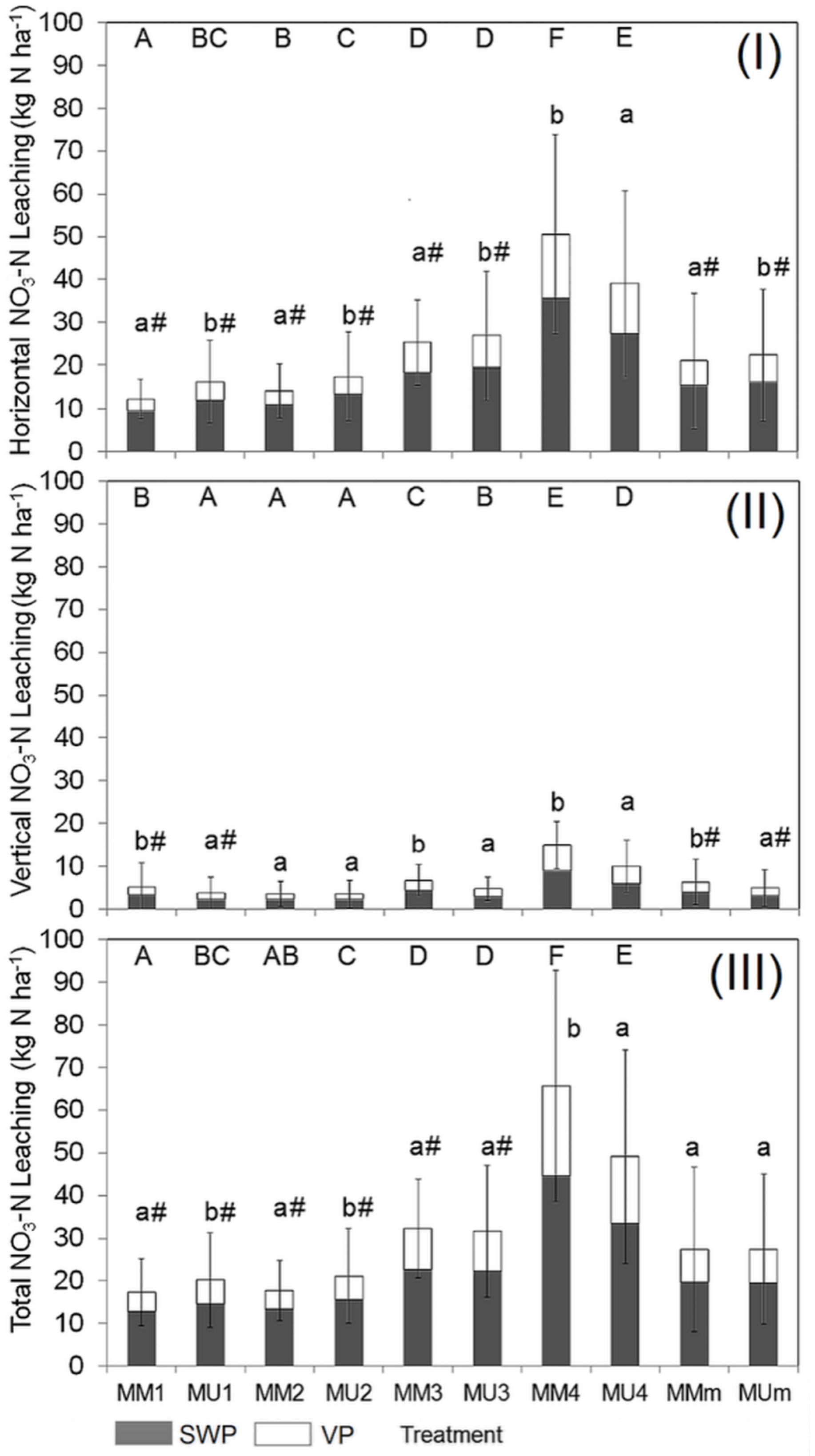

*Fig. 6.5: Simulated horizontal (I), vertical (II), and total (III) NO_3-N leaching (kg N ha^{-1}) for each treatment including the means of monoculture (MMm) and bi-cropping (MUm) split into vegetation period (white bar) and seepage-water period (grey bar) from 11/1996 to 04/2002. Total bar size corresponds to the annual NO_3-N leaching as mean values within SD. (Letters a and b were indicators of significant differences between monoculture and corresponding bi-cropping treatment based on ANOVA (**α = 5%**; a < b) or non-parametrical test (Wilcoxon-Rank sum test; **α = 2.5%**; # marked cases where median values (not shown) were compared because homogeneity of variances was not given; #a < #b); capitals show subgroups without significant differences between arithmetic mean values (ANOVA + Tukey test, **α = 5%**; A < B < C < D < E < F).)*

Table 6.5: Mean, maximum (framed), and minimum (gray-shaded) quartile coefficient of variation (CV) of the NO_3-N leaching in particular treatments including the means of monoculture (MMm) and bi-cropping (MUm) for different aggregation periods.*

Output variable		**Horizontal NO_3-N leaching**			**Vertical NO_3-N leaching**			**Total NO_3-N leaching**		
Period		Nov.–April (SWP)	May–Oct. (VP)	Year	Nov.–April (SWP)	May–Oct. (VP)	Year	Nov.–April (SWP)	May–Oct. (VP)	Year
***CV** (%) for**	MM1:	18	29	21	38	47	38	18	29	20
	MU1:	26	56	30	58	80	64	23	54	30
	MM2:	24	32	25	22	39	25	25	30	26
	MU2:	29	41	34	34	46	32	25	35	29
	MM3:	27	33	26	52	58	51	29	33	35
	MU3:	22	23	22	28	38	26	19	23	23
	MM4:	11	27	19	24	28	27	14	27	21
	MU4:	23	39	22	54	48	38	23	46	26
	MMm:	**20**	**30**	**23**	**34**	**43**	**35**	**22**	**30**	**26**
	MUm:	**25**	**40**	**27**	**43**	**53**	**40**	**23**	**39**	**27**

Increased NO_3-N leaching between 32 kg N ha^{-1} year^{-1} (MM3 and MU3) and 60 kg N ha^{-1} year^{-1} (MM4) were determined for treatments with organic-N input. Obviously, seasonal changes in weather conditions influenced leached N amounts more than particular cropping systems. In general, NO_3-N leaching from April to the end of October was approx. 28% of annual total-N losses for the investigated site. Schiermann (2004) and NLWKN (2012) also confirmed significant NO_3-N leaching on sandy soils during the vegetation period because of considerable precipitation between July and October.

Comparison to leached N amounts proposed by other authors for this site was helpful to validate the results of this study. But reasons for discrepancies between different methods to calculate NO_3-N leaching were numerous, *e.g.*, differences in methodology and empirical algorithms, and possible problems in data homogenization as well as in processing. The calculated NO_3-N leaching as stated by Büchter (2003) was based on measured NO_3-N concentrations below the rooting zone (approx. 60 cm of depth) and an estimated annual seepage-water amount and declined from average 19 kg N ha^{-1} year^{-1} in monocultures to 10 kg N ha^{-1} year^{-1} in bi-cropping systems during the SWP. Consequently, such results were not representative for the total NO_3-N leaching because of potentially dissolved-N amounts below the rooting zone and inconclusive results regarding determination of NO_3-N leaching by means of NO_3-N concentrations in defined soil depths. Kayser et al. (2011) applied the same methodology on maize monoculture at a similar site, a deep-plowed Gleyic Podzol with 6–7% organic matter in the topsoil, in Northwest Germany and calculated a significantly increased NO_3-N leaching of 78–176 kg N ha^{-1} year^{-1} with similar N-fertilizer input. By contrast, this study considered N flows to 135 cm of depth but NO_3-N leaching > 100 kg N ha^{-1} year^{-1} as shown by Herrmann et al. (2005b) to 60 cm of depth for the same treatments were not reproducible. Bleken et al. (2009) stated simulation results between 31 kg N ha^{-1} year^{-1} (MM1) and 75 kg N ha^{-1} year^{-1} (MM4) that were more comparable to our findings for maize monocultures because of aggregated leaching losses to a depth of 120 cm.

Reasons for partially minor differences between monoculture and corresponding bi-cropping system on average (*cf., Fig. 6.5*) were also found in the temporal aggregation of NO_3-N leaching. Total NO_3-N leaching specified for each modeled SWP and VP were at maximum in highly fertilized treatments not only in SWP99/00 after a dry summer but also during SWP01/02 with precipitation above-average in previous summer (*Fig. 6.6)*.

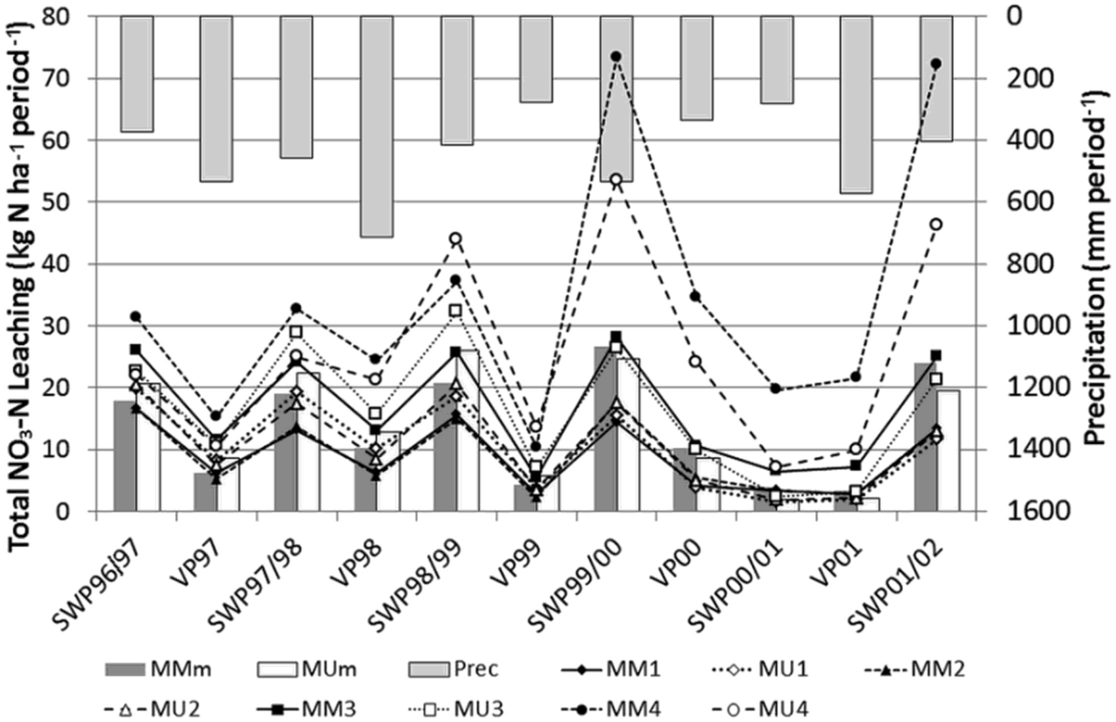

Fig. 6.6: Simulated total NO_3-N leaching in particular seepage-water and vegetation periods between 1996 and 2002 for each treatment including the means of monoculture (MMm) and bi-cropping (MUm) systems as well as the corresponding rainfall. (Results of significance tests on seasonal NO_3-N leaching for each periods and corresponding precipitation can be found in Table A.3.)

Comparison between monoculture and corresponding bi-cropping treatment indicated divergent results for total NO_3-N leaching mainly dependent on applied N amounts during the whole simulation period. Modeled N loss was long-lasting in bi-cropping systems and often higher than for maize monoculture from November 1996 to March 1999. Simulation results also showed that NO_3-N leaching of treatments with mineral-N fertilization (MM2, MU2) mostly corresponded to pattern of unfertilized conditions (MM1, MU1), and one reason was already found in underestimated SMN contents for corresponding monocultures. It must, however, be assumed that deviating from field experiments the implementation of undersown grass before 1998 possibly also influenced the outcome of the period from November 1996 to November 1998 on both N levels. Treatments fertilized with slurry seemed to be at disadvantage regarding NO_3-N leaching, and reasons for relatively high N losses in modeled treatments fertilized with slurry (MM3, MU3) were possibly the overestimated availability of organic-N accompanied by unconsidered NH_3 losses of 15–18% via volatilization in case of applied cattle slurry. The relatively dry period from May 1999 to April 2001 was apparently responsible for diminished NO_3-N leaching in the majority of all treatments. However, elevated NO_3-N leaching was often modeled after dry periods, *e.g.*, SWP99/00 and SWP01/02.

Obviously, sufficient precipitation in summer and mild temperatures during winter can lead to an increased N release by mineralization of stored N in litter and root residues. The strong relationship between the temporal distribution of precipitation, seepage-water and drainage amount, plant evapotranspiration, soil properties, and the resulting seasonality of NO_3-N leaching was also stated in Bakhsh and Kanwar (2011), Peratoner et al. (2013), Randall and Goss

(2008), Strock et al. (2004), and Tauchnitz et al. (2015). For instance, Carlson et al. (2013) stated that 70% of all N lost through tile drainage in the period between April and June was predominantly determined by climatic and plant-related impacts. Kuo et al. (2001) as well as Malone et al. (2014) suggested that fall-planted ryegrass used as cover crop during winter was most effective in reducing NO_3-N leaching in case of dry and mild weather during fall. In this case, residual soil-N contents remained near-surface, and thus an extended N uptake and ryegrass growth before winter was supported. Results of long-term studies about 15 years showed positive effects of ryegrass used as catch crop on reduced SMN contents and NO_3-N leaching between winter wheat and maize during the SWP (Constantin et al., 2012; Constantin et al., 2010). In detail, both SMN contents increased by 13 kg N ha^{-1} after maize harvest and an elevated NO_3-N leaching of 16%, corresponding to 10 kg N ha^{-1} $year^{-1}$, were observed in the fallow period after maize without ryegrass catch crop (Constantin et al., 2010).

Intra-annual comparison of NO_3-N leaching was more comprehensive than the evaluation on basis of periods because problematic months with excessive N losses might be identified. Increased NO_3-N leaching was found between February and May in the majority of all tested N levels and regardless of the cropping system (*Fig. 6.7*). Proportions of 52–63% of total NO_3-N leaching occurred in these four months (*cf.*, Bakhsh et al., 2007), and slightly greater shares of 5–9% were calculated for bi-cropping systems.

Doubtless, N uptake by crops reduced the average NO_3-N leaching considerably by a factor of 2–3 from June until harvest compared with the SWP. General significant reduction of NO_3-N leaching in bi-cropping systems was not found for all presented N levels. Monthly results showed that the potential of undersown grass to limit leaching losses in maize cultivations was greatest with average 25% in the highly fertilized treatment (MU4) that was in line with above-mentioned results (*cf., Fig. 6.5* and *Fig. 6.6*). The number of months with increased NO_3-N leaching in bi-cropping compared with monoculture systems varied between zero (MU4) and two (MU3) when organic-N fertilizer was applied. In contrast, problematic months regarding NO_3-N leaching ranged from February to June in unfertilized (MU1) and exclusively mineral-N fertilized (MU2) treatments. Nevertheless, monthly NO_3-N leaching was increased by a factor of 2–3 and was more variable in treatments with applied slurry. Silage maize fertilized with organic-N was possibly more vulnerable to N losses through subsurface drainage than maize fertilized exclusively with mineral-N because of uncertain mineralization time of slurry (*cf.,* Bakhsh et al., 2005). Comparison between average results for monoculture (MMm) and bi-cropping (MUm) regarding monthly NO_3-N leaching showed not only increased N losses of 2–25% from February to May but also less N amounts of 0–33% from September to January in bi-cropping systems (*Fig. 6.7*, bottom chart).

Undersown grass can serve as catch crop during fall and winter as shown for highly fertilized treatments in this study but physiologically young plants are often subject to increased decomposition, especially after plowing in spring. Therefore, reason for insignificant differences between monoculture and bi-cropping systems in SWP and VP was mainly the compensatory effect between particular months or even periods.

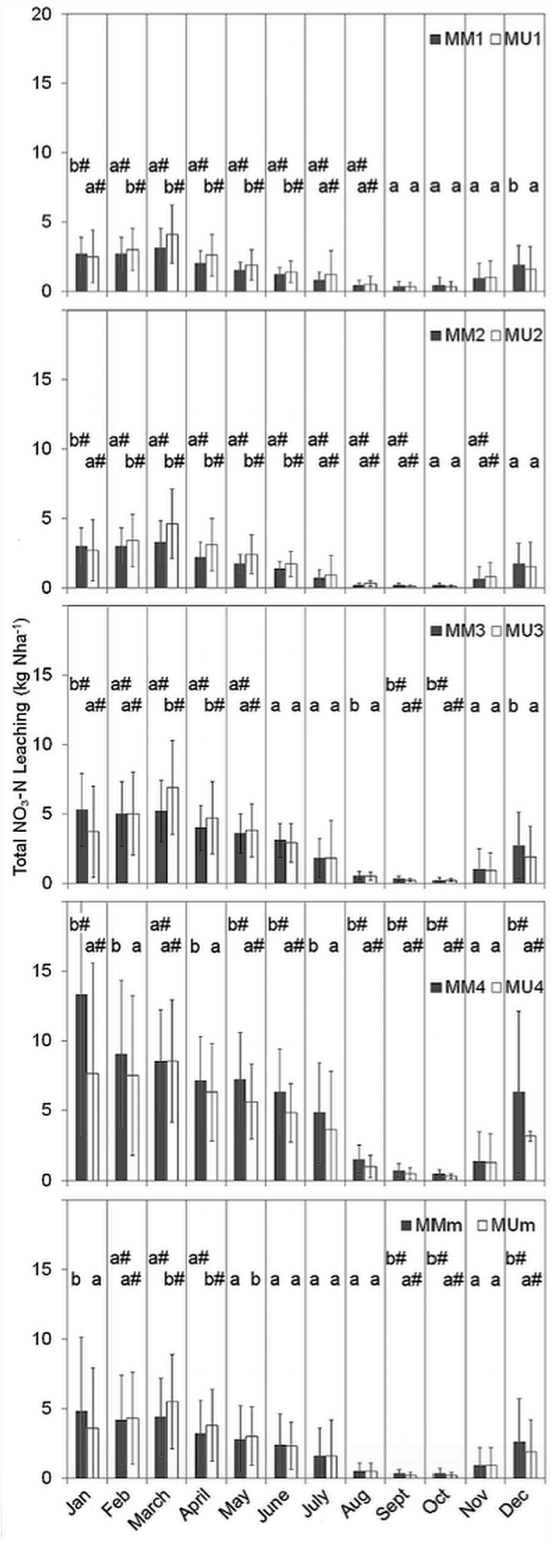

Fig. 6.7: Comparison between simulated monthly total NO_3-N leaching in particular monoculture and corresponding bi-cropping treatments as well as the mean of monoculture (MMm) and bi-cropping (MUm) within SD. (Letters a and b were indicators of significant differences between monoculture and corresponding bi-cropping treatment based on ANOVA (α = 5%; a < b) or non-parametrical test (Wilcoxon-Rank sum test; α = 2.5%; # marked cases where median values were compared because homogeneity of variances was not given; #a < #b).)

The phenomenon of elevated NO_3-N leaching during the SWP for undersown grass might be explained by different *C:N* ratios of the simulated litter pool in soil covered with dormant grass (*M* = 23, *SD* = 3) and in bare soil (*M* = 68, *SD* = 42). The total litter pool in maize monocultures contained old maize residues with *C:N* > 30 resulting in an increased C:N ratio of soil litter, not only after harvest but also during the VP (*M* = 32, *SD* = 2) compared with bi-cropping systems (*M* = 24, *SD* = 2) (see Chapter 7). These results suggested that NO_3-N leaching caused by mineralization of harvest residues might be prevented in continuous maize cultivation despite uncovered soil surface during winter. Justes et al. (2012) concluded that the C:N ratio of litter can be increased in late fall by mulching of chopped maize stubbles but with divergent results regarding NO_3-N leaching. In contrast, root residues of physiologically young grass plants were characterized by *C:N* < 20 that may support the mineralization process clearly (Norton and Schimel, 2011). Büchter (2003) and Volkers (2005) also assumed that incorporated undersown grass was able to lower the C:N < 25 leading to potentially higher mineralization rate. In addition, the application of slurry decreased the C:N ratio of soil litter further and might accelerate both mineralization and NO_3-N leaching as shown in this study.

Van Dam (2006) stated that 10–40% of organic-N in catch crops was released during the first year after incorporation because of significant N mineralization below 5 °C. Benefits from almost total decomposed grass to the next crop were concluded in general when the catch crop was incorporated two or three months before next sowing occurred (Constantin et al., 2015; van Dam, 2006; Volkers, 2005). Another practicable choice might be the removal of above-ground ryegrass before plowing in spring to improve the N balance in addition to reduce NO_3-N leaching (Zavatarro et al., 2012).

As concluding remark, the uncertainty of simulated N leaching had to be also discussed. Presented results were based on statistical measures, *e.g.*, mean value, corresponding standard deviation, and the quartile coefficient of variation. The first two measures are indicators for the random error/uncertainty and give information about the best estimate and the accuracy of this estimate. Furthermore, the accumulated relative uncertainty of the NO_3-N leaching can be also determined from these measures. The relative total uncertainty of NO_3-N leaching according to Eq. 6.1 and Eq. 6.2 varied between 23% (MM4) and 48% (MU3) with average errors of 90% and 82% for monoculture and bi-cropping system, respectively. Major share of simulated total uncertainty originated from an increased uncertainty regarding the SMN content (average of 73%) followed by the drainage water amount (14%) during the SWP as well as the VP. In contrast, relative total errors of NO_3-N leaching calculated according to Büchter (2003) varied from 120% (MM2) to 166% (MU1) and were on average 143% and 156% for monoculture and bi-cropping system, respectively. In that case, increased total uncertainty was caused by high shares of approx. 60% regarding measured NO_3-N concentrations. These significant differences indicated less total uncertainty arising from particular variables as SMN and water contents in the CoupModel approach compared to highly variable NO_3-N concentrations.

6.4 Conclusions

In this study, plausible but highly variable results of simulated NO_3-N leaching for silage maize cultivations were obtained because biomass and N uptake of plants as well as soil mineral-N (SMN) contents were modeled plausibly and according to observations considering both measured and modeled variability. The NO_3-N leaching rose clearly with increasing fertilization in monoculture and bi-cropping systems. The importance of elevated N losses through subsurface drainage between November and April (SWP) was also shown. A general significant reduction of NO_3-N leaching under maize undersown with grass was not provable because of different seasonal climatic conditions and associated processes in plant and soil. Presented results suggested that wet and mild periods usually increase the NO_3-N leaching considerably, and unfertilized or moderately fertilized bi-cropping systems can only benefit after dry periods. Especially bi-cropping of maize and undersown grass at the highest N level (> 200 kg N ha^{-1} $year^{-1}$) showed in most cases reduced NO_3-N leaching compared with maize monocultures. The evaluation on monthly basis confirmed this pattern of variable NO_3-N leaching and highlighted moreover problematic months regarding NO_3-N leaching from February to May for all treatments. Results also suggested that incorporation of physiologically young grass into soil extended the period of NO_3-N leaching until the moment when the following silage maize was able to take up sufficient mineral-N from soil, *i.e.*, from June to August. However, the uptake of catch crop N by the following crop was highly variable affected by the die-back during winter as well as subsequent mineralization before next seeding. Finally, the number of problematic months regarding NO_3-N leaching was mainly dependent on the N fertilization, N uptake, and the mineralization potential of harvest residues and plowed catch crop.

Furthermore, the risk of NO_3-N leaching often increases in case of additional fertilization before sowing and in combination with low N demand of the succeeding maize. This 'fertilizer-value' of catch crop N must be considered in the applied N input of the succeeding crop to limit excessive SMN contents as well as elevated NO_3-N leaching. Therefore, the most important task in agriculture is to fertilize with adequate N amounts especially for crops with late harvest date and high mineralization potential before winter. It is obvious that N applications greater than 250 kg N ha^{-1} $year^{-1}$ characterize highly fertilized treatments that often cause significant enrichment of easily available nutrients in soil, low N efficiency of plants, and an increased risk of NO_3-N leaching. Volkers (2005) concluded an optimal level of N fertilization between 100 and 150 kg N ha^{-1} $year^{-1}$ for silage maize undersown with ryegrass catch crop on sandy-humic soils, but N applications of 80 kg N ha^{-1} $year^{-1}$ seem to be more sustainable especially in combination with organic-N fertilizers and humic soil.

Multiple interactions between soil processes determined by microbial composition, plant, and climate are complex and cannot be predicted with sufficient reliability yet. Therefore, improvements of models are still required. The high variability of modeled NO_3-N leaching suggests that many complex processes in soil and plant have a constitutional variability and often vary with season and site resulting in the fact that universal amounts of NO_3-N leaching are difficult to determine.

Acknowledgments

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Chapter 7
Influencing factors regarding NO_3-N leaching in silage maize cultivations

Significant spatial heterogeneity of dissolved-N or, in particular, nitrate concentrations is caused by different flow paths in the soil profile mainly determined by soil texture and associated hydraulic properties. Further initial factors for highly variable NO_3-N leaching are usually found in above- and below-ground processes related to biomass and soil organic matter (SOM). Amount and quality of soil litter are most important for the formation of humus, however, long-term stability of SOM is depending on various influencing factors such as chemical structure of formed humic substances and environmental conditions, *e.g.*, temperature, moisture, and oxygen contents. As already mentioned in Chapter 6, soil management and associated fractions of harvest residues usually determine SOM dynamics by means of litter formation. To summarize, site-specific factors such as soil-particle size, the pH value, soil temperature, and moisture dynamics are as important as the C:N ratio of plant residues for C decomposition accompanied by N mineralization (Ottow, 2011).

The C:N ratio is often used to characterize the potential of decomposition and mineralization of organic substances in soil. Therefore, optimum C:N ratios are 10–15 to 1 achieved by microbial degradation of fresh dead plants but with significant dependence on species, component, and age of particular plants. It means that remaining harvest residues, applied organic fertilizers, *e.g.*, farmyard manure and slurry, and catch or undersown crops can provide significant sources of SOM. However, the particular effect of each of these sources on humus stability varies dependent on their C:N ratios. In this modeling study, elevated NO_3-N leaching was found below undersown grass during the seepage-water period (SWP) that can be explained by lower C:N ratios of 21–26 in the litter pool compared with bare soil (C:N ratio = 33–118) (*Table 7.1*). In the latter case, remaining roots and harvest residues of old maize plants showed C:N ratios > 30 possibly resulting in decelerated decomposition as opposed to young undersown grass with C:N ratios < 20 during winter. Justes et al. (2012) concluded that mulching and incorporation of chopped maize stubbles in fall increased the C:N ratio of the litter pool and reduced both simulated NO_3-N concentrations in drainage water by 5–10% and NO_3-N leaching by −5 kg N ha^{-1}. This reduction of NO_3-N leaching was not modeled for treatments with maize mulch that was similar to results in this study regarding investigated bi-cropping systems with present grass cover. The application of organic-N as slurry lowered the C:N ratio of soil litter further and might accelerate both N mineralization and NO_3-N leaching as shown in Chapter 6. In addition, the more organic-N fertilizer was applied, the more the C:N ratio of soil litter converged during winter. As opposed to that, C:N ratios were minor different during the vegetation period (VP), and slightly increased C:N ratio in litter was calculated for monocultures during the VP that might diminish subsequent decomposition and mineralization processes.

Table 7.1: Simulated C:N ratio in total litter pool, litter-C amounts, changes of total soil organic matter (SOM) pool (in%), and the comparison between simulated total denitrification with calculated amounts for the investigated site during five years (04/1997–03/2002).

Treatment	MM1	MU1	MM2	MU2	MM3	MU3	MM4	MU4
C:N ratio in total litter pool (–; mean values):								
SWP Mean (11–04; (11–12))	88 (41)	26 (24)	118 (38)	21 (20)	35 (36)	23 (21)	33 (33)	21 (21)
VP Mean (05–10)	35	25	32	25	32	22	29	23
Litter-C amount (kg C ha^{-1} $period^{-1}$; accumulated mean values, 04/1997–03/2002):								
SWP Mean (11–04)	32	570	72	520	83	715	100	710
VP Mean (05–10)	1120	1840	2280	2915	2880	3575	3580	3940
Annual amount	1152	2410	2352	3435	2963	4290	3680	4650
Changes in the total SOM pool between 04/1997 and 03/2002 (% of total SOM on April 1st, 1997):								
Total soil organic-C amount[a]	−2.5 (−2.9)	−0.3 (−0.2)	−1.4 (−1.9)	+0.2 (+0.2)	0 (−0.8)	+2.3 (+2.1)	+0.4 (−0.6)	+3.0 (+2.9)
Total soil organic-N amount[a]	−5.3 (−5.5)	−3.5 (−3.6)	−4.2 (−4.4)	−2.7 (−2.8)	−2.5 (−2.9)	−0.8 (−1.0)	−0.8 (−1.3)	+1.4 (+1.3)
Total denitrification (kg N ha^{-1} $year^{-1}$; accumulated mean values, SD within parentheses):								
CoupModel	2.4 (0.2)	2.7 (0.4)	2.6 (0.4)	2.5 (0.3)	3.8 (0.3)	3.2 (0.4)	5.1 (0.4)	4.1 (0.5)
Bleken et al. (2009)	17.0	–	19.1	–	18.8	–	22.8	–

[a] Values in parenthesis represent the change (in%) related to the total SOM amount on November 1st, 1996.

The release of CO_2 is one key parameter to characterize the metabolism of organisms such as plants and soil microorganisms. Simulated total respiration of CO_2 represents the sum of respiration from soil organics and plant roots (maintenance respiration only). Differences between monoculture and corresponding bi-cropping treatment were significant during VP and SWP (*Fig. 7.1*). This finding was accompanied by an elevated C respiration with increasing biomass amount in fertilized treatments. Total respiration was significantly higher during the VP than the SWP because of activities such as plowing, harvest, and, to minor extent, organic-N fertilization that took place from the end of April to October in each year (*Table 7.1*).

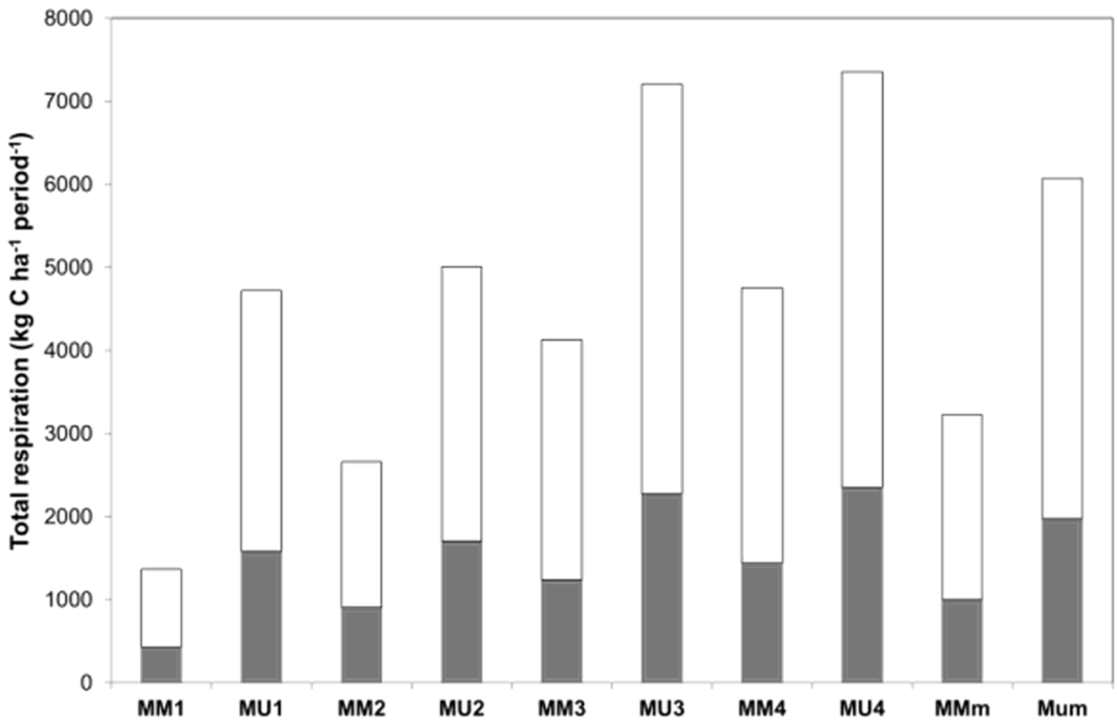

Fig. 7.1: Mean total respiration in seepage-water (gray bar) and vegetation period (white bar) of particular monoculture and corresponding bi-cropping systems including their means (MMm, MUm).

Reasons for up to more than three times greater respirated C in bi-cropping treatments might be the additional organic-C input by plowing up of annual grass in spring with peak values between 30 and 60 kg C ha^{-1} of CO_2. This result was comparable to C amounts released by respiration after harvest in unfertilized treatments or even more in fertilized trials. Comparison between modeled respiration and laboratory measurements for basal respiration in monoculture treatments MM1 and MM2 between March 1999 and March 2000 (Karrasch, 2005) was questionable. The laboratory test was a standardized procedure for disturbed soil samples measuring the oxygen consumption at 25 °C with optimum water content during 7 days for a 15 cm depth increment. Modeled outcome represented the total respiration for the whole soil profile and reflected more the natural variability regarding soil temperature and moisture dynamics. Simulated weekly C respiration varied significantly from 1.5 g C m^{-2} (March 2000) to 4.0 g C m^{-2} (August 1999) for the unfertilized treatment (MM1) and between 3.0 and 7.0 g C m^{-2} in the exclusively mineral-N fertilized trial (MM2). However, these simulated differences between both N levels were not confirmed by Karrasch (2005) with measured basal respiration from 4.6 (November 1999) to 6.0 g C m^{-2} (March 1999) up to 30 cm of depth without significant differences between MM1 and MM2. Reason for this deviation was possibly the simulated litter-C pool that rose considerably during the VP (*Table 7.1*) with highest amounts in highly fertilized treatments.

Accumulated litter-C amounts of unfertilized and mineral-N fertilized treatments changed between 1150 and 3430 kg C ha^{-1} $year^{-1}$ for MM1 and MU2 (*Table 7.1*), respectively. This outcome was plausible according to measured harvest and root residues of approx. 1740 kg C ha^{-1} $year^{-1}$ for maize reported by Engels et al. (2010). Kuzyakov and Domanski (2000) presented highly variable amounts of below-ground C translocated by cereals and grass species of 1000–2250 kg C ha^{-1} $year^{-1}$ for cereals and 840–4432 kg C ha^{-1} $year^{-1}$ for ley grass such as *Lolium perenne* L., confirming simulated outcome of this study. Finally, these results were also plausible for bi-cropping systems because the CO_2 release rose with increasing amount of litter remaining after harvest used as green manure or after plowing. Temporal C dynamics of litter, humus formation, and respiration showed significant differences between particular fertilization levels and between monoculture and corresponding bi-cropping systems (*Fig. 7.2*). It has to be noted that litter-C depended significantly on produced biomass and was mainly formed at harvest. However, smaller amounts of litter-C were also simulated during plant growth, at the turn of the year, and on the day of plowing.

As already stated, more biomass, litter, and humus as well as CO_2 were built with increasing fertilization and in bi-cropping systems. Comparison between simulated total litter and observed above-ground harvest residues in particular treatments showed significant deviations because modeled root biomass was also transferred to the litter pool after harvest. Measured plant residues greater than 2 mm between 0–30 cm of depth (Karrasch, 2005) were more comparable to simulated litter-C amounts in unfertilized and mineral-N fertilized monocultures (MM1 and MM2); even though only single observations were available in fall 1999. Reason for missing significant differences regarding observed stubble amounts (Herrmann, 2006) between particular treatments was possibly found in the constant cutting height unlike defined litter fractions of simulated biomass in the model setup. Associated N dynamics also showed significant impacts of soil management and fertilization on litter, humus-N formation, and NO_3-N leaching on daily basis (*Fig. 7.3*). Elevated N input and undersown grass increased both litter-N amounts and humus-N formation, but also N leaching differed considerably with significant dependence on fertilization. Daily dynamic of NO_3-N leaching differed clearly between SWP and VP but only slightly between monoculture and bi-cropping without uniform pattern regarding leached amounts. Short-term peak values as well as long-lasting NO_3-N leaching occurred in both monoculture and bi-cropping with significant influences of precipitation conditions that was already discussed in Chapter 6.

Changes of the SOM pool were also determined between April 1997 and March 2002 as well as for the whole simulation period (start date: November 1st, 1996) (*Table 7.1*) indicating that particular changes (in%) were greater for total organic-N (SON) than for organic-C (SOC) amounts. Maximum negative changes were found in unfertilized monocultures because of nutrient removal by harvest, whereas undersown grass was able to reduce the loss of SOC significantly.

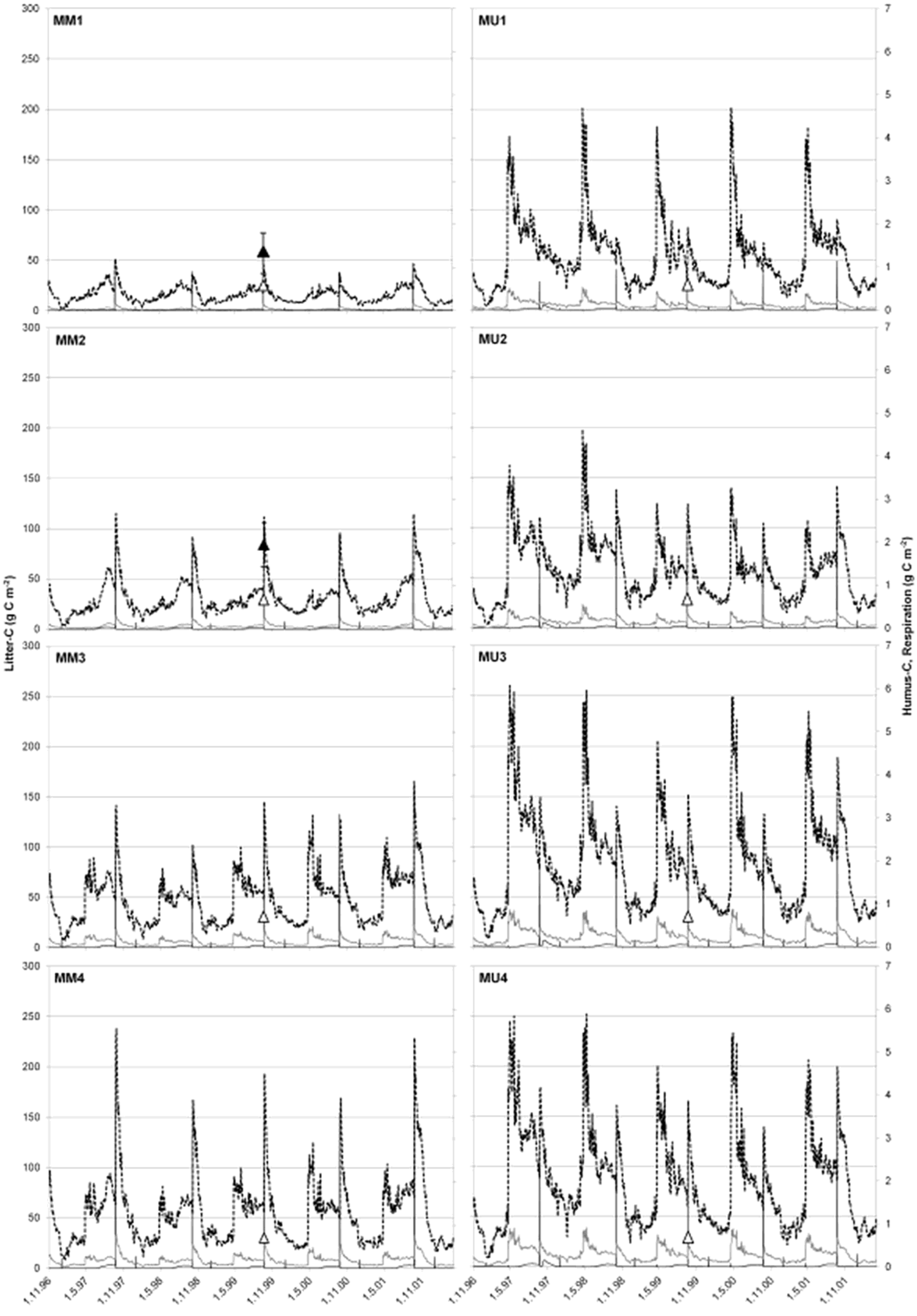

Fig. 7.2: Simulated litter-C amounts (▬), humus-C formation (▬), and total respiration (- - -) of particular treatments from November 1996 to March 2002 in comparison with observed average above-ground harvest residues (maize stubbles, ∆; Herrmann, 2006) and measured plant residues (> 2 mm) in 0–30 cm of soil depth (mean within SD, ▲; Karrasch, 2005).

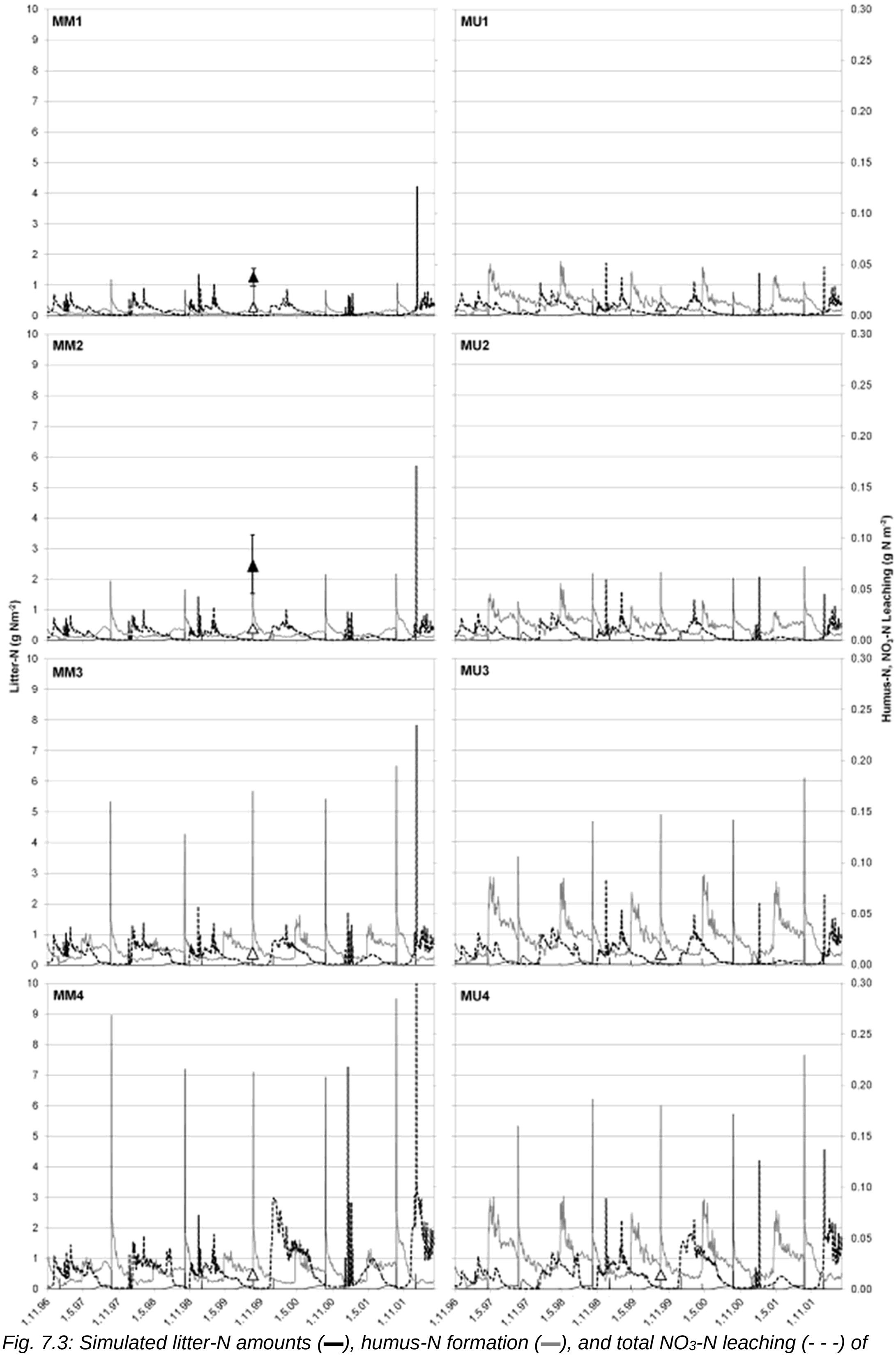

Fig. 7.3: *Simulated litter-N amounts (▬), humus-N formation (▬), and total NO_3-N leaching (- - -) of particular treatments from November 1996 to March 2002 in comparison with observed average above-ground harvest residues (maize stubbles, ∆; Herrmann, 2006) and measured plant residues (> 2 mm) in 0–30 cm of soil depth (mean within SD, ▲; Karrasch, 2005).*

Furthermore, the more fertilizer was applied, the more positive the change of SOC was accounted for, and already the application of 150 kg mineral-N ha^{-1} year^{-1} led to positive SOC changes during five years of investigation. The loss of organic-N was remarkable, and the only treatment with positive SON changes was bi-cropping at the highest fertilization level (MU4). Finally, it can be discussed, whether or not mineralization of soil organic matter was overestimated by the model and simulated NO_3-N leaching showed thus insignificant results between particular cropping systems, except for the highly fertilized treatment. However, five years of investigation were clearly too short for reliable statements regarding the SOM development without observations. The most common method to evaluate the potential of particular crops to improve SOM contents was proposed by the VDLUFA (Körschens et al., 2005). Silage maize is insensitive to overfertilization and can take up large N amounts resulting in decreasing SOM amounts in case of insufficient compensation strategy regarding humus depletion. A loss of −560 to −800 kg humus-C ha^{-1} year^{-1} (Körschens et al., 2005) or even more variable amounts dependent on the quantification method of humus reproduction (Engels et al., 2010) were recommended for silage maize. Maximum simulated loss of −490 kg organic-C ha^{-1} year^{-1} was thus plausible for unfertilized monocultures (detailed data not shown). Reason for the moderate decline of organic-C amounts under unfertilized maize at this site was possibly found in high total SOC contents of 7.5% in the upper soil layers (cf., *Table 6.1*) because of regular fertilizer supply during previous years. Post et al. (2007) presented modeling results confirming observations of decreasing SOM contents between 0–20 cm of depth for long-term crop rotations (> 30 years) without fertilizer input. Furthermore, exclusively mineral-N fertilized maize monoculture (MM2; 150 kg N ha^{-1} year^{-1}) showed also negative SOM changes over five years in this study confirmed by Post et al. (2007). In contrast, Taube (2013a) concluded insignificant differences between long-term maize monocultures and crop rotations with/without maize regarding significant SOM changes based on 67 fields in Schleswig-Holstein. Although, the SOM amount was approx. 20% lower than under permanent grassland.

Stabilization of SOM by means of regular inorganic fertilizer application possibly resulted from the efficiency of mineral-N to increase biomass yields. As a result, considerable plant residues can remain after harvest at field as potential humus compensation (Leithold, 2008). Positive influences of organic fertilizer application on SOM contents, as shown in this study, and humus reproduction in arable farming systems were evident (Engels et al., 2010; Post et al., 2007). However, significant changes regarding SOC contents were only conclusive for periods of 50–100 years. High variability of measured SOC contents and a minimum analysis error of 0.1% for single observations can only result in general information about the site-specific situation of SOM dynamics (Reinhold, 2008). In addition, positive effects of catch crops and temporary grassland on SOM contents was stated by Post et al. (2007). Taube (2013b) concluded that silage maize in crop rotations showed significantly lower yields especially by reduced fertilization but with long-term benefits for humus reproduction. The potential N supply of temporary grass or clover/grass can amount to +100 kg N ha^{-1} compared to monocultures resulting in reduced additional N fertilization. Positive changes in SOC were also found in this study for fertilized bi-cropping systems indicating an increased potential of undersown grass to stabilize SOM by means of elevated litter amounts. As already mentioned before, not only the quantity of litter is important for SOM formation but also its quality, *i.e.*, the C:N ratio and the related mineralization or immobilization potential. Long-term application of combined slurry/mineral-N in combination with organic-N storage in undersown grass (MU4) during the SWP seemed to be most effective to improve SOM and to reduce NO_3-N leaching in conventional maize cultivations. According to recommended values for humus reproduction proposed by the VDLUFA (Körschens et al., 2005), temporary storage of organic-C and organic-N in undersown crops can amount to 200–300 kg humus-C ha^{-1} $year^{-1}$, as long as this biomass was not removed. On the other hand, N fertilization > 250 kg N ha^{-1} $year^{-1}$ can cause significant nutrient enrichment, low plant-N efficiency, and increased NO_3-N leaching loss in soils.

Discrepancies were found for simulated denitrification loss, especially for fertilized treatments, that was possibly underestimated compared with approximate values of 6–20 kg N ha^{-1} $year^{-1}$ for arable land in Germany (Schneider and Haider, 1992). Elevated denitrification rates of approx. 44 kg N ha^{-1} $year^{-1}$ were also reported for arable sites fertilized with organic-N (Nieder et al., 1989). These results cannot be confirmed in this study with at most 5 kg N ha^{-1} $year^{-1}$ (*Table 7.1*). In contrast, the denitrification potential is often reduced in soils with low SOM content below 30 cm of depth and subsurface drainage system because of increased N mineralization under aerobic conditions (Colbourn and Harper, 1987; Jahangir et al., 2012; Kaluli et al., 1999). The investigated field area was surrounded and partially crossed by artificial drainage pipes (Karrasch, 2005) with unknown depth. This can result in both an incomplete transformation from mineral-N to N_2O and lowering of denitrification between 10 and 30 kg N ha^{-1} $year^{-1}$ (Müller and Raissi, 2002). Furthermore, modeled denitrification was set to decrease linearly with depth, and thus denitrified-N amounts originated from upper soil because denitrification in saturated soil horizons (below the saturation level) was neglected. Comparison to observed N_2O emissions of approx. 2 kg N ha^{-1} $year^{-1}$ from silage maize cultivations at the same site (Wienforth et al., 2012) showed that denitrification originating from surface-near management, *e.g.*, plant residues and fertilization, was simulated plausibly in this study. Higher N_2O emissions of 1–14 kg N ha^{-1} were measured for silage maize on sandy-loamy soil in Northern Germany with maximum N_2O losses for pig slurry (440 kg N ha^{-1}) as a result of higher soil moisture at particular water tensions (Dittert and Mühling, 2009). Matschullat et al. (2013) concluded that emitted N_2O amounts varied between 1–2 kg N ha^{-1} $year^{-1}$ in arable soils with increased proportion of total denitrification in case of elevated NO_3-N contents accompanied by significant mineralization potential in temporary saturated soil. Consequently, modeled denitrification had to be interpreted with caution because of its more simple quantification in the model and uncertainties arising from parameterization.

Chapter 8 Conclusions

8.1 Summary of key findings

The main objective of this thesis was the model-based quantification of NO_3-N leaching in agricultural soils. For this, a sequential methodical approach was presented to elaborate suitable model structures regarding particular soil water and nitrogen dynamics dependent on available data and additional information. The key results are summarized according to the four research questions as follows:

(I) Is the process-based model CoupModel able to reproduce temporal dynamics of discharge and NO_3-N leaching by drainage?

Detailed and reliable description of complex soil processes within process-based modeling adapted to site-specific conditions was necessary to obtain conclusive findings for the NO_3-N leaching. The general applicability of the CoupModel to reproduce temporal dynamics of water discharge and NO_3-N leaching in a well-studied artificial drainage system was shown exemplary for an organic crop rotation consisting of winter wheat and undersown red clover catch crop. The manual calibration based on daily measurements and literature values provided plausible temporal N dynamics, even though deviations from observations occurred sporadically in periods with increased mineralization. This finding suggested that manual calibration may ignore sources of uncertainty arising from model structure, input parameter values, and measured data. However, particular soil-related processes are usually also subject to greater variation under natural conditions, and repeated measurements, especially related to soil issues, often show a high variability.

In the course of comprehensive sensitivity analyses, input parameters with variable sensitivity regarding important model output, *e.g.*, the NO_3-N leaching by drainage, were identified and partially used for further investigations. The question was if the adaptation of present model structures on new conditions can be made more efficiently by assuming particular input parameter uncertainties. For this, the following question was answered:

(II) Can stochastic optimization methods such as the Bayesian calibration and the GLUE approach be used for parameter estimations to achieve reliable results for the NO_3-N leaching?

To consider the presumed natural variability just as uncertainties arising from model parameterization, two different optimization approaches were applied. Basically, particular input parameters were selected to vary within defined ranges, and a number of up to 20,000 simulations or rather parameter combinations were carried out. Both optimization methods were based on the Bayesian theorem of conditional likelihoods and aimed at most plausible model realizations that reproduced the behavior of the system in a satisfactory manner. The selection of the most plausible simulations was done by means of defined objective function(s) that were calculated for the considered validation variables of each model realization. Therefore, the plausibility of particular model results was verified on a broad basis according to corresponding measurements (multi-objective calibration). The NO_3-N leaching below the root zone (60–65 cm of depth) of mown permanent grassland was simulated satisfactorily in both cases. However, model performance given by traditional statistic measures, *i.e.*, R^2, *RMSE*, and *ME* values, varied considerably between the tested levels of N fertilization. In addition, parameter dispersion of the accepted simulations, *i.e.*, the coefficient of variation (*CV)*, resulting from Bayesian calibration was slightly increased in case of high N fertilization compared with results obtained from the GLUE optimization. Single parameters governing decomposition and mineralization of litter and humus showed elevated dispersion, beside the scaling coefficient for the thermal conductivity in the upper soil, independent on the optimization method. However, cumulative frequency distribution of accepted input-parameters values, realized with the GLUE, showed neither indication for normal or logarithmic distribution nor general pattern regarding significant differences between both N levels (*Fig. A.1* and *Fig. A.2*). Main reason for that was certainly the insufficient number of accepted simulations, even though maximum dispersion (CV value) was found for parameters governing the decay of humus and litter among these few simulations. These results emphasized the importance of transformation processes regarding soil organic matter and their impact on the N leaching. The consideration of parameter uncertainties can thus improve the understanding and reproduction of complex soil-related processes in modeling at plot scale. Nevertheless, reliable statements on statistical basis are needed and can only be achieved with a large number of plausible simulations.

As the GLUE approach was identified as more robust optimization method and, moreover, resulted in satisfying model results for grassland in general, this invers uncertainty assessment method was used for further model applications. Exemplary, the extensive cultivation of silage maize was chosen to investigate impacts of model uncertainty on variations of input parameters and particular model output. The natural variability in observations whether produced by errors in the measuring itself or resulting from spatial and temporal variations in underlying natural processes had to be considered in the model optimization, too. Consequently, a certain variation had to be also assumed regarding the model results. The 'LogLikelihood' measure, which also considers the measured variability or mean error, was used as main objective function to select the most plausible simulations. The elaboration of an appropriate selection sequence was thus required to balance the importance of different available validation variables against each other. As the basic model structure already existed on the basis of previously presented results, only few site characteristics, *e.g.*, for soil texture and plant growth, had to be adjusted to silage maize cultivations. Due to this fact, special attention was paid to plant growth dynamics of particular crops that has to be parameterized as realistic as possible. The importance of produced biomass and associated harvest residues for modeled soil water and N dynamics was already stated. The match between observed and simulated maize biomass was the priority in this optimization process. Further traditional statistic measures to evaluate the model performance confirmed the plausible model parameterization regarding abiotic and biotic processes partially. The uncertainty of selected input parameters was reduced significantly after optimization resulting in quartile coefficients of variation (*CV**) < 25% for 36% and 26% of selected parameters in monoculture and bi-cropping systems, respectively. The *Fig. A.3* shows the distribution of accepted parameter values within the predefined ranges. This overview indicated only few parameters with significant differences between monoculture and bi-cropping systems, *e.g.*, efficiency of humus decay, radiation use efficiency, and particular plant allocation parameters. Based on subsequent selection of the most plausible simulations for different silage maize treatments, following two joined research questions can be answered:

(III) Does undersown annual grass affect the soil water balance under silage maize negatively?

Based on plausible results for modeled soil temperatures, water contents and potentials, and the groundwater level, particular results for the soil water balance including main components and soil water storage to 30 and 90 cm of depth were evaluated. The *CV** values of evapotranspiration and total runoff varied between 0 and 26% and 8–21%, respectively, on half-yearly basis, and significant differences between the cropping systems were stated. Undersown grass reduced the total runoff but slightly increased the evapotranspiration (ETI) from November to April (SWP). Differences between monoculture and bi-cropping were in parts insignificant for particular periods despite the high variability of modeled results on half-yearly basis. Nevertheless, the annual soil water balance was positive for all treatments indicating that present climate conditions indicate rather certain water surplus that can be also stored in soil below 30 cm of depth. Both silage maize and grass can show maximum root depths of more than 1 m and are able to obtain soil water from subsoil. However, young undersown grass could be at disadvantage before maize harvest because of insufficient root density and depth resulting in a lack of growth. Finally, model results suggest that bi-cropping of silage maize and undersown annual grass resulted in only minor water stress during five years of investigation.

On the basis of plausible model results regarding soil water dynamics, simulated soil N dynamics were also tested for plausibility. For this, particular account was taken for the NO_3-N leaching and its potential leakage pathways to answer the last research question:

(IV) Can the NO_3-N leaching be reduced by bi-cropping of silage maize and annual grass considering sources of uncertainty?

An accompanying problem is often the choice of the reference level that should be determined carefully to calculate the N leaching into or from water bodies and drainage systems. The determination of N losses in a particular soil depth, *e.g.*, below the root zone in 60–65 cm of depth, is certainly not incorrect, but it may neglect potential lateral NO_3-N flows into drainage and/or surface water above this level. Consequently, the total NO_3-N leaching considering losses by drainage and deep percolation (in 135 cm of depth) was determined within modeling.

The predictable variance between total N leaching and particular 'uncertain' input parameters showed most dominant parameters governing the litter decomposition in maize monoculture and additional parameters related to plant growth in bi-cropping. Increased uncertainty regarding determined NO_3-N leaching was also found indicated by considerable data dispersion, *i.e.*, *CV** values between 11–80%, especially in bi-cropping treatments. Modeled NO_3-N leaching was just as variable as or more different than estimations based on more simple calculations (*cf.*, Büchter, 2003). Annual NO_3-N leaching differed significantly between the pathway by horizontal drainage and by deep percolation. Not surprisingly, maximum NO_3-N leaching was found in highly fertilized maize treatments during the SWP mostly dominated by horizontal drainage. Undersown annual grass can reduce the N leaching, even though significant reduction was not demonstrable during the SWP but was exclusively stated for the highly fertilized bi-cropping treatment. In general, problematic periods with an elevated NO_3-N leaching ranged predominantly from February to May that is usually associated with increasing soil temperatures and high mineralization potential. Significantly decreased NO_3-N leaching in bi-cropping systems was determined in and after periods with below-average precipitation and from September to January with reductions of 0–33%. Consequently, NO_3-N leaching is highly influenced by weather conditions, and significant differences were mostly identified in case of changing amount of precipitation. The increased risk of NO_3-N leaching in case of sufficient rainfall, permeable soils, artificial subsurface drainage, and excessive N fertilization was shown in this thesis for the investigated sites.

Finally, following summary of simulated NO_3-N leaching during the SWP is given for the investigated cultivation systems in Table 8.1. Simulated results confirmed significant impacts of both N fertilization and the 'fertilizer value' of preceding crops or, in other words, their harvest residues for litter production on the N leaching. In contrast, modeled NO_3-N leaching from May to October (VP) was usually significantly lower than during the SWP. Leached N amounts by horizontal drainage varied between 3–15 kg N ha^{-1} during the VP with highest amounts in the highly fertilized maize monoculture. The NO_3-N leaching of grassland and ecological crop rotations was at most 5 kg N ha^{-1} during summer regardless of the reference depth. Presented results demonstrated both significant impacts of site conditions and N management as well as the general uncertainty to calculate N transformation processes in soil conclusively.

Table 8.1: Summary of simulated NO_3-N leaching dependent on crop, farming system, N fertilization, number of SWPs, and the reference depth.

Crop	**Farming system**	**Mean fertilization rate (kg N ha^{-1})**	**NO_3-N leaching (kg N ha^{-1})**	**Number of SWPs**	**Reference depth**
Red clover	Ecological	0	8	2	Drainage
Grassland	Conventional	0	11	5	60–65 cm
Silage maize	Conventional	0	10–12[a]	6	Drainage
Silage maize	Conventional	150 (mineral-N)	11–13[a]	6	Drainage
Silage maize	Conventional	120 (slurry-N)	18–19[a]	6	Drainage
Winter wheat	Ecological	0	22	1	Drainage
Silage maize	Conventional	270 (mineral/slurry-N)	27[b]–36	6	Drainage
Grassland	Conventional	300 (mineral-N)	74	5	60–65 cm

[a] Differences between monoculture and bi-cropping regarding modeled NO_3-N leaching were insignificant.
[b] Modeled NO_3-N leaching in the corresponding bi-cropping system.

There is no doubt that N fertilization adapted to temporal plant-N demand is most important to limit NO_3-N leaching in agriculture. Complete prevention of leaching processes may be impossible especially during the SWP confirmed by these model results. The application of organic fertilizer as slurry posed an additional risk to N leaching because of uncertain mineralization time compared with treatments exclusively fertilized with mineral-N. Therefore, the 'fertilizer value' of slurry is comparatively prolonged resulting in significantly increased NO_3-N leaching during the SWP. This was confirmed by the model results in spite of less applied organic-N compared with mineral-N amounts and slightly overestimated N removal by above-ground maize biomass in the corresponding treatments. Furthermore, the risk of NO_3-N leaching was also increased before sowing and in combination with low N demand of the succeeding maize plant in spring. The amount of both N fertilizer and SOM may stimulate various processes such as formation of more stable organic matter, decomposition, mineralization, denitrification, but also NO_3-N leaching simultaneously. The 'fertilizer value' of preceding (catch) crops must be considered in the applied N input of the succeeding crop to limit excessive SMN contents and NO_3-N leaching. The amount of harvest residues of maize with C:N ratio > 30 as well as destroyed and plowed annual grass with comparatively low C:N ratios < 25, for instance, seemed to be most important for temporal dynamics of N mineralization and corresponding N losses in bi-cropping. The potential of denitrification to limit NO_3-N amounts in the upper soil was also stated without clear identification of the final products because of model simplifications. On the other hand, sandy-humic soils may provide only suboptimal conditions regarding complete transformation into gaseous N (N_2) in the vadose zone, and instead greenhouse gases such as nitrous oxides (N_2O) may be formed.

Finally, much evidence suggests that the NO_3-N leaching is a product of highly variable processes in soil mainly determined by N fertilization and the sequence of plant growth, decomposition of litter, and mineralization during the year. Many processes in the unsaturated soil are usually non-linear; therefore stochastic simulations, *e.g.*, Monte-Carlo computations, might result in more reliable results because of consideration of uncertainties arising from non-linear relations between different variables.

8.2 Capability and limitations

In the course of this thesis, the applicability of the process-based model CoupModel was tested successfully for different sites and crops in Northern Germany to provide plausible results regarding the NO_3-N leaching. However, highly variable model results were obtained mainly determined by site-specific conditions. This influence is understandable and has to be considered in case of reproduction of observed data at plot scale. During the last decade, the model has been developed further aimed at the consideration of sources of uncertainty. For this, special attention was paid to model uncertainty arising from parameterization that may also represent the existing variability of natural processes. It was assumed that complex interactions between soil, plant, and atmosphere regarding water and nitrogen dynamics in the unsaturated soil were described properly when multiple modeled results matched corresponding observations plausibly. This hypothesis also included the consideration of certain variation regarding particular results and may improve the understanding of natural processes in ecosystems. And even spatial and temporal/seasonal variations of natural processes are the normal case especially in upper soil zone, and hence, modeled variations may provide more realistic indications for leached N amounts. Therefore, consideration of variations can be helpful to adapt calibrated models on different sites. In this context, following limitations regarding presented results, model structure, and particular applications were still detected:

(I) First of all, the significant influence of site characteristics on particular soil processes may hinder the development of universal model structures. The CoupModel has been improved continuously and was applied to specific sites and research issues. Reproduction of particular results may be also hampered by improvements and adaptations of model algorithms. Results of manual calibration presented in Chapter 2 were not verified by means of the GLUE application in the course of this thesis. This step was necessary in fact to check the general model structure including the influence of selected input parameters. Because of indications that manual calibration seems to be meaningless in case of highly parameterized models, the question cannot be answered sufficiently whether or not changes in the parameterization because of defined site-specific conditions, *i.e.*, selection of specific input parameters and their particular value(s), influenced the modeled outcome to a certain extent.

Furthermore, significant impacts on soil-N status and NO_3-N leaching from legume cultivation by means of temporary grown red clover including its plowing up were not validated because of the limited opportunity to parameterize symbiotic-N fixation based on plant physiology in CoupModel.

(II) Indications for possible interactions between parameter uncertainty and variations of particular modeled outcome can be derived from results presented in Chapters 3 and 4. Different optimization approaches were tested on mown pure grassland focused on the quantification of NO_3-N leaching below the root zone, but not by drainage as presented in Chapter 2. Secondly, defined ranges of selected input parameters were defined differently, even though a high number of same parameters were selected in both optimization approaches assumed to be uncertain. For example, influences arising from uncertain conditions of subsurface drainage were only considered in the GLUE optimization. In contrast, a number of corresponding parameter values was fixed in the Bayesian calibration. Regarding the last mentioned approach, additional limitations resulted from both insufficient consideration of different initial values and more restricted parameter ranges in the setup, compared to the GLUE setup. All these issues possibly reduced the simulated uncertainty regarding NO_3-N leaching. Finally, only limited management options, *i.e.*, pure grass stand, multiple cuttings, exclusive mineral-N fertilization, were tested for permanent grassland. Consequently, presented results for simulated NO_3-N leaching might not be representative for grassland consisting of clover-grass mixtures and/or fertilized with slurry despite its high relevance in Northern Germany.

The extensive cultivation of silage maize was chosen exemplary to investigate effects of an undersown grass catch crop on soil water and nitrogen dynamics. Altogether, plausible results were found for maize monoculture and bi-cropping systems regarding the soil water balance, their components, and the NO_3-N leaching including different leakage pathways. However, selection of the 'best' simulations was conducted stepwise mainly with the help of biomass data because of its high quantity as well as quality. In this context, it must be noted that the presented sequential selection procedure was highly subjective, hence it describes rather a semi-automated optimization method. Secondly, the selection on the basis of the '*LogLikelihood*' (*LogLi*) value might not be comparable to other results achieved with more traditional statistic measures, *e.g.*, R^2, *RMSE*, *ME*, and *NSE*, but mean errors of measurements were emphasized stronger by the *LogLi* value. The reproduction of observed SMN contents and NO_3-N concentration in soil water was still a challenge for the model against the background of scarce data availability regarding long-term and frequent measurements. This also indicates that nitrogen dynamics in soil underlie greater variation than soil water or temperature conditions at plot scale. Following limitations were identified in respect of particular research questions:

(III) The statement in this thesis that undersown grass influenced the soil water balance only minor and water stress is, thus, negligible, was made on the basis of half-yearly results without considering effects of particular years.

Consequently, the question might arise whether or not the bi-cropping in periods with below-average precipitation, *e.g*., VP99, VP00, and SWP00/01, can result in negative soil water balance and increased water stress for plants. The same deficit might be mentioned for different runoff components, *i.e*., discharge by drainage or deep percolation. However, particular results were available but not presented in detail due to limit extent of content in the published article (*c.f*., Chapter 5). Secondly, increased variability of components regarding the soil water balance was caused only partially by limited reduction of particular parameter ranges in bi-cropping. The resulting inconsistent pattern of this adjusted parameterization could raise the question concerning appropriate model structure and sufficient parameter ranges.

(IV) Regarding modeled NO_3-N leaching in silage maize cultivations, detailed investigations for different aggregation periods were carried out. Differences regarding N leaching between monoculture and bi-cropping were not significant when only average annual results were considered in contrast to results regarding particular levels of N fertilization. The detailed view on distinct periods with specific precipitation and significant plant-N demand was more suitable to identify distinct pattern of NO_3-N leaching under winter-mild, humid conditions. The same question on the impact of the selection procedure and accepted parameter values on the variability of the N leaching arises here because of an increased data dispersion or variability in bi-cropping. Further limitation regarding applied organic fertilizers might originate from unconsidered ammonia losses in the model structure resulting in increased NO_3-N leaching compared to exclusive mineral-N fertilization. In this way, effects of low-emission application of organic fertilizers on N dynamics can be simulated because higher shares of organic-N may possibly remain in upper soil layers resulting in less ammonia volatilization but potentially increased mineralization.

8.3 Outlook

Altogether, presented results regarding modeled soil water and nitrogen dynamics in the unsaturated soil at plot scale confirmed the high potential of process-based modeling. The CoupModel can be used to improve the knowledge regarding detailed C and N flows in agricultural ecosystems (Nylinder et al., 2011), even though underlying processes are also representative for more natural systems such as forest, peatland (Gärdenäs et al., 2011; Metzger et al., 2015), and mountain areas (Khoshkhoo et al., 2015; Marmy et al., 2016). Considering various sources of uncertainty can, thus, help to apply existing model structures on different sites and plant species.

The need for conclusive calibration procedures including meaningful objective functions is evident, but traditional statistic measures to evaluate the model performance are widely used. However, these measures and their possible combination usually work best in case of long-term and regular data that are more often available for hydrologic issues, *e.g*., discharge and nitrogen load in surface water (Pfannerstill et al., 2014; Haas et al., 2016) compared with soil-related observations.

More attention has to be paid to investigations of relationships between input parameters and particular modeled outcome. For this and in the context of uncertainty assessment, extensive computation resources are necessary to perform the GLUE, for instance, comprehensively.

However, this thesis has presented first steps regarding the potential of conclusive CoupModel applications. For example, the important influence of organic fertilizers has to be investigated further to show effects of N dynamics in soil, especially below permanent grassland, and potential losses into near-surface groundwater (Tsuchiya et al., 2012). Another task is the implementation of legume plants because of their high relevance in organic farming and to reduce artificial N supply in agriculture in the future. According to Taube (2012, 2013b), evident results could offer sustainable solutions also in maize-based crop rotations. Furthermore, expanded crop rotations including maize, cereals or grass species as well as undersown/catch crops could be simulated to investigate, for instance, potential growth risks for particular crops in the context of climate change. Compensative effects of undersown and/or catch crops could be determined by modeling to support divers agricultural crop rotations in the future.

In addition, long-term simulations are necessary to validate the model results in a greater context, *e.g.*, regarding the formation of soil humus or greenhouse gas emissions (He et al., 2016). Benefits of catch crops on reduced NO_3-N leaching in the unsaturated soil have to be also simulated over longer periods to consider the influence of different moisture and nutrient conditions comprehensively.

Finally, impacts on the quality of near-surface groundwater still cannot be evaluated with the model because processes in saturated soil depths as dispersion and denitrification are not currently considered in the model structure. This could be achieved by linked model approaches.

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Supplementary material

Table A.1: List of fixed parameters different from default values.

Parameter	Description	Value	Unit	Source
a) Common abiotic responses:				
SaturationActivity, $p_{\theta Satact}$	Parameters for soil moisture response function	0.8	–	Calibrated
ThetaLowerRange, $p_{\theta Low}$		18	Vol.%	Calibrated
b) Drainage and deep percolation:				
DrainLevelLowerB, z_{p2}	Drainage depth for deep percolation	−2	m	Assumed, Karrasch 2005
DrainSpacingLowerB, d_{p2}	Distance between the drainage system for deep percolation	85	m	Assumed, Karrasch 2005
EmpGFLevBase, z_2	Base and peak levels for groundwater flow to diffuse sink	−1.4	m	Calibrated
EmpGFLevPeak, z_1		−0.3	m	Calibrated
EmpGFlowBase, q_2	Base and peak values for the maximal rates of groundwater flow to diffuse sink	2	mm d^{-1}	Default
EmpGFlowPeak, q_1		8	mm d^{-1}	Calibrated
GWSourceLayer, q_{Sol}	Layer for groundwater source flow	12	#	Assumed
c) Soil hydraulic:				
Sensitivity, h_{sens}	Matric conductivity function	0.85	mm d^{-1}	Calibrated
d) Snow pack:				
MeltCoefAirTemp, m_T	Empirical snow melt function	4.0	Kg °C^{-1} m^{-2} day^{-1}	Calibrated
e) Surface water:				
SoilCover, i_{scov}	Soil infiltration reduction	0.01	–	Assumed
f) Plant:				
TempSumCrit, t_{crit}	Threshold values for air temperature sum calculation	8	°C	Assumed
TempSumStart, t_{start}		40	°C days	Assumed
g) Interception:				
WithinCanopyRes, r_{sint}	Surface resistance for potential evaporation function	1.0	s m^{-1}	Calibrated
h) Plant water uptake:				
CritThresholdDry, Ψ_c	Critical pressure head for reduction of potential water uptake	800	cm water	Calibrated
i) External N input:				
Dep N WetConc, p_{cwet}	N concentration in precipitation deposition	1.5	mg L^{-1}	Lehmhaus et al. 1998
Dep NH4 FracWet, $p_{fNH4,Wet}$	NH4N fraction in wet deposition	0.7	–	ditto
Dep NH4 FracDry, , $p_{fNH4,Dry}$	NH4N fraction in dry deposition	0.7	–	ditto
j) Decomposition process:				
Init H Depth, $i_{h,d}$	Initial depth for humus distribution	−0.3	m	Karrasch 2005
Init H N Tot, $i_{h,N}$	Initial N amount in humus pool	1000	g m^{-2}	Karrasch 2005
Init L1 CN Tot, $i_{l1, CN}$	Initial C:N ratio of litter pool 1	64	–	Karrasch 2005
Init L1 Depth, $i_{l1,d}$	Initial depth for litter pool 1 distribution	−0.3	m	Karrasch 2005
Init L1 N Tot, $i_{l1,N}$	Initial N amount in litter pool 1	1.0	g m^{-2}	Karrasch 2005
Init L2 CN Tot, $i_{l2, CN}$	Initial C:N ratio of litter pool 2	50	–	Karrasch 2005
Init L2 Depth, $i_{l2,d}$	Initial depth for litter pool 2 distribution	−0.3	m	Karrasch 2005
Init L2 N Tot, $i_{l2,N}$	Initial N amount in litter pool 2	0.3	g m^{-2}	Karrasch 2005
i) Nitrification process:				
NUptMaxAvailFrac, f_{Nupt}	Fraction of mineral-N for plant uptake	0.1	d^{-1}	Calibrated
NitrificSpecificRate, n_{rate}	Specific nitrification rate	0.26	d^{-1}	Calibrated
k) Soil management:				
Ploughing Day, $m_{p,day}$	Plowing day	110/113	#	Assumed
Ploughing Depth, $m_{p,depth}$	Plowing depth	−0.27	m	Karrasch 2005
SurfaceCultDay, $m_{s,day}$	Surface cultivation day	100	#	Assumed

Table A.2: List of fixed plant-related parameters different from default values.

Parameter	Description	Maize	Grass	Unit	Source
a) Albedo vegetation:					
Start/Optimum/End Day	Parameters for the albedo calculation	121/210/280	160/200/320	#	Assumed
Start/Optimum/End Value		25/20/40	20/20/25	–	Assumed
b) Size of growing plant (dynamic growth):					
Max Height, p_{hmax}	Maximum height	3.0	0.3	m	Assumed
Root LowestDepth, p_{zroot}	Parameters for root depth calculation	−1	−0.5	m	Calibrated
Root IncDepth, $p_{incroot}$		−0.05	−0.01	m	Calibrated
c) Spatial orientation:					
XcenterPos, x_j	Canopy surface cover	0.5	0.13	m	Assumed
d) Surface canopy cover:					
Max Cover, p_{cmax}	Canopy surface cover	0.9	0.7	m^{-2} m^{-2}	Assumed
e) Potential transpiration:					
CondMax, g_{max}	Maximum conductance of fully open stomata	0.02	0.012	m s^{-1}	Calibrated
f) Allocation to grain parameters:					
C Leaf to Grain, $a_{C,lg}$	C from leaf to grain	0.013	0.01	–	Calibrated
C Stem to Grain, $a_{C,sg}$	C from stem to grain	0.018	0.02	–	Calibrated
C Root to Grain, $a_{C,rg}$	C from root to grain	0.01	0.01	–	Calibrated
N Leaf to Grain, $a_{N,lg}$	N from leaf to grain (MM1, MU1, MM2, MU2)	0.02	0.01	–	Calibrated
	(MM3, MU3, MM4, MU4)	0.013	0.01	–	Calibrated
N Stem to Grain, $a_{N,sg}$	N from stem to grain (MM1, MU1, MM2, MU2)	0.025	0.02	–	Calibrated
	(MM3, MU3, MM4, MU4)	0.018	0.02	–	Calibrated
N Root to Grain, $a_{N,rg}$	N from root to grain (MM1, MU1, MM2, MU2)	0.022	0.01	–	Calibrated
	(MM3, MU3, MM4, MU4)	0.01	0.01	–	Calibrated
g) Growth Stage:					
Sow Tth	Threshold temperatures for sowing date, emergence time, and grain maturing	6	4	°C	Assumed
Emerge Tth		8	6	°C	Assumed
Mature Tth		10	10	°C	Assumed
Mature Tsum	Temperature sum for grain maturing	800	450	°C days	Assumed
Grain Step, g_{step}	Step length for grain filling	0.06	0.02	–	Assumed
h) Litter fall:					
Leaf Tsum1, t_{L1}	Threshold temperature sums for the lower (index 1) and higher (index 2) litter formation rate of leaf, stem, grain, and root pool	1500	1600	°C days	Assumed
Leaf Tsum2, t_{L2}		1600	1700	°C days	Assumed
Stem Tsum1, t_{S1}		1500	1600	°C days	Assumed
Stem Tsum2, t_{S2}		1600	1700	°C days	Assumed
Grain Tsum1, t_{G1}		1500	1600	°C days	Assumed
Grain Tsum2, t_{G2}		1600	1700	°C days	Assumed
Root Tsum1, t_{R1}		1500	1600	°C days	Assumed
Root Tsum2, t_{R2}		1600	1700	°C days	Assumed
i) C:N ratios:					
CN Ratio Max Litter,	Maximum C:N ratio in the leaf litter pool	150	100	–	Calibrated
CN Ratio Min Stem, $cn_{MinStem}$	Minimum C:N ratios for stem, leaf and coarse root pool	25	20	–	Calibrated
CN Ratio Min Leaf, $cn_{MinLeaf}$		25	20	–	Calibrated
CN Ratio Min Coarse Root, $cn_{MinCRoot}$		25	20	–	Calibrated

Table A.3: Results of significance tests on seasonal NO_3-N leaching for each periods and corresponding precipitation.

Treatment	MM1	MU1	MM2	MU2	MM3	MU3	MM4	MU4	Mean MM	Mean MU	Prec (mm period^{-1})
Total NO_3-N leaching:											
SWP 1996/97	a# B	b# C	a# B	b# CD	a# A	b# D	b# E	a# CD	a#	b#	371
VP 1997	a A	b B	a# A	b# BC	a# D	a# C	b# E	a# BC	a#	b#	533
SWP 1997/98	a# A	b# B	a# A	b# B	a# C	b# C	b D	a C	a#	b#	457
VP 1998	a# A	b# B	a# A	b# B	a# C	a# C	a D	a D	a	b	712
SWP 1998/99	a A	b B	a# A	b# B	a C	b D	a E	b F	a	b	414
VP 1999	a AB	b B	a# A	b# B	a C	b D	a# E	b# F	a#	b#	277
SWP 1999/00	a# A	b# AB	a B	a B	a C	a C	b# E	a# D	a	a	534
VP 2000	a AB	a A	b C	a BC	a D	a D	b F	a E	a	a	335
SWP 2000/01	b BC	a A	b# C	a# B	b# D	a# AB	b E	a D	b#	a#	280
VP 2001	b A	a A	b# A	a# A	b B	a A	b D	a C	b#	a#	572
SWP 2001/02	b A	a A	a A	a A	b# B	a# B	b D	a C	a#	a#	404

(Letters a and b are indicators of significant differences between monoculture and corresponding bi-cropping treatment based on ANOVA (comparing mean values, $\alpha = 5\%$) or non-parametrical test (Wilcoxon-Rank sum test; two-sided, $\alpha = 2.5\%$; # marked cases where median values were compared because homogeneity of variances was not given (therefore ANOVA was not allowed)), and capitals show subgroups without significant differences between arithmetic mean values (ANOVA + Tukey test, $\alpha = 5\%$) with increasing mean: $A < B < C < D < E < F$.)

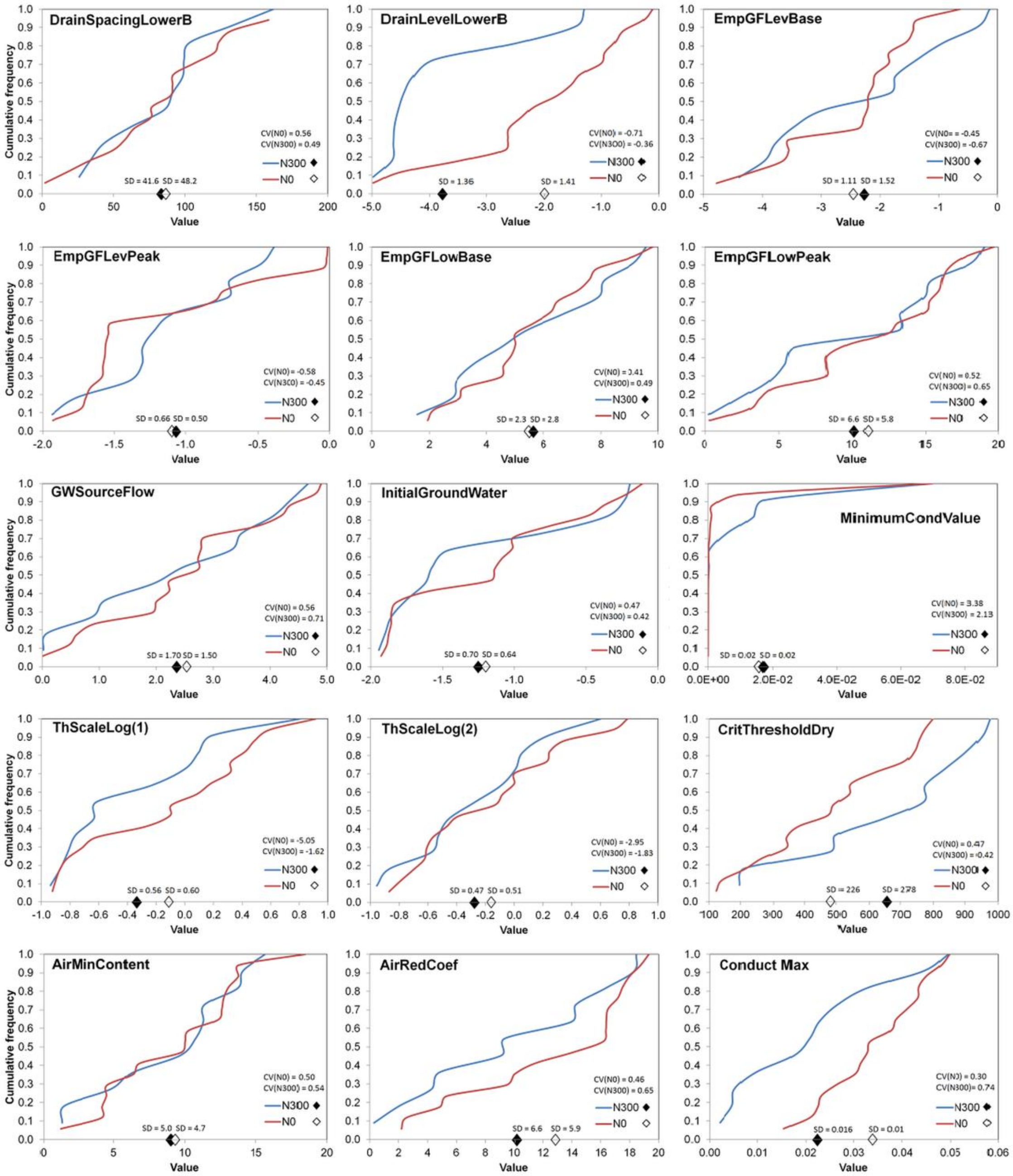

Fig. A.1: Cumulative parameter distribution of selected uncertain input parameters of all accepted simulations for non-fertilized (N0; $n_{accepted}$ = 17) and highly fertilized (N300; $n_{accepted}$ = 11) grassland at the Karkendamm site including means and standard deviation (SD) as well as the coefficient of variation (CV).

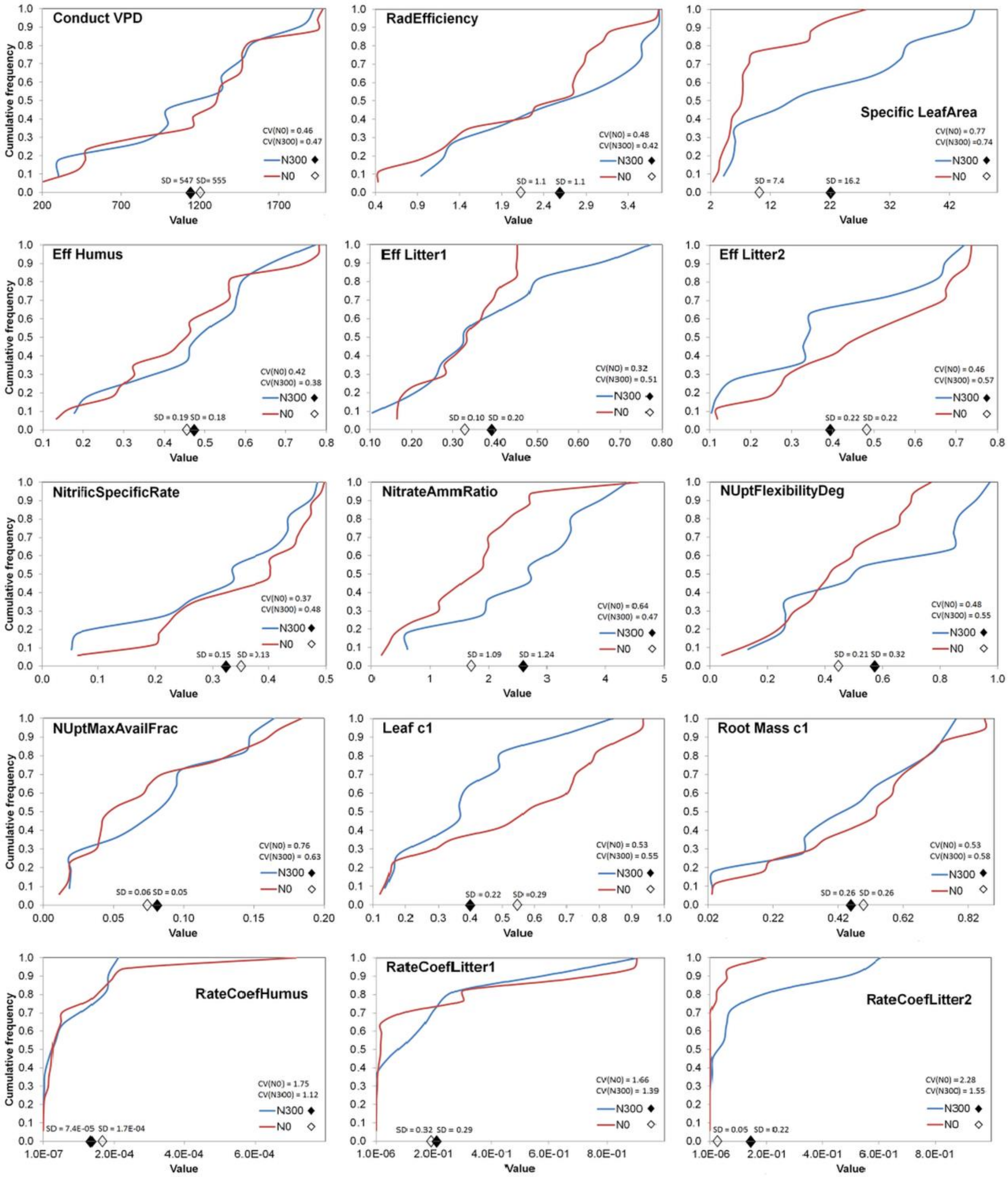

Fig. A.2: Cumulative parameter distribution of selected uncertain input parameters of all accepted simulations for non-fertilized (N0; $n_{accepted}$ = 17) and highly fertilized (N300; $n_{accepted}$ = 11) grassland at the Karkendamm site including means and standard deviation (SD) as well as the coefficient of variation (CV).

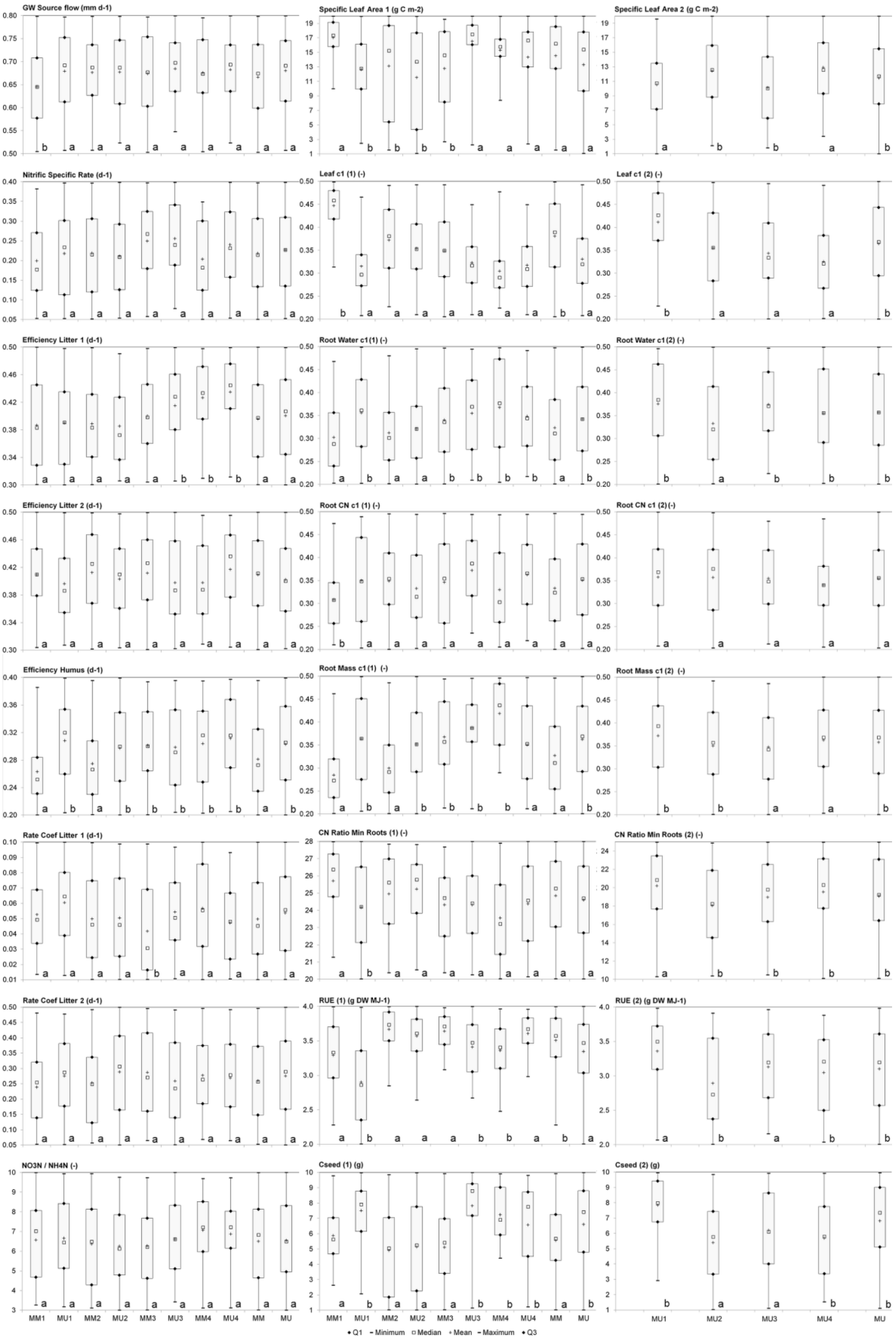

Fig. A.3: Box-whisker plots of selected input parameters of all accepted simulations for different silage maize cultivations including results of significant differences between monoculture and corresponding bi-cropping system for non-plant-specific (left column) and maize-related parameters (index 1; middle) and between maize and grass (index 2; right column) in bi-cropping trials (i.e., compare corresp. MU in middle and right column) as well as between means of monoculture (MM) and bi-cropping (MU) systems (Wilcoxon-Rank sum test, α = 2.5%).

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Eidesstattliche Erklärung

Ich erkläre hiermit, dass ich die vorliegende Arbeit „*Model-based quantification of nitrate-nitrogen leaching considering sources of uncertainty*“ selbständig und nur unter Zuhilfenahme der angegebenen Quellen und Hilfsmittel verfasst habe.

Diese Arbeit war weder in gleicher noch in ähnlicher Fassung ein Bestandteil eines Prüfungsverfahrens. Die Artikel aus den Kapiteln 2, 3, 4, 5 und 6 wurden in den dort angebenenen Fachzeitschriften veröffentlicht bzw. befinden sich noch in der Begutachtung.

Diese Arbeit ist unter Einhaltung der Regeln zur Sicherung guter wissenschaftlicher Praxis der Deutschen Forschungsgemeinschaft erstellt worden.

Kiel, 02.03.2017