Modelling of nitrogen cycles in intensive winter wheat–summer maize double cropping systems in the North China Plain

- Site specific optimisation of nitrogen fertilisation with regard to nitrogen losses, water protection, productivity and regionalisation -

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Summary

The North China Plain (NCP) is one of the most productive and intensive agricultural regions in China. High doses of mineral nitrogen (N) fertiliser, often combined with flood irrigation, are applied, resulting in N surplus, groundwater depletion and environmental pollution. Among methods such as technical field methods like for example reducing N fertiliser rate, applying chemical stabilised fertiliser, using drip or sprinkler irrigation and educational approaches, simulation models can help to assess the N cycle and water use to reduce losses in soil-plant systems. In the NCP models were used to find optimal N fertiliser and irrigation rates especially in the often cultivated winter wheat (*Triticum aestivum* L.)–summer maize (*Zea mays* L.) double crop rotation. For simulations in this thesis the process-based agro-ecosystem model HERMES was used.

The objectives of this thesis were to use the HERMES model to simulate the N cycle and show the performance of the HERMES model, of the new ammonia volatilisation sub-module and of the new nitrification inhibition tool in the NCP. Further objectives were to assess the models potential to save N and water on plot and county scale, as well as on short and long-term. Additionally, improved management strategies with the help of a model-based nitrogen fertiliser recommendation (NFR) and adapted irrigation, should be found.

To achieve this a field experiment with six reduced N-treatments during five seasons of winter wheat–summer maize (2.5 year) were used as basis for model calibration and validation. On two treatments a real-time model-based NFR was performed on plot scale in Quzhou County, NCP as the main location among others. Four approaches to simulate ammonia volatilisation and a tool for nitrification inhibition were implemented into the HERMES model. In long-term (31 years) simulations, regional N losses and the fate of water at county scale in a winter wheat–summer maize double-crop rotation were assessed and model-based best management options were elaborated for two out of six N fertiliser and irrigation management scenarios.

Results showed that the HERMES model performed well under growing conditions of the NCP and was able to describe the relevant processes related to soil–plant interactions concerning N and water. No differences in grain yield between the real-time model-based NFR and the other treatments of the experiments on plot scale in Quzhou County could be found. Simulations with increasing amounts of irrigation resulted in significantly higher N leaching, higher N requirements of the NFR and reduced yields, while the impact of

weather variation on model-based NFR was smaller. In the best-practice scenario simulation on plot-scale, N input could be reduced to 17.1 % of conventional farmers' practice, irrigation water to 72.3 % and N leaching below 0.9 m to 1.8 % and below 2.0 m soil depth to 0.9 % within 2 years.

Also the calibrated and validated ammonia volatilisation sub-module of the HERMES model worked well under the climatic and soil conditions of northern China. Although, for some fertilisation events ammonia volatilisation was overestimated under warmer weather conditions. Simple ammonia volatilisation approaches gave satisfying results with a mean absolute error (*MAE*) across all sites and treatments of 1.8 and 1.4 in % of applied N, respectively, compared to process-oriented approaches, with a *MAE* of 2.2 and 1.9 in % of applied N, respectively.

The test of the nitrification inhibition tool of the HERMES model showed satisfying simulation results. Ammonia volatilisation was higher in the Ammonium sulphate Nitrate with nitrification inhibitor (ASN_{DMPP}) fertiliser simulation (2.39% of applied NH_4) than in the NH_4 fertiliser simulation without nitrification inhibitor (0.52% of applied NH_4), while nitrate leaching in the ASN_{DMPP} fertiliser (248 kg N ha^{-1}) was lower than in the NH_4 fertiliser simulation without nitrification inhibitor (280 kg N ha^{-1}). Differences in denitrification amount could not be found.

Results of the simulated annual long-term N losses in whole Quzhou County in Hebei Province were 296.8 kg N ha^{-1} under common farmers practice treatment and 101.7 kg N ha^{-1} under optimised treatment including NFR and automated irrigation (OPTai) which were 57 % and 40 % of the applied fertiliser N, respectively. Spatial differences in simulated N losses throughout Quzhou County, could only be found due to different N inputs among the 10 townships, which were based on survey results. Simulations of an optimised treatment, applied to wheat–maize double-crop rotations in Quzhou County, could save on average more than 260 kg N $ha^{-1}a^{-1}$ from fertiliser input and 190 kg N $ha^{-1}a^{-1}$ from N losses and around 115.7 mm a^{-1} of water, compared to farmers practice. Additionally, the OPTai worked best on clay loam soil except for a high simulated denitrification loss, while the simulations using farmers practice irrigation could not match the actual water needs resulting in yield decline, especially for winter wheat. However, the optimised treatments did not seem to be able to maintain the soil organic matter pools, even with full crop residue input.

HERMES is a relatively simple model, with regard to data input requirements, to simulate the N cycle. On plot scale the model-based NFR in combination with adapted irrigation had the highest potential to reduce nitrate leaching, compared to farmers practice and mineral N (N_{min})-reduced treatments. During short-term plot-scale best-practice simulations high N reductions were achieved, which were probably possible due to the high initial soil N contents. As the amount of irrigation has a significant impact on leaching and yield, conventional flood irrigation as currently practiced by the farmers bears great uncertainties and exact irrigation amounts should be known for future simulation studies.

Simple ammonia volatilisation approaches also reached good results, while process-oriented approaches better displayed environmental influences. However, simulated changes in topsoil pH need further verification with measurements.

Although the nitrification inhibition tool worked well, simulations need further verification with measurements. Nitrification-born nitrous oxide emissions should be considered in the model in the future.

Long-term simulation results showed compared to the above mentioned short-term simulations, lower N and water saving potential compared to farmers practice. This underlines the necessity of long-term simulations to overcome the effect of high initial N stocks in soil. Management of N and water on clay loam needs a precise adaption to actual weather conditions and plant growth needs. Additionally, extra organic inputs seem to be required to maintain soil quality in the optimised treatments. Other nutrients such as phosphate, nitrification-born nitrous oxide emissions and cation exchange capacity, among others, could be included into HERMES to improve its performance under the conditions of the NCP.

The HERMES model can offer interpretation of management options on plot, on county and regional scale for extension and research staff. Also in combination with other N and water saving methods the model promises to be a useful tool.

Zusammenfassung

(Titel: Modellierung von Stickstoffkreisläufen in intensiven Winter Weizen–Sommer Mais Doppelfruchtfolgen in der Nordchinesischen Tiefebene - Standortspezifische Optimierung der Stickstoffdüngung im Hinblick auf Stickstoffverluste, Gewässerschutz, Produktivität und Regionalisierung -)

Die Nordchinesische Tiefebene (NCP) ist eine der produktivsten und intensivsten Agrarregionen Chinas. Große Düngermengen an mineralischen Stickstoff (N) und der oft in Kombination genutzten Überflutungsbewässerung, resultieren in Stickstoffüberflüssen, Grundwasserabsenkung und Umweltverschmutzung. Zusammen mit anderen Methoden, zum Beispiel technische Feldmethoden wie die N-Düngerate zu reduzieren, chemisch stabilisierte Dünger auszubringen, Tröpfchen- oder Sprinklerbewässerung zu nutzen und Ausbildungsansätze, können Simulationsmodelle helfen den N-Kreislauf und die Wassernutzung zu erfassen, um Verluste im System Boden-Pflanze zu reduzieren. In der NCP wurden Modelle benutzt, um optimale N- und Bewässerungsraten zu finden, besonders in der oft angebauten Winter Weizen (*Triticum aestivum* L.)–Sommer Mais (*Zea mays* L.) Doppelfruchtfolge. Für die Simulationen in dieser Arbeit wurde das prozessbasierte Agrarökosystem-Model HERMES genutzt.

Ziel dieser Arbeit war die Simulation des N-Kreislaufes mit HERMES, sowie dessen Modellgüte, die Modellgüte des neuen Ammoniak-Verflüchtigungsmodules und des neuen Ansatzes zur Simulation von Nitrifikationsinhibitoren in der NCP aufzuzeigen. Weitere Ziele waren das Potential des Modells aufzuzeigen, um N und Wasser, mit Hilfe einer modellbasierten N-Düngeempfehlung (NFR) und angepassten Bewässerungsstrategien einzusparen. Dies erfolgte auf Schlag- und Countyebene wie auch in Kurzzeit- und in Langzeitsimulationen, um verbesserte Management-Strategien zu finden.

Hierzu wurde ein Feldexperiment mit sechs reduzierten N-Behandlungen über fünf Winter Weizen–Sommer Mais Doppelfruchtfolgen (2.5 Jahre) als Grundlage zur Modellkalibrierung und Validierung genutzt. Für zwei Behandlungen wurde auf Schlagebene in Quzhou County, NCP als eines der Hauptversuchsgebiete, unter anderen, eine modellbasierte Echtzeit-NFR durchgeführt. Vier Ansätze zur Simulation von Ammoniak-Verflüchtigung und ein Simulationsansatz für Nitrifikationshemmung wurden ins HERMES Modell implementiert. Während einer Langzeitsimulation (31 Jahre),

wurden regionale N-Verluste und der Verbleib von Wasser auf Countyebene in Winterweizen–Sommermais Doppelfruchtfolgen erfasst und modellbasierte optimierte Bewirtschaftungsoptionen wurden für zwei von sechs N-Düngungs- und Bewässerungsmanagement-Szenarios berechnet.

Die Ergebnisse zeigten, dass das HERMES Modell gut unter den Wachstumsbedingungen der NCP funktioniert und alle relevanten Boden-Pflanze-Interaktionen in Bezug auf N und Wasser beschreiben konnte. Es konnten keine Ertragsunterschiede zwischen Echtzeit modellbasierter NFR und anderen Behandlungen auf Schlagebene in Quzhou County festgestellt werden. Simulationen mit steigenden Bewässerungsgaben ergaben signifikant höheren N-Austrag, höheren N-Bedarf der NFR und reduzierte Erträge, während der Einfluss der Wettervariation auf die modellbasierte NFR kleiner war. In der optimierten („best-practice“) Szenariosimulation auf Schlagebene konnte die N-Düngung auf 17.1 % der konventionellen Düngung, die Bewässerung auf 72.3 % und der N-Austrag in 0.9 m Tiefe auf 1.8 % und in 2.0 m auf 0.9 % innerhalb von 2 Jahren gesenkt werden.

Auch das kalibrierte und validierte Ammoniak-Verflüchtigungs-Modul des HERMES Modells funktionierte gut unter den Klima- und Bodenverhältnissen in Nordchina. Trotzdem wurde die Ammoniak-Verflüchtigung für ein paar Düngeereignisse mit wärmeren Wetter überschätzt. Einfache Ammoniak-Verflüchtigungs-Ansätze gaben zufriedenstellende Ergebnisse mit einem mittleren absoluten Fehler (*MAE*) für alle Versuche und Behandlungen von jeweils 1.8 und 1.4 % der gedüngten N-Menge. Im Gegensatz dazu hatten die prozessorientierten Ansätze einen *MAE* für alle Versuche und Behandlungen von jeweils 2.2 und 1.9 % der gedüngten N-Menge.

Der Test des Nitrifikationshemmungsansatzes zeigte befriedigende Ergebnisse. In der Simulation mit der Ammonsulfatsalpeter mit Nitrifikationsinhibitor (ASN_{DMPP}) Düngung war die Ammoniak-Verflüchtigung höher (2.39% des gedüngtem NH_4^+), als in der Simulation ohne Nitrifikationshemmer (0.52% des gedüngtem NH_4^+), während das Ergebnis für Nitratauswaschung umgekehrt war (ASN_{DMPP} 248 kg N ha^{-1}; ohne Nitrifikationshemmer 280 kg N ha^{-1}). Denitrifikationsunterschiede konnten nicht gefunden werden.

Jährliche simulierte Langzeit N-Verluste im ganzen Quzhou County in Hebei Province waren 296.8 kg N ha^{-1} unter konventioneller Düngung und 101.7 kg N ha^{-1} unter optimierter Düngung inklusive NFR and automatischer Bewässerung (OPTai). Dies waren jeweils 57 % und 40 % der gedüngten N-Menge. Räumliche Unterschiede von simulierten N-Verlusten in Quzhou County konnten nur aufgrund von unterschiedlichen N-

Düngemengen gefunden werden. Diese Unterschiede in den 10 Gemeinden innerhalb des Counties basierten auf einer Umfrage. Simulationen einer optimierten Behandlung, angewandt auf einer Weizen-Mais-Doppelfruchtfolge in Quzhou County, könnten im Durchschnitt mehr als 260 kg N $ha^{-1}a^{-1}$ an N-Düngung und 190 kg N $ha^{-1}a^{-1}$ an N-Verlusten und ungefähr 115.7 mm a^{-1} an Wasser, im Vergleich zur konventionellen Behandlung, einsparen. Dazu kommt, dass auf tonigem Lehm Simulationen mit konventioneller Bewässerung nicht den aktuellen Wasserbedarf decken konnten, welches zu Ertragseinbußen insbesondere für Winterweizen führte, während die OPTai Behandlung, bis auf hohe simulierte Denitrifikationsverluste, am besten funktionierte. Trotzdem schienen die optimierten Behandlungen, trotz voller Strohrückgabe, die organische Bodensubstanz nicht zu erhalten.

HERMES ist ein relativ einfaches Modell, im Hinblick auf die Anforderungen an die Eingangsdaten, um den Stickstoffkreislauf zu simulieren. Auf Schlagebene hatte die modellbasierte NFR in Kombination mit angepasster Bewässerung, im Gegensatz zu konventioneller und mineralischen N (N_{min})-reduzierter Behandlung, das höchste Potential Nitratauswaschung zu reduzieren. Während der Kurzzeitsimulationen unter optimierter Behandlung und auf Schlagebene konnte eine hohe N-Reduzierung erreicht werden, welche vermutlich aufgrund der hohen Anfangs-N-Gehalte im Boden möglich war. Da die Höhe der Bewässerung einen signifikanten Einfluss auf N-Auswaschung und Ertrag hat, birgt die konventionelle Überflutungsbewässerung wie sie derzeitig von den Landwirten praktiziert wird große Unsicherheiten und genaue Bewässerungsmengen sollten für zukünftige Simulationsstudien bekannt sein.

Einfachere Ammoniak-Verflüchtigungsansätze erreichten auch gute Ergebnisse, während prozessorientierte Ansätze Umwelteinflüsse besser darstellen konnten. Des Weiteren sollten die simulierten Veränderungen des pH-Wertes im Oberboden mit weiteren Messungen verifiziert werden.

Obwohl der Nitrifikationsansatz gut funktionierte, sollten die Simulationen mit weiteren Messungen verifiziert werden. Von der Nitrifikation stammende Lachgas Emissionen sollten in Zukunft im Modell berücksichtigt werden.

Die Langzeitsimulationsergebnisse zeigten im Vergleich zu den oben erwähnten Kurzzeitsimulationen niedrigeres N- und Wasserreduktionspotential im Vergleich zur konventionellen Behandlung. Dies unterstreicht die Notwendigkeit von Langzeitsimulationen um den Effekt von hohen Anfangs N_{min}-Gehalten im Boden zu berücksichtigen. Das Management von N und Wasser auf tonigem Lehm in zukünftigen

Simulationen braucht eine genaue Anpassung an aktuelle Wetterverhältnisse und Pflanzenwachstumsbedürfnisse. Außerdem scheinen zusätzliche organische Düngergaben wahrscheinlich notwendig, um die Bodenfruchtbarkeit in den optimierten Behandlungen zu erhalten. Andere Nährstoffe wie z.B. Phosphat, von der Nitrifikation stammende Lachgasemissionen und Kationenaustausch könnten ins HERMES Modell eingebaut werden, um die Güte des Modells in der NCP weiter zu verbessern.

Das HERMES Modell ermöglicht Beratern und Wissenschaftlern Managementoptionen auf Schlag-, County- und Regionalebene anzuwenden. Auch in Kombination mit anderen N- und Wasser-Einsparmethoden verspricht das Modell ein nützliches Instrument zu sein.

1 Introduction

1.1 Background and main objective

Motivation

Agriculture faces the challenge to feed a growing world population on limited land. The combination of population growth and a growth in per-capita consumption was estimated to increase global food demand by 70 % (FAO 2009) and by 100–110% (Tilman et al. 2011) from 2005 to 2050 or as recently updated by 63 % (FAO 2017). From 1961 to 2005 production of maize, wheat and rice as three of the most produced crops in the world increased already around 200 % (FAOSTAT 2019). Main reasons were e.g. for maize an increase in crop area and generally the additional application of synthetic nitrogen (N) fertiliser (Galloway et al. 2004). Nitrogen as an abundant element on earth and being important for humans and animals as a component of protein, is also one of the plant nutrients which plays a major role to achieve high yields. However, to further increase crop production for doubling food production by 2050, average annual growth rates in crop production of 2.4% (non-compounding rate) would be required, but only about half of this growth rate was currently achieved (Ray et al. 2013). Considering the increasing pressure on land due to a growing demand for food, feed, fibre and bio energy, this increase in crop production has, according to a selected climate change scenario, to be achieved from more (4.8 million km^2) but less suitable agriculturally area compared to today (Zabel et al. 2014). This requires an improvement in production efficiency, which would according to Davis et al. (2016) increase the total environmental burden of food production, otherwise it would be insufficient. Increasing food demand and with this an increase in agricultural production requires a more intensive use of N-fertilisation (Cassman et al. 2003). Anthropogenic perturbation of the global N cycle is of increasing concern and N surplus and N loss related to irrigation water use in intensively managed agricultural systems is a globally known problem (Galloway et al. 2004; Bouwman et al. 2005). Forms of N can emit to the atmosphere, accumulate in soil, pollute water systems, decrease crop productivity, contribute to hypoxia, loss of biodiversity, and habitat degradation in coastal ecosystems (Galloway et al. 2003; Gruber and Galloway 2008; Canfield et al. 2010). Additionally, nitrogen pollution has a negative impact in enhancing climate change through producing greenhouse gas emissions (Kanter 2018).

Global synthetic fertiliser and manure production increased from 78 Tg N a^{-1} in 1961 to 215 Tg N a^{-1} in 2014 (FAO 2018). While in Europe the agricultural N balance decreased from 2000 till 2015 and thereafter stagnated (EEA 2018), due to a decrease in N fertiliser consumption, N fertiliser consumption in Asia increased steadily (FAO 2018). Yan et al. (2003) stated that for crop production in East, Southeast and South Asia, more than half of global produced synthetic N fertiliser is consumed.

In many countries world wide non-point source N pollution is seen as a major source of water body eutrophication and groundwater contamination (Seitzinger 2008). For example Seitzinger et al. (2005) estimated that about 21% of the 24.8 Tg a^{-1} dissolved inorganic N at coastal zones globally resulted directly from synthetic fertiliser. These N leaching losses can be considered in different ways. Zhou and Butterbach-Bahl (2014) assessed N leaching losses via a yield-scale basis in wheat maize systems in linking N losses with yields in a given cropping system, while Wang et al. (2019) introduced with increasing N input increasing emission factors. Thus in their study an annual N input of 300 kg N ha^{-1} resulted in an annual leaching of about 30 kg N ha^{-1} and an N input of 400 kg N ha^{-1} in a leaching of about 60 kg N $ha^{-1}a^{-1}$.

Bouwmann et al. (2002) estimated in the 1990ies the global loss of ammonia-N (NH_3-N, here named NH_3) in agricultural systems to be 11.2 Tg N a^{-1} from synthetic fertiliser and 7.8 Tg N a^{-1} from animal manure, which was 14 and 23% of the applied N, respectively. A slightly higher result was found by Pan et al. (2016) who estimated a loss of 18% of applied synthetic fertiliser. Agriculture is an important source of greenhouse gasses. Beside methane, which has, regarding agriculture, its source mainly from livestock and rice production, nitrous oxide (N_2O) sources from N fertilisation (IPCC 2006; Smith et al. 2012; Hénault et al. 2012). The global N_2O emissions from agroecosystems in 1990 were estimated to be less than half of the NH_3 emissions, 6.2 Tg N a^{-1} (Mosier and Kroeze 2000) and 5.3 Tg N a^{-1} (Syakila and Kroeze 2011).

The North China Plain

The North China Plain (NCP) with Beijing in the north and the yellow river crossing the southern part is the largest agricultural region in China (about 330000 km^{-2}; figure 1.1). The soils are mainly silty textured, mean annual temperature is about 13 C° and annual precipitation around 500 mm of which more than 60% fall in summer. It's most common intensive cropping system is a winter wheat (*Triticum aestivum* L.)–summer maize (*Zea* *mays* L.) double crop rotation but also cotton mono crop got more space during the last years. Already in 1990 the NCP had partly more than 80% cropland (Li et al. 2001). Due to few precipitation in spring the increasing water requirement in winter wheat led to an increase in irrigation from 100 mm a^{-1} in the 1950s to 300 mm a^{-1} in the 1980s (Zhang and You 1996; in Wang et al. 2001). Thus excessive use of irrigation has led to over-exploitation of groundwater (Jiao 2010) and decreasing aquifer levels by 1m a^{-1} over a 40-year period in some areas (Liu et al. 2001), which was verified by Shu et al. (2012). In the part of Hebei province, which lies in the NCP, annual grain yield (wheat+maize) increased from about 15 Tg in 1978 to about 26 Tg in 2006, while chemical fertiliser production at the same time increased from about 0.7 to 3.1 Tg. Statistical grain production (wheat+maize) reached a plateau in the late 1990ies/early 2000s in the Hebei province part of the NCP, while fertiliser application only increased slightly at that time as resourcing of chemical fertilisers have been constrained (Mo et al. 2009). However, for the whole of China maize grain yield in kg ha^{-1} stagnated, while the yield of wheat in kg ha^{-1} continued to increase after stagnation in the late 1990ies/early 2000s (Grassini et al. 2013). During the past decades problems through N losses became urgent in the intensive agriculture of the NCP as many farmers, to achieve high crop yields, use high rates of fertiliser and irrigation water without taking environmental consequences into account (Ju et al. 2009).

The project framework and Quzhou County

This thesis was based on the sub-project “Model based optimisation of nitrogen and water management - Regionalisation of management schemes” (Bundesministerium für Bildung und Forschung – Projektträger Jülich: FKZ: 0330800 F) as a part of the Sino-German cooperation project “Innovative nitrogen management technologies to improve agricultural production and environmental protection in intensive Chinese agriculture”, lasting from 2008 till 2012 (TU München 2012). The Leibniz Centre for Agricultural Landscape Research aimed with its partners to find strategies to improve agricultural production in the NCP with regard to reduce N fertilisation and thus, reduce environmental pollution without decreasing yields but improve farmers incomes. One of the main locations within the project is Quzhou County (around 36°50' N, 114°70' E; figure 1.1), which is located in the South of Hebei Province in the NCP. Further description of the county can be found in chapter 5 and supplement figures A.4–A.6 and specific study sites in chapter 2 and Hartmann et al. (2014), as well as supplement figures A.4 and A.6. Two additional, external sites which are described more detailed in chapter 3 are “Dongbeiwang” experimental station of the China Agricultural University, Haidian District, Beijing (39° 55' N 116°20' E) (Mack et al. 2005) and a field experiment in Shunyi District, Beijing (40°11' N 116°33' E) (Heimann et al. 2015), which were used to adapt and to calibrate the HERMES model (Michalczyk et al. 2014; 2016)(figure 1.1).

The **main objective** of this thesis is to use the HERMES model to simulate the N cycle on field and county scale and to draw N and water losses and their saving potential for improved management strategies.

Figure 1.1: China (dark red) with the North China Plain (NCP, dark blue striped, small picture) and the NCP (dark blue dashed) with province boarders (orange), province names (red) and Quzhou County (green). Data Sources: Esri Data and Maps 2014, digitised NCP boarder manually adapted from (Bareth 2003; in Binder 2007), Quzhou County from the GADM database, collaborative work with H.-P. Dauck, final compilation H.-P. Dauck

1.2 State of the art

Nitrogen in Chinese intensive agriculture

Around 1950, millions of small scale farmers in China received land during a land reform. After that agricultural production continuously increased but was slowed down by natural disaster, a big famine, induced partly because the rural population work power was needed for steel production and infrastructure projects instead of crops, while agriculture was run under collectivism and the cultural revolution (Delvaux de Fenffe 2008; Zank 2012). Thereafter private arable plots were allowed again and agricultural intensification started in the 1980ies (Zhou 2013) in regions like the North East, the NCP and the South. To achieve high yields to feed a growing population, high amounts of N fertiliser application were emphasised, leading to N losses. Average statistical wheat and maize yields in Hebei Province reached 5834 and 5481 kg N ha^{-1} a^{-1} in 2013, respectively (MOA 2014). Nitrogen surplus in China was steadily increasing from 1961 (11.62 kg N ha^{-1} a^{-1}) to 2009 (249.64 kg N ha^{-1} a^{-1}), having a decreasing tendency at least till 2011 (202.59 kg N ha^{-1} a^{-1}) (Zhang et al. 2015a). Lassaletta et al. (2014) even calculated an N balance of 270.1 kg N ha^{-1} a^{-1} for 2009. In a survey from 1993 and 1994 including 14 cities and counties across parts of the NCP annual N application rates of more than 500 kg N ha^{-1} in many counties were found. This led to a heavy groundwater contamination in wells (14–150 m depth) and other sources with nitrate contents exceeding allowable contents of drinking water including two mineral waters (Zhang et al. 1996). In recent studies by Zhou et al.(2016) as well as by Ju and Zhang (2017) NO_3 leaching and NH_3 volatilisation was still identified as the main N loss pathways in a wheat–maize system in southern China.

Huge amounts of nitrate leached out of the root zone, accumulated in deeper soil layers under farmers practice management (Dai et al. 2016), especially when common farmers flood irrigation occurred close to heavy rainfall events (Fang et al. 2013). Estimates of N fertiliser induced leaching were as high as 0.88 ± 0.23 Tg N for 2008 in China (Gao et al. 2016). For the NCP Ju et al. (2009) estimated that 2.7 and 12.1% of applied N for wheat and maize, respectively, leached out during growing seasons and Gu et al. (2013) calculated a leaching rate of 7–10 kg N ha^{-1} a^{-1} from croplands. Liu et al. (2005) did a regional differentiation of groundwater contamination with nitrate in Huantai County, Shandong province, NCP analysing a large number of groundwater samples and found, beside an increase in N concentration within four years, that distribution of nitrate was mainly influenced by groundwater flow in horizontal direction.

Intensive agriculture was a main emitter and recipient at the same time as about 44% of inorganic N deposition in Guangdong province in southern China results from agricultural NH_3 emissions (Huang et al. 2015). For the whole of China numerous estimates of NH_3 emissions exist. Kang et al. (2016) estimated the NH_3 emissions to rise from synthetic fertiliser from 2.1 Tg in 1980 to 4.7 Tg in 1996 and then decline to 2.8 Tg in 2012 with regional emission rates of over 20 kg N ha^{-1} from all sources in Hebei Province. Fu et al. (2015) estimated 3 Tg from agricultural fertilisers only in 2011. While Zhang et al. (2018a) calculated 5.05 Tg from fertiliser in 2008 and Ouyang et al. (2018) 5.21 Tg from synthetic N fertiliser in 2013 for China, Xu et al. (2016) estimated for eastern China rates of 65 kg N $ha^{-1}a^{-1}$ also from agricultural fertiliser. Similar to Kang et al. (2016) for NH_3, Yan et al. (2003) estimated the N_2O, nitrogen monoxide and NH_3 emissions to more than 3, 1.5 and 30 kg N ha^{-1} a^{-1} in the NCP.

Similar to the estimations of NH_3 emissions in China, the N_2O emission factors for wheat-maize systems differed between research groups (Ha 2015). Ju et al. (2011) described for different N rates emission factors from 0.08 to 0.46, while Hu et al. (2013) and Li et al. (2010) found emission factors from 0.19 to 0.36 and 0.96, respectively. These large differences were due to the fact that N_2O emissions highly depend on the type of management (fertiliser type and rate, irrigation, tillage, application timing) and environmental conditions (soil, precipitation, temperature).

The N recovery in the NCP from farmers practice fertilisation was only about 31% for winter wheat and 25.5% for summer maize (Ju et al. 2009). This is supported by He et al. (2018) who found that during the 1980ies till the 2000s nitrogen use efficiency (NUE) of cropland decreased in the NCP and thereafter in the 2010s increased again. This increase after the 2000s probably fits to the fact that C and N footprint for staple foods in the NCP, lay in a medium field compared to other regions in China (Xia et al. 2016). Perhaps a further increase in NUE is possible as Xiao et al. (2019) during a 4-year experiment in Shouguang Province increased NUE by 79.3% and irrigation water use efficiency by 61.7% by reducing N and irrigation water without reducing winter wheat–summer maize yields.

Methods and strategies to improve N management and reduce N and water losses

Approaches to reduce N losses and increase nitrogen use efficiency were advanced on different levels, ranging from suggesting political instruments (Ju et al. 2004) and enhancing the N recycling rate (Bai et al. 2016; Roelcke et al. 2016; Yu et al. 2019) to experiments on plot scale (Yin et al. 2019). Engaging small-holder farmers to adopt recommendations, an educational approach was introduced by Cui et al. (2018). Components of this were to establish a decision support program which includes model simulations (Chen et al. 2011) and an educational approach where agricultural scientists live in villages among farmers to enhance and develop participation and technology transfer using the decision support program (Zhang et al. 2016). Xu et al. (2014) developed based on a large number of academic field research results fertiliser recommendations for hybrid maize and Chuan et al. (2013) for wheat, which is based on yield response and agronomic efficiency. This is a fertiliser recommendation method where partly a model is used. Ju et al. (2016) suggested to increase farm size in small-scale farm dominated areas in order to decrease high labour costs, increase machinery level as well as the effect of fertiliser pricing.

The field experiments of Hartmann et al. (2015) proved that, based on crop demand and soil mineral N (N_{min}) status, reduced N application rates, as well as sub-surface banded N application and chemical stabilisation of urea and ammonium (NH_4)-based fertilisers can increase N recovery and agronomic N efficiency, while maintaining crop yield. For NH_4 based fertilisers, nitrification inhibitors can reduce N_2O emissions, denitrification and N leaching losses (Ju et al. 2011; Soares et al. 2012). Zhou et al. (2016) supposed application and incorporation of manure to decrease total environmental N loss and enhance N retention in soil.

To prevent leaching Ju et al. (2007) mentioned deeper rooting crops as an option to catch residual N from previous intensive cropping. The use of different fertilisers (Yang et al. 2011) such as biogas slurry (Du et al. 2019) and controlled release fertiliser (Shi et al. 2018) are further alternatives.

Han et al. (2014) suggested to separate N fertiliser and water with alternating furrow irrigation to reduce NH_3 emissions in maize. Also applying manure (Zhang et al. 2018b), reducing inorganic N-rates, deep placement and split applications of fertiliser N, as well as using slow release fertiliser and urease inhibitors can reduce NH_3 emissions (Huang et al. 2016; Li et al. 2017). Globally seen a 100% conversion to organic agriculture, where no inorganic fertiliser should be used, could reduce N-surplus and pesticide use but needs more land than conventional agriculture (Muller et al. 2017). Anyhow, Zhang et al. (2018b) also found that manure application increased N_2O emissions.

Proper irrigation is also important for saving N, as it has effects on N movement in soil, N movement from soil to atmosphere and, as about one third of reclaimed water is used for agriculture in China (Wang et al. 2017), is a N source. Generally it is necessary to save irrigation water as agricultural water use in winter wheat–summer maize double crop rotation led to depletion of groundwater resources. Thus Meng et al. (2017) introduced a maize-maize double cropping system, different cultivars, planting dates and densities to reduce water use.

Wei et al. (2005) suggested a rise in water price combined with training and extension service to improve agricultural system sustainability, although the effect on N use efficiency and N leaching is low. Using techniques such as drip or sprinkler irrigation instead of commonly used flood irrigation could reduce water use (Li 2006; Zhang et al. 2006), increase N accumulation in soil (Lu et al. 2019), as well as productivity (Zhang et al. 2019). However, drip irrigation is applied more frequently and in smaller amounts which could influence soil water content and soil temperature, which has an effect on soil respiration and therefore may increase CO_2 emissions (Guo et al. 2017). Kendy et al. (2004) proposed to reduce irrigation water use by reducing the actual evapotranspiration (ETA) from agricultural crops through reducing crop area. This was specified in the studies of Sun et al. (2011) and Yang et al. (2015) who suggested a shift from double to single crop per year, which may achieve a positive groundwater balance in future. Zhang et al. (2003) suggested that three times irrigation instead of four (wheat) and straw mulching (wheat–maize) could reduce irrigation water use, while Hu et al. (2005), also with regard to depleting groundwater levels, proposed to schedule irrigation so that one irrigation event takes place at jointing stage and a second only if necessary at heading stage. Similar to their study Fang et al. (2010) suggested for winter wheat to postpone over 50% of irrigation from planting to later sensitive growth stages. But this assumes that irrigation is available exactly when needed, which is often not the case.

Modelling approaches for N and water saving in China

Measurements of N pools in plant-soil systems are often cost and time consuming and thus spatially and temporally limited. Especially when results need to be extrapolated to regional scale and over long term the heterogeneity of N activity in the soil can be a big challenge (Deng et al. 2011). To face these problems one dimensional process-based agro-ecosystem simulation models have been developed for the past four decades and can help to evaluate the impact of N management practices to prevent and reduce N losses. These models describe main dynamic processes of N, water and plant growth.

At national scale N leaching in one baseline and three N management scenarios was simulated for China with the DNDC model by Qiu et al. (2011) to find policy options for balancing N. In the NCP the WNMM model (Li et al. 2007) was used to simulate crop yield, N leaching and NH_3 volatilisation at county scale. It requires detailed data input. For a two year study in North China Li et al. (2014) calibrated the DNDC model to simulate and quantify N leaching. For soil organic carbon (C_{org}) only, the same model was used in Quzhou County, NCP to find farm management options to increase carbon sequestration (Liu et al. 2006). Although the DNDC model was extended with water leaching fluxes from tile drainage lines, the soil profile depth was limited to 50 cm (Li et al. 2006).

The RZWQM(2) was used to investigate interactions between N and irrigation management regarding N leaching on plot scale at different sites in the NCP (Fang et al. 2008; Sun et al. 2018). To quantify crop yield and N management on long term Fang et al. (2013) used the same model on 15 locations in the NCP. Using the SPACSYS model Zhang et al (2018c) suggested that no-till in combination with N fertiliser application and straw return has a positive effect on C and N stocks and reducing CO_2 and N_2O emissions. Umair et al. (2017) used the CropSyst model to identify soil evaporation losses in a wheat-maize system at Luancheng station, NCP and Wang et al. (2009) used the APSIM model and Zhou et al.(2018) the CERES-Wheat model to investigate the effect of irrigation on crop growth in the NCP. Several research groups used the DNDC model on plot scale. Li et al. (2010) identified best management practices concerning greenhouse gas emissions at one site in Quzhou County, while Zhang et al. (2015b) used the model to find agronomic and environmental critical N rates for maize at another site. Zhang et al. (2018d) suggested during long-term simulations at Liucun, Xushui, Hebei Province that intercropping of soybean and maize had a higher agronomic efficiency than crop monoculture. Using long-term simulations as well Zhang et al. (2017) investigated the effect of N fertiliser and straw application rate on crop yield and C_{org} contents in soil at Hengshui City, Hebei Province. Some of the above mentioned models were already used as integrated components within decision support systems. For example Hybrid-Maize simulation model was integrated in a soil–crop system management approach (Chen et al. 2011) and the QUEFTS model operates within the nutrient expert environment (Chuan et al. 2013; Xu et al. 2014).

However, none of the above mentioned studies included a real-time model-based numerical nitrogen fertiliser recommendation (NFR). It has so far never been applied in the NCP; neither have NFR supported best management practices been derived from scenario simulations in China. Model-based NFR can give a recommendation for a specific real-time situation and location and can save time compared to the N_{min} method and scenario simulations. Furthermore, an NH_3 volatilisation simulation approach which fits to the needed requirements (see table 1.1 and chapter 3) could not be found. The same was true for a nitrification inhibition approach, which was probably not yet used in model simulations in the NCP. Some of the mentioned models require complex input data. In addition, nobody has addressed all main N and water inputs and losses together with detailed crop modelling on a specific defined soil and varying spatial management within Quzhou County, Hebei Province, nor used model-based soil type specific N fertiliser recommendation on county scale using average county management to find out best practice options, with long-term simulations in a winter wheat–summer maize double-cropping system.

Thus, the nitrogen advisory model HERMES (Kersebaum 2011) was used to perform such an integrative approach. It is able to simulate N dynamics under limited input parameter conditions to account for robust practical agricultural applications

1.3 Overview of the HERMES model

The HERMES model

The process-based agro-ecosystem model HERMES (Kersebaum and Nendel 2014) was used for all simulations in this thesis. It simulates N and water dynamics as well as crop growth and consists originally of five main processes (Kersebaum 1995) or sub-modules which are N transport, N mineralisation, denitrification, water transport and plant growth with N uptake. These processes are briefly described in chapter 2.2 or more in detail by Kersebaum and Beblik (2001) and (Kersebaum 2011). In chapter 3 (Michalczyk et al. 2016) an additional NH_3 volatilisation sub-module was incorporated that includes urea hydrolysis and nitrification (figure 1.2) to adapt the model to Chinese conditions. The one dimensional model operates at a daily time-step. It was made for practical use as it can run under limited data availability and is able to estimate N fertiliser recommendations (Kersebaum and Beblik 2001). HERMES has a generic crop module and is so far

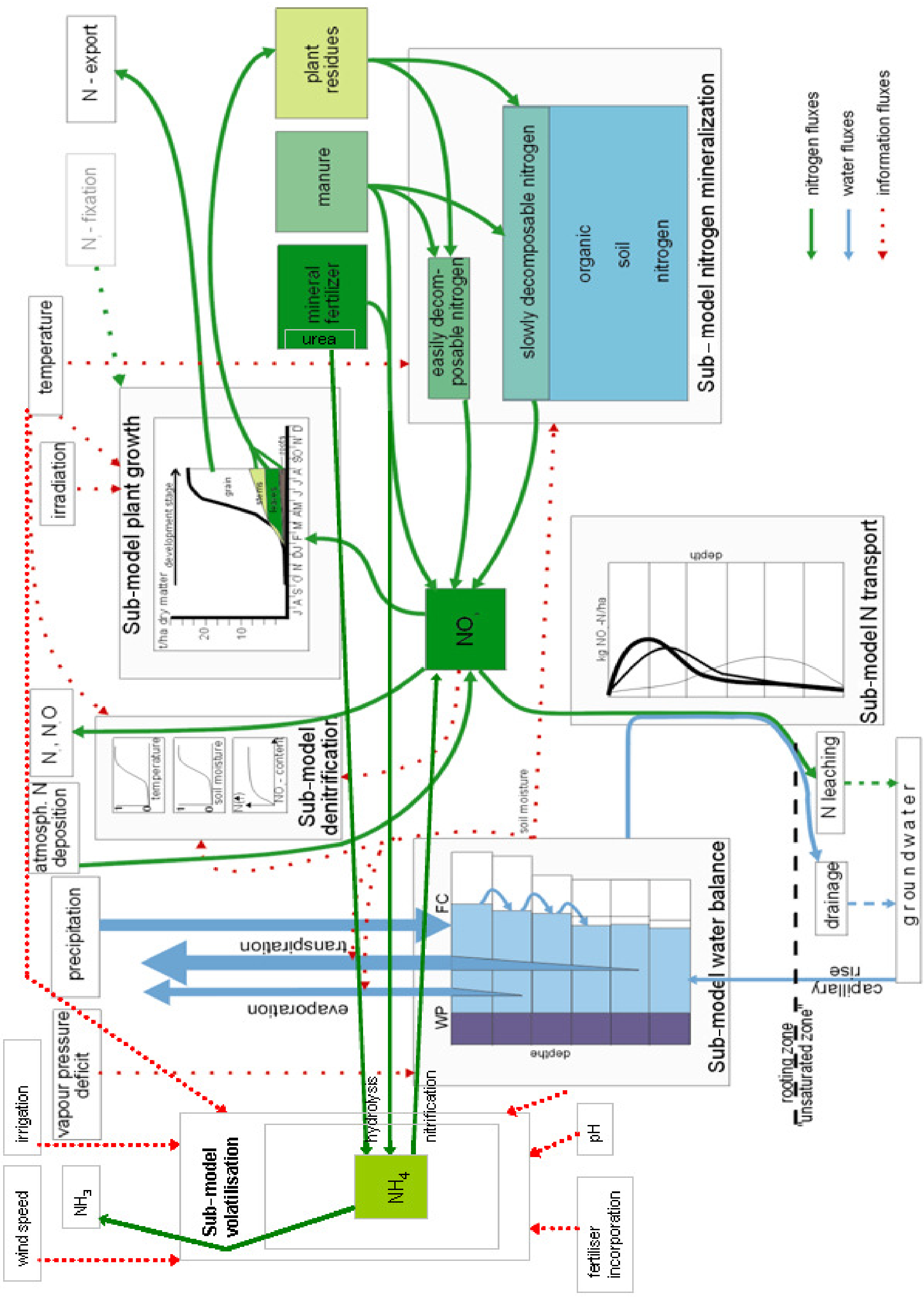

Figure 1.2: Overview of main HERMES sub-modules, adapted from Kersebaum (2009, unpublished)

parameterised to simulate grain crops like wheat and maize, root crops like sugar beet and potatoes, catch crops like phacelia and mustard as well as oil seed rape and grass/pasture. In global and European model inter-comparisons HERMES was performing well (Palosuo et al. 2011; Asseng et al. 2013; Bassu et al. 2014; Yin et al. 2017a). According to individual needs the model was modified and extended with applications such as a solar radiation correction factor to simulate topographic shading (Reuter et al. 2005), CO_2

response algorithms to simulate expected climate change effects (Nendel et al. 2009), a simple drain flow component to simulate subsurface drainage (Malone et al. 2017) or coupled to a geographic information system (GIS) for site-specific fertiliser recommendation (Kersebaum et al. 2005). The model showed a good sensitivity to variable site conditions (Wallor et al. 2018).

Model-based fertiliser recommendation

The HERMES model-based fertiliser recommendation was used in chapter 2 to predict actual N requirement for winter wheat. For the recommendation the model used site specific weather scenarios derived from long-term meteorological observations to predict the future N uptake of the plant minus the simulated available N content in the soil. The procedure is described in detail by Kersebaum and Beblik (2001).

Modifications of the model within this thesis

Ammonia volatilisation was firstly considered to be a percentage of applied N till an additional sub-module was incorporated to HERMES (chapter 3). Four options to calculate NH_3 emissions existed within the sub-module. Variation 1 and 2 were process-oriented approaches and variations 3 and 4 were simple empirical functions. The processes of urea hydrolysis, nitrification from NH_4-based N fertiliser and changes in soil solution pH were the same. The amount of volatised NH_3 in variation 1 depended on type of fertiliser, amount of NH_4 in fertiliser, temperature, pH, soil water content, amount of irrigation/precipitation, wind speed, plant height and solar radiation. For a detailed description of all processes for the four variations see chapter 3.

Before the decision for the above described method was made, several approaches were studied to find a solution to include NH_3 volatilisation into HERMES (table 1.1). The main prerequisites were that the model was tested for field conditions, has a daily time step, contains processes of urea hydrolysis, nitrification, pH change and has an option for inorganic N fertiliser. Additionally the model should have not too complex input data requirements, so it would fit to the HERMES model. Unfortunately none of the approaches completely matched the needed requirements, thus four approaches of combinations of existing and own approaches were used.

Table 1.1: Overview of selected, mainly process-based NH_3 volatilisation models and their pros and cons for the use as a volatilisation sub-module within HERMES

Model/Authors	Pros	Cons	Reference
DUPAV	Considers soil pH change, pH buffer capacity, soil respiration (CO_2 production), usable for urea fertiliser	Based on laboratory conditions, only diffusive processes, no convective transport included, nitrification not considered, time step is six minutes	Rachhpal-Singh and Nye (1986a)
Fleisher, Kenig, Ravina, Hagin	Considers cation exchange capacity, time step is one day	Based on laboratory conditions, nitrification and pH change not considered sufficiently	Fleisher et al. (1987)
DUPAV	Considers method of urea application	See above	Rachhpal-Singh and Nye (1988)
AMOVOL	Considers CO_2 emission, $CaCO_3$ precipitation, suitable for urea fertiliser	Nitrification not considered, time step variable but two hours or less recommended	Sadeghi et al.(1988)
Roelcke, Han, Li, Richter (based on DUPAV)	As described above, extended for $CaCO_3$ precipitation	Based on laboratory conditions, nitrification not considered	Roelcke et al. (1996), Rachhpal-Singh and Nye (1986a)
MANNER	Only simple input requirements	Simulates NH_3 volatilisation only following manure application, nitrification not considered	Chambers et al. (1999)
Ni (reviewed 30 models)	Most models consider pH change and NH_3 transfer from (manure) surface to air	Simulating NH_3 volatilisation only following manure or slurry application	Ni (1999)
Sommer and Olesen	Considers pH change and slurry application method	Simulates NH_3 volatilisation only following slurry application, time step is one hour	Sommer and Olesen (2000)
Plöchl	Only simple input requirements	Based on different modelling approach (neural network), simulates NH_3 volatilisation only following manure application	Plöchl (2001)
ALFAM	Considers fertiliser application method	Soil pH change not considered, only for slurry fertiliser	Søgaard et al. (2002)
Pacholski (based on DUPAV)	As described above, adapted for use under field conditions	Nitrification not considered, time step is six minutes	Pacholski (2003), Rachhpal-Singh and Nye (1986a-c)
Wu, Nofziger, Warren, Hattey (based on Ismail, Wheaton, Douglass, Potts)	Considers flood irrigation with ponded infiltration sub-model	Simulates NH_3 volatilisation only following liquid fertiliser application, soil pH change and nitrification not considered	Wu et al. (2003), Ismail et al. (1991)
WNMM	Considers urea hydrolysis, nitrification, soil temperature, wind speed	Does not consider pH, ammonium–ammonia equilibrium	Li et al. (2007)
Nyord, Schelde, Søgaard, Jensen, Sommer; (based on Izaurralde, Kissel, Cabrera)	Considers fertiliser injection	Based on laboratory conditions, soil pH change and nitrification not considered	Nyord et al.(2008), Izaurralde et al. (1990)
DNDC (before 2018)	Considers urea hydrolysis, ammonium–ammonia equilibrium, nitrification, pH	Complex input data requirement, for urea hydrolysis and volatilisation soil moisture and temperature not considered	Li et al. (1992)
Volt'Air	Considers pH change, usable for mineral fertiliser	Nitrification not considered, time step is one hour	Garcia et al. (2012), Génermont and Cellier (1997)
RZWQM	Considers urea hydrolysis and nitrification	Complex input data requirement	USDA (2018)

Besides NH_3 volatilisation, an option to simulate the effect of nitrification and urease inhibition was implemented in HERMES during this thesis but urease inhibition was not yet tested. The influence of nitrification inhibitors on the amount of nitrified N in the soil was calculated using a coefficient for nitrification inhibition. This coefficient depended on a fertiliser specific factor defining the temperature sum required to reduce nitrification inhibition to zero, representing the decay of the inhibitor (chapter 4). To make the model available for a broader community of Chinese scientists and extension services a Chinese language graphical user-interface version has already been developed for HERMES.

Spatial application

As spatial models are limited in simulating N processes and have large, difficult to measure input data requirements the HERMES model was used and coupled to a GIS (see chapter 5). The GIS programmes, ArcView, ArcGIS and ERDAS imagine were used to process spatial data and run separately from the HERMES model. As neither HERMES is integrated or embedded in a GIS programme nor the other way round, a coupling method was used to link HERMES with the GIS. Crooks and Castle (2012) defined coupling as the linkage of two stand-alone systems by data transfer and the method used in chapter 5 they called loose coupling. As in their example GIS programmes were used in this thesis to prepare data in chapter 5, which were then used for modelling in HERMES and finally with HERMES simulated data was displayed in a GIS. Describing the method in more detail Hartkamp et al. (1999) calls it linking technique, where results from both, the HERMES model as in this thesis and the GIS model were joined via spread sheet and polygon-ID.

Model performance statistics

To judge on the models performance and its reliability to describe soil-plant interactions regarding nitrogen, modelling statistics were used. One measure which was chosen is the mean absolute error (*MAE*); (Shaeffer 1980):

$$MAE = \sum_{i=1}^{n} \frac{|S_i - O_i|}{n} \tag{1}$$

Where S are the simulated values, O the observed means and n the number of observations. This was selected as it returns a mean value of the scale of difference of simulated and measured values in its corresponding unit. This allows an easy comparison between treatments but does not give the direction of the bias and tell weather the model over (positive result) or under predicts (negative result). For this reason the mean bias error (*MBE*; Addiscott and Whitmore 1987) was included as well:

$$MBE = \sum_{i=1}^{n} \frac{S_i - O_i}{n} \tag{2}$$

As a measure of modelling quality the modelling efficiency (*ME*) according to (Nash and Sutcliffe 1970) was used:

$$ME = 1 - \frac{\sum_{i=1}^{n} (S_i - O_i)^2}{\sum_{i=1}^{n} (O_i - \bar{O})^2} \tag{3}$$

Where $\bar{O}$ is the mean value of the observed variable. This parameter was selected because it returns the performance of the model compared to the variation of the measured values. A result above zero means that the difference of the simulated and the measured values is smaller than the variance among the measured mean values. A value close to one indicates an ideal fit of simulated and measured values. The *ME* is without dimension and is thus good for comparison with other studies using *ME* no matter in which unit the original values are.

1.4 Objectives

With regard to the above mentioned main objective and to the objectives of the research articles (Chapters 2–5) four key questions within two thematic fields were created (model performance and extension; model N and water saving potential) which this thesis aims to answer.

Model performance and extension

Question 1: What is the performance of the HERMES model under practical conditions in the NCP and which model adaptations are required?

Question 2: What is the performance of the newly implemented NH_3 volatilisation sub-module with it's four variations and the nitrification inhibition tool?

Model N and water saving potential

Question 3: What is the model's potential to save N and water on plot scale with help of a model-based fertiliser recommendation and adapted irrigation?

Question 4: What is the model's potential to save N and water on county scale over a long-term period?

1.5 Outline of the thesis

This cumulative thesis includes three peer-reviewed articles (chapters 2, 3, 5) and one short, unpublished report (chapter 4) to draw answers to N pathway and budget in soil-plant-atmosphere with regard to soil and water protection in NCP using a simulation model. The articles were written as research articles and were published or are under review in international, peer-reviewed journals. The underlying working progress of this thesis can be followed in the final project report (TU München 2012). Complete references were given on the first page of chapters 2–5, if applicable. The content of the articles remains original only their style was fit to this thesis. A graphical overview of the thesis is presented in figure 1.3.

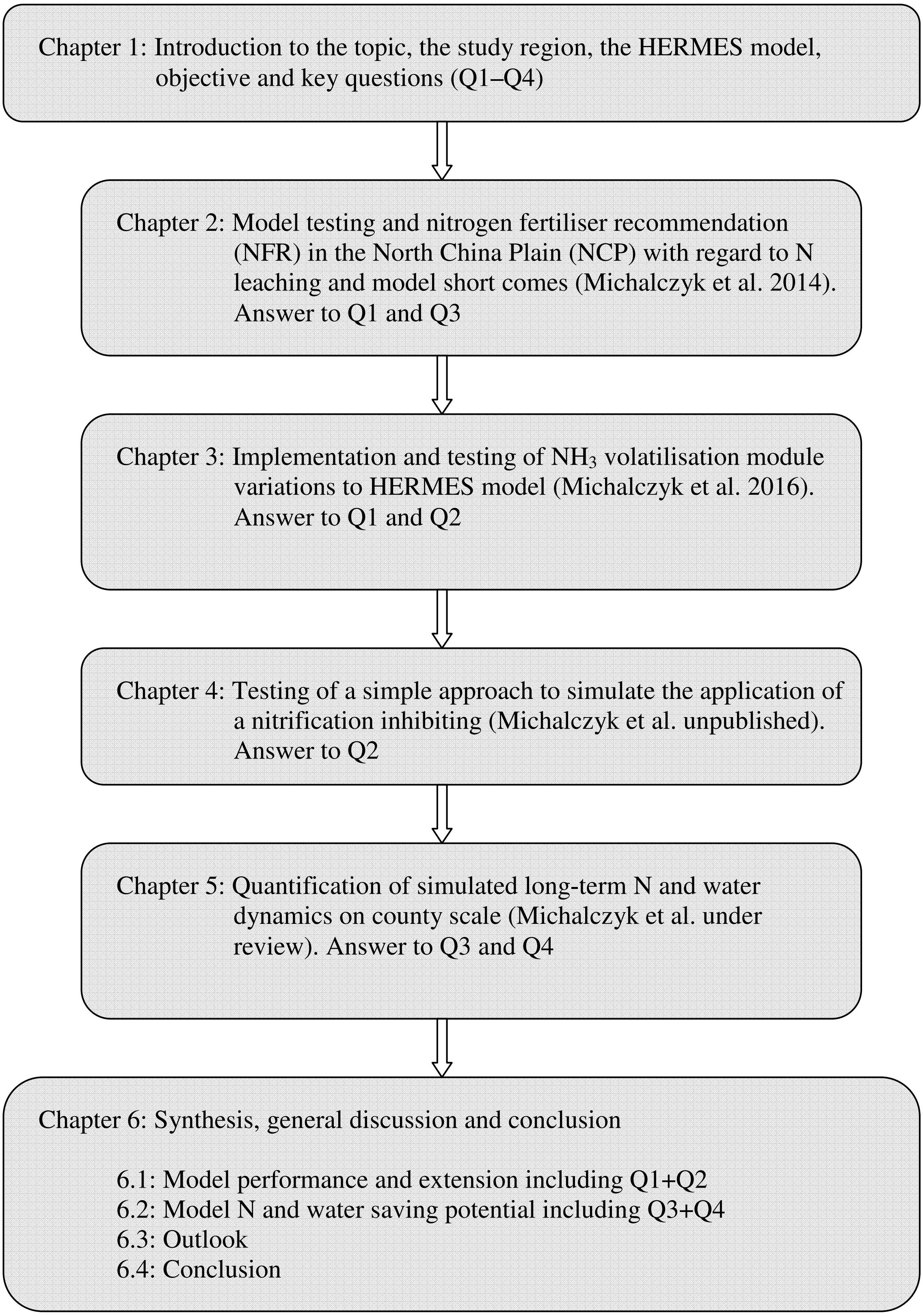

Figure 1.3: Graphical thesis overview. Q1–Q4 = key questions 1–4

Chapter 1

The introduction guides, in presenting the motivation of the thesis, the region of the topic of this thesis and the state of the art, to the four guiding questions.

Chapter 2

This chapter draws a bow from presenting the suitability of the HERMES model on field plot scale in the NCP to a best-practice scenario using model-based recommendations for N fertilisation and irrigation. The model was calibrated and validated on two data sets of field experiments in Quzhou County regarding soil water content, soil N_{min} content, plant N uptake, biomass and yield. For winter wheat 2011 a real-time model-based NFR was applied and an agronomic nitrogen use efficiency was calculated comparing model recommendations with N_{min}-method based fertilisation. The effect of varying irrigation and annual weather variability on model-based NFR was evaluated with model scenarios as well as the optimised best-practice simulation scenario which aimed to highly reduce N losses via leaching. The potential of the model to support best-practice solutions as well as the need to introduce a dynamic NH_3 volatilisation module, which is a relevant N pathway for China to be considered, and conduct long-term simulations was shown.

Chapter 3

Here a new, dynamic volatilisation sub-module including four variations to calculate ammonia losses was established and built into the model HERMES. The variations ranged from simple empirical functions (variation 3 and 4) to process-oriented approaches (variation 1 and 2) including the main processes of NH_3 volatilisation, urea hydrolysis, nitrification from NH_4-based N fertiliser, and changes in soil solution pH. The sub-module was calibrated and validated against four data sets. The performance of the model of matching measured gaseous losses was shown and the results of the four variations were compared. A further need for verification with measurements of simulated changes in topsoil pH was emphasised.

Chapter 4

A simple tool within the NH_3 volatilisation sub-module to describe the application of a nitrification inhibiting fertiliser is shown in this chapter. The nitrification inhibition tool was tested for NH_4 and nitrate pattern in soil, plant N uptake, biomass and yield, as well as for differences in NH_3 volatilisation, denitrification and leaching compared to a fertilization without nitrification inhibitor on one experiment. The performance of the nitrification inhibition tool was shown.

Chapter 5

This chapter describes a long-term regionalisation approach using the HERMES model on county scale in the NCP. For this approach data for a GIS was collected including a ground-truth trail for land use classification. Geographically established weather, soil and farm management data was used to conduct 31 years of long-term simulations in Quzhou County. Six scenarios regarding N application and irrigation water management were simulated: a farmers practice N (FP), a FP + standard deviation, a FP – standard deviation, a FP – 30% N application, a practical (oriented on farmers practice) N and irrigation optimised scenario including NFR and an as much as possible optimised N and irrigation scenario including NFR and model-based irrigation recommendation. The scenarios based on FP were additionally spatially variable according to township specific management. Results of all scenarios were presented and quantitatively and visually compared. The risks of these long-term simulations on regional scale were assessed.

Chapter 6

In the synthesis and general discussion section the general results of the thesis were discussed regarding uncertainties and problems as well as in context with other studies. The four key questions were addressed and general conclusions regarding the state of the art were drawn.

2 Model-based optimisation of nitrogen and water management for wheat–maize systems in the North China Plain

Published as: Michalczyk A, Kersebaum KC, Roelcke M, Hartmann T, Yue SC, Chen XP and Zhang FS (2014) Model-based optimisation of nitrogen and water management for wheat-maize systems in the North China Plain. Nutrient Cycling in Agroecosystems 98**,** 203–222

Abstract

Excessive nitrogen fertiliser application and irrigation in the North China Plain leads to nitrate accumulation in sub-soil and water pollution. HERMES, a dynamic, process-oriented soil-crop model was used to evaluate the effects of improved nitrate and water management on nitrate leaching losses. The model was validated against field studies with a winter wheat (*Triticum aestivum* L.)–summer maize (*Zea mays* L.) double-cropping system. A real-time model-based nitrogen fertiliser recommendation (NFR) was carried out for one wheat crop within the rotation and compared to farmers' practice and soil mineral nitrogen (N_{min}) content-based fertilisation treatments. Consequences of varying irrigation and annual weather variability on model-based NFR and further model outputs were assessed via simulation scenarios. A best-practice simulation scenario with model-based NFR and adapted irrigation was compared to reduced N and farmers' practice treatments and to a dry and a wet scenario. Results of the real-time model-based NFR and the other treatments showed no differences in grain yield. Different fertiliser inputs led to higher nitrogen use efficiency (not significant) of the model-based NFR. Increasing amounts of irrigation resulted in significantly higher N leaching, higher N requirements and reduced yields. The impact of weather variation on model-based NFR was smaller. In the best-practice scenario simulation, nitrogen input could be reduced to 17.1 % of conventional farmers' practice, irrigation water to 72.3 % and nitrogen leaching below 0.9 m to 1.8 % and below 2.0 m soil depth to 0.9 % within 2 years. The model-based NFR in combination with adapted irrigation had the highest potential to reduce nitrate leaching.

The online version of this article (doi:10.1007/s10705-014-9606-0) contains supplementary material, which is shown in the appendix.

Keywords

Nitrogen fertilisation, Irrigation, Fertiliser recommendation, Simulation model, Nitrate leaching

Abbreviations

C_{org}	Organic carbon
ETA	Actual evapotranspiration
EX	Exact experiment
FP	Farmers' practice
HY	High yield treatment
ME	Modelling efficiency
MAE	Mean absolute error
MBE	Mean bias error
NCP	North China Plain
NFR	Nitrogen fertiliser recommendation
N_{min}	Soil mineral nitrogen (nitrate-N (NO_3^--N) + ammonium N (NH_4^+-N))
NH_3	Ammonia
n.s.	Not significant
NUE	Nitrogen use efficiency
NUE_A	Agronomic nitrogen use efficiency of applied nitrogen

2.1 Introduction

The North China Plain (NCP) is one of the most intensive and major grain producing agricultural regions in China. Main cropping systems include winter wheat–summer maize double-crop rotation, cotton and vegetables. Winter wheat is sown in October after tillage and harvested in June of the following year. Immediately thereafter summer maize is sown without tillage; it is harvested as kernel maize at the end of September/beginning of October and used for fodder. Nitrate losses from these intensive cropping systems are a well-known problem in the NCP (Ju et al. 2006). Excessive irrigation and nitrogen (N) fertiliser application cause low water use efficiencies (Fang et al. 2010) and nitrogen use efficiencies (NUE), deeper groundwater tables (Hu et al. 2005) and pollute the environment (Liu et al. 2003). Ju et al. (2009) evaluated several case studies and found that N fertiliser rates higher than those in ''optimised'' treatments (30–60 % less compared to conventional farmers' practice N application rates), could not increase grain yields further. Instead, nitrate pollution of groundwater and eutrophication of surface waters increased considerably (Zhang et al. 2011a). Under improper irrigation nitrate leaching is seen as the major pathway of N losses in winter wheat–summer maize double-crop rotations in the NCP (Fang et al. 2006; Ju et al. 2004; Liu et al. 2003; Zhao et al. 2006). Flood irrigation of commonly more than 100 mm per event and high rainfall during summer monsoon season with events of more than 50 mm per day leach soil nitrate out of the root zone, which accumulates in deeper soil layers. These nitrates may reach shallow ground water (Ju et al. 2004) or adjacent surface waters in a short time. Farmers irrigate according to weather conditions but timing depends on the availability of the pump which has to be shared with other farmers, resulting in great inaccuracies regarding irrigation water amounts.

The N_{min} method (Wehrmann and Scharpf 1986) considers measured soil mineral nitrogen (NO_3^--N + NH_4^+-N; N_{min}) in the root zone prior to fertilisation and expected total N uptake by the crop to calculate optimum fertiliser rates. An ‘‘improved N_{min} method’’ (Chen et al. 2006a; Cui et al. 2008) as well as in-season root zone management (Meng et al. 2012a) and integrated soil-crop system management (Chen et al. 2011; Zhang et al. 2011a) were introduced in the NCP to improve NUE and assure high yields. These modifications consider N recommendations at three plant growth stages and soil depths, N mineralization, N immobilization and N losses, and partly include atmospheric N inputs. The studies by Fang et al. (2008), Hu et al. (2006) and Yu et al. (2006) addressed nitrate leaching losses using the root zone water quality model RZWQM (Ahuja et al. 2000) in the NCP. In their studies N and water management scenarios were evaluated after model calibration. However, a real-time model-based numerical nitrogen fertiliser recommendation (NFR) is not included in RZWQM. Model-based NFR can give a recommendation for a specific real-time situation and location and can save time compared to the N_{min} method and scenario simulations.

Real-time model-based NFR derived from a physiological process model has so far never been applied in the NCP; neither have NFR supported best management practices been derived from scenario simulations in China. The objectives of this study are to (1) verify the application of the HERMES model under growing conditions of northern China in a winter wheat–summer maize double-cropping system, (2) to investigate how a real-time model-based NFR performs compared to common farmers’ practice as well as to the ‘‘improved N_{min} method’’, (3) to assess consequences of varying irrigation management and weather on the model-based NFR and further model outputs, and (4) to determine and evaluate a best- practice management scenario with reduced N fertiliser, irrigation water and nitrate leaching, without decreasing yields.

Table 2.1: Soil characteristics for the study sites. Texture was determined by expert finger testing for exact experiment (EX) as mean of the whole field site and by sieving and sedimentation (Moschrefi 1983) for each '3+x' field site

Site	Depth	Clay[a]	Silt[b]	Sand[c]	Field capacity[d]	Wilting point[d]	pH (H_2O)	Bulk density	C_{org}	C/N
	m	%	%	%	vol. %	vol. %		g cm^{-3}	%	
EX size 2,652 m²	0–0.3	12	67	21	39	12	7.6	1.40	0.90	10
	0.3–0.6	12	67	21	39	12	7.4	1.36	0.60	11
	0.6–0.9	18	64	18	39	21	7.6	1.35	0.50	12
farmer's field #1 size: ~ 375 m^2	0–0.3	7	79	14	37	4	8.3	1.40	0.71	11
	0.3–0.6	4	80	16	37	4	8.5	1.36	0.45	12
	0.6–0.9	7	88	5	37	4	8.4	1.35	0.32	12
farmer's field #6 size: ~ 216 m^2	0–0.3	7	81	12	39	10	8.5	1.40	0.95	11
	0.3–0.6	6	84	10	39	10	8.5	1.36	0.48	12
	0.6–0.9	6	90	4	39	10	8.3	1.35	0.25	12
farmer's field #8 size: ~ 189 m^2	0–0.3	7	78	15	38	8	8.7	1.40	0.82	12
	0.3–0.6	7	80	13	38	8	8.5	1.36	0.45	12
	0.6–0.9	7	87	6	39	10	8.4	1.35	0.32	12

[a] < 2 µm
[b] 2 µm–63 µm
[c] 63 µm–2 mm
[d] According to the German Soil Survey Manual and adapted by model simulations

2.2 Materials and methods

Location and weather data

This study was based on data from two field experiments located at Quzhou County in the southern part of Hebei Province, P.R. China, with a winter wheat (*Triticum aestivum* L.) and summer maize (*Zea mays* L.) double-crop rotation: (1) an exact field experiment (36°520 N and 115°010 E), further denoted as ''EX'', and (2) field experiments on farmers' field sites for demonstration purposes named '3 + x' experiments (36°420 N and 115°550 E), further denoted as '3 + x'. The average annual temperature and the average annual precipitation in Quzhou from 1980 to 2009 were 13.6 °C and 488 mm, respectively, with about 60 % of the annual precipitation occurring during summer. The soils were classified as Cambisol (EX) and Luvisol ('3 + x') with a silt loam or silt texture according to IUSS Working Group WRB (2007). Selected soil characteristics are described in Table 2.1. The relief was flat.

Weather data was obtained from the research station of China Agricultural University (CAU) in Quzhou County at about 500 m distance from EX. The same weather data was used for the '3 + x' sites, which were approximately 20 km away. Precipitation was additionally measured at the '3 + x' location for the growing season 2009. However, precipitation differences were insignificant between the sites, also in comparison to other surrounding weather stations. Thus, precipitation was not further measured at the ‘3 + x’ experiments. Total precipitation in 2009 was 428 mm with no rainfall prior to 10th of April 2009. In 2010 total precipitation was 393 mm with a wet spring, but no precipitation occurred between 4th and 30th of June 2010. Total precipitation in 2011 was 406 mm and 70 mm rain fell on 2nd of July 2011 on a single day.

Field experimental design and crop management

The EX experiment was a Latin rectangle organised in a randomised block design with four replications and eight N level treatments, four of which were used in this study–zero N, conventional farmers’ practice urea (46 % N), reduced (56 % of farmers’ practice) split urea, reduced (56 % of farmers’ practice) urea (reduced N treatment in the following) (Hartmann 2011, personal communication). The varieties used for the winter wheat–summer maize double-crop rotation were *Liangxing99* for wheat and *Zhengdan* for maize. The EX experiment was carried out from summer maize 2009 until summer maize 2011 over five cropping seasons.

The ‘3 + x’ experiments took place on five farmers’ field sites, three of which were selected for evaluation (Table 2.1). The experimental design was laid out in the so-called ‘3 + x’ approach: Each field was split into a conventional farmers’ practice urea (FP treatment), a reduced urea (reduced N treatment) and a zero N plot; as additional ‘x’-treatment, a high yield urea treatment was chosen (HY in the following). The same varieties as in EX were used, except for the HY treatment where Xianyu335 was used for maize (2009 and 2010) and Heng4399 for wheat (2009/10). The ‘3 + x’ experiments lasted from summer maize 2009 until winter wheat 2010/2011 (four cropping seasons).

In both experiments wheat was irrigated twice in spring and maize was irrigated once after sowing according to local farmers’ practice. Approximately 100–300 mm water were pumped up from a nearby canal (EX) or from a groundwater well (‘3 + x’). The nitrate content of the canal water was determined in 2009 and the approximate amount of irrigation water was estimated via pump power and duration. One irrigation event lasting for 4 h was equivalent to about 300 mm of water pumped to the field. Maize straw residues and fertiliser, applied before sowing of the following wheat crop, were incorporated by tillage (0.2 m). Details of the crop management are listed in Table 2.2.

Table 2.2: Site management for the '3+x' site for one farmer's field (#6). RD = reduced N treatment, FP = farmers' practice treatment, HY = 'high yield treatment'

	Summer maize 2009	Winter wheat 2009/10	Summer maize 2010	Winter wheat 2010/11
Sowing date	15th June 09	15th October 09	27th June 10	16th October 10
Fertilisation at sowing date and amount (kg N ha^{-1})	15th June 09; RD=45 FP=45 HY=34	13th October 09; RD=68 FP=128 HY=68	27th June 10; RD=45 FP=45 HY=34	14th October 10; RD=68 FP=128 HY=68
Tillage date and depth (m)	–	14th October 09; 0.2	–	15th October 10; 0.2
First top dressing fertilisation date and amount (kg N ha^{-1})	12th July 09, DP3 [a]; RD=105 FP=138 HY=75	14th April 10, DP3; RD=93 FP=104 HY=93	23rd July 10, DP3; RD=105 FP=138 HY=75	20th April 11, DP3; RD=92 FP=103 HY=92
First irrigation date and amount (mm)	16th June 09; 225	14th April 10, DP3; 225	27th June 10; 225	18th March 11, DP2; 113
Second top dressing fertilisation date and amount (kg N ha^{-1})	2nd August 09, DP4; HY=103	–	2nd August 10, end of DP3; HY=103	–
Second irrigation date and amount (mm)	–	10th May 10, DP4; 225	–	20th April 11, end of DP3; 158
Harvest date	2nd October 09	16th June 10	6th October 10	14th June 11

[a] DP = plant development phases referring to Table 3, if the date is not at sowing or harvest time of the crop

Soil and plant sampling, processing and analyses

Soil was sampled prior to base fertilisation at sowing of the first maize crop, once before top dressing of maize, two or three times after top dressing of maize and once after harvest. During wheat growth soil samples were taken at regreening stage, before top dressing (only '3 + x') and after harvest. The soil samples were taken in three to five replicates per treatment plot in 0–0.3, 0.3–0.6 and 0.6–0.9 m depth increments for the in-season measurements and down to 2.0 m depth for the pre-experiment sampling, and subsequently bulked for each layer. The fresh soil samples were cooled to +4 °C immediately, homogenised, put through a 2 mm sieve, shaken for 1 h in a 0.01 M $CaCl_2$ solution, filtered and stored in a freezer on the sampling day. The extracts were analysed using automated continuous flow analysis (TRAACS 2000 system, Bran and Luebbe, Norderstedt, Germany) for ammonium and nitrate. Gravimetric water contents were determined via drying soil samples at 105 °C for 24 h. Leaching was not directly measured in the field. Plant sampling was done around the same time as soil samples were taken. Plant samples were dried at 70 °C and above-ground dry matter and grain yield was measured. Nitrogen in above-ground plant organs was determined according to the standard Kjeldahl method (Horwitz 1970).

Model structure and NFR tool

The HERMES model is a one-dimensional, dynamic, process-based N simulation model made for practical applications in agriculture under limited input data availability (Kersebaum 1995; Kersebaum and Beblik 2001; Kersebaum 2007). It operates at a daily time step, simulating soil N and water dynamics and its losses, plant N uptake, crop biomass and yield.

The water module is based on a capacity approach using soil texture classes to derive capacity parameters (AG Boden 2005). They are modified by soil organic matter content, bulk density and hydromorphic indices and can be calibrated by the user. Percolation and upward water flow depend on water balance between actual evaporation and precipitation. Capillary rise from shallow groundwater is also considered. Crop specific potential evapotranspiration is calculated using the Penman–Monteith equation according to Allen et al. (1998), which is modified to actual evapotranspiration (ETA) considering root length distribution and available water in each layer. Preferential flow is not considered.

Table 2.3: Selected plant parameters and development stages for winter wheat and summer maize used in this study by the HERMES model

Crop	Parameter	Unit	Value
Winter wheat	Maximum CO_2 assimilation rate	kg CO_2 ha^{-1} and leaf h^{-1}	45
	Maximum effective rooting depth	m	1.5
	Temperature sum development phase 1, sowing till emergence	°C	100
	Temperature sum development phase 2, emergence till double	°C	210
	Temperature sum development phase 3, double ridge to	°C	200
	Temperature sum development phase 4, flowering/begin grain	°C	250
	Temperature sum development phase 5, grain filling	°C	280
	Temperature sum development phase 6, senescence	°C	25
Summer maize	Maximum CO_2 assimilation rate	kg CO_2 ha^{-1} and leaf h^{-1}	80
	Maximum effective rooting depth	m	0.9
	Temperature sum development phase 1, sowing till emergence	°C	70
	Temperature sum development phase 2, emergence till stem	°C	384
	Temperature sum development phase 3, stem elongation till	°C	380
	Temperature sum development phase 4, tassel emergence till	°C	280
	Temperature sum development phase 5, grain filling	°C	400
	Temperature sum development phase 6, senescence	°C	200

The model simulates net N mineralisation from soil organic matter, decomposing plant material and organic fertiliser depending on temperature and soil moisture. Denitrification is simulated via Michaelis–Menten kinetics depending on soil nitrate, water content and temperature in the upper 0.3 m of the soil (Schneider 1991). Nitrate transport in soil is simulated by a convection–dispersion approach using simulated water fluxes. N uptake is simulated as mass flow with the water uptake plus a diffusive radial transport to the roots using root length density and water content in each layer. Ammonia volatilisation from urea to ammonium-based fertilisers was defined by fixed percentages (15 and 10 %, respectively) of total applied N based on studies of Roelcke et al. (2002b) for urea.

The plant growth module is based on the SUCROS model by van Keulen et al. (1982). It simulates biomass production driven by global radiation and temperature (photosynthesis-respiration approach) with minimum growth temperatures of +6 °C for maize and +4 °C for wheat. Phenological development is simulated following the thermal sum approach modified by vernalisation and day length requirements in specific stages. Plant parameters and stages are summarised in Table 2.3. Dry plant biomass is partitioned to crop organs using development stage-specific coefficients. Water stress is simulated when the ratio of actual to potential transpiration falls below a crop-specific threshold for each stage. Accordingly, N stress is simulated when the crop is not able to take up enough nitrogen to keep actual N concentration in the crop above a critical level, determined by crop-specific dilution curves.

The model's NFR tool is described in detail by Kersebaum and Beblik (2001). It predicts the future N uptake by the plant at any time during the growing season and the changes in soil mineral N due to mineralisation, denitrification and leaching using site- specific data of typical weather conditions (predictive weather scenario). The fertiliser recommendation is the difference between the predicted N amount taken up by the crop and the calculated available N in the soil.

Model set up, calibration and validation

The HERMES model has been validated for wheat (Palosuo et al. 2011), maize (Herrmann et al. 2005) spring barley (Rötter et al. 2012) and various crops and crop rotations (Hlavinka et al. 2013) across Europe and other continents (Asseng et al. 2013; Kersebaum et al. 2008). Kersebaum et al. (2005) successfully used the NFR tool for precision agriculture and Kersebaum et al. (2007b) analysed annual variability of NFR with 30 years of weather data.

For this study the model was calibrated against 2 years of data (summer maize 2009 until winter wheat 2010/11) of the EX experiment including four treatments. Initial values for soil water and mineral N contents were taken from pre-experiment sampling. The amount of irrigation water first derived from the duration of the flood irrigation was adopted by inverse modelling in the EX experiment using measured soil gravimetric water content and mineral N contents after irrigation. This resulted in a mean deviation of −17 % from initially calculated amounts for the April and June 2010 irrigation. The other irrigation water amounts remained uncorrected. Soil water capacity parameters were calibrated with measured gravimetric water contents. Plant parameters for winter wheat were taken from the existing model data base and further adapted to the variety Liangxing99 for wheat. For summer maize model parameters were pre- calibrated independently with data from the CAU's experimental site at Dongbeiwang near Beijing (unpublished) and further adapted to the variety Zhengdan. Finally, plant N uptake and soil mineral N was brought together with regard to observed data.

The model was validated against four treatments of the '3 + x' experiments using data sets of three farmers' fields (in the following field #1, #6 and #8) without any further adaptation except for the amounts of irrigation water. First we adjusted the irrigation amount as described above, which resulted in 16–58 % deviations from the initially estimated amount for all farmers' fields equally. Subsequently, an individual adaptation for each field site within ±10 % of the general adapted irrigation was carried out if measured soil water and N contents indicated a further need. An overview of irrigation management is given in Table 2.2.

Model evaluation statistics

To evaluate the model's performance we used indicators usually applied in model inter-comparisons (e.g. Palosuo et al. 2011): (a) the mean absolute error (*MAE*; Shaeffer 1980) which represents the mean deviation between simulated and measured values in its corresponding unit, (b) the mean bias error (*MBE*; Addiscott and Whitmore 1987) that indicates if the model on average over- or underestimates, and (c) the modelling efficiency (*ME*) according to Nash and Sutcliffe (1970) as a measure of modelling quality which returns the performance of the model compared to the variation of the measured values. A value close to one indicates an ideal fit of simulated and measured values.

Real-time model-based NFR

Real-time model-based NFR was calculated using the HERMES model in April 2011 for the top dressing of the final winter wheat crop 2010/11 in the '3 + x' experiments. The NFR were applied on-farm on sub- plots previously used as reduced N and HY plots. Base fertilisation at sowing in autumn 2010 was carried out as described in Table 2.2. For the prediction period of the real-time NFR (from early April 2011 until wheat harvest in mid-June 2011) the irrigation amount and date of fertilisation in the model was set according to farmers' practice. The timing of irrigation was oriented to the predictive weather. According to farmers' practice fertilisation was not split as the model would normally do. Thus the model calculated only one recommendation for the whole period and no iterative improvements could be done. The amount of N fertiliser of the zero N, FP, reduced N and HY treatment was compared to the NFR-recommended N fertilisation amounts. For a further comparison between the treatments the agronomic nitrogen use efficiency of applied N NUE_A (kg grain kg N^{-1}) was calculated as

$$NUE_A = \frac{(Y_F - Y_0)}{F_N} \quad (1)$$

where Y_F is the fertilised grain yield, Y_0 is the unfertilised grain yield of the zero N treatment (in kg ha^{-1}) and F_N is the amount of applied fertiliser N (kg N ha^{-1}). Averages of the three farmers' fields were tested for differences using ANOVA and TUKEY tests.

Effect of irrigation and weather on model-based NFR

The sensitivity of NFR to varying irrigation amounts was tested to assess the uncertainty caused by irrigation. Similar conditions to those for winter wheat 2010/11 of the '3+x' experiments in the reduced N treatment were used to set up the model. This included one fertiliser application on the three farmers' fields and measured weather conditions instead of predictive weather. The irrigation water applied together with the fertilisation and at the second irrigation event 3 weeks later was varied from 0 to 300 mm in steps of 50 mm.

The effect of different seasonal weather conditions was tested in a second scenario for winter wheat 2010/11 on the same three farmers' fields of them'3 + x' experiments. 10 years differing in average precipitation and temperature were selected for the model-based NFR. Precipitation amounts were arranged in decreasing order (Figure 2.8). Actual weather data of 2010/2011 was used until prediction started. Irrigation amounts were kept as in the real-time NFR and just the timing was adapted if necessary.

For both scenarios, the amount of recommended N fertiliser in kg N ha^{-1} and corresponding simulated grain yield in kg ha^{-1}, leaching in 0.9 m depth and denitrification losses in kg N ha^{-1} were compared. ANOVA and TUKEY tests were applied as described above.

Best-practice scenario simulation

A best-practice scenario was simulated for the whole duration of the '3 + x' experiments (summer maizen2009 until winter wheat 2010/11) by optimising the amounts of irrigation water and N fertilisation. Sowing, harvest, fertiliser application and irrigation dates remained unchanged to keep the scenario comparable to the experimental treatments and local practices. The model-based best-practice NFR for winter wheat was calculated in the same way as for the real-time procedure except using observed weather data. For summer maize the required amount of N was determined by step-wise reducing the N dose (starting from farmers' practice amounts) until the simulated grain yield started to decrease due to N stress. The irrigation amounts were calculated by filling the gap between field capacity and simulated soil water content in the major root zone (0–0.9 m depth) at the day prior to irrigation. Nitrogen leaching was simulated for soil depths below 0.9 and 2.0 m.
To evaluate the effect of weather variability on best-practice options, extremely dry and wet weather scenarios for the duration of best-practice scenario simulation were chosen. Three dry years and three wet years were selected for each scenario. Recommended fertilisation, optimised irrigation and simulated grain yield, leaching in 0.9 and 2 m and ETA were compared for the dry, wet and ''normal'' scenarios using ANOVA and TUKEY tests.

2.3 Results

Calibration

The simulation of volumetric soil water contents returned a good fit of measured and simulated values (Figure 2.1). In the reduced N treatment of the EX experiment the upper 0–0.3 m of the soil profile were better simulated (*MBE* −0.38 vol%) than the deeper layers, resulting in a *MBE* from 0 to 0.9 m of −1.09 vol%. This was mainly caused by underestimated soil moisture in October 2009 as well as in March and June 2010 (Figure 2.1).
Above-ground biomass and grain yield simulations also showed satisfying results (Figs. 2, 3, supplement tables A.1, A.2). Both indicated a good correlation, although in the reduced treatment the biomass of maize was underestimated (*MBE* −1,188.6 kg ha^{-1}) and that of wheat slightly overestimated (*MBE* 836.2 kg ha^{-1}). Grain yield for both crops was,

especially on the zero N plot, still somewhat overestimated by the model after calibration in the first year, and slightly underestimated in the second year of the reduced treatment. The plant N uptake (*MBE* 23.6 kg N ha^{-1}, reduced treatment) and soil mineral N in 0–0.9 m (*MBE* −23.4 kg N ha^{-1}, reduced treatment) corresponded well to each other (Figure 2.4), while the model performance parameter indicated a good fit of measurements and simulation. Similar to the soil water content the model simulated the mineral N in the soil in 0–0.3 m depth better than in 0.3–0.6 and 0.6–0.9 m. For further details please see supplement tables A.1 and A.2.

Validation

Soil water content

Across all fields and treatments of the '3 + x' experiments the simulations of soil water content showed a better performance in the 0.6–0.9 m depth than in the upper layers. The positive *ME* in 0–0.9 m depth showed a good agreement of the measured and simulated water contents (Table 2.4, supplement table A.3), especially in the FP treatment (0.29 vol%). On average soil water content was slightly overestimated by 0.75 % in all treatments.

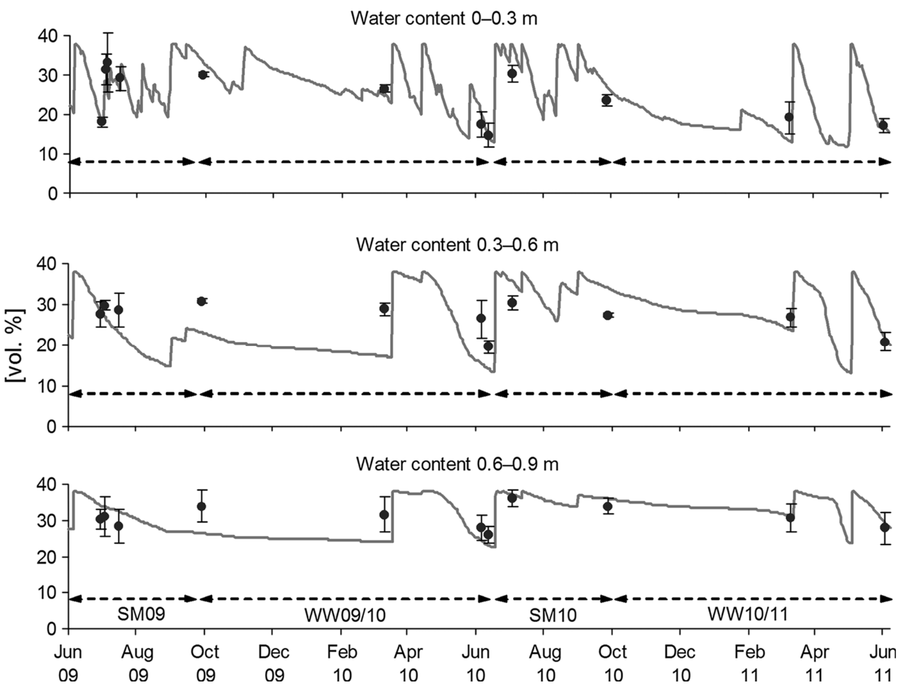

Figure: 2.1 Simulated (*lines*) and measured (*dots*) volumetric soil water contents from June 2009 until June 2011 in 0–0.3, 0.3–0.6 and 0.6–0.9 m depth for the reduced N treatment of the exact field experiment after calibration. *SM* summer maize, *WW* winter wheat. *Bars* show the standard deviation

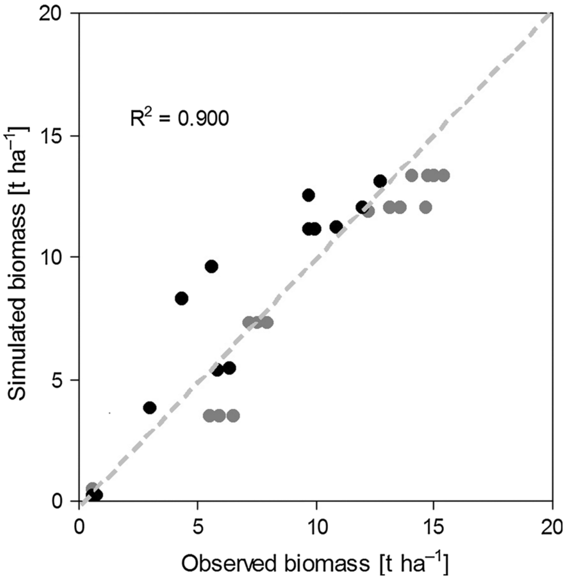

Figure: 2.2 Simulated and measured above-ground biomass in t ha^{-1} for four cropping seasons (summer maize 2009 until winter wheat 2010/11) of the exact field experiment and all treatments after calibration. R^2 coefficient of determination. *Dashed line* 1:1 line. Winter wheat *black dots*, summer maize *grey dots*

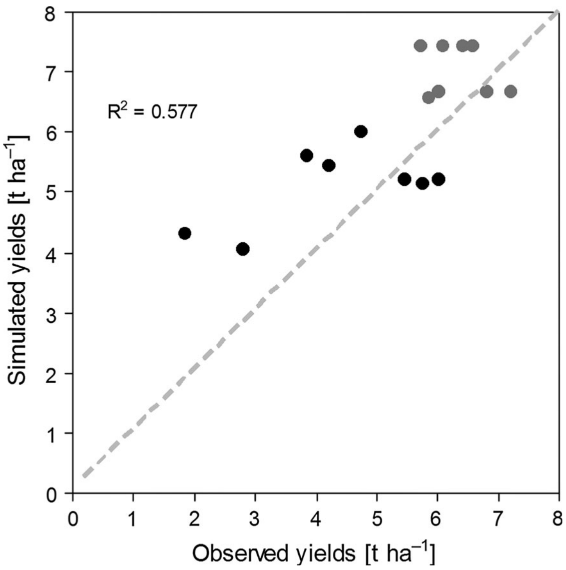

Figure 2.3: Simulated and measured grain yields in t ha^{-1} for four cropping seasons (summer maize 2009 until winter wheat 2010/11) of the exact field experiment and all treatments after calibration. R^2 coefficient of determination. Dashed line 1:1 line. Winter wheat black dots, summer maize grey dots

Above-ground biomass and grain yield

Both above-ground biomass and grain yield were simulated well by the model with low biased and absolute errors (Table 2.4). Across all treatments the *MAE* of above-ground biomass and grain yield were around one ton. Above-ground biomass for winter wheat was underestimated in the reduced treatment and distinctly overestimated in the zero N treatment, with *MAE* markedly higher than one ton. The grain yield was a bit underestimated by the model for both crops. The *MAE* for the grain yield of summer maize in the HY treatment was far above one ton.

Plant N uptake

Across all treatments the *ME* of the N uptake was above zero and showed a satisfying overall model performance (supplement table A.3) with a small overestimation of the N uptake (23.2 kg N ha^{-1}), which corresponded to the underestimation of mineral N in the root zone (−30.0 kg N ha^{-1}). The N uptake by maize was, except for the zero N treatment, overestimated a little, while simulations for winter wheat showed a generally better fit in all treatments (Table 2.4).

Soil mineral N content

Soil N_{min} content showed a good agreement of measured and simulated values across all treatments with a slight underestimation which was related to the overestimation of N uptake (see above) (Table 2.4). The highest underestimation occurred in the zero N plots. In the depths 0.3–0.6 and 0.6–0.9 m the *MAE* was smaller than in the upper soil layer for all treatments (supplement table A.3).

Real-time model-based NFR

The required amounts of N fertiliser calculated by the HERMES model and applied on farmers' fields of the '3 + x' experiments were lower compared to the amounts estimated by the N_{min} method (Figure 2.5). This did not result in significantly different grain yields among the fertilised treatments, but in a higher NUE_A on the model-recommended plots. The worst NUE_A was achieved on the FP treatment as it had the highest N inputs but no higher yields. This held true for each field alone as well as for the mean of all three fields (Fig. 2.5). However, the fertilised treatments showed no statistical differences in NUE_A.

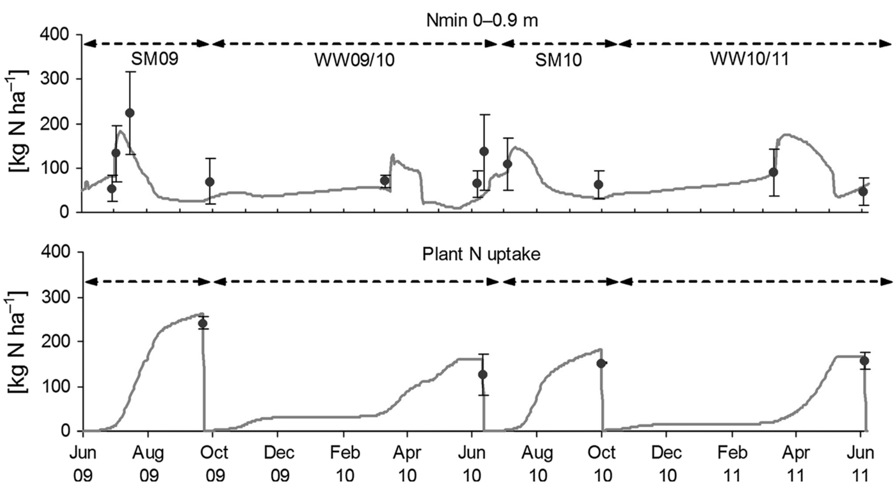

Figure 2.4: Simulated (*lines*) and measured (*dots*) soil mineral nitrogen in kg N ha^{-1} and plant N uptake in kg N ha^{-1} for four cropping seasons (summer maize 2009 to winter wheat 2010/11) and the reduced N treatment in the exact field experiment after calibration. *SM* summer maize. *WW* winter wheat. *Bars* show the standard deviation

Effect of irrigation and weather on model-based NFR

The simulations of varying irrigation levels resulted in NFR to winter wheat ranging from 103 kg N ha^{-1} at 0 mm to 159 kg N ha^{-1} at 300 mm irrigation (Figure 2.6). Irrigation rates higher than 150 mm required higher fertilisation as did irrigation rates lower than 100 mm, except for the zero mm irrigation rate. The average NFR was 129 kg N ha^{-1} with a confidence interval ($\alpha = 0.05$) of 28 kg N ha^{-1}. Grain yield was stable at 5,400 kg ha^{-1} and not statistically different between 300 mm and 150 mm. It started to significantly decrease at irrigation ≤100 mm (Figure 2.7). The mean grain yield of the irrigation variations was 4,200 kg ha^{-1} with a confidence interval ($\alpha = 0.05$) of 3,000 kg ha^{-1}. Leaching was not statistically different from zero (≤2 kg N ha^{-1}) up to 150 mm and increased significantly at higher irrigation rates (Figure 2.7). The confidence interval of leaching (46 kg N ha^{-1}) around the average of 19 was the highest, indicating a huge effect of irrigation variation. Denitrification increased significantly from rainfed conditions to a maximum of 5 kg N ha^{-1} at 100 mm and remained largely unchanged at higher irrigation rates (not significant, n.s.) (Figure 2.7).

The scenarios using variable weather resulted in NFR to winter wheat ranging from 142 kg N ha^{-1} in 2005 to 174 kg N ha^{-1} in 1995. These two extreme years were the only ones with NFR statistically different from all other years (Figure 2.8). The mean of all years was 154 kg N ha^{-1} with a confidence interval of 6 kg N ha^{-1} ($\alpha = 0.05$). Wheat grain yield varied from 5,370 in 2005 to 5,480 kg ha^{-1} in 1995 (n.s., not shown). The average leaching during the ten different weather years was 71 kg N ha^{-1} with a confidence interval of 2 kg N ha^{-1} (n.s., not shown). Denitrification showed the smallest range across years. All investigated variables had the highest value in 1995 and the lowest in 2005. Confidence intervals for all parameters were smaller compared to the irrigation scenario.

Best-practice scenario simulation

The scenario for field #6 with reduced N treatment (74.9 % of FP) led to a reduction of N leaching at 0.9 m depth to 76.9 % (FP = 100 %) but almost no reduction (99.7 %) at 2.0 m depth. Optimized N and water application were estimated to reduce nitrogen leaching to 5 % of FP at 0.9 m and to zero at 2.0 m depth while yields were maintained (Fig. 9). Simulated ETA was not reduced on this field.

On average of the three fields the N input in the best-practice scenario simulation was reduced to

Table 2.4: Mean absolute error, mean bias error and modelling efficiency for soil water content in–0.9 m depth, soil N_{min} in 0–0.9 m depth, N uptake, above-ground biomass and grain yield in the zero N treatment, reduced treatment, farmers' practice treatment and 'high yield' treatment, across farmers' fields of the '3+x' experiments after validation

			Zero N treatment	Reduced N treatment	Farmers' practice treatment	'High yield' treatment	n[a]	Across all treatments
Soil water content 0–0.9 m	vol. %	*MAE*	4.61	4.43	4.23	4.60		4.47
		MBE	1.16	0.76	0.27	0.82	38	0.75
		ME	0.07	0.06	0.29	0.04		0.12
Soil N_{min} 0–0.9 m	kg N ha^{-1}	*MAE*	74.46	65.65	93.44	73.63		76.80
		MBE	-74.46	-27.98	15.66	-33.21	35	−30.00
		ME	-0.48	-0.25	-0.68	-0.51		−0.50
Above-ground biomass maize	kg ha^{-1}	*MAE*	1249.58	954.45	767.39	1445.07		1104.12
		MBE	87.37	-64.92	291.73	-1258.22	24	−236.01
		ME	0.85	0.94	0.96	0.88		0.89
Above-ground biomass wheat	kg ha^{-1}	*MAE*	1703.59	910.70	1088.68	1032.90		1183.97
		MBE	1112.15	-133.97	43.51	130.15	20	287.96
		ME	0.64	0.94	0.90	0.88		0.91
Grain yield maize	kg ha^{-1}	*MAE*	1052.45	825.02	482.55	1835.54		1048.89
		MBE	728.95	-199.07	190.03	-1835.54	6	−278.91
		ME	0.00	0.12	0.47	-1.65		−0.53
Grain yield wheat	kg ha^{-1}	*MAE*	754.27	1038.48	1149.89	986.99		982.41
		MBE	286.42	-989.42	-771.80	-431.62	6	−476.60
		ME	0.17	-4.40	-1.96	-5.21		−1.82
N uptake maize	kg N ha^{-1}	*MAE*	18.16	32.74	40.70	31.39		41.00
		MBE	-12.90	28.21	46.77	24.58	24	21.67
		ME	0.49	-0.28	-1.44	0.05		−0.28
N uptake wheat	kg N ha^{-1}	*MAE*	16.52	25.02	27.03	24.92		31.16
		MBE	12.89	26.81	28.44	26.54	20	23.67
		ME	0.56	0.47	0.35	0.40		0.43

[a] in this column is the number of replications for one treatment. For across all treatments this needs to be multiplied by four

17.1 % and the irrigation water input to 72.3 % which resulted in a strongly reduced leaching to <1.8 and 0.9 % (FP = 100 %) at 0.9 and 2.0 m depth, respectively (Table 2.5). The ETA was only reduced during wheat growth periods and remained at 99.4 %, (not shown). More N was saved during summer maize growth but more water in winter wheat. Nitrogen leaching under summer maize was reduced to zero, and leaching under winter wheat was reduced to 1.8 % of the FP treatment in 2.0 m depth.

Mean simulated grain yields were lower in the wet and dry scenario compared to the ‘‘normal’’ scenario (Table 2.6). The model-based NFR was highest in the wet scenario (maximum for wheat in 2010/11) and lowest in the ''normal'' scenario. This agreed with the average leaching results in 0.9 and in 2.0 m depth being highest in the wet scenario. The ETA was highest in the dry scenario.

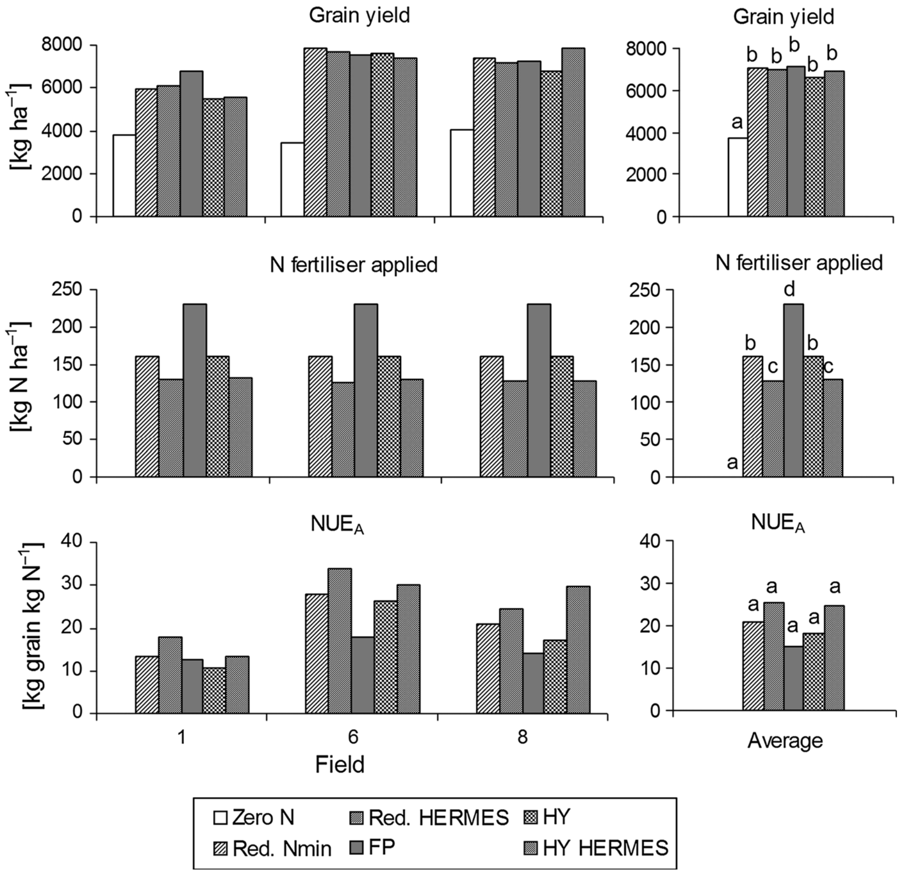

Figure 2.5: Measured winter wheat 2010/11 grain yields in kg ha^{-1} for all treatments with corresponding amounts of fertiliser applied in kg N ha^{-1} and the derived agronomic nitrogen use efficiency (NUE_A) in kg grain kg N^{-1}. Three investigated farmers' fields of the '3 + x' experiments on the left and mean of all three fields on the right side. Zero N = zero N treatment, Red. N_{min} = N_{min} method reduced treatment, Red. HERMES = NFR on former N_{min} method reduced treatment, FP = farmers' practice treatment, HY = 'high yield treatment', HY HERMES = NFR on former 'high yield treatment'. Columns followed by a *different letter* are statistically different (α =5 %)

2.4 Discussion

The HERMES model was able to successfully estimate soil and plant state variables under northern Chinese conditions with mostly small deviations. The real-time NFR recommended lower amounts of N fertilizer compared to the Nmin method while maintaining stable grain yields and low N losses. The derived fertilization recommendations were achieved with no additional labour requirements (only one top dressing application to winter wheat), which suits the current situation of small-scale part-time farmers in the NCP well. This also sets the real-time NFR apart from other approaches such as the ‘‘in-season root-zone N management system’’ recently introduced by Meng et al. (2012a) for maize in the NCP. Regarding water, the main challenge both for the simulations and the recommendations lay in the uncertainties of the actual irrigation amounts applied in the field. Nevertheless, the simulations showed a high water saving potential, especially for the winter wheat crop.

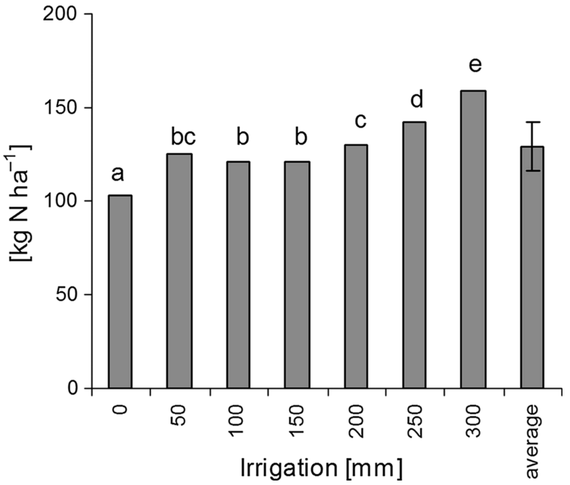

Figure 2.6: Effect of irrigation level on model-based NFR in kg N ha^{-1} on the ‘3 + x’ experiments in average of three farmers’ fields for winter wheat 2010/11, based on reduced treatment. Average NFR of the irrigation variation results with confidence interval. X-axis shows irrigation level in mm. Columns followed by a different letter are statistically different (α = 5 %)

Calibration and validation

Soil water content

In the calibration soil water contents were estimated well with low *MBE* and *MAE* values that corresponded to those observed for calibrated models under experimental conditions (Kersebaum et al. 2007a). Deviations between simulation an observations were higher in deeper layers (mainly 0.3–0.6 m). However, the long error bars indicate that soil water contents were very heterogeneous within the plot due to uneven infiltration. This was caused by irrigation water added to one end of the plots only slowly covering the whole plot area as well as by the imperfectly levelled soil surface. In the validation water content was slightly overestimated in all treatments, although the irrigation amounts had been adapted by inverse modelling. In other studies, irrigations events were 60 or 80 mm up to four times for wheat (Hu et al. 2005) and 60–70 mm five to nine times a year in a fully irrigated plot (Zhang et al. 2006a). Our higher irrigation water amounts per single event may be explained by the lower frequency of irrigation scheduling and with the different geographical location. The history in this region may play a role as well as few decades ago soils were highly salinised and farmers were used to apply more water to leach out salts from the root zone (Shi and Xin 1983, cited in Chen et al. 2006b).

Above-ground biomass and grain yield

Above-ground biomass was simulated well, only the zero N treatment was underestimated during validation. This might have been related to underestimated N_{min} contents and resulting N stress in the model, as discussed below. The overestimated grain yields in the exact experiment after calibration may have been a result of pests and diseases that reduced the grain yield in the field and were not taken into account by the model. This is underlined by the high standard deviation for measured grain yield of wheat 2009/10.

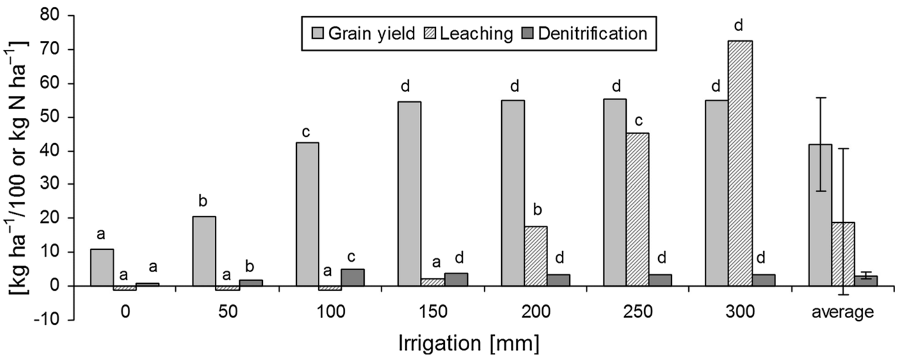

Figure 2.7: Effect of irrigation level on grain yield in kg $ha^{-1}/100$, nitrate leaching and denitrification in kg N ha^{-1} in the '3 + x' experiments on average of three farmers' fields for winter wheat 2010/11, based on reduced treatment. Average grain yield, leaching and denitrification of the irrigation variation results with confidence interval. X-axis shows irrigation level in mm. Columns of the same parameter followed by a *different letter* are statistically different (α = 5 %)

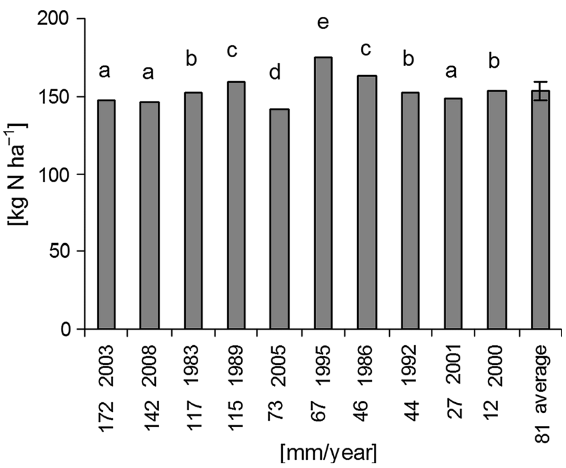

Figure 2.8: Effect of predictive weather on model-based NFR in kg N ha^{-1} in the '3 + x' experiments on average of three farmers' fields for winter wheat 2010/11, based on reduced treatment. Average NFR of the weather variation results with confidence interval. Columns followed by a different letter are statistically different (α = 5 %)

Plant N uptake

Plant N uptake was well simulated after calibration for the exact experiment but overestimated for the '3 + x' experiments during validation, where mineral N in soil was underestimated by the model. This indicates that the simulated extra N taken up by the plants could have been the amount missing in the soil. As these amounts were in the same order of magnitude the overall N budget was met by the model.

Soil mineral N content

Although soil N_{min} contents were displayed well by the model they were underestimated especially in the zero N plots, in particular in the ‘3 + x’ experiments (Table 2.4; Figure 2.4). These high N contents measured in the zero N plot could not easily be explained, even if atmospheric deposition as high as 80 kg N ha^{-1} $year^{-1}$ (Shen et al. 2009; Zhang et al. 2006b, 2008; Luo et al. 2013) and N mineralisation from model calculations were included. A lateral movement from highly fertilized plots in deeper soil layers seems unlikely due to the sub-humid conditions.

Beside the higher N uptake by plants as cause for N_{min} underestimation in the fertilised plots other possible reasons should be discussed as well. Overestimation of ammonia (NH_3) volatilisation by the model–a major pathway of N loss in the NCP next to N leaching–could play a role. In the model NH_3 volatilisation was set to be 15 % of the total applied urea N. Losses of equivalent magnitude as in this study were found in field experiments and studies under similar conditions (Cai et al. 1998, 2002; Pacholski et al. 2006, 2008; Yan et al. 2003; Zhang et al. 2004) while some authors also stated higher rates (Ju et al. 2009; Zhang et al. 2010). A more precise description of NH_3 volatilisation will therefore be included in the model and is the subject of a subsequent paper.

Soils in northern China show a higher potential for N mineralisation than those in the South (Roelcke et al. 2000, 2002a). Nitrogen mineralization in these soils is very rapid especially in summer, despite soil organic carbon (C_{org}) contents in soils being low. Therefore, nitrogen in crop residues of both winter wheat and previous summer maize left on the field after harvest may only be mineralised from late spring to autumn, enhancing the N supply of the summer crop.

Maximum denitrification rate in the model was derived from similar low C_{org} contents (Schneider 1991) to those reported typically for NCP (Cai et al. 2002; Cui et al. 2012; Ding et al. 2007; Fang et al. 2008; Ju et al. 2009; Liang et al. 2012; Zhang et al. 2011b). However, simulated losses were higher than observations (Ding et al. 2007; Ju et al. 2009; Liu et al. 2003; Zhang et al. 2004), and simulations (Fang et al. 2008; Hu et al. 2006) in the NCP and may therefore enhance underestimation of N_{min}. Differences in irrigation techniques and microbial composition might be the reason for the dissimilarities. In addition, losses by nitrification-born N_2O emissions in the NCP as described by Cai et al.

(2002), Cui et al. (2012), Ju et al. (2011) and Zhang et al. (2011b) were not considered by the model.

Real-time model-based NFR and effect of irrigation and weather on model-based NFR

A real-time NFR has never been carried out in the NCP so far. The amounts of applied N and the measured yields were of comparable magnitude to the application rates and yields in the comparative N-level field study of Liu et al. (2003). The NUEA was higher in the real-time NFR than in the recommendation based on the Nmin method (n.s.) (Figure 2.5). However, there is a remaining uncertainty of the input of water and nutrients leaching by flood irrigation. To achieve a better real-time NFR exact amounts of irrigation water applied need to be known.

This is underlined by the strong effect of irrigation level on model-based NFR. A higher N fertilisation seems to be needed to balance the nitrate losses from the root zone which were estimated to increase at irrigation rates of ≥200 mm (Figure 2.7). Although less nitrate is lost at low irrigation rates, lower water contents lead to a reduced water uptake and addition- ally to lower diffusion coefficients in the soil. HERMES considers N transport to the roots by mass flow and diffusion. A compensation through higher N fertilisation is calculated to create a higher gradient for diffusive transport to the root surface (Figure 2.6). Under rainfed conditions water stress limits plant growth; therefore, less N is required for biomass formation. These relationships are among the major causes for the heavy nitrogen over-fertilization prevalent in cropping systems with flood irrigation in the NCP (Fang et al. 2010; Ju et al. 2004; Zhao et al. 2006). The wide range of NFR (Figure 2.6) indicates a high uncertainty for model-based NFR concerning irrigation level which is also supported by the effect of irrigation on simulated grain yield and N leaching. Similar effects of irrigation level on leaching were found by Hu et al. (2006). The amount of 150 mm irrigation seems to be a threshold and an optimum for this study for almost all investigated variables as the NFR was lowest (except for zero irrigation), grain yield was high and leaching low.

The effect of weather on model-based NFR was less than the effect of irrigation amount as the variation in NFR and the confidence interval were both smaller in the weather scenarios (Figure 2.8). This was also found for simulated grain yield, N leaching and denitrification. Simulated yield variation was lower than naturally observed, because (1) only the weather during the main growing period was altered, (2) optimized nitrogen management reduced variability compared to sub-optimal management and (3) other factors like pests and diseases increased naturally observed yield variation.

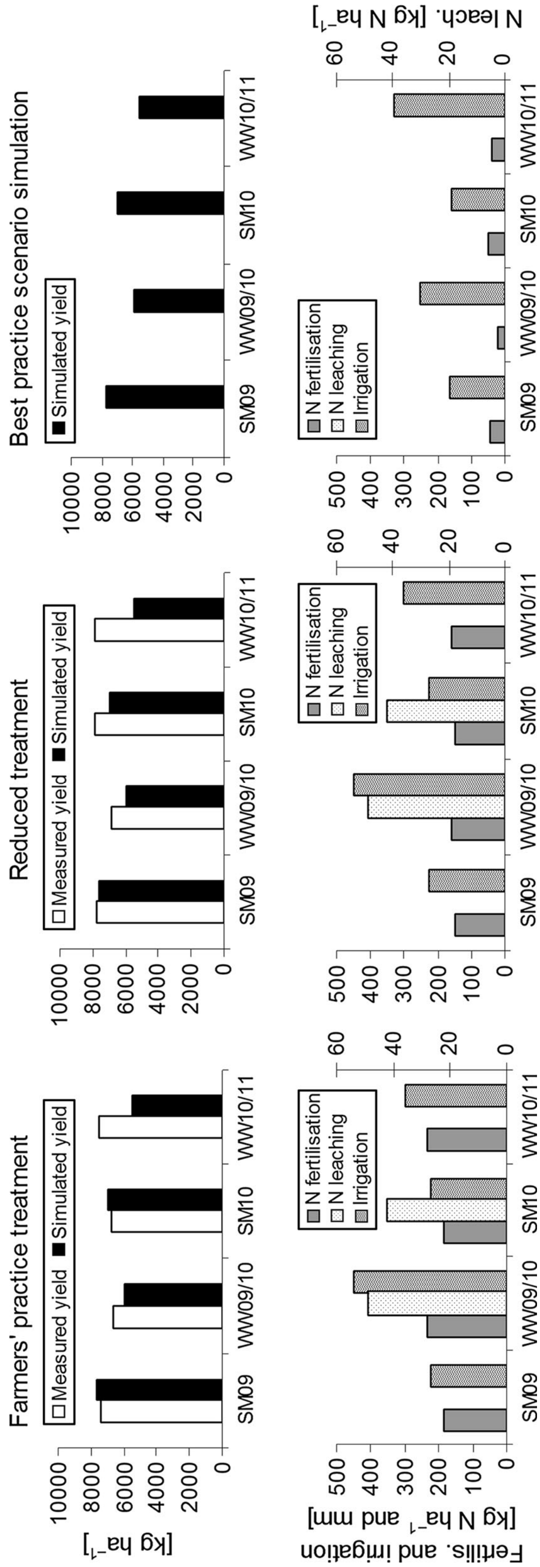

Figure 2.9: Measured and simulated grain yields in kg ha^{-1} and N fertiliser, irrigation water inputs and N leaching (below 2.0 m depth) in kg N ha^{-1} and mm for farmers' practice treatment and reduced N treatment in comparison with simulated grain yields, with N leaching (below 2.0 m depth) and N fertiliser and irrigation water inputs of a best-practice scenario simulation. *SM* summer maize, *WW* winter wheat

Table 2.5: Water and nitrogen inputs and N leaching in 0.9 m and 2.0 m depth for farmers' practice treatment (FP), reduced N treatment (RT) and best-practice scenario results (BP) in the '3 + x' experiments on average of three farmers' fields for two (summer maize 2009 + winter wheat 2009/10 and summer maize 2010 + winter wheat 2010/11) double-cropping seasons

	Precipitation (mm)	Irrigation (mm)	N fertilisation (kg N ha^{-1} $year^{-1}$)	N leaching 0.9 m (kg N ha^{-1} $year^{-1}$)	N leaching 2.0 m (kg N ha^{-1} $year^{-1}$)
2009/10					
FP	433	700	428	216	65
RT	433	700	311	177	65
BP	433	407	63	1	0
2010/11					
FP	448	526	427	47	51
RT	448	526	310	25	50
BP	448	480	84	4	1

Table 2.6: Grain yield, NFR/fertilisation, optimised irrigation, N leaching in 0.9 and 2.0 m and evapotranspiration for summer maize 2009 to winter wheat 2010/11 in the ''normal'', dry and wet best-practice scenario

Parameter	Scenario[a]	Maize 2009	Wheat 2009/10	Maize 2010	Wheat 2010/11	Average
Grain yield (kg ha^{-1})	N	7670a	5890a	6940a	5510a	6500a
	D	7080b	5510b	6820a	5350b	6190b
	W	7750a	4760c	5380b	5410c	5830c
NFR/fertilisation (kg N ha^{-1})	N	31.7a	31.0a	37.0a	46.7a	36.6a
	D	79.0b	20.0a	31.0a	68.0b	49.5ab
	W	19.7a	34.3a	88.3b	104.0c	61.6b
Irrigation (mm)	N	152.7a	254.3a	155.7a	324.0a	221.7ab
	D	164.3a	276.7a	184.3a	422.0b	261.8a
	W	154.7a	261.3a	143.3a	206.7c	191.5b
N leaching 0.9 m (kg N ha^{-1})	N	0.8a	0.2a	3.8a	0.0a	1.2a
	D	173.0b	-9.6a	-7.8a	-12.2	35.8b
	W	60.9a	30.3b	60.3b	19.1c	42.7b
N leaching 2.0 m (kg N ha^{-1})	N	0.0a	0.0a	0.0a	1.0a	0.3a
	D	43.4b	0.0a	0.0a	0.0a	10.8a
	W	2.8a	20.0b	95.1b	55.3b	43.3b
ETA (mm)	N	412.9a	478.4a	370.2a	603.4a	466.2a
	D	425.7b	510.6b	405.9b	547.6b	472.4b
	W	432.4c	487.6a	336.0c	617.3a	468.3a

Numbers followed by a different letter within a column for one parameter are significantly different ($\alpha = 5$ %)

[a] *N* ''normal'' scenario, *W* wet scenario, *D* dry scenario

Best-practice scenario simulation

Nitrogen inputs in the best-practice scenario simulation could be reduced to <20 % and water inputs to <75 % as compared to conventional practice (Figure 2.9). In this scenario, more water was saved in winter wheat compared to summer maize. Winter wheat has a higher water consumption than summer maize and only 20–30 % of total rainfall occur during the winter wheat growing season (Meng et al. 2012b). Hu et al. (2006) used similar irrigation amounts for farmers' practice in their study. However, they were able to reduce irrigation amounts to 50 % and total N fertilisation to a rate of 200 kg N ha^{-1} a^{-1}, which was about 50 % of the FP in this study. Similar reductions were reported in an experimental field study by Wang et al. (2010), where irrigation could be reduced to 60 % and N fertilisation to 55 %. The lesser reduction of irrigation in this study as compared to Hu et al. (2006) was probably due to a slightly higher ETA calculated by HERMES. In the study by Meng et al. (2012b) the measured ETA of summer maize 2009, winter wheat 2009/10 and summer maize 2010 was 294, 408 and 294 mm (conventional treatment) and 300, 324 and 285 mm (optimal treatment) per crop, respectively. This was lower than the scenario simulations by HERMES (382, 495 and 337 mm, respectively). Higher clay contents in the lower soil layers (He et al. 2013) and a different maize variety (Cui et al. 2009; Hu et al. 2006) can explain the differences between the estimations.

Nitrogen leaching was almost reduced to zero kg N ha^{-1} in the best-practice scenario (Figure 2.9) which agrees with the results stated by Fang et al. (2006), Li et al. (2007) and Liu et al. (2003). In their studies, leaching could be strongly reduced by adapting N rates and –in the case of Fang et al. (2006)– also irrigation rates. Leaching in the reduced N treatment was remarkably reduced only below 0.9 m depth but not below 2.0 m depth. This indicates that large amounts of N were accumulated in the 0.9–2.0 m soil layer as have also been found in northern China by Liu et al. (2003), Rees et al. (1997), Roelcke et al. (2000) and Zhao et al. (2006). The high N fertiliser reductions in this best-practice scenario simulation were probably possible due to high amounts of mineral N accumulated in the root zone prior to the experiment, which were used as initial values in the model in the first year (Hu et al. 2006; Zhao et al. 2007). Long-term simulations as described by Fang et al. (2008) are necessary to find out which N rate is required to maintain a stable yield level over the years as well as to take account of climatic variability.

The best-practice scenario simulation demonstrated that N fertiliser and irrigation water can be saved and leaching largely be prevented while yields are maintained. The comparison between wet, dry and ''normal'' scenarios showed that although more N and for the dry scenario also more irrigation water was required, yields could not be maintained at the level of the ''normal'' scenario. The model's NFR reaction to varying weather was comparable to the reaction estimated by Kersebaum et al. (2007b).

2.5 Conclusions

This study was the first to use real-time model-based N fertiliser recommendation (NFR) in the NCP. It shows simulations of local management practice conditions in comparison with other recommended practices. The HERMES model performed well under growing conditions of the NCP and was able to describe the relevant processes related to soil–plant interactions and mineral N. The best-practice scenario exhibits a high groundwater saving potential especially for winter wheat, ensuring a sustainable crop production in the NCP. Conventional flood irrigation as currently practiced by the farmers bears great uncertainties for water and nutrient distribution in the soil profile. Exact irrigation amounts should be known for future simulation studies. Farmers should be enabled to determine irrigation demand according to crop and site-specific requirements and have access to pumps with known capacity. The real-time model based NFR yielded, although not significantly, the highest NUE_A as compared to farmers' practice and the N_{min} method-based treatment. Thus the model can assist in reducing the excessive N fertiliser inputs. The highest potential to reduce N leaching can be exploited when using model-based NFR in combination with optimised irrigation practice. Besides an improved description of ammonia volatilisation a long-term regionalisation approach using this model on county scale in the NCP is currently being pursued. A Chinese language user- interface version has already been developed for HERMES that will be made available to Chinese scientists and extension services.

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3 Simulating *in situ* ammonia volatilization losses in the North China Plain using a dynamic soil-crop model

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Abstract

Ammonia (NH_3) volatilization is an important nitrogen (N) loss pathway in intensive agriculture of the North China Plain (NCP). Simulation models can help to assess complex N and water processes of agricultural soil–crop systems. Four variations (Var) of a sub-module for the deterministic, process-based HERMES model were implemented ranging from simple empirical functions (Var 3 and 4) to process-oriented approaches (Var 1 and 2) including the main processes of NH_3 volatilization, urea hydrolysis, nitrification from ammonium-based N fertilizer and changes in soil solution pH. Ammonia volatilization, plant growth and changes in ammonium and nitrate pools in the soil over several winter wheat–summer maize double-crop rotations at three locations in the NCP were simulated. Results were calibrated with two data sets (Dongbeiwang 1 and Shunyi) and validated using two data sets (Dongbeiwang 2 and Quzhou). They showed that the ammonia volatilization sub-module of the HERMES model worked well under the climatic and soil conditions of northern China. Although the simpler equations, Var 3 and 4, showed lower deviations to observed volatilization across all sites and treatments with a mean absolute error *MAE* of 1.8 and 1.4 in % of applied N, respectively, compared to process-oriented approaches, Var 1 and 2, with a *MAE* of 2.2 and 1.9 in % of applied N, respectively. Environmental conditions were reflected better by the process-oriented approaches. Generally, simulation results were satisfying but simulated changes in topsoil pH need further verification with measurements.

Keywords

NH_3 volatilization, simulation, nitrogen, fertilization, management

Abbreviations

ABC: ammonium bicarbonate (NH_4HCO_3);
DBW: Dongbeiwang experimental station (Haidian District, Beijing);
DTM: Calibrated Draeger-Tube Method;
ETA: actual evapotranspiration;
IHF: Integrated Horizontal Flux;
MAE: mean absolute error;
MBE: mean bias error;
ME: modeling efficiency;
NCP: North China Plain;
NH_3: ammonia;
NH_4^+: ammonium;
N_{min}: soil mineral nitrogen (nitrate-N (NO_3^--N) + ammonium-N (NH_4^+-N));
Var: Variation;

3.1 Introduction

Global ammonia (NH_3) emissions from terrestrial systems due to fertilization increased significantly from 1860 to the mid-1990s (Bouwman et al., 2005) and estimates indicate further increase. Atmospheric NH_3 can cause environmental pollution (Fangmeier et al., 1994), soil acidification (Bobbink et al., 1997) and can damage plants, though most agricultural crops are less sensitive to NH_3 than native vegetation or forests (Krupa, 2003). In 2010 China consumed about one third of the world's total mineral fertilizer nitrogen (N) according to Food and Agriculture Organization of the United Nations (FAO, 2013) statistics (33.1%) and International Fertilizer Association (IFA, 2013) data (31.2%). The mean mineral fertilizer N application rate in China per crop was 180 kg N ha^{-1} in 2010 (China Agricultural Yearbook, 2011). Urea (64.6%; IFA, 2013) and ammonium bicarbonate (NH_4HCO_3, ABC) are among the most commonly used mineral N fertilizers (Price Department of the NDRC, 2006 in Zhang et al., 2011). In China in particular, NH_3 emissions from mineral N fertilizers applied to upland crops were estimated to amount to more than 40 kg N ha^{-1} a^{-1} (Bouwman et al., 2002). The majority of anthropogenic NH_3 in China is emitted from mineral N fertilizers and animal/human excreta (Liu et al., 2011). Compared to other Asian countries, China was the only country where mineral fertilizer was the dominant source of NH_3 and N_2O emissions, with NH_3 losses exceeding those from animal manure (Yan et al., 2003).

The North China Plain (NCP) comprises 313,295 km^2 or 3.3% of the national area of China and is its main grain producing region. Zhang et al. (2011) pointed out that the NCP belongs to the regions in China having the highest NH_3 losses, with ammonia volatilization from this intensively managed cropland estimated to account for 27% of the total NH_3 emissions in China (Zhang et al., 2010). Main reasons for this are high soil surface N balance surpluses, the high soil pH of the alluvial soils of this region (Pacholski et al., 2008), high soil pH buffer capacity (Roelcke et al., 1996) and the excessive application rates of mineral N fertilizer, especially urea and ABC. Besides nitrate leaching, NH_3 losses are the main reason for low nitrogen use efficiencies (NUE) in the NCP (Zhang et al., 2008). Therefore, from both an agronomical and an ecological point of view, reducing NH_3 volatilization and nitrate leaching in cropland are essential tasks.

Improved fertilizer application methods such as incorporation or deep placement techniques, irrigation after fertilization, the use of a different fertilizer type, improved soil mineral N (N_{min})-based N management and urease inhibitors are options to reduce NH_3 volatilization. A range of accurate *in situ* ammonia volatilization measurement methods exists (for a recent comparison, see Ni et al., 2015). However, in particular measurements to compare different agronomical treatments and assess effects of reduction techniques on N losses are costly and time-consuming. Therefore, simulation models can help to estimate NH_3 emissions from cropland and clarify complex interactions concerning N dynamics and management. For the whole of China, Zhang et al. (2011) estimated NH_3 emissions from synthetic N fertilizers via the NARSES model. For the NCP Zhang et al. (2010) estimated NH_3 emissions from agriculture using emission factors recalculated by the RAINS model at a large scale. Pacholski et al. (2008) measured NH_3 losses in situ in a calcareous soil under different treatments on a plot scale near Fengqiu Agricultural Experimental Station, Henan Province. They subsequently simulated the losses using a modification of the deterministic ammonia volatilization model DUPAV by Rachhpal-Singh and Nye (1986a), which was developed based on laboratory experiments. The more complex RZWQM model, able to simulate water and nitrogen in the soil-plant system including NH_3 volatilization, was used at Luancheng Agroecosystem Experimental Station, Hebei Province by Hu et al. (2006) and at Yucheng Integrated Agricultural Experimental Station, Shandong Province by Fang et al. (2008). However, in most of these studies, NH_3 emissions were merely simulated and models were neither calibrated nor validated using wider measurements to check the performance of the model concerning NH_3 volatilization. Li et al. (2007) simulated NH_3 volatilization at Fengqiu Agricultural Experimental Station, Henan Province and Luancheng Agricultural Experimental Station, Hebei Province at a plot and county scale with the WNMM model. Although in their study NH_3 measurements were used for validation, pH change after fertilization and its influence on NH_3 volatilization were not considered in their approach. The WNMM model requires complex input data, while in agricultural practice data availability is usually limited. The nitrogen advisory model HERMES (Kersebaum, 2011) which is able to simulate N dynamics under limited input parameter conditions has recently successfully been applied to simulate N dynamics under field conditions in intensive agriculture of the NCP (Michalczyk et al., 2014). However, so far the HERMES model has considered NH_3 volatilization as a simple empirical non-dynamic fraction defined for each fertilizer type. None of the above mentioned approaches fit our requirements completely as HERMES uses less detailed input data to account for robust practical agricultural applications.

Thus our objectives are (1) to implement variations of a simple, deterministic, process-oriented ammonia volatilization sub-module for HERMES which includes the main processes involved in NH_3 volatilization, urea hydrolysis, nitrification of ammonium from fertilizer and a calculation of changes in soil pH; (2) to calibrate, validate and compare the simulation results of the four variations using four data sets in winter wheat–summer maize double-crop rotations at different locations in the NCP.

3.2 Methods

Experimental sites and data

Data from three experimental sites and four experiments all located in the NCP were used for this study. One field experiment (Heimann, 2013) was located in Shunyi District, Beijing (40°11' N 116°33' E), later referred to as Shunyi experiment. Average annual temperature and precipitation were 11.5°C and 500–700 mm, respectively (Hou et al., 2012). The soil was classified as a “chong ji wu he chao tu”, (cinnamon fluvo-aquic soil on alluvial deposits) according to the Chinese soil classification system (Second Chinese National Soil Survey, 1981) and as Eutric Cambisol with relictic hydromorphic characteristics according to IUSS Working Group WRB (2007) (Heimann et al., 2015). The texture, determined by sieving and sedimentation (Moschrefi, 1983), was a silt loam (Table 3.1). This experiment lasted from spring 2009 to autumn 2010. Maize (*Zea mays* L.) for breeding purposes was grown from mid-May to the end of September in both years, and no winter crop (commonly wheat) was sown in between. The experiment was carried out on two replicate sub-plots (4 m^2 each) located in a larger field. Maize fertilization and sprinkler irrigation management was done according to the local farm manager's practice (Table 3.2). Ammonia volatilization measurements were carried out from July 23 to August 11, 2010 using the calibrated Draeger-Tube Method (DTM) (Roelcke et al., 2002a; Pacholski et al., 2006). Average air temperature during the measurement period was 27.6°C. Soil sampling was carried out three times from March 2009 to March 2010. Soil samples were taken in five replicates per plot to a depth of 2 m and analyzed using automated continuous-flow analysis (TRAACS 2000 system, Bran and Luebbe, Norderstedt, Germany) for ammonium (NH_4^+-N) and nitrate (NO_3^--N). To determine gravimetric water contents soil samples were oven-dried at 105°C for 24 hours. Actual weather data was acquired from the National Climatic Data Center (NCDC) of the National Oceanic and Atmospheric Administration (NOAA, www.ncdc.noaa.gov), whose nearest station (Beijing, no. 545110) was about 20 km away, as well as purchased from the meteorological bureau of Shunyi District. Additionally, precipitation and wind speed were measured at Shunyi experimental site for the duration of the NH_3 volatilization experiment. Two several-year field experiments were conducted at the former experimental station "Dongbeiwang" of the China Agricultural University, Haidian District, Beijing (39° 55' N 116°20' E). The average annual temperature was 11.5°C and the average annual precipitation ranged from 500–650 mm, with about 70% falling during summer (Mack et al., 2005). The soil was classified as Calcic Cambisol (IUSS Working Group WRB, 2007) with a silt loam texture (Table 3.1). Both experiments were conducted in a winter wheat (*Triticum aestivum* L.)–summer maize double-crop rotation having three N level treatments, zero N, optimized N and conventional (farmers' practice) N treatment. Sprinkler irrigation was triggered at 45% to 80% of plant available soil water capacity using time domain reflectometry (TDR) probes (in 0.3 m increments from 0.15 m to 1.35 m) to measure the soil water content every fourth day, representing optimized irrigation. Management data are summarized in Table 3.2. Soil samples were taken in five replicates per plot for the depth increments 0–0.3 m, 0.3–0.6 m, 0.6–0.9 m and subsequently bulked. The soil samples were analyzed as mentioned above to determine nitrate, ammonium as well as soil gravimetric water contents. For winter wheat, plant samples were taken four to seven times and for summer maize about five times per growing season. The plant samples were oven-dried at 70°C and above-ground dry matter and grain yield, plant N content and N uptake were determined. Weather data was measured by the weather station of the experimental station. Experiment 1 (subsequently referred to as DBW 1; Chen et al., 2006) lasted from winter wheat season 1999/2000 to summer maize 2007. Winter wheat variety was Jingdong 8 and summer maize variety was Jingkeng 114. Experiment 2 (Su et al., 2007; later on referred to as DBW 2) lasted from winter wheat 2001/02 to summer maize 2004. Crop varieties, sowing dates, harvest dates and N treatments were generally the same as in DBW 1, but for some application events amounts of N fertilization and irrigation differed slightly (Table 3.2). Ammonia volatilization measurements, published in Su et al. (2007), were carried out five times in the optimized N treatment and six times in the conventional N treatment for a duration of 14 days each after every fertilization event. The NH_3 measurements were made with an automatic wind tunnel system (Braschkat et al., 1993).

A further field experiment was conducted by Li et al. (2002) in Quzhou County in the southern part of Hebei Province (36°52’ N and 115°01’ E) at the Quzhou Experimental Station of China Agricultural University (later on referred to as Quzhou). The average annual temperature and precipitation in Quzhou from 1980 to 2009 were 13.6°C and 488 mm, respectively, with about 60% of the annual precipitation occurring during summer. The soils were classified as Cambisol (IUSS Working Group WRB, 2007) with a silt loam texture (Table 3.1). Weather data was taken from the weather station of the experimental station. The field experiment lasted from summer maize 1999 to the beginning of winter wheat 2000/01, also within a winter wheat–summer maize double-crop rotation. Crop management was done according to local farmers’ practice (Table 3.2). Ammonia volatilization measurements, published in Li et al. (2002), were carried out with an Integrated Horizontal Flux (IHF) micrometeorological method (Denmead et al., 1977) after the top dressing of summer maize in July (1999 and 2000), after basal fertilization of winter wheat in October (1999 and 2000) and, for winter wheat 1999/2000 additionally, after top dressing in April 2000.

Table 3.1: Soil characteristics of the topsoil at Shunyi, Dongbeiwang and Quzhou experimental sites.

Experimental site	Depth	Clay[a]	Silt[b]	Sand[c]	Field capacity	Wilting point	Bulk density	pH (H_2O)	$CaCO_3$	C_{org}	C/N
	m	%	%	%	vol. %	vol. %	g cm^{-3}		%	%	
Shunyi	0–0.2	18	54	28	41	20	1.30	7.0	0.29	0.88	7.4
Dongbeiwang	0–0.3	16	56.5	27.5	37	11	1.33	8.0	5.25	1.33	12
Quzhou[d]	0–0.3	12	67	21	39	12	1.40	7.6	5.82	0.90	10

[a] <2 µm [b] 2 µm–63 µm, for Dongbeiwang 2 µm–50 µm [c] 63 µm–2 mm, for Dongbeiwang 50 µm–2 mm
[d] Soil texture according to expert finger testing and adaptation in the model

Table 3.2: Site management for experimental sites Shunyi, Dongbeiwang 1 (DBW 1), Dongbeiwang 2 (DBW 2), Quzhou.

Site	Crop	Sowing time	Basal fertilization date, amount and type[c, d, f] kg N ha^{-1}	Tillage date and depth[a] m	First top dressing fertilization date, amount and type[d, f] kg N ha^{-1}	First irrigation date and amount in total mm	Second top dressing fertilization date, amount and type[f] kg N ha^{-1}	Second irrigation date and amount in total mm	Harvest date
Shunyi	Maize 2009	May 10, 2009	May 10, 2009, 75 NPK	-[h]	July 13, 2009, 42 NPK	May 9, 2009, 99[g]	-	July 12, 2009, 99	Sept. 28, 2009
Shunyi	Maize 2010	May 10, 2010	May 10, 2010, 30 NPK	July 23, 0.05 Oct. 7, 0.25	July 23, 2010, 150 urea, 0.05[a]	May 9, 2010, 30	-	Aug. 21, 2010, 30	Sept. 28, 2010
DBW 1[b]	Winter wheat 1999/2000–2006/2007	Around Oct. 12	Around Oct. 6 CON=150 urea	Around Oct. 7, 0.25	Around March 24, OPT=16–110 urea; Around April 18, CON=150 urea	0–2 times Oct./Nov., 42–77	Around April 17, OPT=38–85 urea	3–6 times March–May, 131–265	Around June 20
DBW 1[b]	Summer maize 2000–2007	Around June 21, each year	-	-	Around July 13, OPT=10–60 urea; Around July 13, CON=100 urea	0–1 time June, 30–50	Around Aug. 7, OPT=15–90 urea; Around Aug. 7, CON=200 urea	0–2 times July–Aug., 22–65	Around Oct. 3
DBW 2	Winter wheat 2002/2003	Oct. 12, 2002	Oct. 22, 2002, CON=150 ABC	Oct. 23, 2002, 0.05	March 24, 2003, OPT=16–110 urea; April 20, 2003, CON=150 urea	Once Nov. 21, 2002, 42	-	3 times March–May, 2003, 131	June 12, 2003
DBW 2	Summer maize 2003 + 2004	June 18, 2003 + 2004	-	-	July 17, 2003, OPT=20 urea, CON=100 ABC; July 18, 2004, OPT=55 urea, CON=100 urea	July 17, 2003, 15; July 18, 2004, 20	Aug. 4, 2003, OPT=30 urea, CON=200 urea; Aug. 4, 2004, OPT=62 urea, CON=200 urea	Aug. 4, 2003, 15; Aug. 4, 2004, 20	Oct. 3, 2003 + 2004
Quzhou	Winter wheat 1999/2000 + beginning of 2000/2001	After fertilization and tillage (both years)	Oct.8, 1999, 191 ABC; Oct.18, 2000, 210 ABC	Oct. 8 1999, 0.20; Oct. 18 2000, 0.20	April 4, 2000 160 urea	April 4, 2000 100	-	-	June 10, 1999 + 2000
Quzhou	Summer maize 1999 + 2000	June 15, 1999 + 2000	-	-	July 27, 1999, 186 urea; July 18, 2000, 148 urea	July 27, 1999, 100; July 18, 2000, ‘30’[e]	-	-	End of Sept. 1999 + 2000

[a] = Tillage also represents fertilizer incorporation depth in m
[b] = Average dates for all winter wheat and all summer maize seasons, ranges for N fertilizer and irrigation if any
[c] = NPK, compound fertilizer
[d] = ABC, ammonium bicarbonate
[e] = Fertilization applied immediately after 30 mm of rain
[f] = Fertilizer was surface broadcast by hand if no tillage was carried out
[g] = Approximate value as used in simulation
[h] = As done in simulation

General description of the model and new algorithms for NH_3 volatilization

Model description

The one-dimensional, dynamic, process-based agro-ecosystem model HERMES was developed for application in agricultural fields under limited input data availability (Kersebaum, 2011). It simulates nitrogen and water dynamics in the soil and its losses, as well as plant N uptake, plant biomass and yield at a daily time step. Originally the model consisted of sub-modules for water balance, nitrogen mineralization, nitrogen transport, denitrification and crop growth.

Water dynamics are simulated with a capacity approach using soil texture classes and related parameters according to the German Soil Survey Manual (AG Boden, 2005) as default settings which can be adapted by the user. Water stress is assumed when the ratio of actual to potential transpiration falls below a crop- and development stage-specific threshold.

The N mineralization module calculates mineralization of soil organic N, decomposing plant material and organic fertilizer to nitrate according to temperature and soil moisture. Denitrification is considered to depend on soil nitrate content, soil water content and temperature. Ammonia volatilization from ammonium-based fertilizers and urea was so far calculated using a fertilizer-specific percentage loss from the amount of urea N or ammonium N applied with each fertilization. Nitrogen stress for crops is assumed when the crop's actual N concentration in above-ground dry matter falls below a critical level, which is determined by crop-specific dilution curves. The model was successfully applied for real-time nitrogen fertilizer recommendations (NFR) (Kersebaum et al., 2005; Michalczyk et al., 2014).

Crop growth is based on the SUCROS model by van Keulen et al. (1982), where biomass assimilation depends on global radiation and temperature. Phenological development is calculated on the basis of "growing degree days", considering day length and vernalization (e.g. in case of winter wheat) requirements of the specific crop according to Weir et al., (1984). Biomass partitioning to crop organs depends on phenological development as well as kc (crop coefficient) factors calculating crop specific evapotranspiration from a Penman-Monteith based reference grass evapotranspiration (Allen et al., 1998).

Volatilization sub-module

To account for different average temperatures during day- and nighttime, the time step in this new sub-module was divided into two half-day time steps, assuming that fertilizer application always happened during the day. All processes described in this sub-module were restricted to the upper three centimeters (cm) of the topsoil as we assumed that below this depth such processes would no longer take place (Rachhpal-Singh and Nye, 1984a; Pacholski et al., 2007). If no tillage was carried out all fertilizer was present in the top three cm of soil. Fertilizer incorporation, harrowing and ploughing homogenize the soil to tillage depth and consequently dilute the fertilizer N concentration in the upper three cm of the soil. The NH_4^+-N below three cm depth after the tillage event was attributed directly to the soil N_{min} pool by the model and was not further considered for volatilization.

The first process considered in the volatilization sub-module was the hydrolysis of urea to ammonium in the soil (Eq. 1). The amount of newly-formed NH_4^+ depends on the amount of urea applied, the temperature and moisture conditions and the initial soil pH in the upper three centimeters of the topsoil. Urease activity itself was not considered directly as the information is usually not available from standard measurements during field experiments.

$$NH_4Hydr = \frac{U * (Tv + 20) * RpH * RW}{100} \tag{1}$$

NH4Hydr is the amount of NH_4^+ hydrolyzed in mg N $L^{-1}d^{-1}$ in soil solution, *U* is the amount of urea applied in mg N L^{-1}, *Tv* is average day or night temperature of the day (°C) according to the time step, *RpH* (0–1) is the reaction coefficient for initial soil pH (based on Rachhpal-Singh and Nye, 1984b) and *RW* (0–1) the reaction coefficient for soil moisture (adapted from Stange and Neue, 2009).

$$RpH = \frac{\left(-0.6 * (pH_0 - 6.5)^2 + 9\right)}{7} \tag{2}$$

where pH_0 is the pH in the soil from the previous calculation.

$$RW = 1 - e^{-\left(\frac{\theta}{\theta_{crit}}\right)^{10}} \tag{3}$$

where θ is the soil water content of the day and θ_{crit} (= 0.1) is the critical lowest water content in cm^3 cm^{-3}.

Ammonium bicarbonate (ABC) fertilizer is a substance with a high NH_3 partial pressure which decomposes rapidly under high temperature and solar radiation. Therefore, a direct loss of NH_3 from the NH_4^+ fraction of this fertilizer at application time was empirically determined and added:

$$ABCloss = NH_4^+ * \left(1 + \frac{e^{(0.03 + Tv * 0.1 + RAD * 0.1)}}{300}\right) \tag{4}$$

where *ABCloss* is the direct NH_3 loss in kg N ha^{-1}, NH_4^+ is the ammonium part of the fertilizer N in kg N ha^{-1} and *RAD* is the solar radiation of the day in J m^{-2}.

Equations 5 to 9 apply to variation 1 (Var 1) of ammonia volatilization calculation, see sub-chapter 2.2.3 for description of Var 2 to 4.

The relationship between NH_4^+ and NH_3 in soil solution was described by using an adapted equation of Emerson et al. (1975 cited in Freney et al., 1985) and Denmead et al. (1982). It is mainly driven by soil pH and temperature.

$$NH_{3aq}Soil = \frac{NH_x}{\left(1 + 10^{\left(0.09018 + \frac{2729.92}{(Tv + 273.15)} - pH\right)}\right)} \tag{5}$$

where $NH_{3aq}Soil$ is NH_3 solute and NH_x is ammoniacal N (= NH_3-N + NH_4^+-N; from hydrolysis and from ammonium fraction of the fertilizer) solute in soil water in mg N L^{-1}.

To calculate the change from aqueous NH_3 to the gaseous phase another adapted equation by Emerson et al. (1975 cited in Freney et al., 1985) and Denmead et al. (1982) was used.

$$p[NH_3] = \frac{0.488 * NH_{3aq}Soil * (Tv + 273.15)}{10^{(1477.8/(Tv + 273.15) - 1.6937)}} \tag{6}$$

where $p[NH_3]$ is the ammonia partial pressure in Pa.

In a last step the transfer of gaseous NH_3 to the atmosphere was calculated empirically.

$$NH_3loss = p[NH_3] * RWf * WBf \tag{7}$$

where NH_3loss is loss of NH_3 due to volatilization in kg N ha^{-1}, *RWf* and *WBf* are empirical fractions to reduce NH_3 loss due to low or high soil water content and wind speed in combination with plant biomass dry weight, as indicator for plant height, respectively. The *RWf* summarizes the influence of soil water content on diffusive (aqueous and gaseous) and convective movements of ammoniacal N in the soil which partly occur during earlier phases of the volatilization process. These parameters are defined as a series of conditional sentences in the sub-module,

$$RWf \begin{Bmatrix} RWf = 1.0 \; if \; \theta > 0.1 < FC \\ RWf = 0.7 \; if \; \theta > FC \; or \; Prc > 1.6 \\ RWf = 0.5 \; if \; \theta < 0.1 \end{Bmatrix} \tag{8}$$

and

$$WBf\begin{cases} WBf = 1.0 \text{ if } Wind > 1.9 \text{ and } AGB < 100 \\ WBf = 0.8 \text{ if } Wind > 1.9 \text{ and } AGB > 100 < 2000 \\ WBf = 0.8 \text{ if } Wind < 2 \text{ and } AGB < 100 \\ WBf = 0.7 \text{ if } Wind > 1.9 \text{ and } AGB > 2000 \\ WBf = 0.6 \text{ if } Wind < 2 \text{ and } AGB > 100 < 2000 \\ WBf = 0.5 \text{ if } Wind < 2 \text{ and } AGB > 2000 \end{cases} \qquad (9)$$

where *FC* is the field capacity of the soil in cm^3 cm^{-3} and *Prc* the rainfall amount (including irrigation) of the day in cm, *Wind* is the average daily wind speed in m s^{-1}, *AGB* is the above-ground plant dry matter in kg ha^{-1}.

In case ABC fertilizer was used the *ABCloss* from Eq. 4 was added to NH_3loss:

$$NH_3loss = NH_3loss + ABCloss \qquad (10)$$

Nitrification from ammonium-based fertilizer or hydrolyzed urea was adapted from Stange and Neue (2009). First a temperature-dependent reduction coefficient was calculated from an O`Neill function which gives decreasing values when the temperature is below or above a chosen optimum:

$$R_T = \left(\frac{T_{max} - Tv}{T_{max} - T_{opt}}\right)^a * e^{a*\frac{(Tv - T_{opt})}{(T_{max} - T_{opt})}} \qquad (11)$$

where R_T (0–1) is the effect of soil temperature on nitrification, T_{max} is the maximum temperature set to 45°C, T_{opt} is the optimum temperature (= 30°C) and *a* (= 1.8) is a shape parameter of the O'Neill function.

Thereafter, a soil moisture reduction coefficient as first described by Diekkrüger et al. (1995) and later used by Stange and Neue (2009) was included. This function does not reduce the coefficient due to high water contents. As the HERMES model is a capacity model and the water content cannot increase above the field capacity of the chosen soil the following approach was used:

$$R_\theta = 1 - e^{-\left(\frac{\theta}{\theta_{crit}}\right)^b} \qquad (12)$$

where R_θ (0–1) is the effect of soil water content on nitrification, θ is the daily soil water content, θ_{crit} (= 0.1) is the critical water content for nitrification in cm^3 cm^{-3}, and *b* (= 16) is the shape parameter of the function.

Finally, to combine temperature and moisture functions a modified harmonic mean approach as described in Stange and Neue (2009) was used. The amount of N nitrified in kg N ha^{-1} (*NH_4nit*) depends on the amount of available ammonium in soil solution and on the reduction coefficients for temperature and soil moisture:

$$NH_4nit = \frac{0.8 * NH_4fert}{\left(\frac{1}{R_\theta} + \frac{1}{R_T}\right)} \tag{13}$$

where *NH_4fert* is the ammonium from applied fertilizer present in the upper three cm of soil in kg N ha^{-1}.

The pH is a driving force of aqueous NH_3 concentration in soil solution and thus of high importance for NH_3 volatilization. Therefore, a calculation of pH change in the vicinity of the applied fertilizer during the volatilization process was included. To keep the model simple no exact ion balance of the soil was calculated. This would have been difficult as biological ammonium immobilization, NH_4^+ adsorption and fixation, pH buffer capacity of the soil, CO_2 loss and $CaCO_3$ precipitation were not considered in this sub-module. Hence the change in pH the soil surface during NH_3 volatilization processes was solely related to the amounts of hydrolyzed ammonium, volatilized NH_3 and nitrified nitrate, but oriented on the H^+-ion production and consumption based on Rachhpal-Singh and Nye (1986a).

Changes in pH after application of urea were calculated as follows, depending on the amount of hydrolyzed NH_4^+ in mg N L^{-1} d^{-1} (Eq. 1)

$$pH_1 = pH_0 + \left(\frac{NH_4hydrol * 1.92}{1000}\right) \tag{14}$$

where pH_1 is the soil pH after hydrolysis of urea. The pH decrease at the soil surface after NH_3 volatilization depending on the volatilized NH_3 in mg N L^{-1} d^{-1} can be described as:

$$pH_2 = pH_1 - \left(\frac{NH_3lossmg * 1.92}{1000}\right) \tag{15}$$

where pH_2 is the pH after NH_3 volatilization and *$NH_3lossmg$* is the daily NH_3 loss in mg N L^{-1}. After nitrification the pH decrease depending on the nitrified NO_3^- in mg N L^{-1} d^{-1} was estimated as:

$$pH_3 = pH_2 - \left(\frac{NH_4nitmg * 1.92}{1000}\right) \tag{16}$$

Where pH_3 is the pH after nitrification and NH_4nitmg is the daily amount of nitrified nitrate in mg L^{-1}.

Variations for ammonia volatilization calculations

Three additional variations within this sub-module were implemented replacing one or several of the equations five to nine from the previous sub-chapter.

The second approach (Var 2) was according to equilibrium considerations by Avnimelech and Laher (1977) using:

$$NH_{3aq}Soilmol = \frac{1}{\left(-6.64 * 10^{-3} + 19.29 * \frac{1}{NH_x mol}\right)} \tag{17}$$

instead of Eq. 5. Where $NH_3aqSoilmol$ is NH_3 solute in mol L^{-1} and NH_xmol is NH_x in mol L^{-1}. All other equations remained the same.

The third approach (Var 3) was according to Chambers et al. (1999). Here Eqs. 5–9 were replaced by:

$$NH_3loss = \frac{N_{max} * t}{(t + K_m)} \tag{18}$$

Where N_{max} is NH_x*0.33 representing the maximum NH_3 loss in kg N ha^{-1}. The t is time of the day after fertilizer application and K_m is the time in days when NH_3loss is 0.5 N_{max}.

The fourth approach (Var 4) is a simple multiple regression considering environmental conditions such as soil ammoniacal N (NH_x) in kg N ha^{-1}, pH, average air temperature (Tv), wind speed ($Wind$) and above ground biomass (AGB). Again Eqs. 5–9 were replaced by:

$$NH_3loss = 0.3 * NH_x * pH * Tv * \left(Wind * \left(\frac{10^4}{(AGB + 10^3)}\right) + 10\right) * 10^{-4} \tag{19}$$

Calibration, validation, statistics

Crop and soil parameters have previously been calibrated against data from DBW 1 (unpublished), and data of Michalczyk et al. (2014) without the volatilization sub-module using measured soil water contents, soil mineral N contents, above-ground plant biomass, plant N uptake and yield at DBW 1 (winter wheat 1999/2000 to summer maize 2007). The same procedure was repeated with the new model version including the volatilization sub-module using Var 1, where only slight adaptations were necessary. For initial soil water and soil mineral N (N_{min}) contents first measured values from each experiment were used. The active pool of soil organic N for mineralization was set to 17% of N_{org} as in Michalczyk et al. (2014).

The volatilization sub-module in general (using Var 1) was calibrated by means of measured NH_3 volatilization data of the Shunyi experiment (summer maize 2010). All other parameters remained the same as calibrated against data of DBW 1. Variations 2 to 4 were calibrated on the same data set. After calibration the volatilization sub-module (using Var 1) was validated against data of the optimized N and conventional N treatments of DBW 2 (for winter wheat 2002/03, summer maize 2003 and summer maize 2004) and Quzhou (summer maize 1999 until beginning of winter wheat 2000/01). Finally DBW 2 and Quzhou were run with Var 2 to 4 as well. We assumed that the different NH_3 measurement techniques (calibrated DTM, automatic wind tunnel system, IHF micrometeorological method) give comparable results if in case of the wind tunnel conditions of wind speed and precipitation and in case of DTM evenly distributed urea application are taken into account (Mannheim et al., 1995; Pacholski et al., 2008; Ni et al., 2015), and since the DTM had been calibrated against the IHF method under similar agro-climatic conditions in China (Pacholski et al., 2006).

To evaluate the model's performance (for the overall model, DBW 1 and the sub-module, Shunyi, DBW 2, Quzhou) the following statistical measures were used: the mean absolute error *MAE* (Shaeffer, 1980) which is the mean deviation between simulated and measured values in its corresponding unit, the mean bias error *MBE* (Addiscott and Whitmore, 1987) to show if the model over- or under-predicted, and the modeling efficiency *ME* (0–1) according to *Nash* and Sutcliffe (1970) to assess modeling quality, where one represents a perfect fit. Values above zero indicate that the variation within the simulated values is higher than the variation within the measurements.

3.3 Results

Calibration of plant, soil water and N parameters against Dongbeiwang 1 experimental data

The calibration results for above-ground biomass showed a good fit of simulated and measured values in the DBW 1 experiment (Figure 3.1). The *MAE* was slightly greater than one ton in all treatments and the negative *MBE* indicated that this deviation resulted from a small underestimation by the model (Table 3.3). The general model performance for biomass simulation showed good results, with a *ME* of 0.85 over all variants and crops (data not sown).

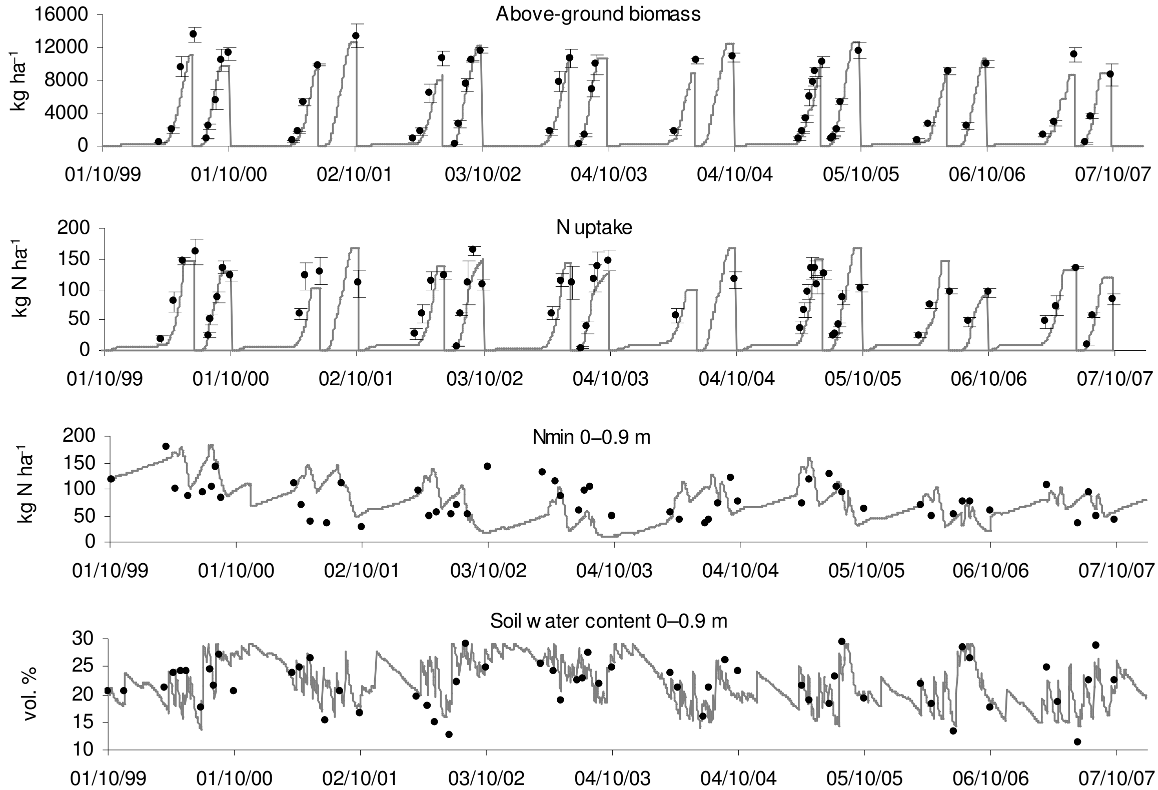

Figure 3.1: Time courses of above-ground biomass in kg ha^{-1}, N uptake in kg N ha^{-1}, N_{min} in 0–0.9 m depth in kg N ha^{-1} and soil water content in 0–0.9 m depth in vol. % for the optimized N treatment for sub-module variation 1 of Dongbeiwang 1 experiment for winter wheat 1999/2000 to summer maize 2007. Error bars show the standard deviation.

For grain yield estimation, the model performance was satisfactory especially in the conventional and optimized N treatments, with *MAE* just above one ton. The positive *MBE* indicated a tendency for overestimated yields (Table 3.3). Over all variants and crops the *ME* for grain yield simulation was 0.41 (data not shown).

The simulated plant N uptake reflected the observations well, especially in the optimized N treatment (Figure 3.1). The negative *MBE* indicated a small underestimation of plant N uptake in all treatments by the model (Table 3.3). Over all variants and crops the *ME* was 0.92 (data not shown).

Table 3.3: Mean absolute error (*MAE*), mean bias error (*MBE*) and modeling efficiency (*ME*) of above-ground biomass and grain yield in kg ha^{-1}, plant N uptake and soil N_{min} in kg N ha^{-1} and soil water content in vol. % for the zero, conventional and optimized N treatments of Dongbeiwang 1 (DBW 1) experiment for sub-module variation 1 from winter wheat 1999 until summer maize 2007.

			Zero N treatment	n[a]	Conventional N treatment	Optimized N treatment	n[b]
Above-ground biomass wheat	kg ha^{-1}	*MAE*	915.01	25	1394.07	1238.84	30
		MBE	428.31		−1380.69	−1220.12	
		ME	0.81		0.83	0.86	
Above-ground biomass maize	kg ha^{-1}	*MAE*	1292.01	20	945.79	920.11	27
		MBE	−1119.22		184.24	−318.86	
		ME	0.70		0.91	0.90	
Grain yield wheat	kg ha^{-1}	*MAE*	877.98	8	417.00	510.21	8
		MBE	877.98		−84.48	−109.72	
		ME	−0.10		0.63	0.41	
Grain yield maize	kg ha^{-1}	*MAE*	1445.16	8	1142.67	861.89	8
		MBE	333.13		740.57	857.39	
		ME	−1.00		0.13	−0.10	
N uptake wheat	kg N ha^{-1}	*MAE*	18.68	25	37.38	28.06	28
		MBE	6.35		−29.26	−16.54	
		ME	0.36		0.09	0.36	
N uptake maize	kg N ha^{-1}	*MAE*	21.01	20	19.83	22.02	27
		MBE	−11.89		7.34	−0.84	
		ME	0.14		0.68	0.62	
Soil N_{min} 0–0.9 m	kg N ha^{-1}	*MAE*	15.71	30	193.24	36.87	52
		MBE	−7.81		175.79	6.53	
		ME	0.11		−2.69	−0.89	
Soil water content 0–0.9 m	vol. %	*MAE*	3.07	35	2.86	2.89	56
		MBE	−2.74		−0.61	−0.58	
		ME	−0.25		0.34	0.25	

[a] Zero N treatment
[b] Conventional and optimized N treatments

The soil mineral N content was mostly well simulated in the optimized N (Figure 3.1) and also in the zero N treatment, while in the conventional N treatment the model performance was not as good (Table 3.3). In the conventional N treatment the upper soil layer was simulated slightly better than the deeper layers (not shown). The *MBE* in the conventional treatment was positive in all layers and indicated an overestimation of soil N_{min} content by the model. In the optimized N treatment *MAE* and *MBE* represented a good fit of measured and simulated values, while the *ME* was not as good (Table 3.3). Due to poorer model performance in the conventional treatment the *ME* over all variants was −2.55 in 0–0.9 m depth (data not shown).

The soil water content was simulated well by the model in the optimized (Figure 3.1) and conventional treatments, while the zero N treatment shows a slight underestimation of measurements by the model (Table 3.3). In all treatments the 0–0.3 m depth was simulated better than the deeper layers (not shown). Over all variants the *ME* was 0.42 in 0–0.9 m depth (data not shown).

Calibration of the NH_3 sub-module against Shunyi experimental data

The calibration of the NH_3 sub-module using Var 1 showed a generally good fit of measured (22.5 kg N ha^{-1}) and simulated (27.7 kg N ha^{-1}, of 150 kg urea-N ha^{-1}) cumulative NH_3 losses (Figure 3.2a). The *MAE* was 8.9 kg N ha^{-1} and the *ME* was −0.98 reflecting a moderate model performance (Table 3.4). A positive *MBE* of 8.9 kg N ha^{-1} indicated an overestimation by the model, which mainly occurred in the first week of the measurement period (Figure 3.2a and b).

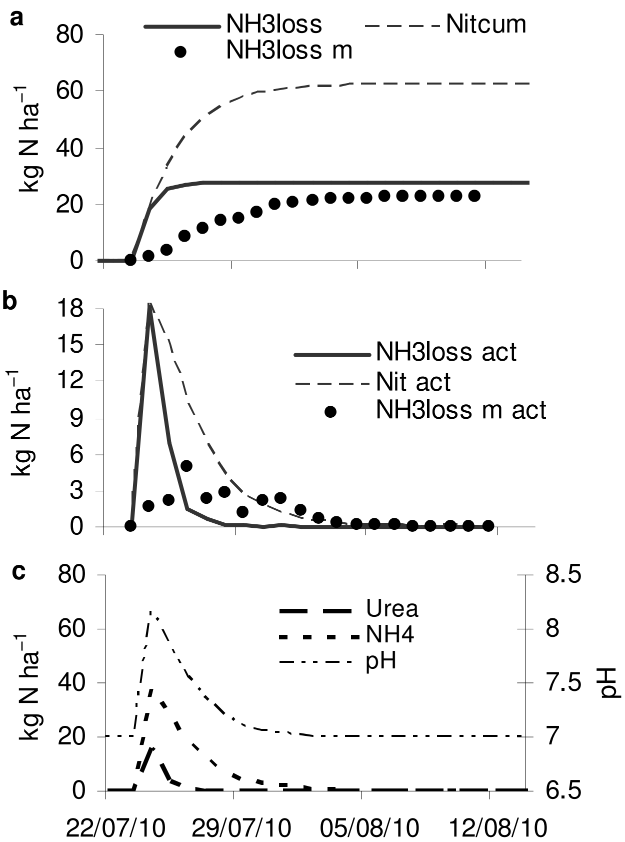

Figure 3.2: (a) Simulated cumulative NH_3 loss (NH3loss) and nitrate from nitrification (Nitcum) in kg N ha^{-1} 0.03 m^{-1} (depth) and measured cumulative NH_3 loss (NH3loss m) in kg N ha^{-1}; (b) simulated daily time course of NH_3 fluxes (NH3loss act) and nitrate from nitrification (Nit act) in kg N ha^{-1} 0.03 m^{-1} d^{-1} and measured daily NH_3 loss (NH3loss m act) in kg N ha^{-1} d^{-1}; (c) simulated urea pool (Urea) in kg N ha^{-1}, simulated NH_4^+ pool (NH_4^+) in kg N ha^{-1} and simulated soil pH in 0.03 m^{-1} (depth) for sub-module variation 1 of Shunyi experiment for the NH_3 measurement period from July 22 to August 11, 2010.

Variation 2 underestimated cumulative NH_3 losses, while Var 3 and 4 simulations fit well to the measurements (Table 3.4). The simulated urea and ammonium pools as well as soil pH were corresponding similarly to the amount of volatilized NH_3 in all variations. The major part of the urea pool in the model was hydrolyzed within two days after fertilization and completely within five days. The majority of remaining simulated ammonium in soil was nitrified within seven days and completely within the first 13 days of the simulation.

The model (Var 1) simulated a rise in soil pH due to urea hydrolysis by 1.16 pH units and thereafter a return to the original level prior to NH_3 volatilization and NH_4^+ nitrification (Figure 3.2c).

Validation of the NH_3 volatilization sub-module against Dongbeiwang 2 and Quzhou experimental data

The volatilization sub-module was first validated against NH_3 measurements in the DBW 2 experiment. Both the conventional and the optimized treatment were generally well simulated by the model. Although in ammonia volatilization Var 1 the deviations in percent of applied fertilizer N of measured and simulated values were lower in the conventional N treatment (Table 3.5) a better model performance was achieved by the optimized N treatment (Table 3.4). In the conventional treatment the model (Var 1) underestimated cumulative NH_3 volatilization after ABC application to winter wheat in October 2002 and to summer maize in July 2003 by 8.3 and 9.6% of the applied fertilizer, respectively (Table 3.5). After urea fertilization to winter wheat April 2003, to maize in August 2003 and to summer maize in July and August 2004, NH_3 volatilization was overestimated by 10.7, 7.7, 12.5 and 25.9% of the applied fertilizer, respectively (Table 3.5). The cumulative NH_3 volatilization in the optimized treatment in winter wheat 2002/03 (April 2003) and summer maize 2003 (two applications, July and August 2003) were underestimated by the model (Var 1) by 34.1, 48.5 and 34.0% of the applied fertilizer, respectively, while the NH_3 loss simulations in summer maize 2004 matched the measurements better (Table 3.5). Variation 2 performed similar as Var 1 (Table 3.4 and 3.5), while the model performance of Var 3 was better than Var 1 and 2 especially in the optimized treatment (Table 3.4). However, similar to Var 1 the Var 3 estimated the absolute NH_3 loss well in the conventional treatment, except for the first two measurements and worse in the optimized treatment (underestimation, Table 3.5). Simulations with Var 4 matched the measured values well in both treatments. The *ME* over both treatments was −0.3, −0.7, −0.3 and 0.6 using the final cumulative values of Var 1, 2, 3 and 4, respectively. The simulated temporal soil pH change using Var 1 after urea fertilization in the DBW 2 experiment was between 0.22 and 0.62 pH units and between 0.23 and 1.35 pH units in the optimized and the conventional treatments, respectively.

Table 3.4: Mean absolute error (*MAE*), mean bias error (*MBE*) and modeling efficiency (*ME*) of NH_3 volatilization for the conventional N treatment of Shunyi, conventional and optimized N treatments of Dongbeiwang 2 (DBW 2), and conventional N treatment of Quzhou experiments for four sub-module variations (Var).

		Conventional N treatment Shunyi	Conventional N treatment DBW 2	Optimized N treatment DBW 2	Conventional N treatment Quzhou	Model variation
n		20	88	74	66	
MAE	kg N ha^{-1}	8.93	24.14	4.26	11.04	Var 1: Emerson et al. (1975) and Denmead et al. (1982)
MBE	kg N ha^{-1}	8.93	21.67	−1.82	3.71	
ME		−0.98	−2.46	−0.37	0.59	
MAE	kg N ha^{-1}	7.08	12.09	5.52	16.54	Var 2: Avnimelech and Laher (1977)
MBE	kg N ha^{-1}	-6.66	-10.75	-5.51	-14.08	
ME		-0.21	-0.18	-1.11	0.28	
MAE	kg N ha^{-1}	1.94	16.11	2.55	17.90	Var 3: Chambers et al. (1999)
MBE	kg N ha^{-1}	1.06	15.40	0.83	9.33	
ME		0.88	-0.78	0.51	0.36	
MAE	kg N ha^{-1}	3.62	8.08	3.25	14.51	Var 4: Simple Regression
MBE	kg N ha^{-1}	-1.04	2.43	−1.09	6.61	
ME		0.72	0.62	0.21	0.54	

At Quzhou experimental site, the model reproduced the measured NH_3 loss well (Table 3.4, Figure 3.3). Using Var 1 in summer maize 1999 NH_3 volatilization was overestimated by 15.3% of the applied urea fertilizer, while in 2000, also in summer maize volatilization was matched well (Table 3.6). Whereas the measurement and simulation of NH_3 volatilization in winter wheat, October 1999, fit well, the NH_3 losses in winter wheat in April and October 2000 were slightly underestimated by the model (Var 1) by 8.0% and 5.7% of the applied urea fertilizer, respectively. The *MAE, MBE* and *ME* were smaller than in the conventional treatment of the DBW 2 experiment (Table 3.4). The model performance of Var 2 to 4 was similar to that of Var 1, showing only a small overestimation, except for Var 2, where the model underestimated NH_3 volatilization (Table 3.4). This could also be found in the absolute values, where only the simulations in October 2002 and 2003 fit the measurements. Contrary to Var 2, Var 3 and 4 overestimated volatilization in October 1999 and 2000, while the other measurements were met well (Table 3.6). The simulated temporal soil pH change after urea fertilization in the Quzhou experiment using Var 1 was between 1.00 and 1.14 pH units.

Table 3.5: Measured[a] and simulated NH_3 volatilization for four sub-module variations (Var) in % of applied fertilizer N for the conventional N and optimized treatments of Dongbeiwang 2 and corresponding amounts of irrigation and fertilization from October 2002 to August 2004.

	Both treatments		- Dongbeiwang 2 - Conventional N treatment									
	Irrigation	Fertilization[b]	NH_3 loss measured		NH_3 loss simulated; Var 1: Emerson et al. (1975) and Denmead et al. (1982)		NH_3 loss simulated; Var 2: Avnimelech and Laher (1977)		NH_3 loss simulated; Var 3: Chambers et al. (1999)		NH_3 loss simulated; Var 4: Simple Regression	
	mm	kg N ha^{-1}	kg N ha^{-1}	% of N applied	kg N ha^{-1}	% of N applied	kg N ha^{-1}	% of N applied	kg N ha^{-1}	% of N applied	kg N ha^{-1}	% of N applied
23.10.02	0	150a	15.2	10.1	2.8	1.9	12.9	8.6	72.2	48.1	12.6	8.4
20.04.03	90	150u	29.9	19.9	46.0	30.7	12.8	8.5	54.9	36.6	27.8	18.5
17.07.03	15	100a	24.1	24.1	14.5	14.5	15.2	15.2	22	22.0	24.2	24.2
04.08.03	15	200u	66.3	33.2	81.7	40.9	12.6	6.3	56.5	28.3	35.9	18.0
18.07.04	20	100u	22.1	22.1	34.6	34.6	7.7	7.7	24.8	24.8	25.3	25.3
04.08.04	20	200u	47.4	23.7	99.2	49.6	15.9	8.0	52.7	26.4	41.6	20.8
			- Dongbeiwang 2 - Optimized N treatment									
23.10.02	0	0	-	-	-	-	-	-	-	-	-	-
20.04.03	90	34u	14.4	42.4	2.8	8.2	2.8	8.2	12.2	35.9	6	17.6
17.07.03	15	20u	11.5	57.5	1.8	9.0	1.3	6.5	5.4	27.0	4	20.0
04.08.03	15	30u	13.2	44.0	3.0	10.0	1.9	6.3	7.9	26.3	4.9	16.3
18.07.04	20	55u	15.1	27.5	12.2	22.2	4.2	7.6	13.5	24.5	13.5	24.5
04.08.04	20	62u	15.9	25.5	14.6	23.4	4.9	7.9	15.5	24.9	11.8	18.9

[a] as given in *Su* et al. (2007) (wind tunnel experiment)
[b] a=ammonium bicarbonate; u=urea

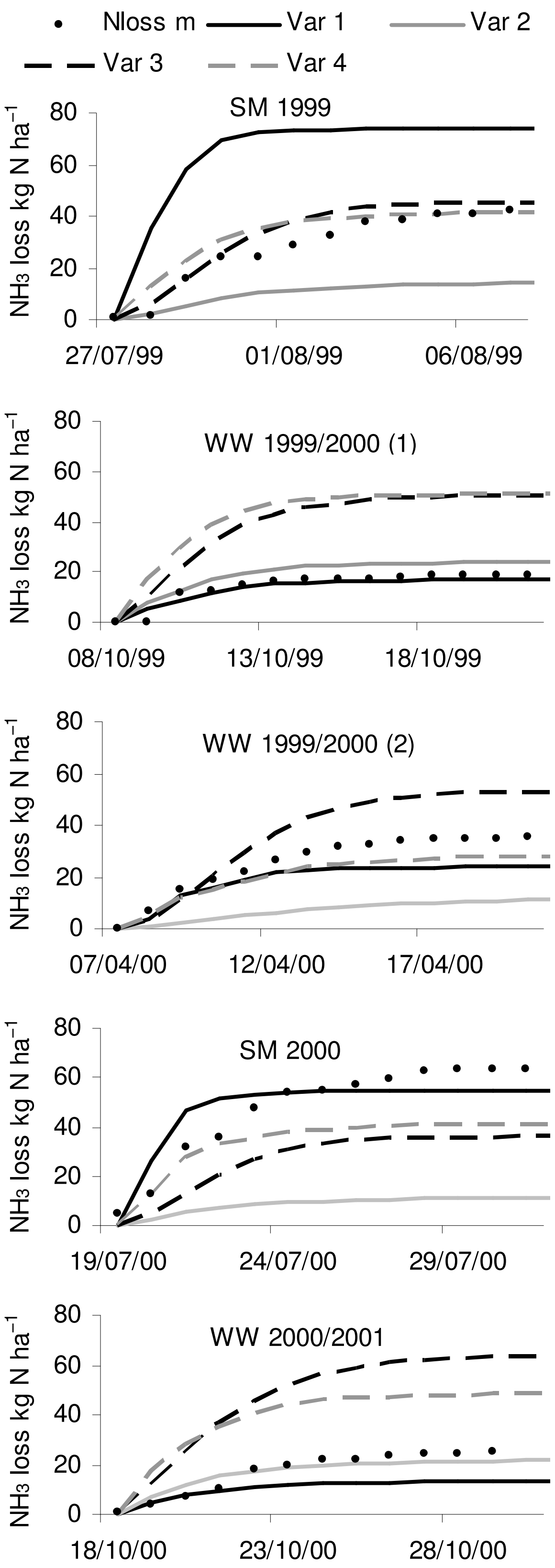

Figure 3.3: Simulated cumulative NH_3 loss (lines) in kg N ha^{-1} for four sub-module variations (Var 1 to Var 4) and measured cumulative NH_3 loss (dots) in kg N ha^{-1}, after N fertilization of Quzhou experiment from summer maize (SM) 1999/2000 to beginning of winter wheat (WW) 2000/2001.

Table 3.6: Measured[a] and simulated NH_3 volatilization for four sub-module variations (Var) in % of applied fertilizer N for the conventional N treatment of Quzhou experiments and corresponding amounts of irrigation and fertilization from July 1999 to October 2000.

	Quzhou Conventional N treatment											
	Irrigation/incorporation	Fertilization[b]	NH_3 loss measured		NH_3 loss simulated; Var 1: Emerson et al. (1975) and Denmead et al. (1982)		NH_3 loss simulated; Var 2: Avnimelech and Laher (1977)		NH_3 loss simulated; Var 3: Chambers et al. (1999)		NH_3 loss simulated; Var 4: Simple Regression	
	mm/m	kg N ha^{-1}	kg N ha^{-1}	% of N applied	kg N ha^{-1}	% of N applied	kg N ha^{-1}	% of N applied	kg N ha^{-1}	% of N applied	kg N ha^{-1}	% of N applied
27.07.99	100/ -	186u	42.9	24.5	74.1	39.8	14	7.5	45.4	24.4	41.2	22.2
08.10.99	0/0.2	191a	18.9	9.9	17.1	9.0	24.1	12.6	50.5	26.4	51.3	26.9
07.04.00	100/ -	150u	35.1	24.0	24.0	16.0	11	7.3	53.1	35.4	28	18.7
19.07.00	30 precipitation/ -	148u	63.5	37.0	54.9	37.1	10.9	7.4	36.1	24.4	41	27.7
18.10.00	0/0.2	210a	25.2	12.0	13.3	6.3	21.5	10.2	63.6	30.3	48.3	23.0

[a] as given in *Li* et al. (2002)
[b] a=ammonium bicarbonate; u=urea

3.4 Discussion

Calibration of plant, soil water and N parameters against Dongbeiwang 1 experimental data

The HERMES model with a NH_3 volatilization sub-module was firstly applied against DBW 1 experimental data in the NCP. The calibration of plant, soil water and N parameters resulted in satisfying outputs providing a good basis for further model use. Above-ground plant biomass was simulated well by the model, although it showed a small underestimation (e.g. *MBE* conventional N, both crops −639.4 kg ha^{-1}, not shown) which corresponds to the slightly underestimated plant N uptake (e.g. *MBE* conventional N, both crops −11.3 kg N ha^{-1}, not shown). Grain yield was simulated satisfactorily by the model. Its positive *MBE* indicated a slight overestimation which might have resulted from yield reduction by pests and diseases *in situ* which were not considered by the model. Soil mineral N contents were simulated well with a low *MAE* except for the conventional treatment where the positive *MBE* indicated an overestimation. This might have occurred due to a simulated convective transport through upward water movement by the model which transported N_{min} upwards that had accumulated in soil layers below 0.9 m. The volumetric soil water content was simulated adequately by the HERMES model, even though it was slightly underestimated (*MBE* 0–0.9 m: −2.7 vol. %, zero N to −0.6 kg vol. %, optimized N).

Calibration of the NH_3 volatilization sub-module against Shunyi experimental data

The calibration of the model against *in situ* NH_3 measurements in the Shunyi experiment was generally satisfying. Zhang et al. (2004) and Pacholski et al. (2006; 2008) measured NH_3 volatilization losses that were in the same range in the NCP, considering weather, soil and management conditions. Simulations by Fang et al. (2008) were equally in a similar range, while model results of Hu et al. (2006) were much lower and those by Li et al. (2007) a bit higher than in this study using Var 1. Results of Var 2 were in the same range as of Hu et al. (2006). Unfortunately the soil pH was not given for the studies of Hu et al. (2006) and Fang et al. (2008) and for Li et al. (2007) a precise site management description was missing.

The HERMES model with NH_3 volatilization sub-module using Var 1 and 4 overestimated NH_3 volatilization during the first week of the Shunyi experiment. In the studies by Roelcke et al. (2002a) in July 1991, Pacholski et al. (2006; 2008) in June/July 1998 and July 1999 and Li et al. (2007) in July 1999 the highest NH_3 losses following urea application occurred during the first few days after N fertilization as well. The main reason for the overestimation in the Shunyi experiment is that urea fertilizer had been uniformly incorporated in 0–0.05 m soil depth immediately following surface broadcast application (Table 3.2). This led to a slight delay (Figure 3.2a) and to lower daily maximum ammonia fluxes (Figure 3.2b), but to no reduction in the overall amount of measured NH_3 volatilization losses (Figure 3.2a). Moist initial soil conditions and the high air temperatures during most of the Shunyi experiment (average 27.6°C) are likely to have carried unhydrolized urea N, as well as part of the urea-derived ammoniacal N, and HCO_3^- ions in soil solution upward with the evaporative water stream (Kirk and Nye, 1991; Roelcke et al., 2002a). Kröbel et al. (2010) discussed an existing upward flow at DBW site as the DNDC model used in their study did not accurately estimate soil water contents. Upward and downward flows were only considered for water and nitrate in the HERMES model so far.

The simulated NH_3 volatilization using Var 2 was lower than the measurements, probably due to the fact that only the processes related to NH_4-NH_3 equilibrium were considered in the study of Avnimelech and Laher (1977), which did not react on changes of temperature and soil pH. According to their study there was no option to further calibrate the equation used, thus it could not be adapted to other related processes such as nitrification.

For high NH_3 volatilization in the first days after urea application a quick urea hydrolysis, as simulated in our study, is required. Such rapid hydrolysis of urea was also found by Rachhpal-Singh and Nye (1984b), Roelcke et al. (2002a) and Denmead et al. (2010) who reported the highest urease activity within the first two days of their laboratory incubation experiment. The fast simulated nitrification of ammonium N resulting from urea hydrolysis was found to be similar in an incubation study by Addiscott (1983). Calcareous soils in northern China typically show very high N mineralization and nitrification rates (Roelcke et al., 2002b; Lan et al., 2013).

The influence of soil cation exchange capacity (CEC) on NH_4^+ adsorption and soil pH buffer capacity on pH were not considered in our model approach. Although cation adsorption by the soil does limit NH_3 losses from surface-applied N fertilizers to some extent, CEC does not efficiently control NH_3 losses at even the highest CEC values (Fenn and Hossner, 1985). Likewise, the effect of NH_4^+ adsorption on NH_3 losses was less important compared to initial soil pH and soil pH buffer capacity in the sensitivity analysis of the DUPAV model by Rachhpal-Singh and Nye (1986c). As described by Rachhpal-Singh and Nye (1986a, b) and Roelcke et al. (1996) the soil pH rises in the first few days following urea application due to hydrolysis and thereafter decreases again, due to protons (H^+) remaining at the immediate soil surface during the volatilization of NH_3. This rise and decline in pH was also described by the HERMES model, though there were differences in magnitude in the study of Roelcke et al. (1996), where surface $CaCO_3$ content was high (10%) which buffered pH change. This suggests that this magnitude may have been overestimated, since soil pH buffer capacity, clay and $CaCO_3$ contents and CO_2 loss was not taken into account.

Validation of the NH_3 volatilization sub-module against Dongbeiwang 2 and Quzhou experimental data

The validation results of DBW 2 showed a generally satisfying model performance in simulating NH_3 volatilization especially for the conventional N treatment. Simulation results matched measured NH_3 losses less well for the optimized treatments in DBW 2, regarding absolute values and the percentage NH_3 volatilization of applied fertilizer (using Var 1 and 2). A similar model performance was found for calibrated NH_3 losses in Fengqiu County for the WNMM model (Li et al., 2007). In the conventional treatment in DBW 2 NH_3 volatilization was underestimated for the first ABC fertilizer application in October 2002; although a direct loss of NH_3 from the ammonium fraction of the fertilizer at application time was included in the sub-module. Reasons for the discrepancy may be a low mean air temperature of 2.9°C during the measurements (ranging from −6.9 to 10.6°C), while the temperature inside the wind-tunnel might have been above the ambient temperature during daytime due to a high daily solar radiation (1181 J cm^{-2} d^{-1} on average during the measurement period October 22 to November 4, 2002). The overestimation of NH_3 losses by the model using Var 1 under conventional fertilization was much higher in August 2004 than in August 2003, even though the same amount of urea had been applied (200 kg N ha^{-1}). A possible explanation might be that the influence of temperature on NH_3 volatilization may have been overestimated by the model; since the mean air temperatures during the first week after fertilizer application in the two experimental periods differed (23.9°C in 2003 and 27.6°C in 2004). This trend could also be found for Var 4 where the influence of temperature on NH_3 volatilization seems to be less pronounced. In the optimized treatment of DBW 2 the lower amount of applied urea in the model might have played a role in underestimating NH_3 loss using Var 1 in April, July and August 2003 as less urea hydrolyzed results in a smaller simulated soil pH rise and thus in lower NH_3 volatilization. Simulated NH_3 losses in July and August 2004, also optimized treatment but with higher N application rates, fit the measured data better. However, some uncertainties may also have been involved related to the wind tunnel measurements in DBW since NH_3 losses were calculated from continuous measurements as daily averages and precipitation was not considered in the experiment. As described by Bouwmeester et al. (1985) and McInnes et al. (1986), light precipitation (<10–15 mm) providing adequate moisture for urea hydrolysis to occur and to desorb ammoniacal N from soil may result in increased NH_3 losses. The simulations with Var 2 showed an underestimation of NH_3 volatilization in DBW 2, which might have occurred due to the same reasons as described in the previous chapter. The missing temperature sensitiveness could have played the major role since especially the NH_3 measurements during summer month were underestimated by the model. The opposite occurred for NH_3 simulations with Var 3, where the simulations fit well the measurements during summer but over predicted in April and October. In this case the N_{max} and K_m value from Equation 20 need to be adapted for colder weather conditions.

The validation at the Quzhou experiment showed better results compared to DBW 2, with smaller deviations of measured and simulated values. This is especially underlined by a good *ME* in the Quzhou experiment compared to DBW for all variations. For Quzhou similar trends like in the previous chapters were found and previous explanations apply accordingly. However, with Var 4, which should be sensitive to temperature, the model still overestimates the NH_3 measurements during October 1999 and 2000. One explanation could be that the amount of ammoniacal N has a too strong influence on the final NH_3 estimation.

The calculated changes in soil pH reflected the theory well in the simulations at all three locations, although they were probably a little overestimated as mentioned before. In the conventional treatment in DBW pH changes were much greater than in the optimized treatment due to a higher N fertilization rate, which was similarly described in the model by Rachhpal-Singh and Nye (1986c). In their sensitivity analysis, the initial pH had the strongest effect on NH_3 losses compared to the other parameters tested. Simulated changes in pH after fertilization, especially after application of urea, should be further investigated using measured data. However, the soil pH has been known to be both difficult to measure and to simulate correctly, in particular in situ, in other studies as well (e.g., Sommer et al., 2003).

General model performance across all simulations

Regarding the general performance of the variations, a simple approach as Var 3 or 4 can give satisfying results with a *MAE* across all sites and treatments of 1.8 and 1.4 in % of applied N, respectively, compared to process-oriented approaches, Var 1 and 2, with a *MAE* of 2.2 and 1.9 in % of applied N, respectively. Considering single volatilization events it seems that approaches only calculating according to a maximum N amount and a rate coefficient (e.g. Var 3) are not sufficient to respond to changing environmental influences. To reflect these conditions approaches as in Var 4 or even additional physical and chemical processes as in Var 1 are necessary.

Even though the results showed some discrepancies between measurements and simulations, HERMES (all variations) was generally able to describe cumulative NH_3 losses, measured on three different sites in the correct order of magnitude, whereby NH_3 losses measured with micrometeorological method could be described better by the model compared to wind-tunnel measurements. The *ME* of −0.08, −0.91, −0.56 and 0.32 over all simulations using final cumulative values in variations 1, 2, 3 and 4, respectively, indicated a sufficient overall model performance, even though its complexity and time resolution is limited compared to other deterministic models designed especially to describe the NH_3 volatilization process. However, the detailed inputs required by these models are often not available in agricultural practice in China.

3.5 Conclusion

The HERMES model, with the new ammonia volatilization sub-module using four variations was able to describe cumulative NH_3 volatilization sufficiently well for practical purpose, considering the data sets of the field experiments. This also includes most other relevant N related processes in a soil–plant system in the NCP with sub-humid climate and alkaline soil conditions. To work well under different environmental conditions, environmental inputs are necessary as in Variation 1, but when input data is limited a simple empirical approach as in Variation 3 could be an option. However, depending on weather conditions, the simulated initial NH_3 fluxes were higher compared to the measured ones, which could generally be a little delayed at the beginning and stronger or longer lasting at the end of volatilization process after urea fertilization. Furthermore, upward and downward movement of ammonium and alkalinity should be included in the model. Cation exchange, pH buffer capacities and pH buffering effects caused by dissolution and precipitation of $CaCO_3$ and CO_2 loss could be optional inputs amongst the underlying physical and chemical processes in the model for future studies. The model is to be further validated with other data sets from the NCP or regions with similar soil and climatic conditions, especially regarding soil pH change.

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4 A simple approach to simulate the application of a nitrification inhibiting fertiliser in the North China Plain

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Abstract

In intensive agriculture in the North China Plain high mineral nitrogen fertiliser applications result in high nitrogen losses causing environmental problems. Nitrification inhibitors are an option to reduce nitrogen leaching losses. Simulation models can help to access complex nitrogen processes, calculate ammonia losses and the influence of nitrification inhibitors on changes in ammonium and nitrate patterns in soil. Therefore, additional algorithms for nitrification inhibition were implemented in the NH_3 sub-module of the HERMES model. Results showed that the nitrification inhibition tool of the HERMES model worked well under the climatic and soil conditions of northern China. N_2O emissions resulting from nitrification processes for improving the denitrification outputs could be included in the model.

4.1 Introduction

High mineral nitrogen (N) application rates in intensive winter wheat-summer maize double crop rotations in the North China Plain (NCP) cause high N losses from the system. In comparison to other Asian countries, China was the only country where mineral fertiliser was the dominant source of NH_3 and N_2O emissions (Yan et al. 2003).

Cai et al. (2002) found that irrigation after fertilization reduced NH_3 losses and deep point placement of fertiliser reduced denitrification as well as NH_3 volatilisation losses. Additionally the use of a different fertiliser type, such as Calcium Ammonium Nitrate or Ammonium Sulphate-Nitrate (Yang et al. 2011) and an adapted crop rotation (Zhou et al. 2008) can reduce N losses. For ammonium based fertilizers, nitrification inhibitors as well as improved soil N_{min}-based N management can reduce N_2O emissions, denitrification and N leaching losses. In a study of Ju et al. (2011) N_2O emissions, resulting mainly from the nitrification process in the NCP, could be effectively reduced by using a nitrification inhibitor.

Measurements *in situ* to assess effects of reduction techniques on N losses require special instruments and accurate experiments are costly and time consuming, thus simulation models can help to clarify complex interactions in N dynamics.

The effect of nitrification inhibitors was estimated on a worldwide scale by Del Grosso et al. (2009) by reducing the nitrification rate by 50% for 2 months after fertilization using the DAYCENT model. Giltrap et al. (2010) used the NZ-DNDC model with a similar approach on a plot scale in New Zealand, to simulate the inhibition of nitrification using the duration and effectiveness of the nitrification inhibitor. The decay rate was expressed as exponential function of the half-time of the inhibitor but their approach was not temperature-dependent. No such approach has been used in the NCP yet.

The agro-ecosystem, nitrogen advisory model HERMES (Kersebaum 1995; Kersebaum and Beblik 2001; Kersebaum 2007) which can simulate N dynamics under limited input data conditions was previously used to simulate N dynamics under field conditions in the NCP (Michalczyk et al. 2014) However, nitrification inhibition was not considered so far.

Thus our objectives were to test the nitrification inhibition tool within the ammonia volatilisation sub-module of the HERMES model and simulate the influence of nitrification inhibitors on the ammonium and nitrate pools in the soil, N losses and plant parameter in a winter wheat–summer maize double-crop rotation in the NCP.

4.2 Methods

The "exact field experiment" later on referred to as Quzhou 1 (Hartmann et al. 2015), took place next to the CAU's experimental station "Quzhou". Weather data was taken from the own weather station of the experimental station. The experiment lasted from 2009 summer maize until 2011 summer maize within a winter wheat–summer maize double-crop rotation. It consisted of eight N level treatments of which only the reduced urea (46% N) and the reduced ASN_{DMPP} (26% N; Ammonium sulphate Nitrate + 3.4-Dimethyl pyrazolephosphate as nitrification inhibitor, ENTEC® 26) fertiliser treatments are considered here. For more details see Hartmann et al. (2015).

The new algorithms for nitrification inhibition, which were implemented into the HERMES model were as follows. The amount of nitrified N in kg ha^{-1} (NH_4nit) depends on the available ammonium in soil solution and on the reduction coefficients for temperature (R_T) and soil moisture (R_θ):

$$NH_4nit = \frac{0.4 * 2 * NH_4fert}{\frac{1}{R_\theta} + \frac{1}{R_T}} * Inh_{nit} \tag{1}$$

Where NH_4fert is the ammonium in the upper three cm of soil from applied fertiliser in kg N ha^{-1} and Inh_{nit} is a coefficient for nitrification inhibition in case a fertiliser with nitrification inhibitor is applied.

$$Inh_{nit} = \frac{(TSF)}{(TSNI)} \tag{2}$$

Where TSF is the cumulative temperature sum since fertilisation and $TSNI$ is a fertiliser specific factor defining the temperature sum required to reduce nitrification inhibition to zero to represent the decay of the inhibitor. See equation no. 11 and 12 of the previous chapter for calculation of reduction coefficients for temperature (R_T) and soil moisture (R_θ). Table 4.1 gives an overview of parameters used and their value.

The simulation of nitrification inhibition was tested on data of Quzhou 1 experiment. For this simulated plant N uptake, biomass, yield, soil water contents and soil ammonium, nitrate and urea contents as well as NH_3 volatilisation, denitrification and nitrification were compared to measured values of the reduced urea and reduced ASN_{DMPP} treatments.

For evaluation of the model's performance the following modelling statistics were used: mean absolute error (*MAE)*, mean bias error (*MBE)* and modelling efficiency (*ME)*. For more details see Michalczyk et al. (2014).

Table 4.1: Model parameters used for the simulation of ammonia volatilisation and nitrification inhibition.

Parameter	Unit	Value
a		1.8
b		16
T_{max}	°C	45
T_{opt}	°C	30
TSNI		1700[a]
θ_{crit}	vol. %	0.1

[a] value for ASN_{DMPP} fertilizer

4.3 Results

Model performance indicators for the nitrification inhibition tool of the HERMES model showed satisfying simulation results (Table 4.2). Measured N uptake and above-ground biomass were slightly underestimated by the model, while yield was a bit overestimated as seen on the *MBE* in Table 4.2. Soil water content was underestimated in 0.3–0.6 m, especially in autumn 2009 (6.8 vol. %) and spring 2010 (17.3 vol. %). While in the soil depth of 0–0.3 m and 0.6–0.9 m the model overestimated the measured soil water contents slightly as seen on the positive *MBE* in Table 4.2.

Table 4.2: Mean absolute error, mean bias error and modelling efficiency of N uptake, above-ground biomass and yield for the ASNDMPP treatment in the Quzhou 1 experiment.

	N uptake	Above ground biomass	Yield	Water content 0–0.3 m	Water content 0.3–0.6 m	Water content 0.6–0.9 m	Water content 0–0.9 m
	kg N ha^{-1}	kg ha^{-1}	kg ha^{-1}	vol. %	vol. %	vol. %	vol. %
MAE	39.30	1060.00	773.40	4.29	6.48	3.57	3.86
MBE	-4.14	-479.54	354.80	0.70	-1.51	0.42	0.01
ME	-0.17	0.93	-3.48	0.41	-2.74	-1.76	-0.30

As the model only calculates ammonium after fertilization in the top 0.03 m and the measurements of NH_4^+ and nitrate were done for the top 0.3 m, no model statistics could be calculated. Total mineral N including nitrate was simulated worse for the ASN_{DMPP} treatment compared to the reduced urea treatment (not shown). Anyhow, the dynamics of the change of NH_4^+ in the topsoil after fertilization was well represented by the model (Figure 4.1). A model run with a similar virtual ammonium fertiliser without inhibition function (Figure 4.1c) resulted in smaller amounts of NH_4^+ in the pool which was nitrified faster compared to the normal ASN_{DMPP} fertiliser simulation run (Figure 4.1a). This fast turnover was also simulated in the reduced urea simulation run (Figure 4.1e). Ammonia volatilisation was higher in the ASN_{DMPP} fertiliser simulation (2.39% of applied NH_4^+, Figure 4.1b) than in the ammonium fertiliser simulation without nitrification inhibitor (0.52% of applied NH_4^+, Figure 4.1d) and highest in the reduced urea treatment (28.84% of applied NH_4^+, Figure 4.1f).

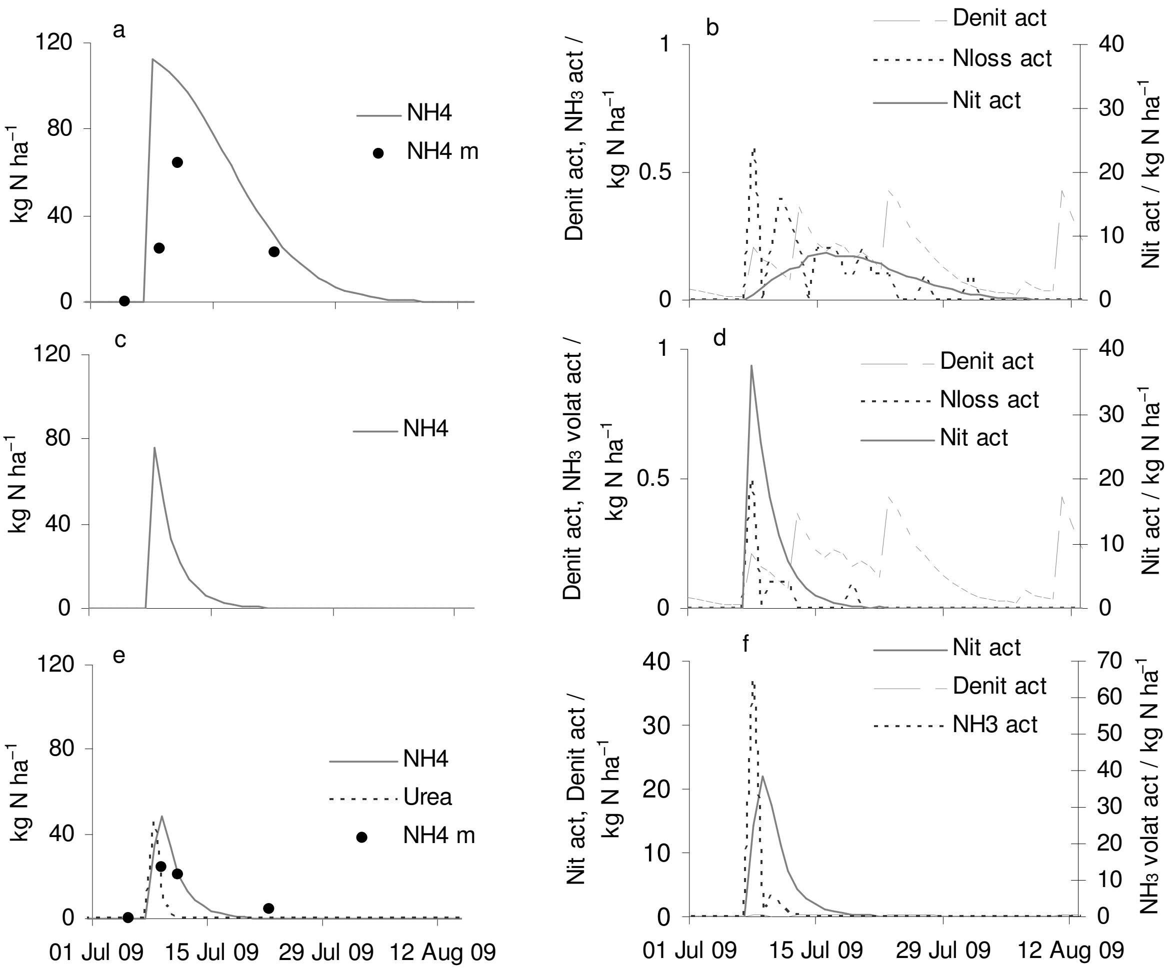

Figure 4.1a-f: Simulated NH4+ (NH4), measured NH4+ (NH4 m), urea (Urea), simulated nitrate from nitrification of ammonium fertiliser (Nit act), daily denitrification (Denit act) and daily NH3 loss (Nloss act) in kg N ha−1 for the first top dressing of summer maize 2009 in Quzhou 1 for the ASNDMPP treatment (a, b, 160 kg N ha−1), the ammonium treatment without nitrification inhibition (c, d, 160 kg N ha−1) and the reduced urea treatment (e, f, 160 kg N ha−1).

No difference in denitrification could be found between the ASN_{DMPP} fertiliser simulation (13.75% of applied N) and the ammonium fertiliser simulation without nitrification inhibitor (13.75% of applied N, Figure 4.1b, d). Denitrification in the reduced urea treatment was simulated slightly lower (12.83% of applied N, Figure 4.1f). Over the whole experimental period nitrate leaching in the ASN_{DMPP} fertiliser simulation amounted to 248 kg N ha^{-1}, which was lower than in the ammonium fertiliser simulation without nitrification inhibitor (280 kg N ha^{-1}); leaching was lowest in the reduced urea treatment (197 kg N ha^{-1}) (not shown).

4.4 Discussion

The soil water content, N uptake, above-ground biomass and yield were simulated well by the model, indicating a generally well model performance for the ASN_{DMPP} treatment. Unfortunately, this treatment could not be compared to an ammonium-based (ASN) fertiliser treatment without nitritrification inhibitor. Urea, the fertiliser used in the "normal" reduced treatment, lets the soil pH rise locally. Thus the ASN_{DMPP} treatment was compared to the reduced urea treatment as well as to a simulation run with a virtual fertiliser similar to ASN_{DMPP} fertiliser but without nitrification inhibitor. The changes in NH_4^+ contents in the topsoil in these three variants show that the model was able to simulate nitrification inhibition sufficiently well. In the ASN_{DMPP} fertiliser simulation the ammonium pool lasted longer in the soil after fertilization and may thus reduce the risk of nitrate leaching as ammonium is much less mobile and less prone to leaching as nitrate. This was confirmed as simulated cumulative leaching was less (32 kg N ha^{-1} difference) in the ASN_{DMPP} fertiliser variant compared to the virtual fertiliser without nitrification inhibition over the whole experimental period. This effect was also found by (Yang et al. 2016). Anyhow cumulative leaching in the reduced urea treatment was even 83 kg N ha^{-1} lower, which might be due to high ammonia volatilisation losses.

Ammonia volatilisation in the ASN_{DMPP} fertiliser simulation was higher compared to the virtual ASN fertiliser simulation run without nitrification inhibitor. This was probably due to larger and longer availability of ammonium in the soil and soil solution as nitrification was inhibited. Similar results were reported by Soares et al. (2012) for a study in Brazil where NH_3 volatilisation was 7% of total applied N higher from urea with nitrification inhibitor than urea without.

No differences in denitrification could be found between the ASN_{DMPP} fertiliser simulation (13.75% of applied N) and the virtual ASN fertiliser simulation without nitrification inhibitor (13.75% of applied N). This was also found in other studies with ASN_{DMPP} (Kleineidam et al. 2011), or where dicyandiamide was used as nitrification inhibitor (Giltrap et al. 2010). The delayed increase of the nitrate pools through nitrification inhibition did not have an influence on final total denitrification losses. However, in a study in the NCP, where N_2O losses from nitrification (nitrifier denitrification) play a very important role (Cai et al. 2002; Zhang et al. 2011; Cui et al. 2012), N_2O emissions could be reduced with an nitrification inhibitor (Ding et al. 2011). Therefore, the model needs to be adapted for N_2O losses from nitrification (nitrifier denitrification) which play a very important role in the North China Plain (Cai et al. 2002; Zhang et al. 2011; Cui et al. 2012).

The nitrification inhibition tool was tested for one experiment only. To verify these results the tool still needs validation on other data sets.

4.5 Conclusion

A tool for nitrification inhibition was implemented and tested for the HERMES model. The model was able to well describe nitrification inhibition, including most other relevant N related processes in a soil–plant system in the NCP with sub-humid climate and alkaline soil conditions.

However, simulations of nitrification inhibition need further verification with measurements.

Changes in ammonium and nitrate (N_{min}) contents in the topsoil and ammonia volatilisation after fertilization with nitrification inhibitor were simulated well by the model but no differences in denitrification amount could be simulated. Thus, processes of nitrification-born N_2O emissions should be considered in the model in the future, which are particularly important under conditions in the NCP.

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5 Quantifying nitrogen loss and water use via regionalization and long-term scenario simulations in the North China Plain

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Keywords: regional modelling, nitrogen and water management, county scale, GIS

Abstract

Intensive winter wheat–summer maize double-cropping systems in the North China Plain often have high nitrogen (N) losses and water use causing harmful threats to the environment. The HERMES model was used to quantify spatial long-term (31 years) N and water losses on county scale in order to find best-practice management applications. Six management scenarios were performed. Results show simulated annual long-term N losses in whole Quzhou County in Hebei Province of 296.8 kg N/ha under common farmers practice treatment and 101.7 kg N/ha under optimized treatment including N fertilizer recommendation and automated irrigation (OPTai) which is a proportion of 0.57 and 0.4 of the applied fertilizer N, respectively. Spatial differences in N losses were found due to survey specific different average N input amounts among the townships. More than 260 kg N/ha/a from fertilizer input and 190 kg N/ha/a from N losses and around 115.7 mm/a on average could be saved when optimized treatments were used instead of farmers practice. On clay loam soil only OPTai could maintain crop yield without drought stress. The optimized treatments had the lowest N inputs and N losses but they did not seem to be able to sustain the organic matter pools. Thus, a precise adaptation of N and water to actual weather conditions and plant growth needs to be done. Especially for simulations on clay loam soil drought resistance parameters in the model might need more adjustment to local wheat (*Triticum aestivum* L.) and maize (*Zea mays* L.) varieties.

5.1 Introduction

Nitrogen (N) surplus and N loss related to inefficient irrigation water use in intensively managed agricultural systems is a known problem in most industrialized countries (Bouwman *et al.,* 2005). During the past decades this problem became urgent in the North China Plain (NCP) where winter wheat (*Triticum aestivum* L.) – summer maize (*Zea mays* L.) double-crop rotation is the major cropping system on this intensely managed arable land. In this system annual N loads of more than 500 kg N/ha combined with flood irrigation of about 350 mm (Kröbel *et al.,* 2010) cause a harmful threat on agricultural ecosystems and to the environment in the region.
Simulation models, among other methods, such as an ''improved, mineral N (N_{min}) method'' (Cui *et al.,* 2008), integrated soil-crop system management which combines model simulation with in-season root-zone N management (Chen *et al.,* 2011), active canopy sensor – based precision nitrogen management (Cao *et al.,* 2017) and optimized fertigation (Zhang *et al.,* 2019) are used in the NCP to assess nitrogen dynamics on plot scale, county scale and regional scale to find solutions for this problem. While agro-ecosystem models on plot scale are able to simulate complex interactions in soil-plant-atmosphere systems, their application at regional scale needs strong generalization of input data to remain feasible in terms of computing capacity, practical use and data accessibility. Such large-scale calculations often investigate only one output variable such as maize production potentials (DNDC, Binder *et al.,* 2008), ammonia (NH_3) volatilization (e.g. NARSES, Zhang *et al.,* 2011) or nitrous oxide (N_2O) emissions (DNDC, Li *et al.,* 2001). Li *et al.* (2007) used the water and nitrogen management model (WNMM) at regional scale in Fengqiu and Luancheng Counties. Their model predicts water movement and soil N dynamics well and has a good GIS application integrated but also requires detailed inputs and high computing power while a more process-oriented denitrification could improve the model. Anyhow the regional application lasted only for one year. That was similar to the two year study of Deng *et al.* (2011) in Sichuan province using DNDC model to calculate N loading in a small watershed. Li *et al.* (2014) used the same model to simulate N leaching in North China which lasted only for two years. A simulation study over 19 years using the same model on regional scale in Quzhou County in the NCP (Liu *et al.,* 2006) as well as a 30 year but plot-scale study using DNDC model at Hengshui, NCP (Zhang *et al.,* 2017) only focussed on soil organic carbon.

Until now nobody has addressed all main N and water inputs and losses together with detailed crop modelling on a specific defined soil and varying regional management within Quzhou County, Hebei Province, nor used model-based soil type specific N fertilizer recommendation on county scale using average county management to find out best practice, with long-term simulations in a winter wheat–summer maize double-cropping system.

In order to perform such an integrative approach the HERMES model was used in the current study (Kersebaum and Beblik 2001) which was widely tested in Europe (Herrmann *et al.,* 2005; Palosuo *et al.,* 2011; Rötter *et al.,* 2012; Hlavinka *et al.,* 2014; Kollas *et al.,* 2015; Salo *et al.,* 2016; Yin *et al.,* 2017), Canada (Kersebaum *et al.,* 2008), USA (Malone *et al.,* 2017) and in China as well (Michalczyk *et al.,* 2014; 2016) as it can operate with minimal data inputs and simulates water and N dynamics satisfactorily.

The aim of the current study was to use HERMES to upscale field-scale simulations on the basis of regional soil, climatic, N and water management and land use classification information to assess long-term regional as well as township management specific differences of N and water dynamics and crop distribution.

The objectives of the study are (1) to calculate long-term regional N losses and the fate of water at county scale in a winter wheat–summer maize double-crop rotation under farmers practice (FP); (2) to find out site specific differences of N dynamics, water dynamics and crop yield regarding soil type and sub regional (township) management; and (3) to elaborate model-based best management options for these conditions.

5.2 Materials and methods

Site description

This study was based in Quzhou County (stretching between 36°58' N, 114°58' E in the north to 36°37' N, 114°57' E in the south, and between 36°46' N, 114°48' E in the east to 36°48' N, 115°12' E in the west) in the southern part of Hebei Province, P.R. China, with an area of about 67000 ha and has a flat relief around 40 m a.s.l.. The mean annual temperature and the average annual precipitation in Quzhou from 1980 to 2009 were 13.6 °C and 488 mm, respectively, with about two thirds of the annual precipitation occurring during summer and an actual evapotranspiration (ETA) of an irrigated wheat–maize rotation between 750 and 950 mm. Dominant soil types in the region are aquatic Cambisols with a loamy texture according to IUSS Working Group WRB (2007). Soils in the North and South-West of the county have mainly a silty loam texture, in the centre and in the Mid-South the dominant soil texture is a clay loam, while in the South-East sandy loam patches occur close to a riverbed (Liu *et al.,* 2006; Table 5.1). The county capital is Quzhou. Main crops are winter wheat–summer maize double-crop rotations, cotton and vegetables. Nitrogen fertilizer applications average around 286 kg N/ha for winter wheat and around 236 kg N/ha for summer maize. Flood irrigation is applied three to five times to winter wheat and two to three times to summer maize.

Spatial and survey data acquisition and processing

All digital information was used in the geographical system WGS84 and projected in UTM50. For data processing Excel spread sheets, ArcGIS, ArcView GIS 3.3 and ERDAS Imagine were used.

A basic topographic map was digitized for Quzhou County. Basic information, such as village borders, buildings, streets and water bodies was taken from digital chart of the world data (DCW), CNES/Spot Image and DigitalGlobe pictures from Google Earth. Townships as administrative units were digitized from a 1:55000 paper map of Quzhou County and adapted to the borders of the soil texture map described below.

A soil texture map with corresponding attribute tables (Liu *et al.,* 2006) complemented by soil profiles measured in 1999 with a geographic reference was used as input for the model (Figure 5.4a).

Agricultural management data was extracted from a questionnaire based farm survey conducted 2007 in Quzhou County including 183 farmers. Data for sowing, harvest, grain yield (dry matter), fertilization and irrigation of winter wheat and summer maize was averaged on basis of ten township sub regions (Figure 5.4a).

Land use classifications were done on basis of two satellite images. One was from the Earth Observing-1 (EO-1) Extended Mission with Advanced Land Imager (ALI) Sensor made on 31 March 2011, which was used for ground truth mission and comparison. The second one, Landsat 5 Thematic Mapper (TM) satellite image from the 8 June 2011 was finally used as simulation input (Figure 5.4a), since the outcome of the land use classification test gave better results, and in the ALI Sensor image a small part in the south-west of the county was missing as well as some clouds occurred in the south-east. A one-week ground truth data collection campaign in Quzhou County was conducted in May 2011 and >1900 locations (in total) were gathered. To obtain a good data quality a multiple documentation approach was used to mark a reference area. A field with the type of crop

on a paper field map was marked first and then a waypoint with a GPS device was taken and documented in a table with a short description of the surroundings. Finally, if the point was of special interest a picture was taken. Reference areas on the field map were digitized, sorted concerning their quality and an attribute table with descriptions of the marked areas was done. The land use classification was made on the basis of a proportion of 0.7 of the reference areas as a supervised maximum-likelihood classification approach (Esri 2018) and aggregated with fuzzy convolution (3x3) kernel (Foody 1999). Signatures for each class were done on the basis of the reference areas. As winter wheat was about to be harvested when the Landsat picture was taken and thus had diverse spectral values its signature was created on the basis of three characteristic lines. The remaining proportion of 0.3 of the reference areas was used for an accuracy assessment test which resulted in an overall accuracy of 82.33% and a Kappa coefficient of 0.7632 (Congalton 1991).
Weather data was obtained from the research station of China Agricultural University located in the northern part of Quzhou County, (36°52' N and 115°01' E) for the period 1980–2011. This data was used for the whole county. Lacking data of this station was filled with data from surrounding weather stations from the National Climatic Data Center (NCDC) of the National Oceanic and Atmospheric Administration (National Oceanic and Atmospheric Administration 2018).

The HERMES model

The HERMES model is a one-dimensional, dynamic, process-based agro-ecosystem model which can operate under limited input data availability (Kersebaum 2011). It consists of six sub-modules including water balance, N mineralization, N transport, denitrification, crop growth and NH_3 volatilization, running at a daily time step. For further model description and application please see Kersebaum (2011) and Kersebaum *et al.* (2005). Previous model applications within the same study region were done by Michalczyk *et al.* (2014; 2016). In the current study HERMES was, according to Hartkamp *et al.* (1999), interfaced with GIS data for regional modelling via linking. That means that HERMES and the GIS operated separately and model results for each modelling unit were joined via spread sheet and polygon-ID.

Model set up and scenarios

The period from 1980 to 2011 was simulated continuously using 1980 as year for initialization, resulting in 31 simulation years. The model was generally set up with plant and soil parameters based on a calibration and validation across winter wheat–summer maize crop seasons of experimental field data in previous studies in Quzhou County (Michalczyk *et al.* (2014; 2016). Initial values for soil water and mineral N (N_{min}) content were estimated based on farmers' field experiments. The soil parameters as well as plant varieties and crop management were not adapted to the conditions in the 1980s but set with intention according to the practice around the year 2010 to demonstrate the long-term effect of recent and current agricultural practice.

Individual modelling units were derived by overlaying the soil texture map with the administrative boundary map to take different regional management practices and the land use classification map into account. Four different soil types were used for modelling which were based on soil texture and measured soil profiles (Table 5.1). All simulations were made for winter wheat–summer maize double-crop rotations. Sowing, tillage, fertilization, irrigation and harvest dates and amounts were set according to unpublished survey results from 2007 which were averaged for each of the ten townships in Quzhou County (Table 5.2). Due to lack of data of Quzhou Township, it represented the average of the whole county.

Six scenarios regarding N fertilization and irrigation were performed, four farmers practice scenarios based on survey results and two optimized scenarios:

1. farmers practice N fertilization as average for each of the ten townships, conventional flood irrigation (FP),
2. farmers practice N fertilization as maximum standard deviation for each of the ten townships, conventional flood irrigation (FP+SD),
3. farmers practice N fertilization as minimum standard deviation for each of the ten townships, conventional flood irrigation (FP–SD),
4. farmers practice N fertilization as average for each of the ten townships reduced by a proportion of 0.3 N, conventional flood irrigation (FP–30),
5. optimized with model-based N fertilizer recommendations for wheat in one dose as in farmers practice, manual N fertilizer recommendations for maize in one dose as in farmers practice and manual irrigation water adaption for average management data of the whole county (OPTfp),
6. optimized with model-based N fertilizer recommendations for wheat in two doses, manual N fertilizer recommendations for maize in two doses and automated irrigation application, for average management data of the whole county (OPTai).

The depth for manual irrigation application calculation in OPTfp was 0.9 m taking major roots and maximum root depths from winter wheat (Zhang *et al.,* 2004) and summer maize

(Zhuang *et al.,* 2001) into account. All irrigation dates were used as in FP just the amounts were adapted using the difference between field capacity and current simulated water content of the soil. Exceptions were made in wet or dry years (Table 5.2). Automated irrigation in OPTai was applied when the plant available water within the top 0.5 m of the soil was < 60%, including precipitation of the application day. Additionally, the precipitation sum of the following two days needs to be < 5 mm, which mimics the use of weather forecast for irrigation scheduling. The amount of automated irrigation was up to 90% of field capacity within the top 0.5 m, but not more than 25 mm per day.

Both crops, winter wheat as well as summer maize received a fertilization at sowing. First split N fertilization in OPTai in winter wheat was applied on 21 March at double ridge (GS 21) growth stage (Julius Kühn-Institut, JKI 2018), as in OPTfp and the following on 26 April around flowering (GS 65) and/or beginning of grain filling (GS 71). Winter wheat fertilizer recommendation was calculated according to Kersebaum and Beblik (2001) using a predictive weather derived from the local long-term weather series. First split N fertilization in OPTai in summer maize was applied on 10 July at stem elongation as in OPTfp and second split N fertilization was applied on 2 August at tassel emergence (GS55). Summer maize fertilizer recommendation was calculated manually. Starting from FP N fertilizer amounts the N doses were reduced in steps of 5 kg N/ha till yield started to decline.

Table 5.1: Soil characteristics for four soil types in Quzhou County

Soil type	Depth	Clay[1]	Silt[2]	Sand[3]	Field capacity[4]	Wilting point[4]	pH (H_2O)	Bulk density[4]	Organic C	C/N
	m	%	%	%	vol. %	vol. %			%	
Sandy loam	0–0.3	10	59	31	38	14	7.6	low	0.58	7
	0.3–0.5	12	71	16	38	12	7.6	low	0.31	10
	0.5–1.0	6	65	29	40	12	7.6	low	0.19	11
	1.0–2.0	2	55	43	40	12	7.6	low	0.09	11
Silty loam	0–0.2	4	87	9	42	13	7.9	low	0.82	10
	0.2–0.8	6	88	6	42	13	7.9	low	0.40	11
	0.8–1.4	38	60	2	45	28	7.9	low	0.59	12
	1.4–2.0	5	87	9	42	13	7.9	low	0.14	12
Medium loam	0–0.2	16	66	18	38	12	8.2	low	0.89	10
	0.2–0.5	21	60	18	41	20	8.2	low	0.59	11
	0.5–1.2	17	67	17	38	12	8.2	low	0.28	12
	1.2–2.0	14	78	9	38	12	8.2	low	0.23	12
Clay loam	0–0.2	33	62	5	45	28	8.4	low	0.99	7
	0.2–1.1	53	45	2	47	31	8.4	low	0.53	10
	1.1–1.2	34	62	4	45	28	8.4	low	0.44	11
	1.2–2.0	12	82	6	39	11	8.4	low	0.32	11

[1] < 2 µm
[2] 2 µm–50 µm
[3] 50 µm–2 mm
[4] According to the German Soil Survey Manual and adapted by model simulations

Table 5.2: Site management for winter wheat (WW) and summer maize (SM) as average per township and year in Quzhou County. Fertilization and irrigation amounts as in farmers practice

Township	Crop	Sowing date	Fertilization at sowing date, type[1] and amount kg N/ha	Tillage date and depth[2] m	First irrigation date and amount[3] mm	First fertilization date, type and amount kg N/ha	Second irrigation date and amount[4] mm	Third irrigation date and amount mm	Straw return proportion	Harvest date
Anzhai	WW	17th Oct.	15th Oct.; NPK 165	16th Oct.; 0.2	18th Oct.; 150	21st March; URE 130	22nd March; 150	20th April; 150	1	9th June
	SM	13th June	13th June; NPK 76	-	14th June; 150	10th July; URE 172	11th July; 150	-	0. 85	20th Sept.
Baizhai	WW	12th Oct.	10th Oct.; NPK 159	11th Oct.; 0.2	13th Oct.; 150	21st March; URE 142	22nd March; 150	20th April; 150	0.88	8th June
	SM	14th June	14th June; NPK 87	-	15th June; 150	10th July; URE 149	11th July; 150	-	1	25th Sept.
Dahedao	WW	07th Oct.	5th Oct.; NPK 167	6th Oct.; 0.2	8th Oct.; 150	21st March; URE 131	22nd March; 150	20th April; 150	0.94	8th June
	SM	15th June	15th June; NPK 72	-	16th June; 150	10th July; URE 128	11th July; 150	-	0.94	22th Sept.
Henantuan	WW	13th Oct.	11th Oct.; NPK 157	12th Oct.; 0.2	14th Oct.; 150	21st March; URE 137	22nd March; 150	20th April; 150	1	8th June
	SM	13th June	13th June; NPK 125	-	14th June; 150	10th July; URE 142	11th July; 150	-	0.95	23th Sept.
Houcun	WW	17th Oct.	17th Oct.; NPK 130	16th Oct.; 0.2	18th Oct.; 150	21st March; URE 159	22nd March; 150	20th April; 150	0.75	8th June
	SM	12th June	12th June; NPK 57	-	13th June; 150	10th July; URE 147	11th July; 150	-	0.75	23th Sept.
Huaiqiao	WW	16th Oct.	16th Oct.; NPK 134	15th Oct.; 0.2	17th Oct.; 150	21st March; URE 130	22nd March; 150	20th April; 150	1	11th June
	SM	14th June	14th June; NPK 80	-	15th June; 150	10th July; URE 134	11th July; 150	-	1	23th Sept.
Liyue	WW	16th Oct.	16th Oct.; ABC 170	15th Oct.; 0.2	17th Oct.; 150	21st March; ABC 146	22nd March; 150	20th April; 150	0.91	9th June
	SM	14th June	14th June; NPK 95	-	15th June; 150	10th July; NPK 130	11th July; 150	-	0.82	25th Sept.
Quzhou[5]	WW	13th Oct.	13th Oct.; NPK 145	12th Oct.; 0.2	14th Oct.; 150	21st March; URE 141	22nd March; 150	20th April; 150	1	8th June
	SM	13th June	13th June; NPK 83	-	14th June; 150	10th July; URE 153	11th July; 150	-	1	23rd Sept.
Situan	WW	13th Oct.	13th Oct.; ABC 143	12th Oct.; 0.2	14th Oct.; 150	21st March; URE 126	22nd March; 150	20th April; 150	0.82	8th June
	SM	13th June	13th June; NPK 110	-	14th June; 150	10th July; URE 171	11th July; 150	-	1	24th Sept.
Yizhuang	WW	03th Oct.	3rd Oct.; NPK 106	2nd Oct.; 0.2	4th Oct.; 150	21st March; URE 181	22nd March; 150	20th April; 150	1	5th June
	SM	8th June	6th June; NPK 42	-	9th June; 150	10th July; URE 168	11th July; 150	-	0.75	23th Sept.

[1] NPK = compound fertilizer, URE = urea, ABC = ammonium bi-carbonate
[2] as used in model
[3] in wet years no irrigation carried out in October
[4] WW: in dry years 150 mm in end of February/beginning of March additional or replacing the irrigation in April; SM: 150 mm on 11th July only in dry years
[5] due to lack of data, Quzhou Township represents the average of the whole county

Calculation of soil organic carbon and groundwater use

Soil organic carbon (C) is not calculated directly by HERMES, but it simulates fast (N_{fast}) and slowly (N_{slow}) decomposable organic N pools at certain times. While N_{slow} is initially calculated as a fraction (0.17) of total organic N, N_{fast} and a smaller portion of N_{slow} depend on the residue composition from the previous crop. To calculate organic C (in kg C/ha in the upper 20 or 30 cm, depending on the size of the upper soil layer) the inert organic N pool initially calculated by the model is added to the two dynamic pools and the sum was multiplied by the initial C/N-ratio.

Organic C = (N_{slow} + N_{fast} + $N_{passive}$) * C/N

Mass% of organic C was calculated using the bulk density of the upper soil layer. Average annually groundwater use was calculated using the simulated percolation at 120 cm depth (groundwater recharge) and irrigation (groundwater withdrawal).

5.3 Results

Long-term regional N losses and groundwater use

Nitrogen losses in general

Total simulated N loss resulting from nitrate leaching, ammonia (NH_3) volatilization and denitrification for the whole county under winter wheat–summer maize double-crop rotation were under FP almost three times higher than under OPT treatments (Table 5.3). Cumulative N losses are shown in Figure 5.1. That would result in a total loss of 289397.5 t N under FP or between 99021.8 (OPTfp) and 494701.9 t N (FP+SD) in 31 years.

Across all treatments averaged N losses increased with increase of clay content in soil texture from 198.2 on sandy loam to 243.1 kg N/ha on clay loam. If an optimized treatment was used instead of FP this would save more than 6000 t N from N fertilizer application or more than 8000 t N annually from N loss in Quzhou County.

Table 5.3: Average annually simulated N loss sum per N treatment for whole Quzhou County for winter wheat (WW)–summer maize (SM) double-crop rotation 1980–2011

Treatment	Annually N loss sum	N loss	Proportion of applied fertilizer N
	t N	kg N/ha	
FP	9335.1	296.8	0.57
FP+SD	15958.1	507.3	0.67
FP−SD	3917.5	124.5	0.43
FP−30	5402.5	171.7	0.47
OPTfp	3194.3	101.5	0.43
OPTai	3198.2	101.7	0.40

Nitrogen leaching, volatilization and denitrification

Average annual N leaching, volatilization and denitrification were generally closely related to the magnitude of fertilizer N input, which was FP+SD>FP>FP−30>FP−SD>OPTai>OPTfp (Table 5.4). An exception was the leaching under OPTai which had slightly higher N inputs but clearly lower, close to zero leaching compared to OPTfp. Another exception was the volatilization under the OPTfp treatment which was higher than FP-SD under silty, medium and clay loam. The uppermost exception was denitrification under OPTai, which was in a similar range as the denitrification of FP+SD.

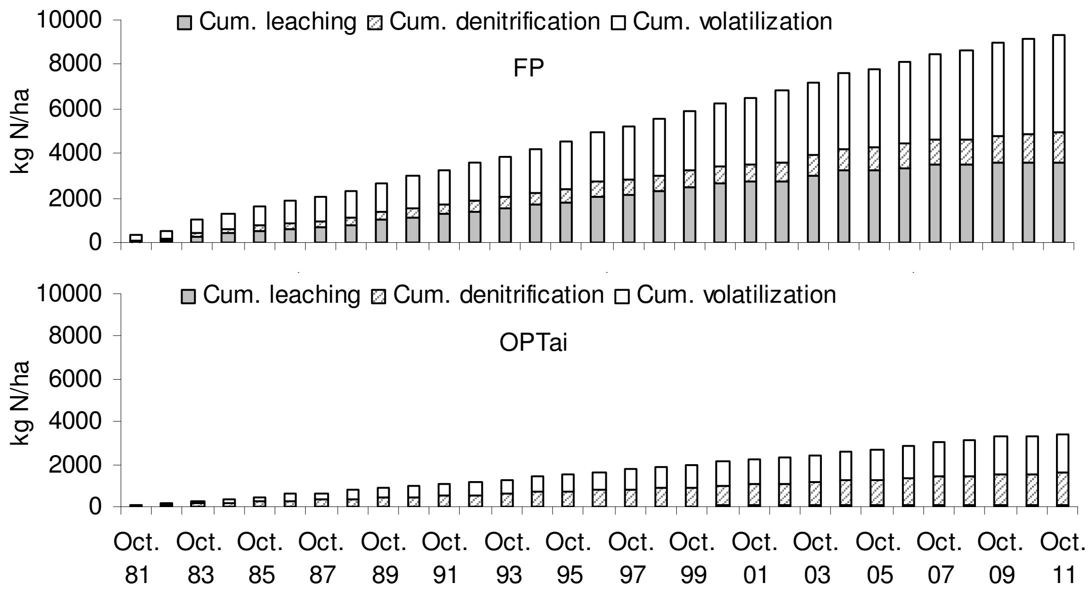


Figure 5.1: Simulated cumulative N leaching (at 120 cm soil depth), volatilization and denitrification under FP for average county management and OPTai treatment on medium loam in Quzhou County for 1980–2011

Mineral nitrogen and organic carbon pools and grain yield

The actual organic C pool at last maize harvest in 2011 before residue incorporation (complete) was generally higher with higher fertilizer N input and higher clay content; anyhow there was almost no difference between the FP+SD and the FP treatment (Table

5.4). On silty and medium loam the initial values (16347.1 and 17764.7 kg C/ha, respectively) were reached in all N treatments except on medium loam, OPTai treatment, while on sandy loam the initial value (11562.4 kg C/ha) was reached in none of the treatments. On clay loam only the FP treatments reached the initial value (19760.6 kg C/ha) again. Similar to the organic C pool the N_{min} pool at the end of simulation period in 0–120 cm depth decreased with decreasing N fertilizer input. The N_{min} content decreased with increasing clay content, which was opposite to the organic C with little exceptions. There was almost no difference in grain yield (dry matter) between the N treatments for sandy, silty and medium loam. On clay loam the yield was lower except for OPTai.

Table 5.4: Average annual simulated fertilizer N input, N losses, N_{min} and organic C pools at the end of simulation period, total annual grain yield (winter wheat + summer maize, dry matter) and nitrogen use efficiency (NUE) for 1980–2011 for average county management[1] in Quzhou County

Treatment[2]	Texture	Fertilizer N input	Leaching[3]	Volatilization	Denitrification	N_{min} 0–120 cm Oct. 2011	Organic C 0–20 cm Oct. 2011[4]	Grain yield	NUE[5]
-	-	kg N/ha	N_{min} kg N/ha	N_{min} kg N/ha	N_{min} kg N/ha	N_{min} kg N/ha	kg C/ha	dry matter kg/ha	kg grain /kg N
FP+SD	Sandy loam	756	291.0	174.3	37.0	1354.5	11398.6	12145.5	16.1
FP+SD	Silty loam	756	259.7	175.5	53.6	1358.4	17499.1	12093.2	16.0
FP+SD	Medium loam	756	236.3	226.3	45.5	999.1	20514.7	12017.7	15.9
FP+SD	Clay loam	756	248.7	197.9	91.3	894.3	20896.7	10238.1	13.5
FP	Sandy loam	522	160.8	95.3	34.7	665.3	11393.4	12144.5	23.3
FP	Silty loam	522	131.7	100.0	49.6	577.0	17491.1	12092.3	23.2
FP	Medium loam	522	117.1	139.5	41.2	401.4	20449.7	12017.4	23.0
FP	Clay loam	522	119.7	120.7	81.7	378.1	20891.8	10238.1	19.6
FP-30	Sandy loam	366	82.1	47.7	30.9	246.9	11329.5	12142.6	33.2
FP-30	Silty loam	366	58.3	53.7	43.3	155.2	17313.1	12091.3	33.0
FP-30	Medium loam	366	58.3	82.4	35.8	121.6	19952.7	12015.5	32.8
FP-30	Clay loam	366	56.1	72.2	68.1	113.0	20464.8	10237.4	28.0
FP-SD	Sandy loam	288	52.0	31.0	27.8	112.7	11163.4	12138.4	42.1
FP-SD	Silty loam	288	33.4	36.6	39.0	68.9	16878.1	12090.0	42.0
FP-SD	Medium loam	288	37.9	59.5	32.5	69.4	19276.7	12010.3	41.7
FP-SD	Clay loam	288	34.8	52.0	60.5	60.4	19877.5	10236.8	35.5
OPTfp	Sandy loam	215	10.6	28.8	25.3	52.2	10930.5	11983.9	55.7
OPTfp	Silty loam	240	7.7	42.9	36.3	39.5	16425.1	12032.6	50.1
OPTfp	Medium loam	263	7.3	74.2	31.9	33.5	18888.7	11781.3	44.7
OPTfp	Clay loam	236	4.0	61.5	54.8	19.9	19539.4	10061.9	42.6
OPTai	Sandy loam	224	3.0	18.3	38.7	19.7	10940.8	12374.8	55.2
OPTai	Silty loam	243	1.7	25.9	52.8	17.6	16359.1	12374.8	50.9
OPTai	Medium loam	268	3.3	59.7	46.9	17.6	17709.7	12379.4	46.2
OPTai	Clay loam	276	3.1	51.6	80.0	14.4	18544.0	12291.9	44.5

[1] According to farm survey Quzhou County 2007
[2] The original N and water management in FP is the average of the county
[3] At 120 cm depth
[4] Before full residue incorporation
[5] NUE = grain yield (kg/ha) / applied N (kg N/ha)

Mineral nitrogen and organic carbon dynamic

Having a look at the N dynamics under FP during the simulation period from year to year the N loss was low when N_{min} content in the soil was high and precipitation was low, and vice versa. The organic C pool under FP with full residue input in 0–20 cm at maize harvest in October, before residue incorporation, increased from 18564.7 in 1981 to 20865.7 kg C/ha in 1989 and thereafter decreased a bit to 19920.7 kg C/ha in 2007. During he final four years until 2011 it slightly increased again to 20449.7 kg C/ha, which is greater than the initial value. The organic C pool under FP with a proportion of 0.75 residue input showed the same dynamics with 4–10% lower values (Figure 5.2).

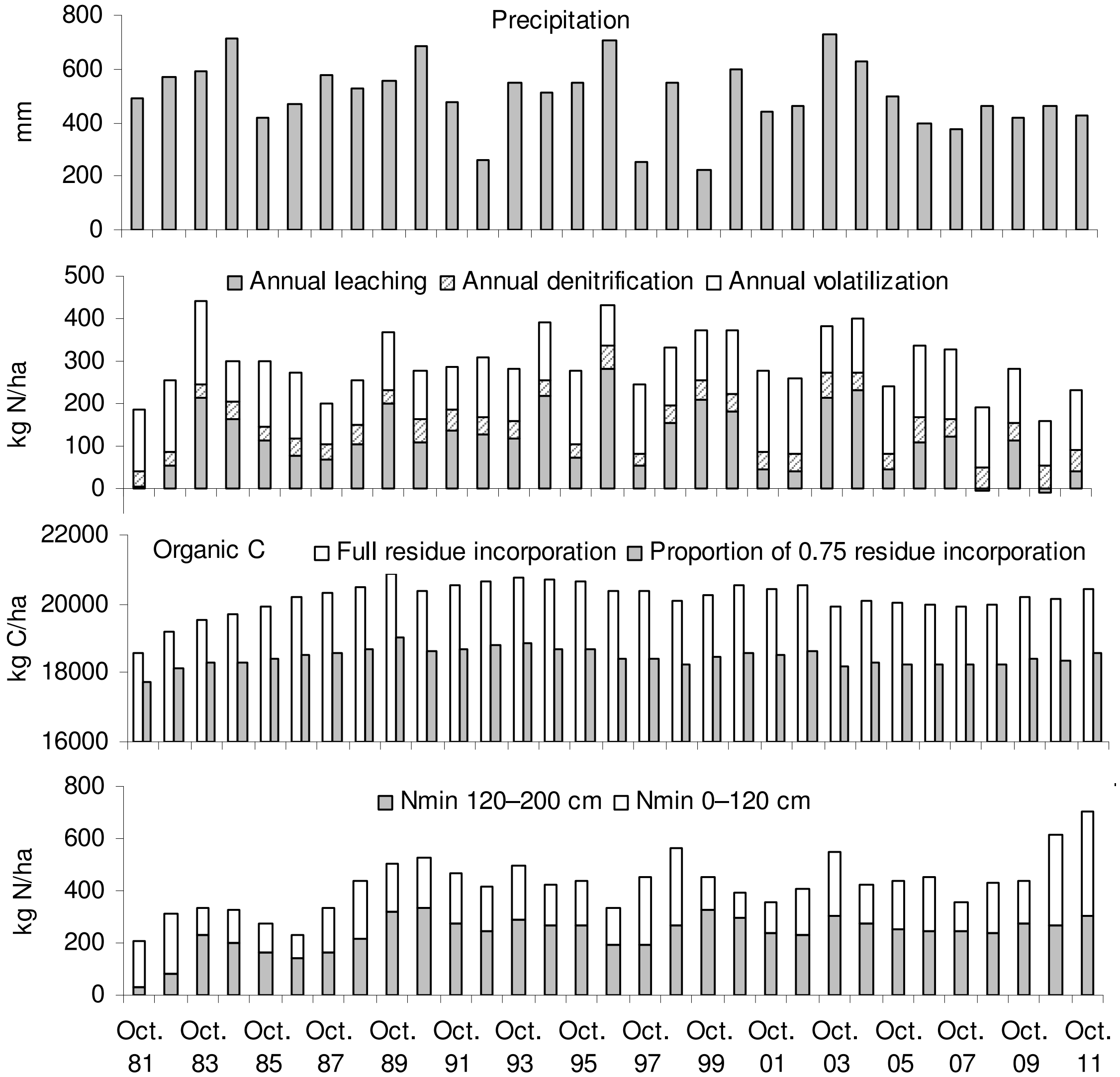


Figure 5.2: Annual precipitation, N leaching (at 120 cm soil depth), volatilization, denitrification, organic C (0–20 cm, full residue incorporation and at a proportion of 0.75) and N_{min} pools at maize harvest, before residue incorporation under FP treatment for average county management on medium loam in Quzhou County for 1980–2011

As a yearly average the organic C pool with full residue input is 19067.9 (1.10.80–30.9.81) and 21206.7 (1.10.10–30.9.11) kg C/ha. The organic C pool in 0–20 cm and N_{min}

pool in the root zone (0–120 cm) did not show a trend but in the N_{min} pool underneath the root zone (120–200 cm) a slight accumulation of N was visible.

Groundwater use

Groundwater use in winter wheat–summer maize double-crop rotations over the whole county was 433 mm for FP, FP+SD, FP−SD, FP−30; 424 mm for OPTfp and 489 mm for OPTai. Although less irrigation water was taken from groundwater in the OPT variants, the distinct decrease of percolation counterbalanced the groundwater saving effect.

Average annual percolation was highest on clay loam soil and for the four farmers practice treatments (Table 5.5). Low percolation and high irrigation from groundwater especially on clay loam resulted in high groundwater use. Average annual actual evapotranspiration (ETA) was similar in all FP and in the OPTfp treatment. Only in OPTai the ETA was slightly higher especially on clay loam.

Table 5.5: Annual irrigation, percolation water, actual evapotranspiration (ETA) and irrigation water use efficiency (WUE) for winter wheat (WW)–summer maize (SM) double-crop rotation 1980–2011 in Quzhou County

Treatment[1]	Texture	WW−SM area	irrigation sum	percolation water[2]	ETA	WUE[3]
-	-	ha	mm/a	mm	mm	kg/ha/mm
FP+SD	Sandy loam	888.8	579	123.3	978.5	11.2
FP+SD	Silty loam	14768.9	579	123.0	978.5	11.2
FP+SD	Medium loam	6835.9	579	134.1	967.4	11.1
FP+SD	Clay loam	8962.2	579	204.1	897.0	9.5
FP	Sandy loam	888.8	579	123.3	978.5	11.2
FP	Silty loam	14768.9	579	123.0	978.5	11.2
FP	Medium loam	6835.9	579	134.1	967.4	11.1
FP	Clay loam	8962.2	579	204.1	897.0	9.5
FP-30	Sandy loam	888.8	579	123.3	978.5	11.2
FP-30	Silty loam	14768.9	579	123.0	978.5	11.2
FP-30	Medium loam	6835.9	579	134.1	967.5	11.1
FP-30	Clay loam	8962.2	579	204.1	897.0	9.5
FP-SD	Sandy loam	888.8	579	123.4	978.5	11.2
FP-SD	Silty loam	14768.9	579	123.0	978.4	11.2
FP-SD	Medium loam	6835.9	579	134.1	967.5	11.1
FP-SD	Clay loam	8962.2	579	204.1	897.0	9.5
OPTfp	Sandy loam	888.8	478	30.3	972.3	12.2
OPTfp	Silty loam	14768.9	497	42.3	977.9	12.0
OPTfp	Medium loam	6835.9	464	31.0	956.8	12.2
OPTfp	Clay loam	8962.2	415	53.5	884.9	11.0
OPTai	Sandy loam	888.8	506	16.7	1011.8	12.3
OPTai	Silty loam	14768.9	502	15.5	1008.5	12.3
OPTai	Medium loam	6835.9	516	25.9	1012.9	12.2
OPTai	Clay loam	8962.2	573	82.9	1009.8	11.4

[1] The original N and water management in FP is the average of the county

[2] At 120 cm depth

[3] WUE = grain yield [kg/ha] / (precipitation [mm] + irrigation [mm])

Over the years under FP treatment annual percolation and annual ETA were varying around the averages of 134.1 mm and 967.5 mm, respectively. Percolation was higher in years with high rainfall and ETA was lower (Figure 5.3).

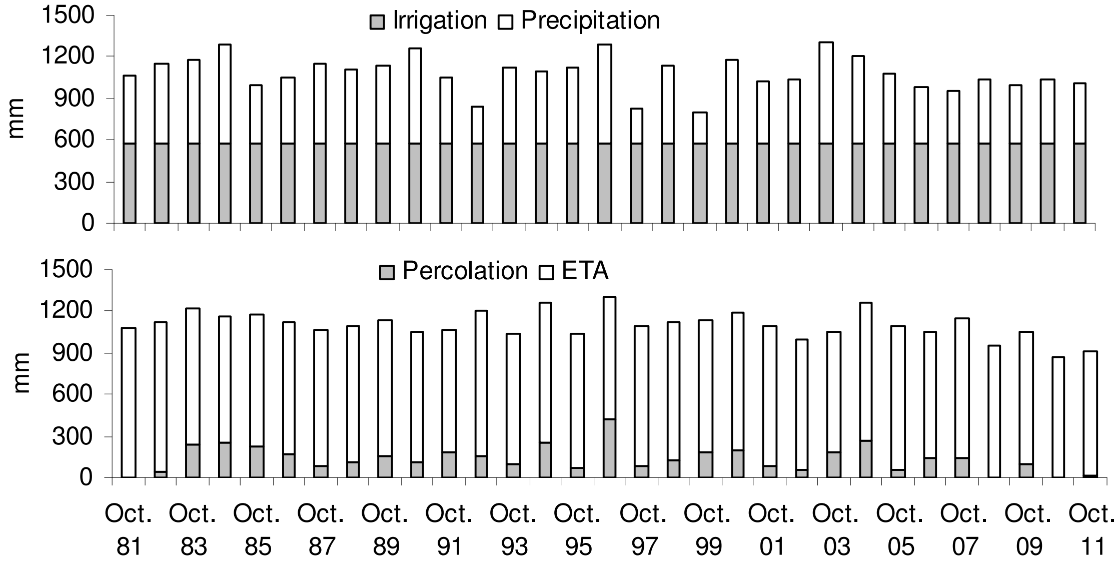


Figure 5.3: Annual irrigation, precipitation, percolation (at 120 cm soil depth) and ETA under FP treatment for average county management on medium loam in Quzhou County for 1980–2011

Site specific differences and their spatial distribution of N, water and yield

Land use classification

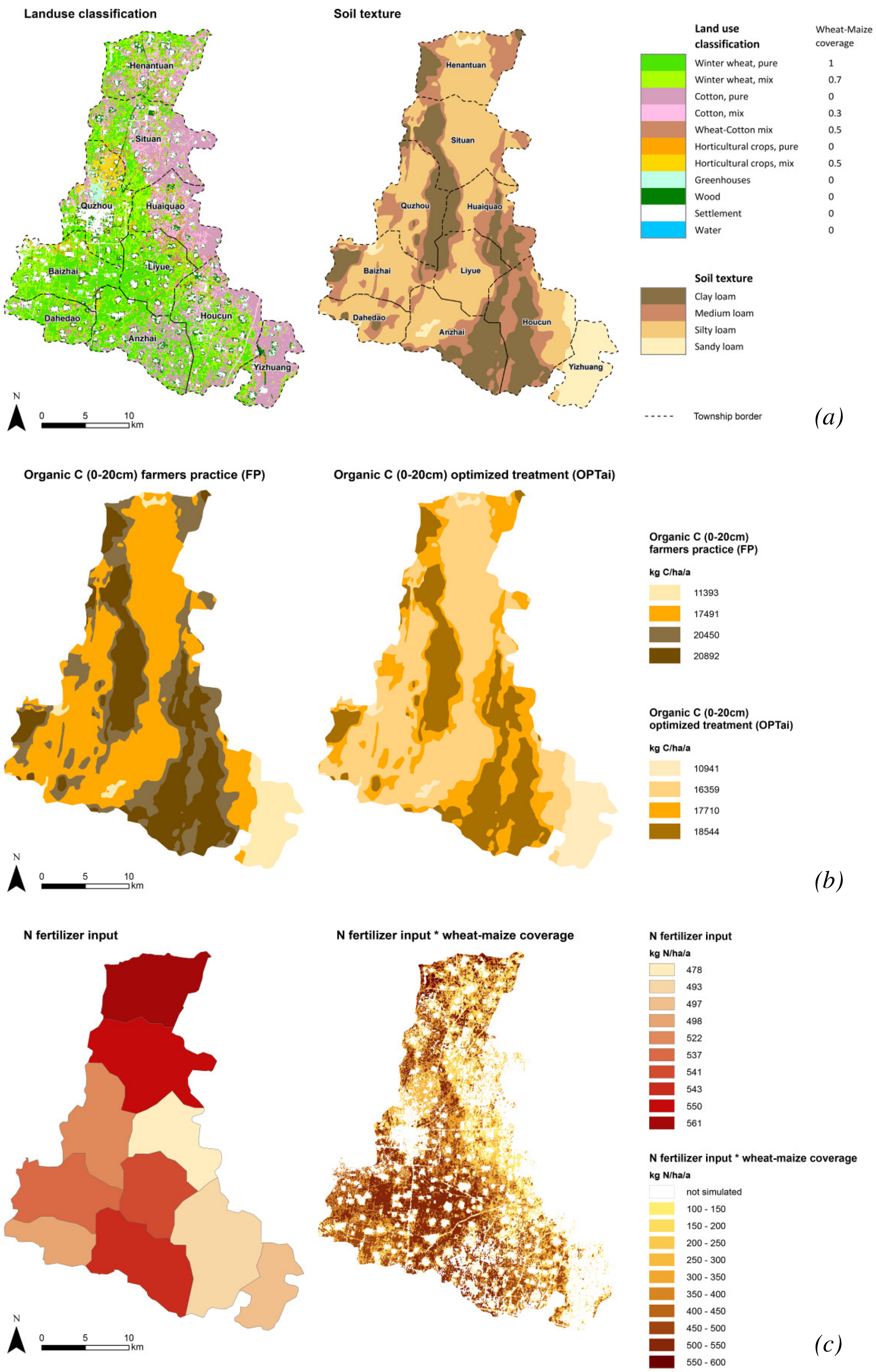
According to the land use classification a proportion of 0.83 of Quzhou County was agricultural land and 0.45 of the agricultural land was under winter wheat–summer maize double-crop rotation, while 0.34 were covered with cotton and 0.04 planted with horticultural crops. Winter wheat and summer maize was mostly grown from the north-west to the south-west of the county, while cotton was mainly grown along the eastern border. Parts of the middle north and middle south were wheat–maize and cotton mixed areas. Horticultural crops (both open field and in greenhouses) were mainly located north of Quzhou town (Figure 5.4a).

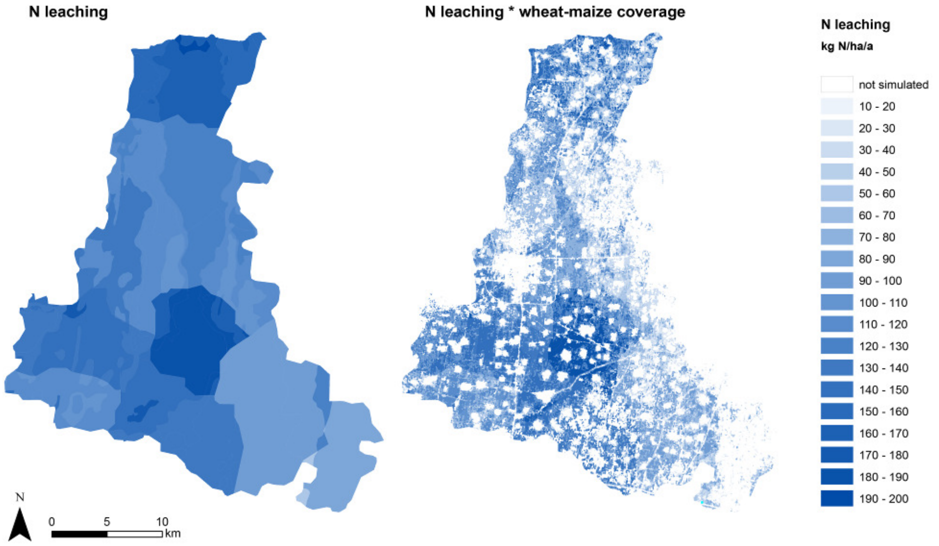
Nitrogen fertilizer input

Annual N input via fertilization for FP according to a survey for winter wheat–summer maize rotations was highest in Henantuan, Situan, Anzhai, Liyue, Baizhai, Quzhou, Dahedao, Yizhouang, Houcun and Huaiquao townships in descending order with values from 561 to 478 kg N/ha for both crops together. Generally average N input per ha was higher in the north-west of the county, while in the south-east average N inputs were less (Figure 5.4c).

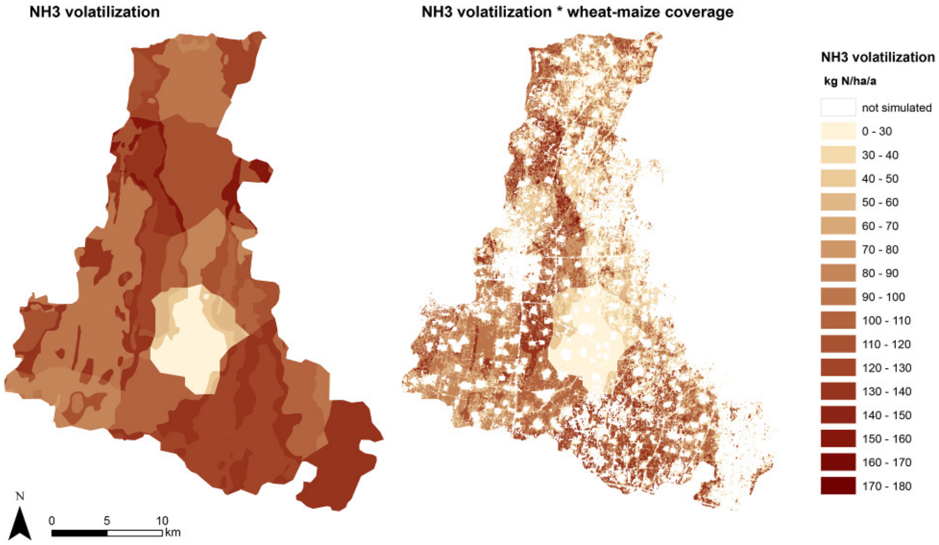
Nitrogen leaching, NH_3 volatilization and denitrification

Simulated nitrogen leaching under FP in kg N/ha/a was highest on sandy and lower in descending order on silty, clay and medium loam. According to the township borders Liyue and Henantuan had the highest N leaching, while Houcun and Yizhuang had the lowest. Generally the area south of Quzhou had higher N leaching (Figure 5.4d). Ammonia volatilization in kg N/ha/a was highest on medium loam, then descending in the order of clay, silty and sandy loam. The township with the lowest NH_3 volatilization was Liyue, while Situan has the highest. All other townships were in between and without a visible pattern. The township Liyue displayed low volatilization losses (Figure 5.4e) but high N_{min} contents in the soil and high leaching losses, compared to other townships. Denitrification in kg N/ha/a was highest on clay loam and silty loam, while it was lower on medium and sandy loam. In Huaiquao and the southern parts of the county denitrification was lower (Figure 5.4f). When N losses from leaching, volatilization and denitrification were averaged per township and summed up, the N loss sum showed a similar pattern as the N input via mineral fertilizer (not shown).

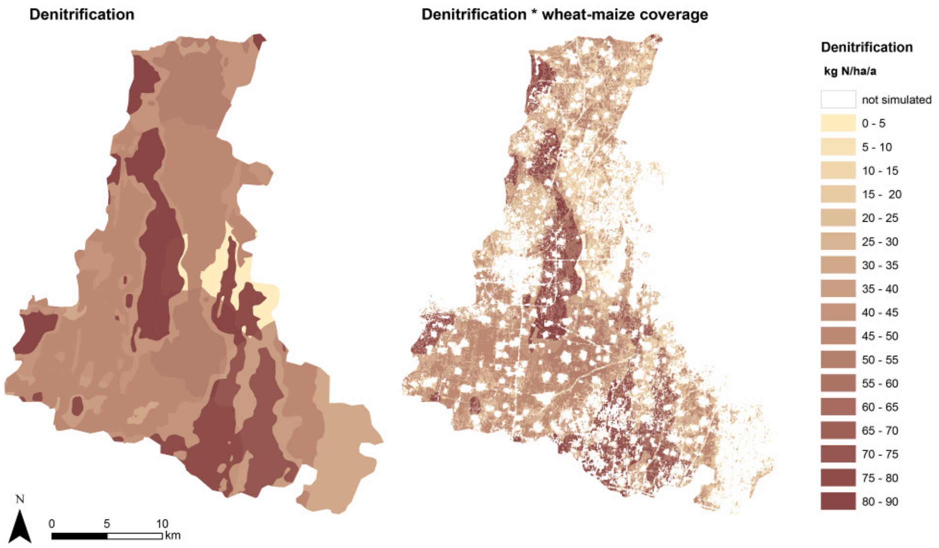

Landuse classification
Soil texture
Henantuan
Situan
Quzhou
Huaiquao
Liyue
Baizhai
Dahedao
Houcun
Anzhai
Yizhuang
Land use classification
Wheat-Maize coverage
Winter wheat, pure 1
Winter wheat, mix 0.7
Cotton, pure 0
Cotton, mix 0.3
Wheat-Cotton mix 0.5
Horticultural crops, pure 0
Horticultural crops, mix 0.5
Greenhouses 0
Wood 0
Settlement 0
Water 0
Soil texture
Clay loam
Medium loam
Silty loam
Sandy loam
Township border
N
0 5 10 km
(a)
Organic C (0-20cm) farmers practice (FP)
Organic C (0-20cm) optimized treatment (OPTai)
Organic C (0-20cm) farmers practice (FP)
kg C/ha/a
11393
17491
20450
20892
Organic C (0-20cm) optimized treatment (OPTai)
kg C/ha/a
10941
16359
17710
18544
(b)
N fertilizer input
N fertilizer input * wheat-maize coverage
N fertilizer input
kg N/ha/a
478
493
497
498
522
537
541
543
550
561
N fertilizer input * wheat-maize coverage
kg N/ha/a
not simulated
100 - 150
150 - 200
200 - 250
250 - 300
300 - 350
350 - 400
400 - 450
450 - 500
500 - 550
550 - 600
(c)


N leaching
N leaching * wheat-maize coverage
N leaching
kg N/ha/a
not simulated
10 - 20
20 - 30
30 - 40
40 - 50
50 - 60
60 - 70
70 - 80
80 - 90
90 - 100
100 - 110
110 - 120
120 - 130
130 - 140
140 - 150
150 - 160
160 - 170
170 - 180
180 - 190
190 - 200
N
0
5
10
km

(d)


NH3 volatilization
NH3 volatilization * wheat-maize coverage
NH3 volatilization
kg N/ha/a
not simulated
0 - 30
30 - 40
40 - 50
50 - 60
60 - 70
70 - 80
80 - 90
90 - 100
100 - 110
110 - 120
120 - 130
130 - 140
140 - 150
150 - 160
160 - 170
170 - 180
N
0
5
10
km

(e)


Denitrification
Denitrification * wheat-maize coverage
Denitrification
kg N/ha/a
not simulated
0 - 5
5 - 10
10 - 15
15 - 20
20 - 25
25 - 30
30 - 35
35 - 40
40 - 45
45 - 50
50 - 55
55 - 60
60 - 65
65 - 70
70 - 75
75 - 80
80 - 90
N
0
5
10
km

(f)

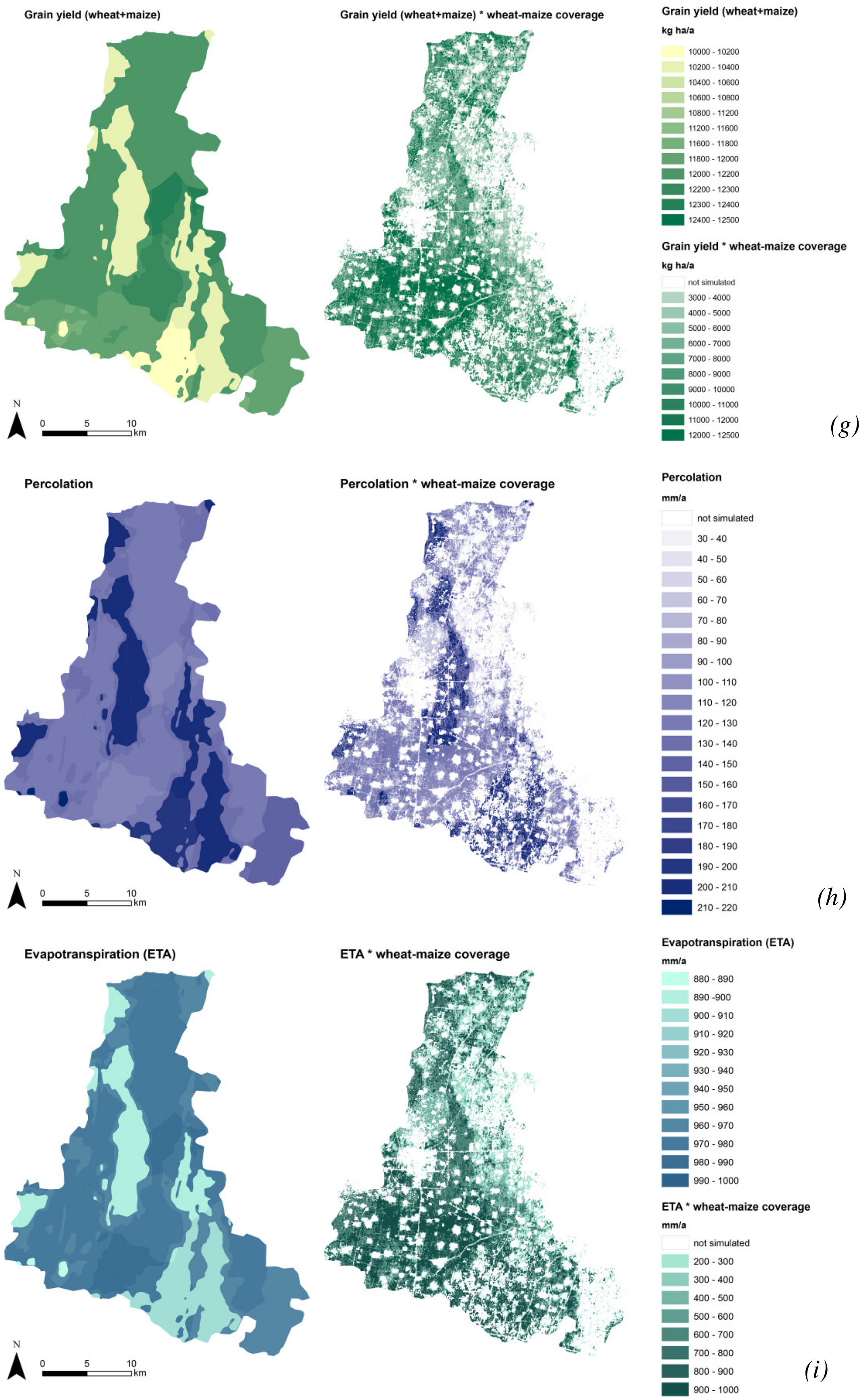


Figure 5.4: Quzhou County with township names and borders, soil texture, land use (*a*), annual averages of N fertilizer input (*c*), N leaching (*d*), NH_3 volatilization (*e*), denitrification (*f*) in kg N/ha, grain yield (g) in kg/ha (dry matter), percolation (*h*) and ETA (*i*) in mm for farmers practice from 1981 to 2011. For the left

column (*c–i*) a complete coverage with winter wheat–summer maize was assumed and in the right column values were multiplied by the fraction of actual winter wheat–summer maize share. For both figures of organic C (*b*) in kg C/ha in 0–20 cm depths at maize harvest in 2011 before residue incorporation, a complete coverage with winter wheat–summer maize was assumed. The left figure shows farmers practice based on average county N management and the right OPTai N treatment

Grain yield, Percolation and ETA

Grain yield in kg/ha/a (dry matter) was higher on silty loam compared to clay loam, while yields on medium and sandy loam were in between. The townships around Quzhou town and the townships of Situan, Huaiquao, Liyue and Baizhai had higher yields compared to the remaining townships (Figure 5.4g).

Percolation and ETA in mm/a under FP showed differences mainly according to soil texture. While percolation was higher on clay loam than on silty loam, for ETA it was vice versa (Figures 5.4h, 5.4i). As irrigation was the same for FP in the whole county it showed only differences when area weighted by wheat–maize coverage (not shown).

Spatial differences in general

No spatial north–south gradient or similar trends in management like higher N fertilizer application amounts in the north than in the south or earlier sowing dates in the south than in the north across the county could be observed based on the survey inputs. The reactions of the outputs due to different soil texture differed from the reactions due to different township management. Differences in leaching and volatilization between the townships resulting from different management were, according to standard deviation, higher than differences due to soil texture under FP. For differences in denitrification, plant biomass, grain yield, percolation and ETA, it was the other way round.

Spatial differences under optimized treatments

Site-specific differences under optimized treatments did only exist due to soil texture and magnitude of wheat–maize cultivation area. Under OPTai wheat and maize on sandy and silty loam needed less and also lost less N and irrigation water than on medium and clay loam, while yields were similar. This resulted in higher N inputs and losses in the middle and southern parts of the county where the clay loam soils are located as well as a high percentage of wheat-maize land cover existed. The same was true for OPTfp, except that the N input and grain yield (dry matter) on clay loam were lower than under OPTai, mainly due to drought stress. In some years, simulated yield is additionally reduced for about three days after irrigation by 1 or 2% due to oxygen deficiency. Compared to FP the OPTai treatment showed lower organic C values throughout the county with the highest values on clay loam and the lowest on sandy loam (Figure 5.4b).

Best-practice management options

Best-practice options in general

Results of the OPT scenarios showed that water and N could be saved in comparison to the FP scenarios. This reduction of inputs was possible, with a few exceptions, without reducing yields. If average FP management of the township Huaiquiao would have been used in the whole of Quzhou County instead of FP management of Henantuan this would have resulted in a saving potential of 83.0 kg N/ha/a fertilizer input or 56.2 kg N/ha/a N losses. If an optimized treatment would have been used in the whole county instead of FP this would have saved in average more than 260 kg N/ha/a from fertilizer input and 190 kg N/ha/a from N losses on winter wheat–summer maize cropland.

Comparing N treatments and soil textures to each other under a county-average management (Table 5.4), the model-based recommended fertilizer N input of OPTfp treatment on sandy loam resulted in the lowest N input of all treatments without yield reduction. Fertilizer N input and N loss (from leaching, volatilization, denitrification) in both OPT treatments increased with clay content, except for N input under OPTfp on clay loam where yield (dry matter) was also lower due to drought stress and to a very small amount to oxygen deficiency. OPTai had slightly higher yields than the other treatments on all soil types, especially on clay loam. Nitrogen use efficiency (NUE = grain yield [kg/ha, dry matter] / kg N [applied/ha]) as Partial factor productivity of applied N was best under the OPT treatments, especially on sandy loam (Table 5.4).

Nitrogen leaching, NH_3 volatilization and denitrification

Leaching of nitrate N under OPTai was the lowest of all treatments and almost reduced to zero in comparison to FP (Figs 1 and 5). In some years it even showed negative leaching due to upward movement of nitrate from deeper soil layers. The lowest volatilization was under FP−SD, OPTfp and OPTai treatments with higher values on medium loam and lower on sandy loam. Denitrification was lowest under OPTfp, while under OPTai treatment it was as high as in FP+SD. When summing up the three N loss pathways, OPTai treatment generally had the lowest loss except on clay loam, where OPTfp was lower.

The N loss under OPTai from year to year amounted to 28.3–129.1 kg N/ha/a and was thus much lower compared to FP with 107.2–149.5 kg N/ha/a. Years with highest N losses had average precipitation, since in those years volatilization was especially high and relatively large N_{min} pools accumulated.

Mineral nitrogen and organic carbon pools

The organic C pool (0–20 cm) under OPTai treatment at maize harvest, before residue incorporation, varied around 17800.0 during the first years of simulation, decreased to 17357.7 in 2004 and thereafter increased slightly to 17709.7 kg C/ha in 2011 again. As a yearly average the organic C pool amounted to 21567.0 at the start (1.10.80–30.9.81) and 20772.1 kg C/ha in the end of the simulation period (1.10.10–30.9.11). Compared to FP organic matter pools under OPTai were smaller (organic C, Figure 5.4b). The organic C pool under OPTai did not reach the initial value again, showing a slight downward trend. The soil N_{min} pool under OPTai in 120–200 cm depth was with initially 20.4 kg N/ha on the last day before maize harvest in October 1981 to 38.2 kg N/ha before maize harvest in October 2011 much smaller than under FP, but it indicated a small accumulation over the simulation period as well (Figure 5.5).

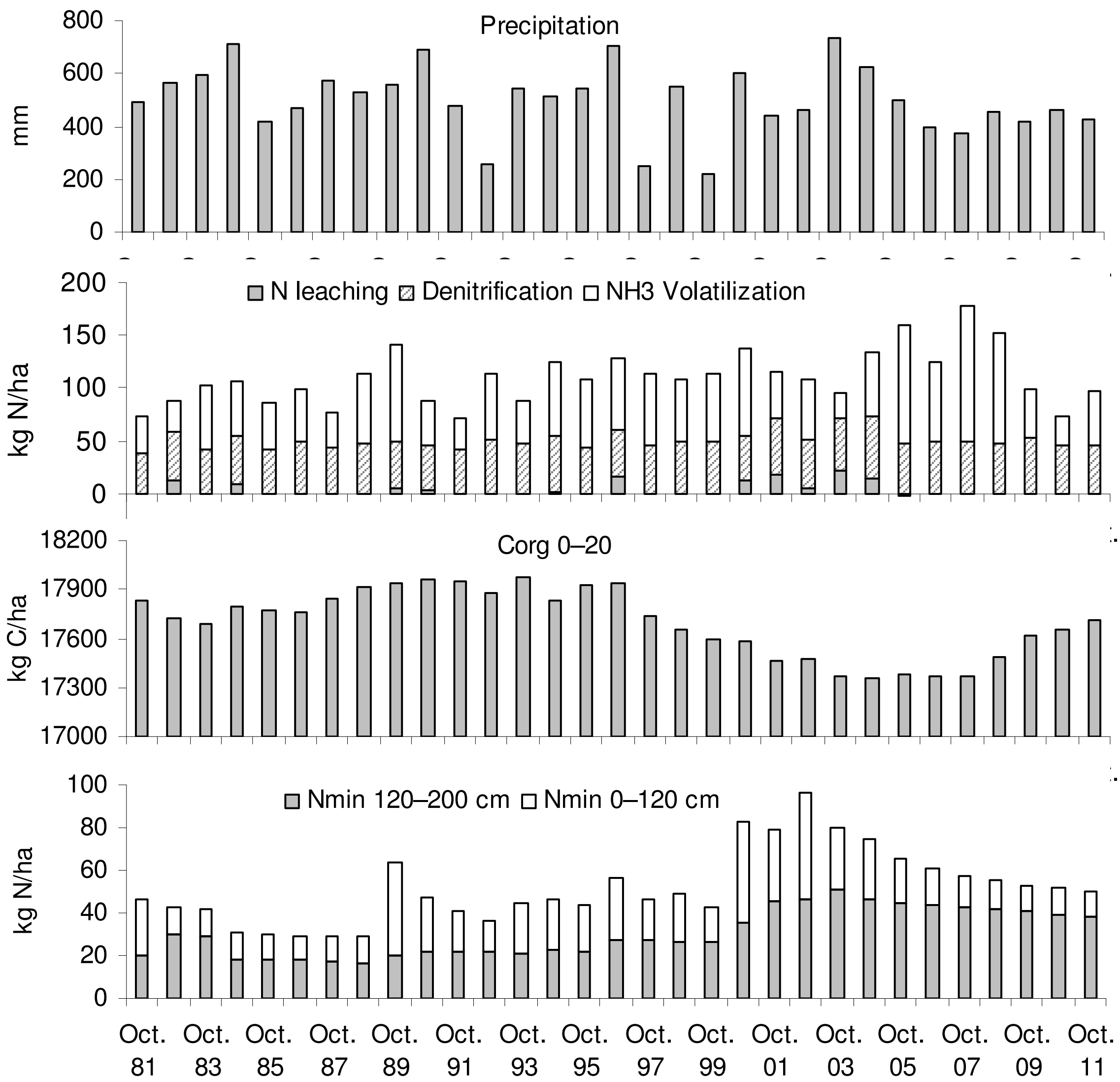


Figure 5.5: Annual precipitation, nitrate N leaching (in 120 cm), NH_3 volatilization and denitrification, organic C (0–20 cm) and N_{min} pools at maize harvest before residue incorporation under OPTai treatment on medium loam in Quzhou County for 1980–2011

Groundwater use

Irrigation amounts were lower in the optimized treatments except on clay loam. If OPTfp treatment would be used in the whole county instead of FP this could save around 115.7 mm/a or 35.6 million m^3/a for the whole of Quzhou County. On clay loam and under OPTai irrigation was as high as under farmers practice treatments but, in contrast to all other treatments, had almost no yield (dry matter) reduction due to drought stress. The irrigation water input in the OPTfp treatment was the lowest on sandy loam with an average of 478 mm/a without reducing yield (see also previous chapter). Percolation under OPTai was reduced to zero in many years while irrigation was reduced only slightly, resulting in higher ETA, higher soil water contents and higher groundwater use than in the FP treatments (Figs 6 and 7). The inter-annual variability of total water inputs (irrigation + precipitation) was lower in OPTai (Figure 5.6).

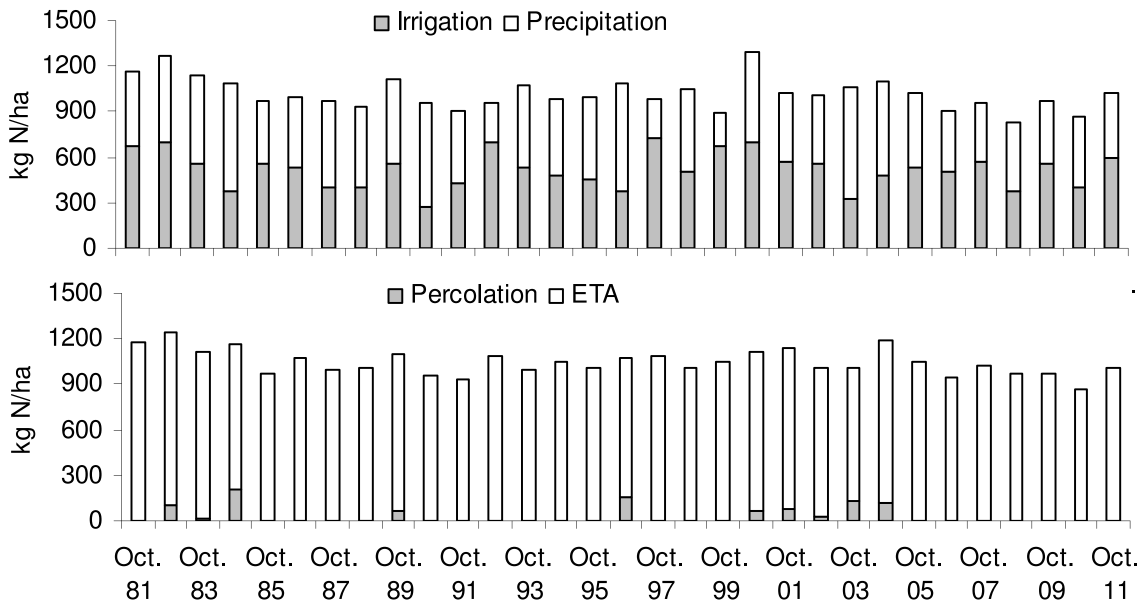


Figure 5.6: Annual irrigation, precipitation, percolation and ETA under OPTai treatment on medium loam in Quzhou County for 1980–2011

Figure 5.7 shows that the soil layers beneath the root zone dried out between October 2007 and October 2011 under OPTai irrigation because precipitation amounts were not enough to reach the 120–200 cm layers. While under FP irrigation the irrigation amounts in February 2009 and March 2011 were enough to refill these layers up to field capacity. Regarding the irrigation water use efficiency (WUE = grain yield [kg/ha, dry matter] / (precipitation [mm] + irrigation [mm]) there were no differences between treatments and soils except for FP treatments and OPTfp treatment on clay loam (Table 5.5).

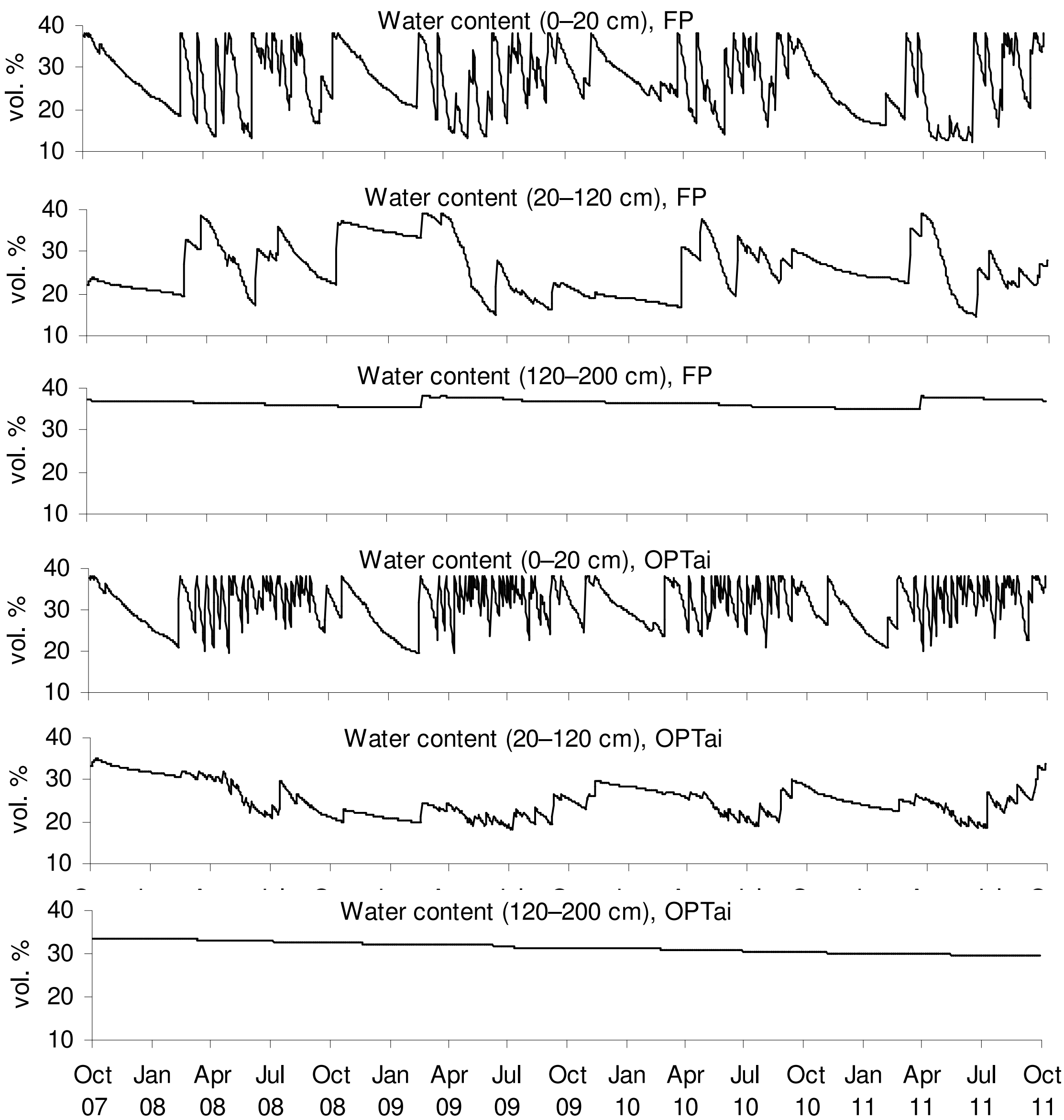


Figure 5.7: Actual water contents under average county management for farmers practice (FP) and model-based optimized with automated irrigation (OPTai) treatments on medium loam in Quzhou County for October 2007–September 2011

5.4 Discussion

Long-term regional N losses and groundwater use

The N losses in the current study under FP treatment, compared to FP treatment in other studies in the North China Plain appear quite high. For example another study conducted in Quzhou County by Li *et al.* (2010) calculated a cumulative N_2O loss of 4.9 kg N/ha with 270 kg N/ha fertilization from October 2005 to October 2006. In the current study, for the same period and under similar conditions, HERMES simulated 42.4 kg N/ha loss from total denitrification. This huge difference might have resulted firstly because the current study calculated total denitrification and not only N_2O but also from a higher irrigation in the current study and uncertainties in the interpolation method used to calculate annual emission rates by Li *et al.* (2010). However, this overestimation might be another evidence that the model should be further calibrated regarding N_2O emissions from denitrification as already discussed in Michalczyk *et al.* (2014). Additionally nitrification-born N_2O emissions should be implemented as a majority of N_2O in the NCP might be released that way (Ju *et al.,* 2011). Leaching might also have been a little higher, as irrigation amounts in other studies were a bit lower but with a higher frequency (Zhang *et al.,* 2003; Sun *et al.,* 2011). On the other hand the simulation results using the RZWQM2 model by Sun *et al.* (2018) were in a similar range; 400 mm irrigation with 400 kg N/ha resulted in leaching of a proportion of 0.48 of applied N. The higher volatilization under OPTfp treatment with lower N input compared to FP–SD was due to lower irrigation amounts under OPTfp because the model reduces NH_3 volatilization if irrigation amounts given at the time of fertilization are high (Michalczyk *et al.,* 2016). When comparing NH_3 losses of the current study from 1999 and 2000 under FP treatment with measurements by Li *et al.* (2002) and simulations by Li *et al.* (2019), results fit quite well.

The reaction of the organic C pool resulting from the amount of N input was also found by Liu *et al.* (2006) who simulated organic C with the DNDC model in Quzhou County. Their results of around 20 t C/ha on medium loam for a farmers practice treatment were similar to the results of the current study although they assumed a lower straw return proportion in their study. An increase of organic C during long-term studies was also found by Zhang *et al.* (2017) in Hengshui City, Hebei Province in NCP using the DNDC model (1981: 18.9 t C/ha; 2011: 28.9 t C/ha) and very strong increase by Niu *et al.* (2011) in Quzhou County during a field experiment (1985: 19.9 t C/ha; 2001: 37.3 t C/ha) both in 0–20 cm depth, using high inorganic N fertilization and residue return. These strong increases compared to the current study might be due to different soil characteristics. Also the results of Yan *et al.* (2012), 32.6 t C/ha in Quzhou County and Qin *et al.* (2013), 22.5 t C/ha in upland cropping systems in the NCP in 0–30 cm fit to the range of the results in the current study. In opposite to the current study HERMES simulated a decline in organic C from 85 to 77 t/ha in a soil depth of 0–30 cm from 1980 to 2007 in a study in Czech Republic (Hlavinka *et al.,* 2014), which may probably have resulted from less residue in put than in the current study. However, it is not clear whether the organic C pool will be maintained only with chemical fertiliser and residue input under these conditions on an even longer run.

In contrast to the organic C pool the N_{min} pool under OPTai treatment showed a slight accumulation which has been simulated due to heavy rainfall events. This indicates that under this climatic setting only natural perennial vegetation without N fertilization would totally impede leaching.

The yield gap on clay loam soil under all FP treatments and OPTfp mainly was due to drought stress during grain filling (GS71–79) in winter wheat at the end of May or with less intensity during grain filling (GS71–79) in summer maize end of August. When the soil water content was close to field capacity after irrigation an oxygen deficit occurred for one to three days resulting in a slight yield decline of 1–2%. However, this happened more often under OPTai irrigation than under FP irrigation. Only the management of OPTai was able to close the yield gap with continuous and field capacity-related irrigation but it resulted in slightly higher N losses compared to OPTfp, particularly for denitrification. On sandy, silty and medium loam the results fit to the results of Wang *et al.* (2001) who, at that time, supposed a lower irrigation frequency to reduce soil evaporation. But on clay loam soil this might not hold true due drought stress and resulting yield reduction, especially in winter wheat. Thus the results of the current study suggest that irrigation timing is essential especially on soils with higher clay contents to fill the yield gap. An effect of soil type on maize yields was also found by Zhao *et al.* (2015).

As groundwater is assumed to be used for irrigation, the higher groundwater use under OPTai was due to lower percolation amounts, but relatively high irrigation amounts resulting from a higher irrigation frequency with lower amounts and thus a higher ETA. This consequently led to a reduced groundwater recharge, which may even become worse if it is accompanied by a water rebound effect (Song *et al.,* 2018). All FP and OPTfp treatments were irrigated in average 3.4 times per year, while in the OPTai treatment during the same period between 12.3 (silty loam) and 14.4 (clay loam) irrigation events per year took place (successive days with irrigation were counted as one event). A higher ETA with a higher irrigation frequency was also found by Dar *et al.* (2017).

Mo *et al.* (2005) found a slightly lower potential ET (1060 mm/a) in summer maize in 1992 and winter wheat in 1993 in a large part of Hebei province (108 counties including Quzhou) as in the current study (1095 mm/a). The actual ET showed a similar trend with 750–900 mm/a and 825–952 mm/a, respectively. This difference might be a result of a higher irrigation (549–663 mm/a, five applications, OPTfp) compared to the study of Mo *et al.* (2005), (360 mm/a, six applications). In the study of Sun *et al.* (2011), the ETA of a wheat-maize rotation at one site in Quzhou County was more than 100 mm/a lower than in the current study on comparable soil during the same period, probably for the same reason. Both studies used Penman–Monteith equation to calculate ETA. Thus one reason for the difference might be that the crop (Kc) and the soil adjustment coefficient (Ks) were calculated in a different way.

In general the simulations bear a risk to have worse results compared to measured or survey data due to fixed sowing, harvest and, in part, fertilization and irrigation dates. This could have been the case for grain yield 2007. When comparing grain yields the simulated results (whole county average for FP, 2007) were only slightly lower with 5.6 t/ha for winter wheat and 6.9 t/ha for summer maize, but were in a similar range as the average yield resulting from the survey in 2007 with 6.6 t/ha for winter wheat and 7.2 t/ha for summer maize. Anyhow, the grain yield results for the sum of four harvests, winter wheat 2005 to summer maize 2006, of 22.3 t/ha fit well to the results of Sun *et al.* (2011), with about 23 t/ha.

Site specific differences and their spatial distribution of N water and yield

Technically the coupling of the GIS with the HERMES model might not be the best solution, resulting in much manual simulation work. Other authors found better coupling solutions like Li *et al.* (2007) which were, however, fixed to a certain GIS system. General risk may have resulted from overlaying maps from different sources in GIS as borders did not exactly fit to each other. Also, being a one-dimensional model, HERMES does not consider horizontal flows and thus, does not calculate water and nutrient exchange between modelling units.

Similar to the cropping pattern found by Liu *et al.* (2006) in 2001/02, wheat–maize was mainly grown in the north-west and south of the county in the current study in 2011 as well. This was despite the share of wheat–maize and cotton area to total sown area, with a proportion of 0.95, being bigger than in Liu *et al.* (2006), which had only more than 0.7. Thus land use patterns might have shifted towards wheat–maize and cotton during the last decade. This was underlined by Zhao *et al.* (2015) who found that the area of classified maize in Quzhou County increased over time from 62.55 km^2 in 2007 to 150.0 km^2 in 2013. However, the wheat–maize area of the current study for the year 2011 was 314.56 km^2, which may be due to the fact that in the current study the winter wheat area was classified in end of May, assuming that summer maize was planted on all winter wheat fields, with mainly one satellite image only, while Zhao *et al.* (2015) used four per year.

However, the current study used >1300 ground truth data locations (a proportion of 0.7 of total locations), while Zhao *et al.* (2015) used 65 only.

The accuracy of the land use classification was satisfactory although there were a lot mixed pixels as the pixel size of Landsat5 (1000 m^2) satellite images can exceed the field plot size of a farmer in this region, which according to the survey in 2007 is on average about 3.6 mu or 2400 m^2. These land use classification problems due to small-scale differences were also found by Liu *et al.* (2006).

The lower N fertilizer inputs according to the survey in 2007 in the south-east of the county might result from the sandy soil in the far south-east and the related high proportion of cotton cultivation along the eastern border of the county, as cotton in China prefers sandier soils. There were no other spatially different management trends like a north–south trend within the county as, for example in the study of Binder *et al.* (2008) who simulated the whole NCP. This may be due to the small size of the county with, except for soil texture, similar crop growing conditions within the county, especially climatic conditions which were the same for the whole county. Li *et al.* (2014) up-scaled the DNDC model to a region larger than the NCP using counties as the smallest unit in 2009. They found an average N leaching under full irrigation between 127.66 and 132.12 kg N/ha for N inputs around 423 kg N/ha/a which fits the results of the current study quite well. Anyhow for Quzhou County their simulation resulted in only 0–50 kg N/ha leaching, which may be due to the lower fertilizer N input of <150 kg N/ha. Their spatial differences were mainly driven by differences in N and water input, whereas for the current study also soil texture plays an important role. For example grain yield under N saturated conditions like under FP in this study is more dependent on soil texture, as this determines the plant water availability. The low volatilization losses in Liyue were due to the use of ABC (ammonium bi-carbonate) fertilizer (17% N) in cooler autumn and spring weather and NPK (compound) fertilizer (15% N) in summer instead of urea which is often used in the other townships.

Best-practice management options

In the current study the N saving potential was 450 kg N/ha/a when management was changed from FP to OPT, resulting in a reduction of 52–54% N fertilizer and 9–20% groundwater irrigation, which is, in case of N fertilizer, quite high compared to other studies. Xiao *et al.* (2019) was able to reduce N fertilizer by 43% and groundwater input by 28% when a recommended farming management was used instead of FP. In a five year study in Beijing Zhang *et al.* (2015) suggested a N rate based on the DNDC model between 150–240 kg N/ha for maize with regard to "acceptable" yield and N leaching, while the lowest possible N rate in the current study for maize ranged only between 100–130 kg N/ha. This may be due to lower long-term yields and the summer maize–winter wheat double crop rotation in the current study. Wang *et al.* (2017) found a threshold of 185 kg N/ha, regarding acceptable yield and N losses, for winter wheat on six sites in the NCP in two and three years, while N application in the OPT treatments ranged from 115–153 kg N/ha around the average of 134 kg N/ha, which is probably for the same reason as for summer maize mentioned above. Anyhow the model-based N fertilizer recommendation using HERMES gave good results when tested in real-time against field data in Quzhou County (Michalczyk *et al.,* 2014). In a four-year study on winter wheat at Luancheng, Zhang *et al.* (2018a) found that 100 kg N/ha and two irrigation events of 60 mm each could maintain high yield (7500–9200 kg/ha). Unfortunately they did not specify soil N_{min} status before the experiment and the amount of pre-sowing irrigation. According to the Ministry of Agriculture of People's Republic of China, the recommended nitrogen application rate for wheat in North China Plain ranged between 106 and 141 kg N/ha for yields <5630 kg/ha, which was the lowest yield category (Wang *et al.,* 2017). This indicates that the N recommendation in the current study was in a reasonable range since the long-term winter wheat yield was at around 5000 kg ha^{-1}. Again taking the differences in grain yield into account the following studies also match to these results. Using the DNDC model at Doncun farm, Shanxi Province in Northern China, Cui *et al.* (2014) found a possible reduction to 366 kg N/ha/a and 300 mm/a in a winter wheat summer maize double-crop rotation without reducing grain yield. In a study of Zhang *et al.* (2018b) based on the same field experiments as those by Wang *et al.* (2017) optimal N rates considering yield and environment of 202 kg N/ha for winter wheat and 179 kg N/ha for summer maize were found, with yields of 6527 and 7915 kg/ha, respectively. According to regional N rate guidelines, developed for the NCP by Cui *et al.* (2013) on basis of residual mineral N, the N rates for yields of 6 and 9 t/ha for wheat and maize should be 154 to 159 and 164 to 171 kg N/ha, respectively.

Using supplementary irrigation in a similar irrigation regime as under OPTai, Wang *et al.* (2015) found 210 kg N/ha to be the optimal N rate for wheat at Shandong Agricultural University Experimental Station, NCP, which was higher than in the current study but they also achieved a higher yield. Sufficient irrigation was higher in the current study than in most other studies mentioned here; this may lead to the fact that crop drought resistance, especially of winter wheat, should be even more adapted in the model parameters as in Michalczyk *et al.* (2014).

There is a risk of bias as one soil type was represented by one fixed soil profile. For example denitrification was higher on silty loam than on medium loam due to a clay band in 80 to 140 cm depth in the soil profile. This profile had been chosen as clay bands in deeper layers seemed quite normal in the region according to survey data.

When only N input and output is considered OPTfp seems to be the best option. But if yield is taken into account OPTai might be the best management scenario as it closed the drought yield gap on clay loam with the disadvantage of higher denitrification. Even higher differences in denitrification on soil with a low and a high clay content were found by Fang *et al.* (2013). Although the OPTai scenario seems to be the best option according to N use, N losses and water use it may have a negative effect on soil organic matter pools, as the initial organic C content was not reached even when straw residues were completely returned. Thus future work should contain an irrigation management adapted precisely to weather, soil type and crop needs. In order to support a good organic matter regime N management should be optimized but compared to this study not too low and include manure-based fertilization (Gai *et al.,* 2018).

In late 2014, China had announced a policy of "zero growth of chemical fertilizer use and zero growth of pesticide use" by the year 2020, which has been implemented since early 2015 (Jin and Zhou 2018). In the field of mineral fertilizers, besides the abolition of some former national preferential policies such as reduced energy prices for fertilizer production or reduced tariffs for fertilizer transport by rail, this has led to strong efforts by provincial governments to reduce fertilizer use. As a result, per hectare application rates of mineral N and phosphorus fertilizers have already been declining in many provinces since 2016. In applied research, an increasing number of field experiments are now dealing with reducing mineral fertilizer application rates (Liu *et al.,* 2016; Wang *et al.,* 2017). A well parameterized and locally adapted advisory model such as HERMES may therefore offer an additional powerful tool for assessing the potential effects of fertilizer application rate reductions on grain yield and the environment.

5.5 Conclusion

Probably no other study in the North China Plain, has simultaneously investigated N and water losses in a winter wheat–summer maize cropping system and their best management options with the help of model recommendations on county scale. Simulated annual long-term total N losses from nitrate leaching, NH_3 volatilization and denitrification summed up to 296.8 kg N/ha under FP and to 101.7 kg N/ha under OPTai treatment, corresponding to a proportion of 0.57 and 0.4 of the applied fertilizer N. Spatial differences in N losses, beside differences due to land use and soil texture, throughout Quzhou County could only be found due to different N inputs among the townships, which were based on survey results. Compared to farmers practice an optimized treatment could save on average more than 260 kg N/ha/a from fertilizer input and 190 kg N/ha/a from N losses and around 115.7 mm/a of water. The OPTfp treatment on sandy loam had the lowest fertilizer N and irrigation water input without reducing yield, while N losses were lowest under OPTai. On clay loam soil OPTai worked best, except for a high simulated denitrification loss, while the simulations based on farmers practice could not match the actual water needs which resulted in yield decline, especially for winter wheat. Although the optimized treatments had the lowest N inputs and N losses, they did not seem to be able to maintain the soil organic matter pools, even with full crop residue input. Additional organic inputs would be required, preferably from animal sources. Thus, especially for simulations on clay loam soils, management of N and water needs a precise adaption to actual weather conditions and plant growth needs. Additionally, drought resistance parameters in the model might need more adjustment to local wheat and maize varieties. Using the HERMES model is a relatively simple method to quantify N losses and N saving potentials via N fertilizer and irrigation water recommendation on spatial scale.

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Conflicts of Interest

The authors declare there are no conflicts of interest.

Ethical Standards

Not applicable.

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6 Synthesis, general discussion and conclusion

6.1 Model performance and extension *(answers to Q1 and Q2)*

Performance

The research presented in this thesis shows that the HERMES model generally performed well under the experimental conditions of the NCP (chapter 2). It reached similar results as other recent studies, e.g. for calibrated wheat–maize biomass the coefficient of determination (R^2) was 0.90 compared to 0.88 for wheat achieved by Zhou et al. (2018). Validated wheat biomass had a modelling efficiency (*ME*) of 0.91 in this thesis versus 0.75 in Zhou et al. (2018). A study (Zhang et al. 2017) focussing on wheat–maize grain yield and C_{org} achieved higher *ME* values (wheat grain 0.82, maize grain 0.69) than this thesis, chapter 2 (from validation, wheat grain −1.82, maize grain −0.53), however calibration and evaluation of Zhang et al. (2017) took place on the same experiment only with different treatments. The C_{org} content was in a reasonable range as in (Cong et al. 2014), although it was not clear whether it may be maintained on an even longer run than 31 years, while the ETA seemed to be a little overestimated (chapter 5, discussion) for wheat–maize rotations. Malone et al. (2017) came to a similar result and suggested that this was in their case due to a lacking reduction of soil evaporation under surface residue cover, which would fit to this thesis as the average straw return was between 75 and 100 % throughout the county. Simulations on Dongbeiwang 1 experiment, conventional treatment (chapter 3) on the one hand indicated an overestimation of N_{min} contents by the model, which might have been due to an upward water movement, that transported N_{min} upwards from deeper soil layers. The idea of upward water movement in this region was also supported by Kröbel et al. (2010). On the other hand the high measured soil N_{min} contents were a bit underestimated by HERMES, which was a bit difficult to explain (‘3 + x’ experiments, chapter 2). One explanation might be that the NH_3 volatilisation was overestimated, as it was set to 15% of applied urea N based on local expert knowledge. This made a dynamic volatilisation sub-module necessary, which was for this reason implemented in chapter 3. In agreement with the findings in chapter 3, NH_3 overestimation probably occurred especially with high N application rates and on application dates with low temperatures in the more simpler (variations 3 and 4) NH_3 volatilisation approaches.

Extensions

The solutions for NH_3 volatilisation (chapter 3) gave good results with daily cumulative average *ME* values between –0.81 and 0.52 or between –0.91 and 0.32 over all simulations using final cumulative values. These were in a similar range as found by Li et al. (2019) using the DNDC model also for simulated experiments in the NCP or by Li et al. (2007) for calibrated NH_3 losses in Fengqiu County using the WNMM model. Fang et al. (2008) simulated NH_3 volatilisation with the RZWQM-CERES model with comparable absolute values than in this thesis. They did not calculate the model performance for NH_3 volatilisation but *ME* values e.g. for wheat and maize biomass were with 0.74 and 0.77, respectively, in a similar range. Absolute NH_3 volatilisation values of chapter 3 and also long-term regionalised NH_3 values of chapter 5 fit to the range of recently measured (Yang et al. 2019) as well as simulated (Li et al. 2019). Whereas Huo et al.(2015) measured lower values for urea (12.0% ± 3.1% of applied N). Four model approaches are available and therefore, make the model suitable for more complex conditions as well as circumstances with limited input data availability. For some events with variation 1 under warmer weather conditions NH_3 volatilisation was overestimated. This might be explained by an overestimation of the influence of temperature on NH_3 volatilisation by the model (see chapter 3). In chapter 3 it was also pointed out that simple approaches such as variation 3 or 4 can also give satisfying results, having advantages in requiring less inputs. However, they were not sufficient to respond to changing environmental influences, which made the implementation of underlying physical and chemical processes necessary (variations 1 and 2).

The nitrification inhibition tool within the HERMES model (see chapter 4) performed well under the experimental conditions. However, it should be further tested and validated. The effect of the nitrification inhibitor on simulated leaching, NH_3 volatilisation and denitrification was well displayed by the model. It resulted in a longer lasting NH_4 pool and consequently in lower N leaching, which was also found by (Yang et al. 2016). However, a longer lasting NH_4 pool also resulted in higher NH_3 volatilisation that was also described by Qiao et al. (2015). No differences in denitrification could be found for simulations with and without nitrification inhibitor. Though, a nitrification inhibitor may decrease N_2O emissions via nitrifier denitrification (Wu et al. 2018). Therefore, the model needs to be adapted for N_2O losses from nitrification. Thereafter the HERMES model with the nitrification inhibition tool could well contribute to further N and water saving calculations.

Modelling risk

The quality of available data is essential for sensitivity analysis and validation of models, thus it is important to take care for measurement errors in field data since data quality is effected by them (Shaeffer 1980). Measurement of soil water contents in chapter 2 indicate that they were very heterogeneous within the plot due to uneven infiltration. The same can be true for observations of soil N_{min} which can have a large spatial variance that can sometimes be even larger than expected from model calculations (Kersebaum et al. 2005).
Kollas et al. (2015) stated that a multiple-model ensemble reduces error in simulating European cereal crop yield compared to a single-model. Which in turn means that single model studies such as in this thesis bear a higher failure risk. Also Yin et al. (2017a, b) give the evidence that the mean of several models predicts European grain N better than one single model.
As also mentioned by Hoffmann et al. (2016), soil aggregation like using one representative soil profile for one of the four soil types in Quzhou County as in the regionalisation study chapter 5 bears uncertainty, especially when spatial yield patterns were assessed. However the study of Fu et al. (2015) used the same soil texture for one 36 km*36 km grid cell to calculate NH_3 emissions for whole China and Li et al. (2014) used counties as the smallest modelling unit to calculate leaching in Northern China, compared to these studies, simulations in chapter 5 were more detailed bearing lower risk. In flat, homogenous landscapes a resolution of 50–100 km for weather data is sufficient (Zhao et al. 2015). Therefore, using data from one single weather station for the whole county (chapter 5) was adequate.
In chapter 2 it was indicated that there was an uncertainty of the input of water and nutrient leaching by flood irrigation. This was also true for the irrigation amount sensitive model-based NFR. Thus exact irrigation amounts should be known for future studies.

Possible improvements for HERMES

Most N fertilisation studies do not consider other nutrients such as phosphor (P) as well as HERMES in this thesis. In a long-term fertilisation study on wheat-maize cropping systems in China Duan et al. (2014) stressed the importance of P supply especially for wheat. Li et al. (2005) found out that P has the potential to increase the resistance of crops to droughts, while one of the results of Wen et al. (2016) was that balanced application of N with P significantly reduced soil residual nitrate compared with only N fertiliser application. Thus not considering P holds the risk that, if P is not fertilised sufficiently, P might be the limiting factor at least in field experiments (van der Velde et al. 2014). In the simulations of this thesis P could not influence crop growth and thus synergy effects, as mentioned above and by Wen et al. (2016), could not be studied. However, apart from P, runoff and pests and diseases, HERMES does consider major environmental factors. Although, nitrification-born N_2O emissions should be additionally implemented into HERMES as a majority of N_2O in the NCP might be released that way (Ju et al. 2011).

Hou et al. (2018) found that for upland areas in China surface N runoff increased by 31% since 1990, but also stated that the up-scaling of the model led to uncertainties of 40% as coefficient of variation of N runoff due to up-scaling. HERMES does not consider N runoff, which was probably not relevant for this thesis as the farmers in the experiments made a little wall around their fields for irrigation. If at all, surface N runoff probably would have happened only to a small extend as we only simulated on plot and county scale. Additionally a decreased irrigation could have offset the impact of high N fertilisation on N runoff trends (Hou et al. 2018). Wang et al. (2014) concluded that the modelling risk of runoff N loss was one tenth of the risk for leaching.

To further improve the NH_3 volatilisation upward and downward movement of NH_4 and alkalinity should be included in the model as mentioned in chapter 3. Also cation exchange, pH buffer capacities and pH buffering effects caused by dissolution and precipitation of $CaCO_3$ and CO_2 loss could be optional inputs as already suggested by Roelcke et al. (1996). However, such measurements are not commonly available in practice. In order to better display local wheat and maize varieties, drought resistance parameters in the model could be adjusted as discussed in chapter 5.

6.2 Model-based N and water saving potential on plot scale, long term and regional scale (*answers to Q3 and Q4*)

Saving potential on plot scale

A prerequisite to use a model to find out its potential to help with calculating optimised N rates is that it has a high modelling performance as discussed in the previous chapter. Assuming this generally, the model-based NFR in combination with optimised irrigation practice has the highest potential to reduce N losses.

N input and fertilisation rate

The average model-based NFRs for winter wheat and summer maize in this thesis on plot scale and short term (chapter 2) was only 63 for 2009/10 and 84 kg N $ha^{-1}a^{-1}$ for 2010/11 for optimised N and optimised irrigation. For winter wheat with high irrigation it was 126 kg N ha^{-1}. This was on the one hand comparably low, e.g. Manevski et al. (2016) recommended with the help of the DAISY model 100 kg N ha^{-1} for maize and 200 kg N ha^{-1} for wheat with yields of 8 and 6.5 t ha^{-1}, respectively during four and six years at Luancheng station in the NCP. On the other hand Liu et al. (2003) recommended similar, to the winter wheat in this thesis with high irrigation, low N rates in their two year study. Also Hu et al. (2006) recommended about 100 kg N ha^{-1} and crop in a 2.5 year study, while winter wheat yield was even best with an N rate of 50 kg N ha^{-1} and crop. However, Zhang et al. (2018e) calculated N rates of 202 kg ha^{-1} for wheat and 136 kg ha^{-1} for maize for highest economic benefit considering environmental cost. This rate was said to result in soil nutrient mining under maize, as an input of 43 kg N ha^{-1} was necessary to make the soil N balanced and was thus not enough to maintain soil fertility in long term.

Leaching and irrigation rate

In the best-practice management modelling scenario in chapter 2 leaching was reduced almost to zero, while yields were maintained. However, there is a remaining uncertainty of the input of water and nutrients leaching by flood irrigation especially when soil N accumulation is high as described in chapter 2. Although Wang et al. (2014) stated for the Baiyangdian Basin, which is around 250 km north of Quzhou County, that leaching risk below crop root zone in a period up to 10 years was low, and the nitrate contamination of groundwater not yet reached a critical level due to the thickness of the unsaturated zone.

In this soil-plant system irrigation practice also plays a role regarding nitrogen and groundwater contamination via leaching. An irrigation rate of 150 mm per crop (two events, 75 mm each) at beginning of double ridge and beginning of flowering seemed to be best as the need for more N fertilisation as well as leaching started to increase at higher rates, while at a lower rate yield decreased (chapter 2). Even though a critical irrigation rate could be identified, risk for modelling uncertainties remains as Mack et al. (2005) found that after harvest of winter wheat the water transfer to the atmosphere was increased. That bears the possibility that some nitrate might move upward again with soil water and become available for plants. This was also simulated by HERMES especially under hot and dry weather, e.g. 6 June, 33.4 kg N ha^{-1} and 6 July 1988, 32.9 kg N ha^{-1} leaching resulting in 0.5 kg N ha^{-1} upward movement within one month.

Volatilisation and denitrification

HERMES simulated changes in NH_3 volatilisation according to management changes well, and thus can contribute to the models N saving potential. While in chapter 2 NH_3 volatilisation was a fixed amount of 15% of applied fertiliser N and thus proportional changing with the change of fertiliser N input, in chapter 3 NH_3 volatilisation was simulated dynamically (table 6.1). As discussed above similar uncertainties occur for NH_3 volatilisation and denitrification concerning irrigation water input.

Table 6.1: Average N fertilisation, average NH_3 loss measured and average NH_3 loss simulated per treatment in kg N ha^{-1} and their reduction between the treatments in % of Dongbeiwang 2 experiment (chapter 3)

	Average N fertilization kg N ha^{-1}	Average NH_3 loss measured kg N ha^{-1}	Average NH_3 loss simulated[a] kg N ha^{-1}
Conventional N treatment	150.0	34.2	33.6
Optimised N treatment	40.2	14.0	7.2
Reduction from conventional to optimised N treatment in %	73.2	59.0	78.5

[a] average across all fertilization events and the four NH_3 model variations

Saving potential on long term, regional scale

N input and fertilisation rate

A key issue of this thesis was to find best management options including the lowest possible long-term N rate for wheat and maize on regional scale concerning crop yield and soil quality. In this thesis it ranged only between 100–130 kg N ha^{-1} for maize and between 115–153 kg N ha^{-1} for wheat, which was comparable to other studies when differences in yield were considered (Zhang et al. 2018f; Zhang et al. 2018b) (chapter 5). The range of summer maize yield throughout the NCP found by Binder et al. (2008) was similar to the yield found in this thesis although they used a slightly higher N rate (140 kg N ha^{-1}). However, if quality such as grain protein content is considered higher N rates (208–230 kg N ha^{-1}) might be necessary as in the study of Liu et al. (2016). In chapter 5 it was discussed that C_{org} could be maintained under farmers practice (522 kg N ha^{-1} a^{-1} input) but not under optimised practice (about 246 kg N ha^{-1} a^{-1} input). Thus, additional organic input preferably from animal sources or compost (Liang et al. 2012; Roelcke et al. 2016) might be necessary. This is supported by Zhang et al. (2017) who found an optimal N rate based on yields, soil fertility, and greenhouse gas emissions with continuous inorganic fertilization combined with straw incorporation of 300 kg N ha^{-1} at Hengshui City, Hebei Province in NCP.

One reason, beside lower yield in this thesis, for these low N rates on county scale might be a synergy effect of simultaneously optimisation of N rate and irrigation rate (K. C. Kersebaum personal communication 9.9.2018). Although this effect cannot be simulated by the HERMES model, the assumption of Wang et al. (2018) would fit to the synergy effect. They stated that there is an effect on soil improvement and nutrient availability through a larger number of big macro-aggregates and higher C_{org}, total N and biological activity, as a result of long-term N fertilisation, which can make lower N fertilisation rates possible. The combination of chapter 2 and 4 allows further conclusions beyond the already mentioned. The regional long-term results of chapter 5 with its low soil N_{min} contents and higher recommended N inputs, might be the evidence to the already in chapter 2 discussed phenomena: The lower recommended N rates in the experimental fields might be a result of initially high observed N contents in the soil. In agreement to this, field experiments have shown higher N content in wheat straw due to N over fertilisation (Yue et al. 2012) which is supported by a high N mineralisation potential (Roelcke et al. 2000; Roelcke et al. 2002; Hartmann et al. 2014).

Leaching and irrigation rate

Simulated annual long-term N losses due to leaching in this thesis were lower than simulated leaching losses in the study of Fang et al. (2013) under similar conditions. However, N losses in total were similar, because losses from volatilisation and denitrification in this thesis were higher. One reason for these differences might be the use of different types of N fertiliser. Leaching losses were generally higher due to higher N input (Dai et al. 2016) and higher sand content in soil as well as higher nitrate content in fertiliser (chapter 5), when farmers practice flood irrigation was applied. In case of model-based automated irrigation application this was not true, since leaching was reduced almost to zero (on average 2.8 kg N $ha^{-1}a^{-1}$). Automated irrigation was applied by the model

according to soil moisture content, but not more than 25 mm per day, which resulted in numerous smaller doses and less amount in total, compared to flood irrigation.
Under similar conditions as under best-practice treatment in short term (see previous section and chapter 2), long-term simulations resulted in average leaching of 7.4 kg N $ha^{-1}a^{-1}$ in 120 cm depth. This is finally more than the 5.7 kg N $ha^{-1}a^{-1}$ in 90 cm depth and 0 kg N $ha^{-1}a^{-1}$ in 200 cm depth on short term, which underlines the necessity of long-term studies.

Volatilisation and denitrification
In this thesis (chapter 5) average simulated NH_3 emissions for Quzhou County ranged around 109 kg N ha^{-1} in 2000, 106 kg N ha^{-1} in 2008 and 99 kg N ha^{-1} in 2011, which is in a similar range than in the study of Xu et al.(2016) who estimated 74 kg N ha^{-1} in 2008 for the NCP from agricultural fertiliser. However this thesis exceeded the estimates of Kang et al. (2016) which were >30 kg N ha^{-1} in 2000 and < 20 kg N ha^{-1} in 2012 due to a reduction in the use of ammonium bi-carbonate fertiliser. This difference resulted probably from the different estimation methods as Kang et al. (2016) used emission factors on large scale which did not include changes due to wind speed and temperature for 16 kinds of crops, while in this thesis only the wheat–maize double cropping system was considered. Another reason might be that management conditions in this thesis (chapter 5) were based on current farmers practice and not adapted to former conditions when the simulation started (1980ies) as in Kang et al. (2016) and for example in Fu et al. (2015).
When changing from farmers practice to optimised N treatment a reduction between 55 and 66% NH_3 emissions on average for Quzhou County could be obtained in this thesis. However, in a global study on reduction potential of NH_3 emissions in general which took more aspects than water and N management into account, such as different fertiliser type and deep placement techniques, possible reductions of up to almost 100% compared to a control with urea fertiliser were found (Ti et al. 2019).
Denitrification in this thesis was higher on clay loam than on sandier soil. An even higher difference in denitrification on soil with different clay content was found by Fang et al. (2013). HERMES calculates total denitrification, while other studies only consider N_2O. Still, compared to other studies (e.g. Ding et al. 2007; Fang et al. 2008; Li et al. 2010) denitrification in this thesis seemed a bit high (see also chapters 2 and 4). This could be due to the limited availability of easily available organic carbon in NCP soils (Cai et al. 2002; Cui et al. 2012), which is not directly considered for the denitrification process in

HERMES and therefore has no declining effect. However, maximum denitrification rate in the model was derived from similar low C_{org} contents (Schneider 1991). Thus, processes involved in denitrification and production of N_2O emissions, should be investigated further using the HERMES model in the NCP. Nitrification born N_2O emissions (Ju et al. 2011) should be included into HERMES. However, the reaction of lower N input on denitrification was in a reasonable range in Quzhou County in this thesis with an N input of 756 kg N $ha^{-1}a^{-1}$ and an average denitrification loss of 57 kg N $ha^{-1}a^{-1}$ and N input of 239 kg N $ha^{-1}a^{-1}$ and a loss of 37 kg N $ha^{-1}a^{-1}$, compared to Ju et al. (2011). This also holds true for the effect of a higher irrigation frequency on denitrification. Here the N input was 253 kg N $ha^{-1}a^{-1}$, which resulted in 55 kg N $ha^{-1}a^{-1}$ denitrification loss.

Chances of implementation and adoption of N and irrigation water saving and recommendation methods

As mentioned in chapter 1.2 (subchapter methods and strategies…) numerous N and water saving methods such as technical field methods like reducing N fertiliser rate, applying chemical stabilised fertiliser or manure, using deep placement techniques, cultivation of deeper rooting plants or different plant cultivars in a different system like shifting from double to single crop per year, using drip or sprinkler irrigation as well as schedule irrigation do exist (Hu et al. 2005; Li et al. 2006; Ju et al. 2007; Sun et al. 2011; Hartmann et al. 2015; Huang et al. 2016; Meng et al. 2017; Zhang et al. 2018b). But there also have been suggestions on policy level or educational approaches as combining a rise in water price with training and extension, increase machinery level and the effect of fertiliser pricing through increase in farm size, as well as using a decision support program and establishing farmers participation and education approaches in villages (Wei et al. 2005; Chuan et al. 2013; Xu et al. 2014; Ju et al. 2016; Zhang et al. 2016).

A combination of these methods and model simulations as for example mentioned in chapter 1.2 (subchapter modelling approaches…), which are already part of some approaches, may lead to promising results which could convince farmers to adopt and thus, bear a great potential. To increase the number of model users a Chinese user interface for HERMES was introduced, but for adoption of the model probably more professionalism through larger farms and extension service might be necessary.

However, in the study of Böhm and Bergmann (2012) over 60% of farmers mentioned established habits and tradition (关系 guānxi) as being most important for decision making, in terms of fertiliser and manure management. This might be true for irrigation practice as well and will make the implementation of new ideas, promoted by extension service or scientific staff, even more difficult. Additionally, the timing of irrigation may depend on the availability of the pump which has to be shared with other farmers, resulting in great inaccuracies regarding irrigation water amounts.

This and the small-scale farm structure make a wider or nationwide application of N and water saving methods unlikely. Hartmann (2014) discussed prerequisites for improving N management in China and listed the education of farmers as the most important and also introduced a strategy to first cut the N rate in short term in using for example a simple recommendation method based on crop N demand (Hartmann et al. 2012). Then as an intermediate step the N application techniques and the extension service should be improved and finally on long term a balanced N fertilisation regime should be implemented. For mid and long term the above mentioned decision support systems and educational approaches such as “Science and Technology Backyard platforms” which involve local extension service as well as farmers (Zhang et al. 2016) could be an option, along with structural changes (Trappel 2015) like carefully enhancing farm sizes. Here, although model use for calculating high-yield systems was established already, the additional and more comprehensive use of the HERMES model could be integrated to further improve the method especially in terms of NFR. This was so far done manually via N_{min} probes.

Finally, important for the success of changes is the awareness and support of the Chinese Ministry of Agriculture who introduced in 2015 an action plan of “zero growth of chemical fertiliser use and zero growth of pesticide use” by the year 2020 (Jin and Zhou 2018).

This might be another step towards the “European Nitrates Directive” (European Commission 1991).

6.3 Outlook

The following prospects that arose during this thesis might be addressed in future research. Regarding the further use of HERMES in the NCP, nitrification born N_2O emission should be included into the model, as well as further possible implementations mentioned under chapter 6.1. A more exact input of irrigation water amount should be emphasised.

On the basis of this thesis HERMES could be applied and validated in other counties with different texture, weather and management for winter wheat–summer maize rotations, and also on alternative cropping systems in the same region to help to cope with climate change (Meng et al. 2017). This thesis was limited in using urea, ammonium bi-carbonate, ASN_{DMPP} and NPK (compound fertiliser) as fertiliser. Reducing NH_3 volatilisation with urease inhibitors seems to be also a promising option (Li et al. 2017) and could be tested in using HERMES. The same applies for a deeper investigation of nitrification inhibitors.

The C_{org} content was simulated for mineral fertiliser and straw return only. One question that came up was that from this thesis it was not evident whether solely inorganic fertiliser application with straw return could maintain C_{org} levels under NCP conditions.

Another related question arises whether a partly replacement of chemical fertiliser with manure would have under the conditions of this thesis a more positive long-term effect on C_{org} as well as the resulting long-term effect on model-based fertiliser recommendation and N rate.

Manure application in the NCP was found to increase wheat and maize yield under recent climate change simulations (Liang et al. 2018). This would fit into current announcements of the Chinese Ministry of Agriculture to save mineral fertilisers in using manure within crop- and region-specific rates (Hou 2017) and to the action plan of Chinese Ministry of Agriculture of “zero growth of chemical fertiliser use and zero growth of pesticide use” (Jin and Zhou 2018).

Generally the further, extensive use of the HERMES model in China would make sense, as it was carefully tested within this thesis, generating good results and as discussed in the previous section, could supplement the already existing model applications in the decision support systems for N and water strategies, also already a Chinese user interface for the model exists.

Another question arose was: What happens with drainage water on long-term and its eventually nitrate content beneath the root zone when groundwater level is far away like in the NCP? This would require extensive field studies on fate of water and N perhaps with N15 as also suggested by Hartmann et al. (2014) to be used for subsequent modelling.

As a projection for China prognoses a decrease in N surplus from 38 (2010) to 11 Tg N a^{-1} (2050) (Zhang et al. 2015) and additionally Chinas agriculture seems to face structural changes from smallholder farming to commercial and industrial agrarian production (Trappel 2015), changes of N and water management and of production potentials can be expected. To describe and evaluate these changes using a simulation model can play a major role.

6.4 Conclusion

The HERMES model performed well under the growing conditions of the NCP and was able to describe dynamics of the relevant processes related to soil–plant interactions and N_{min} within a winter wheat–summer maize cropping system. This was the first time a real-time model-based N fertiliser recommendation was used to improve nitrogen and irrigation water management in highly intensive agriculture of the NCP, where the model calculates the amount of needed nitrogen fertiliser at predefined fertilisation dates. During the short-term plot-scale best-practice simulations N reductions of 85 and 80% were achieved. These were probably possible due to the high initial soil N contents. However, despite displaying the N cycle well, the model might have slightly overestimated denitrification and ETA. Additionally, the current farmers practice of flood irrigation released uncertainties for model simulations with regard to soil water and mineral N. To decrease these insecurity, exact irrigation amounts should be known for future simulation studies.
The four newly implemented variations for calculating NH_3 volatilisation worked well under the conditions of the field experiments. As the HERMES model is a widely tested and established model the successful implementation of the dynamic NH_3 volatilisation sub-module is a benefit for future use. Nevertheless, in some cases especially with higher temperatures, simulated initial NH_3 fluxes were higher compared to the measured ones, depending on weather conditions.
Like NH_3 volatilisation, the HERMES model described nitrification inhibition with the newly implemented nitrification inhibition tool for ammonium-based fertiliser well compared to measured data. However, simulations of nitrification inhibition need further verification with measurements and processes of nitrification-born N_2O emissions should be considered in the model in the future.
Furthermore, temperature dependency of NH_3 volatilisation should be carefully checked for future simulations. Upward and downward movement of NH_4 and alkalinity, cation exchange, pH buffer capacities and pH buffering effects caused by dissolution and precipitation of $CaCO_3$ and CO_2 loss could be implemented in the model. However, these changes would require much more detailed data not only regarding soil properties, but also of the exact timing of fertiliser application and tillage operations during the day. Additionally, other nutrients such as P and surface N runoff could be included into HERMES to improve its performance under the conditions of the NCP.

The regionalisation of detailed N transformation processes and losses within a winter wheat–summer maize cropping system on specific defined soil and varying regional management within Quzhou County, gave good results. The model-based soil type specific N fertiliser and irrigation recommendation on county scale, within long-term simulations in the NCP, also performed well. When changing from farmers practice treatment to an optimised treatment, N fertiliser input could be cut down to on average 50%, N losses from nitrate leaching, NH_3 volatilisation and denitrification to 34% and irrigation water input to around 80% of farmers practice input on long term. This underlines the necessity of long-term simulations to overcome the effect of high N stocks in soil on short-term simulations. Thus, especially the combination of model-based N and irrigation recommendation bears a high potential to save N and water particularly in terms of leaching. The model could support best-practice solutions on plot scale as well as on county scale in terms of nitrogen and water use.

However, on clay loam crop water needs could not be reached by farmers practice irrigation. Thus, future simulations on clay loam soils require a precise adaption of management to plant N and water needs regarding actual weather conditions and probably also a better adjustment of drought resistance parameters in the model to local wheat and maize varieties.

Additionally, the optimised treatments did not seem to be able to maintain the C_{org} pools, even with full crop residue input. Thus, extra organic inputs would be required, preferably from animal sources or compost to maintain soil quality.

This thesis, in combining findings of chapter 2, 3, 4 and 5, operates between practical applications on plot scale with farmers and extension or research staff; and estimations on large (national, continental, global) scale. It, thus can offer, beside simulations on plot scale, further interpretation on county and regional scale for extension and research staff. In combination with other N and water saving methods and the prerequisite of stakeholder participation the HERMES model promises to be a useful tool.

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Appendix

Supplements for chapter 2

Table A.1: Mean absolute error, mean bias error and modelling efficiency for soil mineral nitrogen in 0–0.9 m, 0–0.3 m, 0.3–0.6 m and 0.6–0.9 m depth and above-ground biomass in the reduced N treatment of the exact experiment after calibration

		MAE	*MBE*	*ME*	n
Soil N_{min} 0–0.9 m	kg N ha^{-1}	34.68	–23.36	0.23	11
Soil N_{min} 0–0.3 m	kg N ha^{-1}	13.00	1.92	0.82	12
Soil N_{min} 0.3–0.6 m	kg N ha^{-1}	17.62	–15.66	–1.30	11
Soil N_{min} 0.6–0.9 m	kg N ha^{-1}	14.26	–9.79	–1.13	11
Above-ground biomass all	kg ha^{-1}	1223.27	–288.69	0.90	9
Above-ground biomass maize	kg ha^{-1}	1188.60	–1188.60	0.92	5
Above-ground biomass wheat	kg ha^{-1}	1266.61	836.19	0.83	4
N uptake all	kg N ha^{-1}	23.57	23.57	0.66	4
Grain yield all	kg ha^{-1}	953.33	368.85	0.29	4

Table A.2: Measured values, simulated values and their differences of N uptake and grain yield in the reduced N treatment of the exact experiment after calibration. Numbers following measured values show standard deviation

		Measured	Simulated	Difference [a]	n
N uptake maize 2009	kg N ha^{-1}	241.47 ±12.66	262.40	20.93	1
N uptake maize 2010	kg N ha^{-1}	152.17 ±2.08	181.80	29.63	1
N uptake wheat 2009/10	kg N ha^{-1}	125.55 ±46.57	160.20	34.65	1
N uptake wheat 2010/11	kg N ha^{-1}	158.45 ±18.47	167.50	9.05	1
Grain yield maize 2009	kg ha^{-1}	6571.67 ±328.05	7450.00	878.33	1
Grain yield maize 2010	kg ha^{-1}	7222.78 ±585.87	6670.00	–552.78	1
Grain yield wheat 2009/10	kg ha^{-1}	3843.98 ±1163.58	5610.00	1766.02	1
Grain yield wheat 2010/11	kg ha^{-1}	5766.19 ±524.29	5150.00	–616.19	1

[a] Simulated−Measured

Table A.3: Mean absolute error, mean bias error and modelling efficiency for soil water content in 0–0.3 m, 0.3–0.6 m and 0.6–0.9 m depth, soil N_{min} in 0–0.3 m, 0.3–0.6 m and 0.6–0.9 m depth, N uptake, above-ground biomass and grain yield in the zero N treatment, reduced N treatment, farmers' practice treatment and 'high yield' treatment, across farmers' fields of the '3+x' experiments after validation

			Zero N treatment	Reduced N treatment	Farmers' practice treatment	'High yield' treatment	n[a]	Across all treatments
Soil water content 0–0.3 m	vol. %	*MAE*	5.32	5.06	5.29	5.22		5.22
		MBE	0.05	-0.33	-0.65	0.12	38	–0.20
		ME	-0.02	-0.01	0.15	-0.03		0.03
Soil water content 0.3–0.6 m	vol. %	*MAE*	5.37	5.89	5.19	5.97		5.61
		MBE	2.10	2.44	1.80	1.73	38	2.02
		ME	-0.12	-0.40	0.00	-0.27		–0.20
Soil water content 0.6–0.9 m	vol. %	*MAE*	4.96	4.28	4.59	4.24		4.52
		MBE	1.31	0.18	-0.35	0.62	38	0.44
		ME	-0.06	0.21	0.27	0.07		0.13
Above-ground biomass all	kg ha^{-1}	*MAE*	1488.45	949.58	934.96	1278.13		1162.78
		MBE	582.42	-97.61	179.12	-628.19	44	8.94
		ME	0.78	0.94	0.93	0.88		0.43
Grain yield all	kg ha^{-1}	*MAE*	903.36	931.75	816.22	1411.27		1015.65
		MBE	507.69	-594.24	-290.89	-1133.58	12	–377.75
		ME	0.12	-1.11	-0.16	0.18		0.00
N uptake all	kg N ha^{-1}	*MAE*	17.72	29.90	35.13	29.07		37.28
		MBE	-0.78	28.28	39.02	26.14	44	23.17
		ME	0.55	0.23	-0.17	0.27		0.18
Soil N_{min} 0–0.3 m	kg N ha^{-1}	*MAE*	34.62	35.42	66.08	36.31		43.11
		MBE	-34.18	-1.32	21.41	-12.68	35	–6.69
		ME	-0.80	-0.07	-1.32	-0.48		–0.71
Soil N_{min} 0.3–0.6 m	kg N ha^{-1}	*MAE*	26.84	33.60	36.05	29.70		31.55
		MBE	-25.79	-17.81	-7.57	-13.78	35	–16.24
		ME	-1.02	-1.06	-1.92	-1.43		–1.41
Soil N_{min} 0.6–0.9 m	kg N ha^{-1}	*MAE*	26.37	25.03	24.19	31.34		26.74
		MBE	-14.49	-8.84	1.82	-6.74	35	–7.06
		ME	0.17	-0.11	0.04	-0.33		–0.04

[a] in this column is the number of replications for one treatment. For across all treatments this needs to be multiplied by four

Supplements for chapters 1 and 4

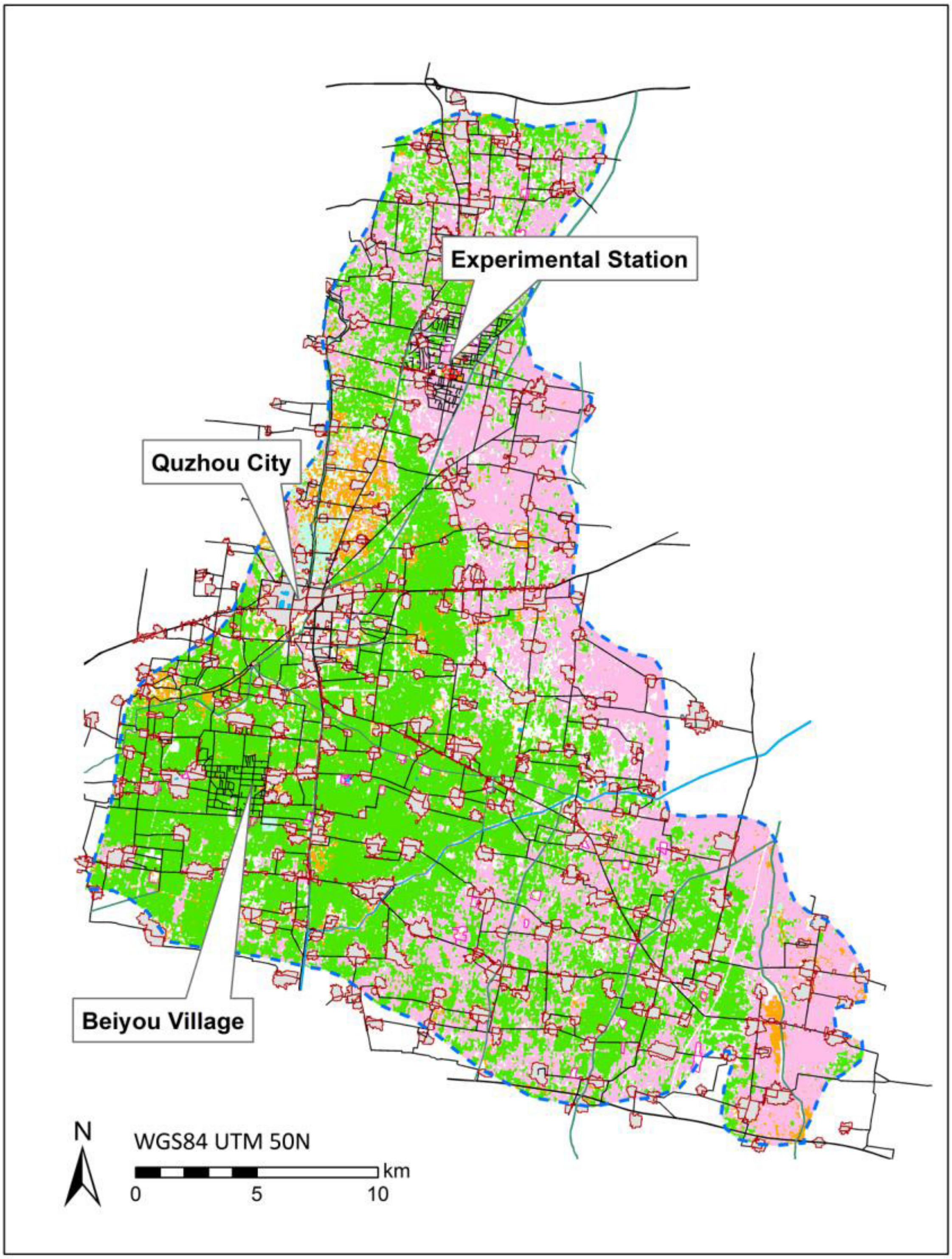

Figure A.1: Quzhou County with "Topo-GIS", manually digitised featured such as villages and streets and land use classification as background, green = wheat, pink = cotton. Close to experimental station was the exact experiment located (chapter 2 and 4) and close to Beiyou village was the 3+x experiment located (chapter 2). Made by H.-P. Dauck

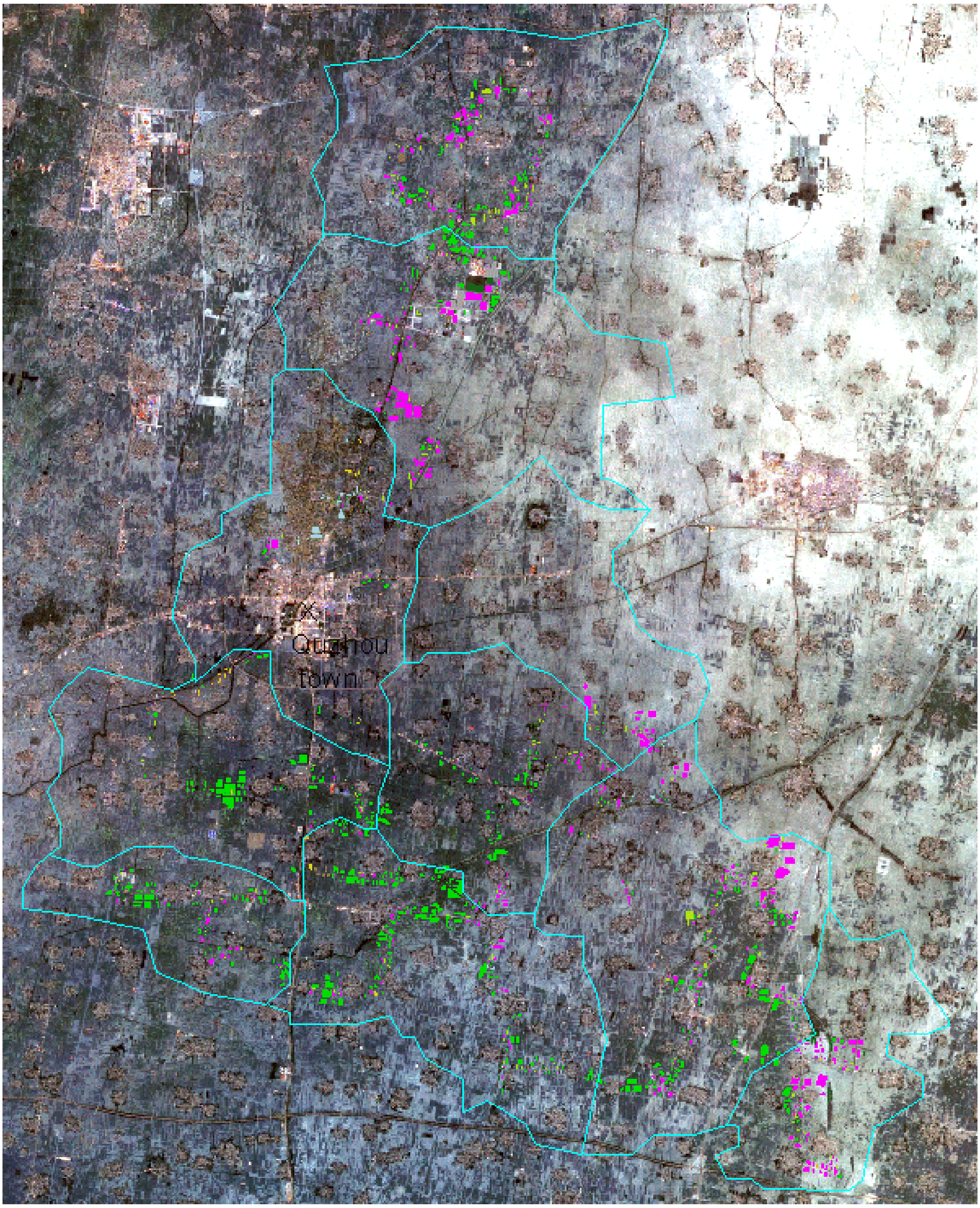

Figure A.2: Quzhou County with township borders (blue), ground truth areas (coloured) and Landsat 5 satellite picture as background. Prepared partly by H.-P. Dauck

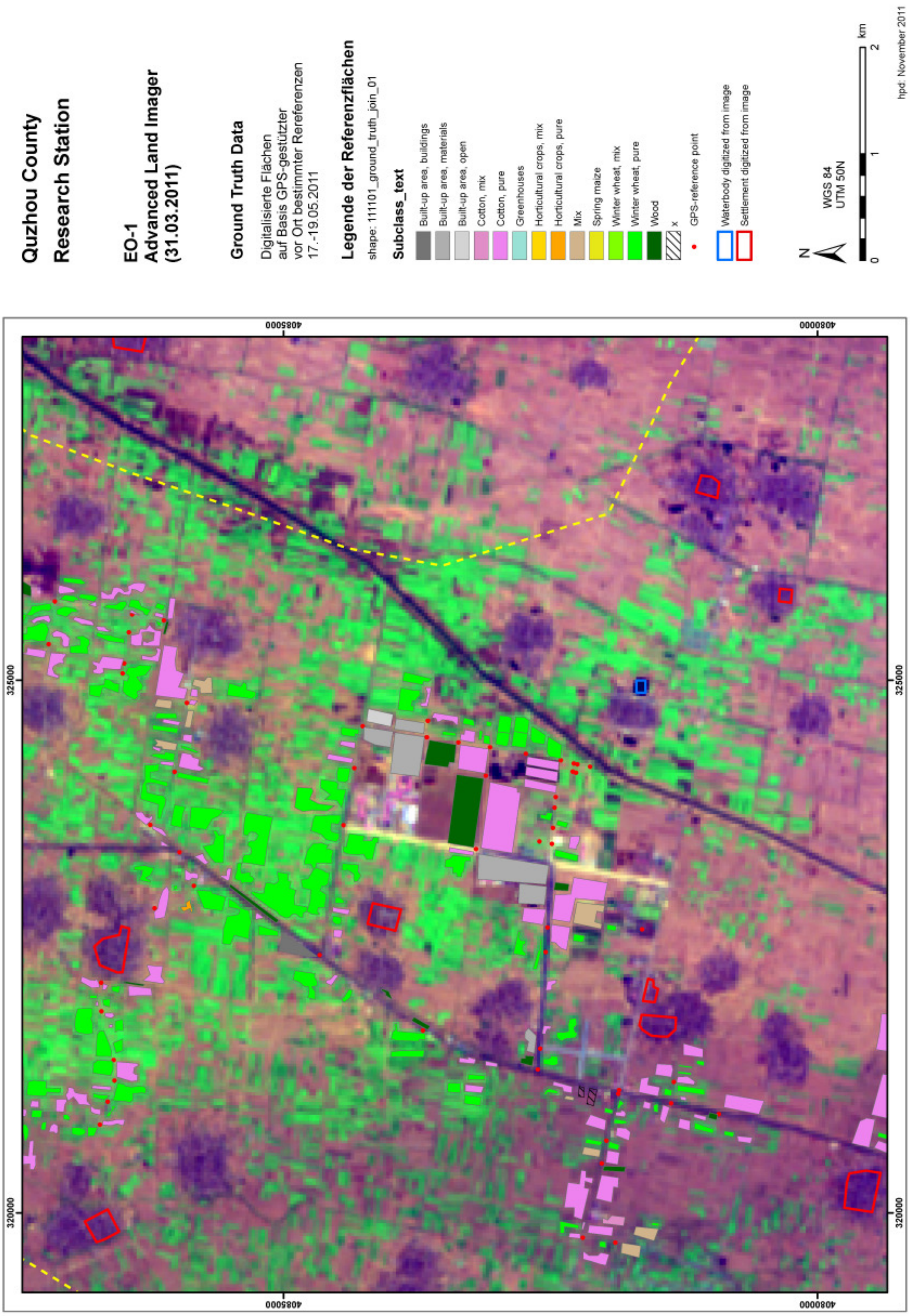

Figure A.3: Extract of the area around Quzhou experimental station. Full bright colours show manually *in-situ* digitised ground-truth patches, lines digitised from image. Satellite picture of EO-1 Advanced Land Imager as background

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