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Drivers of yield and nitrogen-loss tradeoffs: Cropping system evaluations with process-based modeling

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Drivers of yield and nitrogen-loss tradeoffs: Cropping system evaluations with process-based modeling

by

Rafael A. Martinez-Feria

A dissertation submitted to the graduate faculty
in partial fulfillment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

Major: Crop Production and Physiology

Program of Study Committee:
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The student author, whose presentation of the scholarship herein was approved by the program of study committee, is solely responsible for the content of this dissertation. The Graduate College will ensure this dissertation is globally accessible and will not permit alterations after a degree is conferred.

Iowa State University
Ames, Iowa
2018

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The Midwest is one of the most productive agricultural regions, but mitigating loss of nitrogen (N) from cropland is needed to improve environmental quality. Tradeoffs between crop yield and N loss have been linked largely to the inefficient use of N fertilizers, but the contributions of more systemic factors such as soil characteristics, crop sequences and genotypes have not been thoroughly studied. This dissertation examines and quantifies the impact of various genetic, environmental and management drivers of crop yield and N-loss tradeoffs in the maize and soybean cropping systems of the US Midwest, and identifies potential management strategies to lessen these tradeoffs. To this end, a system analysis framework was employed, which used field data from small plots, long-term experiments, publicly available databases, and process-based modeling. The approach allowed for full exploration of the soil-plant-atmosphere continuum and extrapolation of the behavior of cropping systems across a wide range of weather, soil, and management. Findings from these studies indicate the prominent role of crop sequences and residue dynamics in driving tradeoffs. In maize-soybean systems, it was estimated that a majority (55%) of N losses originated from the release of native soil N into the environment due to asynchrony between soil mineralization and crop uptake. Including a rye cover crop in rotations was shown to be an effective way of improving soil N retention and reducing losses, while seldom resulting in yield tradeoffs. However, the most effective strategies also required simultaneously choosing appropriate genotypes, timely planting, and optimizing N inputs to better match crop requirements. Research also aimed to advance knowledge and modeling of various crop-soil processes.
including: maize, soybean and rye growth; water and N cycling; and a novel algorithm to simulate grain dry down of maize and soybean.
CHAPTER 1. GENERAL INTRODUCTION

Background

With world population expected to reach 9.7 billion by 2050, a 33% increase from 2015 levels (UN, 2015), pressure is rising on agricultural systems to deliver more goods to meet the needs of growing populations. Meanwhile, environmental impacts of crop production continue to mount (Altieri, 2009). Given the various societal and ecological constraints to expansion of cultivated lands, increasing production will likely be achieved by the further intensification of agricultural systems, that is the use of external inputs to boost productivity per unit of land area (Giller et al., 1997). Productivity gains, however, need to be accompanied by major improvements to environmental quality: the ‘grand challenge’ of 21st century agriculture (Robertson and Swinton, 2005). These principles have been articulated as the sustainable intensification strategy (Pretty, 1997; Tilman et al., 2002)

In already-intensified areas, current efforts toward this goal have focused on mitigating environmental impacts without adversely affecting crop productivity levels or reducing profitability. Yet, given complex biophysical controls on agroecosystem processes, tradeoffs between production and environmental cropping system outcomes often arise (Basso et al., 2016; Jarchow et al., 2015; Kelly et al., 1996; Robertson et al., 2014). In this dissertation, the tradeoff between system productivity and environmental nitrogen (N) loss is examined. Several studies have shown that tradeoffs are not unavoidable, and win–win scenarios can be possible through the more efficient management of inputs and ecosystem processes (Davis et al., 2012; McLellan et al., 2018; Power, 2010). However, the most effective strategies for balancing tradeoffs often require relatively more changes to the existing production systems (Robertson et al., 2014). Owing to a number of economic,
societal and institutional factors, the potential for widespread adoption of these alternatives is limited (Roesch-McNally et al., 2018). Thus, evaluating scenarios within the socio-ecological context in which current production systems operate (i.e. annual cycle, rainfed, intensive input use, cash-crop purpose) is needed to offer feasible and scalable pathways for improvement.

**Context: Cropping systems of the US Midwest**

The Midwest is one of the most intensified rainfed agricultural regions on earth. During the period of active crop growth, gross primary productivity in the region surpasses that of the Amazonian forests (Guanter et al., 2014; Mueller et al., 2016). Once expansive prairie grasslands, today the cultivation of maize (*Zea mays* L.) and soybean (*Glicyne max* L. [Merr.]) dominates the landscape, with dwindling areas devoted to perennial forages and other crops (Alter et al., 2018; Lin and Henry, 2016; Wright and Wimberly, 2013).

Benefiting from a unique combination of warm, humid summers and deep, fertile soils, monoculture of maize or rotational maize-soybean cropping systems occupy more than 23 million hectares (greater than 90% of cropland in some areas), producing greater than 30% of the global supply of these commodities (USDA-FAS, 2018).

As in other temperate, sub-humid climates, the growing season duration for maize and soybeans is constrained to the frost-free period (May through September). Around two-thirds of moderate annual rainfall is received during this time. Snowmelt and spring rainfalls often provide surplus water early in the season, and its removal is often necessary to allow for timely field operations (e.g. tillage, planting, harvest). To this end, extensive networks of subsurface drainage systems have been installed over the decades, today reaching 80% of cropland under drainage in some areas (Blann et al., 2009).
Crop yield and N loss tradeoffs

The soil and climate characteristics of the US Midwest, while favorable for the production of rainfed maize and soybeans, also pose critical challenges to managing water and N efficiently (Dietzel et al., 2016; Randall and Mulla, 2001). Hence, tradeoffs between crop productivity and environmental N losses are related to the complex, weather-driven cycling of water and N within and beyond agroecosystems. Nitrate ($\text{NO}_3$) is the dominant plant-available form of N in many soils, but N from soil mineralization and atmospheric deposition are seldom sufficient for achieving water-limited yield potential of modern cultivars (Cassman et al., 2002; Farmaha et al., 2015; Sinclair and Rufty, 2012). Thus, exogenous N inputs are regularly applied to non-leguminous crops, but only half of global N fertilizer inputs to farmland can be accounted in harvested yield (Conant et al., 2013; Gardner and Drinkwater, 2009).

The unused NO$_3$ is difficult to store in soils, and thus it is readily lost to the atmosphere via gaseous denitrification, leached into groundwater, or transported by drainage systems into surface water bodies (Dinnes et al., 2002; Gilliam et al., 1999). Nitrous oxide ($\text{N}_2\text{O}$), a byproduct from denitrification, is a greenhouse gas with ~300 times more radiative forcing than CO$_2$ and contributes to stratospheric ozone depletion (Davidson and Kanter, 2014; IPCC, 2014), and at present, agricultural soils are the major contributors to $\text{N}_2\text{O}$ emissions in the US (USEPA, 2013). Accumulation of NO$_3$ in water bodies limits their use as sources of drinking water, and may cause eutrophication and hypoxia, impairing their ability to sustain aquatic life (Carpenter et al., 2011). Increasing N fertilization rates has been found to result in higher $\text{N}_2\text{O}$ fluxes (Li et al., 2016; Linquist et al., 2012) and NO$_3$ losses in subsurface drainage (Zhou and Butterbach-Bahl, 2014).
In the Midwest, the loss of nitrate (NO$_3$) through subsurface drainage has received much attention, both by researchers and the wider public, given its link to the development of seasonal hypoxic zones in the Gulf of Mexico (David et al., 2010). The biophysical controls on NO$_3$ transport to subsurface drainage systems are well understood (Randall and Mulla, 2001). The lack of a strong sink (e.g. a growing plant) during the fallow period (October to May) can lead to NO$_3$ buildup in soils following addition of pre-season N fertilizer inputs or through the decomposition of plant residues and soil organic matter. With the occurrence of spring rainfall events, water fluxes through the soil, flushing NO$_3$ below the root zone or into drainage systems (Randall and Goss, 2008).

The tradeoff between crop N use and NO$_3$ losses is expected to be exacerbated by changing climatic patterns (Bowles et al., 2018). The Midwest has already seen increasing precipitation intensity driven in part by global warming effects and feedbacks from agricultural intensification in the region (Alter et al., 2018; Walthall et al., 2012). Not only the direct hydrologic effects could be increased, but weather variability may also increase uncertainty in the duration of the growing season, or larger spring rainfall events may delay planting operations and affect crop establishment and emergence (Bowles et al., 2018). Meanwhile, increasing soil temperatures may lead to more soil organic matter mineralization during the fallow periods, and hence more release of native soil N. Additionally, the negative impacts of increasing weather variability on crop growth, could affect crop N recovery (Kim et al., 2008). This would lead to greater amounts of residual (i.e. unused) NO$_3$ leftover in the soil after harvest (Bowles et al., 2018).

**The process-based modeling approach for evaluating tradeoffs**

Field experimentation remains the main approach through which alternative system designs and management are evaluated, and experimental findings are often the basis for
recommendations for policy and implementation efforts (Christianson et al., 2017; Zhao et al., 2017). While necessary to refine our understanding of the biophysical controls on crop and soil processes, field experiments are often constrained by time and resources such that only a few factors or environments can be evaluated simultaneously, and extrapolating across weather, soils and management conditions becomes challenging. Hence, experimental approaches are limited to a descriptive capacity (i.e. hindsight). Bridging the gap between current production system outcomes and the goals of sustainable intensification will require more predictive (i.e. insight) and prescriptive (i.e. foresight) levels of understanding (National Academy of Sciences, 2018).

Process-based models have become increasingly valuable tools to help guide decision-making (Jones et al., 2017). In contrast to statistical models, the simulation approach explicitly includes mathematical representations of various crop-soil-atmospheric processes and complex system interactions and dynamics (Wallach et al., 2014). This allows for prediction of the expected changes in the system state in response to weather and management, and how these changes would be affected by other system characteristics (e.g. soil properties). Hence, the specific contributions of various factors to outcomes and tradeoffs can be assessed. System analysis using process-based simulation models can be especially useful to sieve through a universe of potential factors—an approach that is too costly or impractical for field experimentation—and to extrapolate the behavior of the system and narrow down promising alternatives that deserve further examination. Additionally, the explanatory and predictive capacity of simulation models offers numerous opportunities, not only to increase scientific understanding on biophysical processes driving outcomes and
tradeoffs, but also to provide information for supporting decisions and policies (van Ittersum et al., 1998).

Various simulation modeling platforms (e.g. APSIM (Keating et al., 2003), DSSAT (Jones et al., 2003) and RZWQM (Ahuja et al., 2000)) have been shown to successfully replicate the dynamics and outcomes of various cropping systems in the Midwest (Archontoulis et al., 2014; Basche et al., 2016; Dietzel et al., 2016; Gillette et al., 2018; Li et al., 2008; Malone et al., 2007).

However, application of these tools face major limitations in that current models may lack accurate mechanistic processes and model parameters, especially for complex water and N cycling dynamics and environmental losses (Banger et al., 2017; Brilli et al., 2017; Wallach and Thorburn, 2014). We have identified several knowledge gaps that require further investigation to improve and validate mechanisms in the models’ application of Midwestern cropping systems. These include, but are not limited to:

- Crop root growth, depth and interactions with shallow water tables (Ordóñez et al., 2018)
- Amount and variability of biological N fixation of modern soybean cultivars (Cordova et al. 2018)
- Rye cover crop effects on soil temperature, moisture, residue C and N inputs (Chapter 2)
- Grain dry down in the field, thus timing harvesting and crop residue additions (Chapter 3)
- Contribution of NO$_3$ concentrations in shallow water tables to NO$_3$ loads in drainage systems and denitrification losses (Fang et al., 2012; Gillette et al., 2018)
- Residue effects on soil evaporation and other components of the water balance
- Long-term N fertilization effects on crop residue and soil organic matter decomposition (Poffenbarger et al., 2018, 2017)
Rotational effects on the maize yield response to fertilizer N rate (Puntel et al., 2016)

Contribution of shallow water tables to crop water use (Singh et al., 2014)

Winter effects soil hydrology and N transformations (Wagner-Riddle et al., 2017)

Given these uncertainties, calibration guided by site-specific data is required before conducting assessments with an acceptable level of confidence (Baffaut et al., 2017; Banger et al., 2017).

**Objectives**

The overarching goals of this dissertation are to 1) examine and quantify the impact of various genetic, environmental and management drivers of tradeoffs between crop yield and N loss in the maize and soybean cropping systems of the US Midwest, and 2) identify potential management scenarios where these tradeoffs can be minimized or avoided. To this end, studies were conducted to examine the environmental (e.g. weather, soil), management (e.g. crop sequences, inputs, timing,), and genetic (e.g. crop types, cultivars) change in productivity, water and N cycling profiles of these systems. Given the identified knowledge gaps, we analyzed experimental data to fill some of those, particularly for rye cover crop and the timing of grain dry down in the field. The specific objectives of each of the chapters were:

⇒ To quantify the contributions of including a rye cover crop to changes in maize cropping systems dynamics including soil temperature, water use, residue inputs and soil N mineralization, subsurface water drainage flow and NO₃ losses (Chapter 2)

⇒ To develop and parameterize scalable algorithms to more accurately predict timing of maize and soybean grain dry down, so as to more realistically simulate harvest date and
residue decomposition dynamics in long-term (sequential) crop rotation evaluations.
(Chapter 3)

⇒ To develop a theoretical framework to link the efficiency of N input use and soil N retention to environmental N losses across various cropping systems, and compare the derived system index and traditional metrics for use in environmental assessments
(Chapter 4)

⇒ To evaluate the potential of multi-practice management strategies in maize and soybean to reduce agricultural drainage NO$_3$ losses while minimizing tradeoffs with crop yields
(Chapter 5)

**Methodological Framework**

The work presented in this dissertation employs a system analysis framework (Fig. 1.1). The approach used field data collected from small plots, long-term experiments and publicly available databases from experimental sites in Iowa and other locations in the Midwest. Soils at the sites are generally deep and fertile, with sub-humid temperate climate. These data, along with literature information, were used to configure, calibrate, drive and test various process-based models. Chapters 2, 3, and 5 use models within APSIM (Agricultural Production Systems sIMulator). Chapter 3 uses a stand-alone literature model. Once process-based models were shown to replicate experimental conditions satisfactorily, then simulation experiments were conducted following a what-if approach to extrapolate system behavior across weather and management. Simulated data was analyzed with various procedures to synthetize results into meaningful information, and discussed within the context of the experimental data and literature.
Dissertation Organization

This dissertation consists of six chapters (Fig. 1.2). Chapter 1 (this chapter), provides general background on the food security and environmental issues that motivate investigation, and an overview on the known factors driving yield and N loss tradeoffs in the cropping systems of the US Midwest. It also outlines the methodology used, and identifies critical uncertainties and knowledge gaps of implementation. Chapters 2 and 3 aim to fill some of these gaps. Chapter 2 deals with uncertainties surrounding the inclusion of rye cover crops in maize cropping systems, specifically the mechanisms that lead to maize yield penalties and reductions in NO\textsubscript{3} losses in subsurface drainage. Chapter 3 examines the influence of weather factors on grain dry down to develop algorithms to predict post-maturity grain moisture in maize and soybeans. Together, these studies allowed us to better calibrate process-based models, and improve simulation of residue decomposition dynamics, and water and N cycling in simulation experiments. Chapter 4 and 5 include advanced
applications of the APSIM modeling platform to examine drivers of tradeoffs and identify potential solutions. Chapter 4 studies various N cycling processes in maize-soybean systems to explore contributions of N input use and soil N retention to environmental N losses, and outlines a conceptual framework to link the soil and crop components of N-use efficiency at the system level. Chapter 5 evaluates a large number of simulated scenarios of management, weather and soil state variables across a gradient of soil-climatic characteristics in the Midwest to characterize key drivers of the variation in NO₃ losses and crop yield. It also identifies multi-practice management strategies that more effectively reduce NO₃ losses without negatively affecting yields. Chapter 6 (conclusions) provides synthesis of the results reported in the previous chapters and discusses the significance of the contributions presented herein.

Figure 1.2 Schematic of dissertation organization. Text boxes represent the research undertaken, with the main questions addressed in each of the chapters. Chapters 2 and 3 deal with bridging knowledge gaps and improve process-based modeling tools. Chapter 4 and 5 focused on applying these tools to explore yield and N loss tradeoffs. All these studies included analysis of various genetic, environmental and management drivers. Arrows represent information flows.
References


CHAPTER 2. RYE COVER CROP EFFECTS ON MAIZE: A SYSTEM-LEVEL ANALYSIS

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Abstract

Inclusion of a rye cover crop into maize-based systems can offer environmental benefits, but adoption of the practice in the US Midwest is still low. This is related to the possible risk of reduced maize yields following rye. We hypothesized that the magnitude of rye effects on maize yields and drainage water and nitrate (NO$_3$)-N losses would be proportionally related to rye biomass. We tested this hypothesis by analyzing data from continuous maize treatments (with and without cover crop) in Iowa, US, that were fertilized following recommendations from late spring NO$_3$ tests. Dataset included measurements (2009-2014) of soil water and temperature, drainage water and NO$_3$-N losses, soil NO$_3$, rye shoot and root biomass and C:N, and maize yields. We supplemented our analysis with a literature review and the use of a cropping systems model (APSIM) to calculate trade-offs in system performance characteristics. Experimentally, rye cover crop reduced drainage by 12% and NO$_3$-N losses by 20% (or 31% per unit of N applied), and maize yields by 6%. We also found minimal effects on soil temperature, water deficits that reduced yields only during drought years (2012 and 2013), and lower NO$_3$-N losses that were related to reduced NO$_3$-N
concentrations in drainage. Results also revealed a linear relationship between drainage and precipitation ($r^2=0.96$), and rye transpiration and shoot biomass ($r^2=0.84$). Model scenario analysis (4 termination dates × 30 years) indicated that rye cover crop decreases NO$_3$-N losses ($-25.5 \pm 26\%$) but does not always reduce drainage water ($-3.9 \pm 13\%$) or grain yields ($-1.84 \pm 6\%$), which is consistent with experimental and literature results. However, analysis of the synthesized measured and simulated dataset do not support a strong relationship between these variables and rye biomass. These results are valuable for decision-making and add new fundamental knowledge on rye water and N use.

**Introduction**

Inclusion of winter cover crops in high-input rain-fed maize (*Zea mays* L.)-based cropping systems is a conservation practice for enhancing the environmental performance of these systems (Kaspar and Singer, 2011; Thorup-Kristensen et al., 2003). Cover crop shoots protect soil from erosion (Kaspar et al., 2001), and roots take up residual NO$_3$-N from the soil during the fall-to-spring fallow period, reducing the movement of nutrients into surface and ground water (Dinnes et al., 2002; Kaspar et al., 2012, 2007; Salmerón et al., 2010). The use of cover crops also has the potential to provide long-term soil quality benefits such as improving carbon sequestration and soil physical properties (Basche et al., 2016; Blanco-Canqui et al., 2015; Kaspar and Singer, 2011; Moore et al., 2014), and other ecosystem services such as weed and pest suppression and beneficial insect conservation (Schipanski et al., 2014). Water quality degradation, especially NO$_3$ pollution of surface waters, is the most pressing environmental impact of these systems in the US Midwest. Cover crops have been promoted as one of the most viable options for reaching water quality goals set in the Midwest (e.g. Iowa Nutrient Reduction Strategy; IDALS, 2014) because of their lower cost
of adoption compared to built infrastructure such as denitrifying bioreactors and wetlands (Christianson et al., 2013; Dinnes et al., 2002).

Despite the evidence of the benefits of cover crops and the existence of incentives such as cost-share programs, adoption of the practice lags behind targets. Current records indicate that cover crops are used in only 1.55% of Iowa row-crop farmland (National Agricultural Statistics Service). In the Midwest, winter rye (Cereale secale L.) is a commonly used cover crop species (Singer, 2008) because it can withstand harsh winter conditions and has superior growth and N uptake compared to other species (Johnson et al., 1998; Kaspar and Bakker, 2015). Some studies have reported reductions in maize yield following a rye cover crop (Iqbal et al., 2015; Johnson et al., 1998; Kaspar and Bakker, 2015; Krueger et al., 2012, 2011; Pantoja et al., 2015; Singer and Kohler, 2005; Singer et al., 2008), although rye and other grass winter cover crops do not consistently reduce maize yields in the Midwest (Basche et al., 2016; Miguez and Bollero, 2005). Nonetheless, concerns regarding possible negative yield impacts of rye on maize have been found to be an impediment to the adoption of cover crops by producers (Arbuckle and Roesch-McNally, 2015). To promote the adoption of the practice, quantification of the actual risks and the trade-offs associated with cover crop use, along with the development of risk abatement strategies, are necessary (Arbuckle and Roesch-McNally, 2015; Carlson and Stockwell, 2013).

Miguez and Bollero (2005) identified that the effect of grass cover crops on maize yields throughout US studies was neutral, although significant variation existed across these studies. Similarly, rye cover crops generally reduce NO₃-N loss but the magnitude of the leaching-reduction effect also varies widely across years, locations and management (Dabney et al., 2010; Dinnes et al., 2002; Kaspar and Singer, 2011; Thorup-Kristensen et al., 2003).
This indicates that rye effects on the maize system depend on specific combinations of management choices and environmental conditions. Most studies have focused on quantifying rye effects on final maize yields and/or annual NO$_3$-N losses, and many knowledge gaps still exist regarding the mechanisms by which rye affects these systems. Broadly speaking, rye effects on maize can be grouped into biotic and abiotic factors. Biotic factors include pests and disease pressure (Acharya et al., 2016; Bakker et al., 2016) and allelopathy (Dhima et al., 2006; Duiker and Curran, 2005; Raimbult et al., 1991; Tollenaar et al., 1993), and at present are not well understood (Blanco-Canqui et al., 2015). A larger body of evidence exists for abiotic factors, which allowed us to develop a generalized framework of the abiotic effects of rye on the maize system (Fig. 2.1).

Literature findings have shown maize yield reductions following rye cover crop to be related to depletion of soil moisture (Krueger et al., 2011; Mirsky et al., 2015; Raimbult et al., 1991; Unger and Vigil, 1998) and/or plant available N (Crandall et al., 2005; Kessavalou and Walters, 1999; Krueger et al., 2011; Tollenaar et al., 1993), or to a mulching effect that reduces soil temperature and seedling growth (Munawar et al., 1990; Teasdale and Mohler, 1993). More specifically, rye abiotic effects on the maize system can arise from changes in the soil via: 1) the addition of organic C and N (shoot and root); 2) changes in soil surface cover that alter temperature and water dynamics; and 3) changes in the state variables such as inorganic N and soil water at the time of cover crop termination (Fig. 2.1). The magnitude of these changes affects the system differently, which may explain the wide variation in yield and NO$_3$-N leaching responses to rye cover crops across different studies.
Figure 2.1. A generalized diagram showing the abiotic mechanisms by which rye cover crop can affect crop yield and N losses in maize-based systems.

The amount of biomass produced by crops is strongly related to their water and N use (Gastal and Lemaire, 2002; Sinclair and de Wit, 1975; Sinclair and Rufty, 2012). For rye cover crops, this could mean that the greater the biomass, the higher the potential to alter water, N and temperature dynamics, resulting in increases in the potential for both yield penalty and reductions in NO$_3$-N losses. Kruger et al. (2011) and Pantoja et al. (2015) found rye biomass production to have a direct relationship to maize yield penalty, while Malone et al. (2014) found in a modeling study that rye N uptake had a strong relationship with NO$_3$-N losses. In this study, we hypothesized that the magnitude of rye cover crop abiotic effects on
maize yields and environmental performance variables such as drainage water and NO$_3$-N losses would be proportionally related to its biomass production. We tested this hypothesis and examined the underlying crop-soil dynamics that would support such a scenario by analyzing six years of data from a no-till continuous maize (with and without rye cover crop) experiment carried out in central Iowa, US. This dataset was collected over years that crops experienced drought, flood and historically average weather, and included measurements of many system variables shown in Fig. 2.1. We supplemented our analysis by using a calibrated cropping systems model for this site (Dietzel et al., 2016) to better understand growth-limiting factors and soil-crop dynamics with variability in both weather (30 years) and management (four simulated rye termination dates within a year). To our knowledge, current literature lacks a system-level analysis of the effect of rye on maize in which the most important system variables are analyzed simultaneously. Such analysis is necessary to further our understanding of the abiotic mechanisms by which rye impacts maize and the environmental performance of the system, and to provide baselines for quantifying trade-offs and risks associated with this practice.

**Materials and Methods**

**Experimental site and measurements**

**Soil**

The dataset used in this study was derived from observations collected from 2009 to 2014 in the Comparison of Biofuel Systems (COBS) experiment. This experiment was conducted in a 9-ha field that is part of the Iowa State University Agronomy and Agricultural Engineering Research Farm, in Boone County, Iowa (41.92 °N, 93.75 °W). The soil is a Webster silty clay loam (fine-loamy, mixed, superactive, mesic Typic Endoaquoll) and
Nicollet loam (fine-loamy, mixed, superactive, mesic Aquic Hapludoll), characterized by high soil organic matter (~5%) and water holding capacity. Soil at the experiment site was artificially drained with corrugated plastic subsurface drains. For more details about soil characteristics and management we refer the reader to Daigh et al. (2014, 2015), Jarchow et al. (2015) and Dietzel et al. (2016, 2015).

**Weather**

Precipitation, temperature, and radiation were recorded hourly from a weather station at the site. Historical weather data were retrieved from DAYMET (Thornton et al., 2014). The average annual daily temperature for the site is 9.4 °C with an average frost-free growing season of 155 days (April to mid-October). During fallow periods (October to April) the average daily mean temperature is 1.4°C. The average annual precipitation (including melted snow) is 935 mm. During the experiment period, the site experienced flood- and drought-inducing conditions (Fig. 2.2). The year 2010 was among the wettest on record, while 2012 and 2013 included periods of extremely low precipitation during summer. The year 2012 registered one of the lowest annual precipitations on record (656 mm). Even though the year 2013 registered about normal annual precipitation, the rainfall events were heavily concentrated in the May-June period and very dry conditions prevailed during mid-summer and early fall. The winter of 2013-2014 was extremely cold, with 26 days with daily average temperatures below -15 °C. The 2014 growing season remained relatively cool with average daily temperatures about 0.9 °C below the historical average. The site also experienced nearly average weather conditions in 2011 (Fig. 2.2).
Management

The experiment at COBS employed a spatially balanced complete block design with four blocks and six different cropping system treatments (plot size: 27 m × 61 m). In this study, we analyzed observations from the continuous maize system (CC) and continuous maize with rye cover crop system (CCW) treatments. At maize harvest, grain and 50% of the residue (stover) was removed from the system each year from both treatments. The plots were managed without tillage. Weeds and diseases were controlled chemically. Maize was planted in rows spaced at 76 cm at a rate of 79,500 seeds ha⁻¹. Two maize hybrids with 104-day relative maturity were used (Agrigold 6325 VT3 from 2009 to 2011 and Pioneer P0448XR thereafter). Rye cover crop variety ‘Rymin’ was planted a few days after maize stover harvest at a seeding rate of 300 seeds m⁻² and row spacing of 20 cm. Rye was chemically terminated during vegetative growth with glyphosate (N-[phosphonomethyl] glycine, 0.39-0.45 L a.i. ha⁻¹) the following spring before maize plantings. Table 2.1 provides details on management for both crops. Nitrogen fertilization was split-applied between
planting and the maize sixth leaf stage (V6; as defined in Abendroth et al., 2011) following the recommendations from a late spring N test (LSNT; Blackmer et al., 1997) using a critical soil NO₃-N concentration of 25 mg kg⁻¹. Table 2.2 provides details on N fertilization for maize.

**Soil temperature, moisture and nitrate measurements**

Soil temperature and volumetric soil water content were measured from 2009 to 2013 with Decagon 5TE ECH₂O sensors and Em50 data loggers (Decagon Devices Inc., Pullman, WA, US) at 5, 10, 17.5, 35, and 50 cm depths every 30 minutes. The sensors were installed in 2008 at one point per plot (midway between center and border of the plots), resulting in 4 replicates per treatment at each depth. Further details are available in Daigh et al. (2014) and Dietzel et al. (2016). Using these data we calculated average daily soil temperatures for three soil layers: 5-15 cm, 15-30 cm and 30-50 cm, and daily total soil water content (mm) for 0-15 cm, 0-30 cm and 0-50 cm soil profiles (supplemental Fig. S2.1).

Table 2.1. Summary of dates of major field activities for continuous maize (CC) and the continuous maize with rye cover crop (CCW) treatments.

<table>
<thead>
<tr>
<th>Year</th>
<th>Rye†</th>
<th>Maize</th>
<th>Harvest</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Termination§</td>
<td>Planting</td>
<td>Planting</td>
</tr>
<tr>
<td>2009</td>
<td>6-May</td>
<td>6-Nov</td>
<td>8-May</td>
</tr>
<tr>
<td>2010</td>
<td>5-May</td>
<td>4-Oct</td>
<td>6-May</td>
</tr>
<tr>
<td>2012</td>
<td>18-Apr</td>
<td>1-Oct</td>
<td>11-May</td>
</tr>
</tbody>
</table>

† Only for the CCW treatment
§ Total rye biomass (root + shoot) was determined a few days before termination.
£ LSNT: late spring soil nitrate test at maize sixth leaf stage
¶ Total maize biomass (shoot) was determined a few days before grain harvest.
Soil NO₃ measurements were collected to a depth of 30 cm in each plot shortly prior to V6 every year and soil NO₃-N concentration was determined colorimetrically using the cadmium reduction method (Gelderman and Beegle, 2012) and expressed in mg N kg⁻¹ soil, and in kg N ha⁻¹ using the average value of 1.4 g cm⁻³ for bulk density in the top 30 cm soil depth (Dietzel et al., 2016).

**Subsurface drainage water volume and nitrate-N losses**

Subsurface drains were installed at ~1.1 m depth along the center and border of the plots (long-side direction) in the spring of 2009. Effluent from the center subsurface drains (hereafter drainage) was measured and recorded every 5 minutes using in-flow meters throughout the drainage period (i.e., early March to early December). Daily cumulative flow values were calculated and expressed in mm. Water samples were obtained through an orifice that diverted ~0.1% of drained water flow into a plastic container. Samples were collected periodically (twice weekly), stored at 4 °C, and subjected to colorimetric analysis to determine NO₃-N concentrations. Further details about system setup, instrumentation and chemical analysis method were provided by Daigh et al. (2014, 2015). Nitrate-N losses were calculated by multiplying results from colorimetric analysis by the drainage recorded during a given collection period and expressed in kg N ha⁻¹. Annual flow-weighted NO₃-N concentrations in drainage water were calculated by dividing cumulative annual NO₃-N losses by the annual drainage water volume, and expressed in mg N L⁻¹. Additionally, given that N fertilization rates applied to maize were not uniform across the CC and CCW treatments (LSNT-based rates; Table 2.2), NO₃-N losses were also expressed as percentage of N fertilization in kg of N loss 100 kg⁻¹ of N applied.
Table 2.2. Amount of N applied to the continuous maize (CC) and the continuous maize with rye cover crop (CCW) treatments during the experiment. The N fertilizer type was liquid urea-ammonium-nitrate (32%) and was injected to a depth of 7.5 cm.

<table>
<thead>
<tr>
<th>Year</th>
<th>At planting</th>
<th>Side-dressed (at maize sixth leaf stage)</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>CC</td>
<td>CCW</td>
<td>CC</td>
</tr>
<tr>
<td>2008</td>
<td>73</td>
<td>101</td>
<td>174</td>
</tr>
<tr>
<td>2009</td>
<td>84</td>
<td>84</td>
<td>168</td>
</tr>
<tr>
<td>2010</td>
<td>87</td>
<td>36</td>
<td>123</td>
</tr>
<tr>
<td>2011</td>
<td>87</td>
<td>56</td>
<td>143</td>
</tr>
<tr>
<td>2012</td>
<td>87</td>
<td>112</td>
<td>199</td>
</tr>
<tr>
<td>2013</td>
<td>90</td>
<td>112</td>
<td>202</td>
</tr>
<tr>
<td>2014</td>
<td>84</td>
<td>95</td>
<td>179</td>
</tr>
<tr>
<td>Average</td>
<td>84.6</td>
<td>85.1</td>
<td>107.6</td>
</tr>
</tbody>
</table>

**Crop measurements**

Rye biomass samples were collected a few days before rye termination (Table 2.1). Rye aboveground biomass (hereafter shoot) was sampled from four random areas per plot (1.34 m² total). Rye roots were sampled by digging plants with a spade to a 15-cm depth (roots and shoots separated at the crown level) in 2009. In the following years (2010–2013), root mass was determined by collecting four 32-mm-diameter soil cores, two cores on the row and two from between rye rows, at a 30-cm depth. Roots were separated from the bulk soil using a soil elutriator as described by Wiles et al. (1996) and Jarchow and Liebman (2012). Shoot and root samples were dried in a forced-air oven at 60 °C until constant weight. Dry samples were weighed, ground to a fine powder (<1 mm) and concentrations of C and N were determined by combustion analysis at the Soil and Plant Analysis Laboratory at Iowa State University (Ames, Iowa). In 2014, only shoot biomass weight was determined. Rye water use was estimated with a soil water balance difference method. This was done by summing the differences between CC and CCW in soil water (0–50 cm soil profile) and
water loss through subsurface drainage. This estimate should be a good proxy for rye transpiration.

Maize grain yields were measured from the center 12 rows of each plot using a John Deere 9550 combine harvester. Maize aboveground biomass was measured a few days before harvest by collecting eight representative plants from each plot (~1 m² area). Plants were dried at 60 °C, and weighed. Biomass samples were not collected in 2014. Maize yields and biomass are both expressed on dry matter basis (0% moisture). Maize grain samples were collected to determine N concentration in 2008 (establishment year), 2009, and 2013.

**Modeling analyses**

**APSIM model and testing**

The Agricultural Production Systems sIMulator (APSIM, Holzworth et al., 2014; Keating et al., 2003) is a field-scale cropping system model that operates on a daily time step. Inputs to the model are daily weather, soil, management, cultivars and crop or crops in rotation. Outputs from the model are many soil-plant-atmosphere variables, including crop growth processes, soil water, soil temperature, N and C cycling, and residue dynamics. Details about APSIM and its performance across a range of environments can be found at [www.apsim.info](http://www.apsim.info) and in the following studies for Iowa: Malone et al. (2007); Hammer et al. (2009); Archontoulis et al. (2015, 2014a,b); Dietzel et al. (2016); and Basche et al. (2016).

Recently, Dietzel et al. (2016) provided a comprehensive calibration and testing of the APSIM model at the COBS site, including the CC and CCW treatments. We built on this work and further tested and improved the model by using additional datasets that included maize grain yields in 2014, maize grain N concentration, and high-resolution measurements (daily from 2009 to 2014) of drainage water volume and NO₃-N losses in subsurface drainage during the drainage period. Our focus was to further improve the representation of
rye in the model, given that APSIM, like many other cropping systems platforms (e.g. RZWQM, Malone et al., 2014), does not have a specific rye model and the representation of rye growth and development is through the wheat model with ad-hoc modifications (Basche et al., 2016; Dietzel et al., 2016). Additionally, we modified two key parameters in the maize model to better reflect growth and N uptake in modern maize hybrids. Details about changes in the specific parameter values in the rye and maize models and their underlying rationale are summarized in Table 2.3. No changes were made in the soil model. All these changes maintained or improved the version published by Dietzel et al. (2016).

Table 2.3. Details of the improvements made to the APSIM model version published by Dietzel et al. (2016).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Change</th>
<th>Rationale and significance</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specific area of residues of wheat (ha kg(^{-1}))</td>
<td>0.005 to 0.0005</td>
<td>Rye residue surface area at termination (Zadoks stage 25) consists of leaves and young stems, and is very different from that of dry mature stems in wheat residue after harvest (Zadoks stage 99, default value). Reduced soil cover per unit of biomass.</td>
</tr>
<tr>
<td>Transpiration efficiency coefficient of wheat (kPa)</td>
<td>6.0 to 4.5</td>
<td>Better fit to estimated values of rye water use (Fig. 7). It suggests that rye is less efficient than wheat in using water.</td>
</tr>
<tr>
<td>Maximum rooting depth (cm)</td>
<td>90 to 120</td>
<td>Better fit to rye biomass and NO(_3)-N leaching data and better reflection of the putative role of rye as a catch crop. These changes increased the ability of rye roots to extract water and nutrients from deeper soil depths.</td>
</tr>
<tr>
<td>Soil/root water extraction coefficient for wheat (KL, d(^{-1}))</td>
<td>From 0.08 to 0.1 for 0 to 40 cm soil layers; from 0.05 to 0.08 for 40 to 90 cm soil layers; 0.04 for 90 to 120 cm soil layer</td>
<td></td>
</tr>
<tr>
<td>Critical grain N concentrations (g kg(^{-1}))</td>
<td>15 to 12</td>
<td>Better fit to measured grain N content data (Fig. 9) and NO(_3)-N leaching (Fig. 6).</td>
</tr>
<tr>
<td>Root penetration resistance coefficient (XF, unit less)</td>
<td>1.0 to 0.5 in soil layers below 60 cm</td>
<td>Improved simulation of NO(_3)-N leaching in years 2012, 2013 and 2014.</td>
</tr>
</tbody>
</table>
Scenario analysis

We used the improved version of the APSIM model to explore the long-term effect of rye biomass production on maize yields, subsurface drainage and NO$_3$-N losses. To create variability in rye biomass at termination day, we simulated four different termination dates: 13 April, 25 April, 5 May and 15 May during 30 weather years (1985-2014). These dates reflect the variability in rye termination dates in this region. Maize plantings were 10 days after rye termination using average management practices for this region (Tables 1 and 2), including 50% residue removal, which was specific for the COBS experiment. It should be noted that in the scenario analysis we used the same N-rate (190 kg N ha$^{-1}$ yr$^{-1}$) in both CC and CCW. Rye planting was 20 Oct every year, which also reflects the average planting date for this region. Simulated results of this analysis were synthesized by calculating relative treatment differences between CC and CCW using the following formula:

$$y = 100 \left( \frac{CCW - CC}{CC} \right)$$

(Equation 1)

where CCW and CC are the simulated values of maize yields, annual cumulative drainage or NO$_3$-N losses for each simulation treatment. In this scale, positive values represent increases associated with the rye cover crop, while negative values indicate decreases.

Literature review data collection

To better understand rye effects on N cycling, we synthesized literature data with our measurements and simulations to develop a relationship between rye shoot and root biomass and C:N. Aiming to capture a range of environmental and management conditions, we selected studies conducted within the last 20 years across the US reporting results on a year-
treatment-location basis. For studies reporting solely N concentration, C:N ratios were calculated assuming 40% and 33% C content for the shoot and root, respectively, which was based on our experimental findings. Each point in this dataset represented a site-year-treatment observation.

To compare APSIM-simulated relative changes to experimental measurements, we searched for publications reporting rye effects on maize yield, cumulative drainage and/or NO$_3$-N losses. Relative treatment differences were computed analogously to simulated results from the scenario analysis (Eq. 1), using a control value on a year-location basis.

**Statistical analyses**

**Crop and drainage data**

Statistical analyses were conducted using R statistical software version 3.2.1 (R Core Team, 2015). To test treatment effects in the measured crop and drainage variables, analyses of variance (ANOVA) were conducted with the Linear Mixed-effects Model (*lme*) function from the Linear and Nonlinear Mixed Effects Model (*nlme*) package (Pinheiro et al., 2015). The effect of treatments, year and their interactions were considered fixed, while the effect of the year within each block (split-plot in time) was considered random. When the interaction of treatment$x$year was significant, simple effects across years were tested using the Test Contrasts of Factor Interactions (*testInteractions*) function from the Post-Hoc Analysis of Interactions (*phia*) package (De Rosario Martínez, 2015). Data tested using this method were rye measurements at termination, soil NO$_3$ test results, maize measurements at harvest, and annual cumulative drainage water volume and NO$_3$-N losses. Drainage data were transformed prior to conducting ANOVAs using the logarithmic transformation because a Bartlett’s test ($\alpha=0.05$) indicated that variances from the different treatments across years were unequal. Simple regression analyses were conducted to test proportionality of the
relationship between rye biomass and changes in yield, cumulative drainage and NO$_3$-N losses, as well as for describing the underlying mechanisms, through relationships between transpiration and rye biomass, and cumulative precipitation and drainage and NO$_3$-N losses. All these tests were conducted using a significance level of $\alpha=0.05$.

**Soil moisture and temperature data**

Time series sensor data were analyzed by conducting ANOVAs at every depth and day of the studied period (analyzed as a completely randomized block design). This method was chosen for its simplicity and ease of interpretation. However, this test may lack power to detect differences (type II error) with days of large variation (e.g. precipitation events) or with missing data. For this reason, we determined it appropriate to use a significance level $\alpha=0.1$ for the soil water data. For the soil temperature data, a significance level of $\alpha=0.05$ was considered appropriate given the relatively low treatment variability in these measurements. These analyses were focused on periods when rye effects were expected to be most relevant, 30 days prior to and 30 days after cover crop termination (soil temperature) or until the end of the maize-growing season (soil water).

**Non-linear regression model for rye C:N versus biomass**

We fitted curves in the form $y = a \times x^b$ to the C:N dataset (see section 2.3.), using the Non-linear Least Squares ($nls$) function from the nlme package in R (Pinheiro et al., 2015). Prediction intervals ($\alpha = 0.2$) were estimated using the linear approximation method described by Bates and Watts (2007), which is comparable to what has been done for studies on wheat (Justes et al., 1994; Ziadi et al., 2010).

**Model goodness of fit**

To assess overall APSIM model fit, we a) fitted linear regressions of observed versus model simulated values, and b) computed the coefficient of determination ($r^2$), the root mean
square error (RMSE) and relative mean square error (RRMSE). To assess fit of non-linear models, only the $r^2$ and RMSE were computed. The equations can be viewed in Archontoulis and Miguez (2013). The $r^2$ reflects prediction ability and the higher the value the better. The RMSE and RRMSE reflect simulation error and the lower the value the better.

Results

Rye shoot and root biomass and C:N

Over the 6-yr period, rye shoot biomass at termination day varied from 120 to 2499 kg ha$^{-1}$ (Table 2.4). The low rye biomass production in 2009 and 2013 coincided with relatively cool spring weather conditions in those years (Fig. 2.2). In 2014, poor growth was related to winterkill, caused by extremely harsh conditions during that winter. On the other hand, the unusually warm temperatures in February and March of 2012 allowed rye to produce the highest biomass over the 6-year period even when it was terminated about 2-3 weeks earlier than all other years (Table 2.1). Measured rye root biomass at termination ranged from 57 to 2093 kg ha$^{-1}$. It should be noted that the biomass recorded for 2009 was widely different to measurements from all other years, probably due to the difference in root sampling method used that year. The corresponding root:shoot for 2010-2013 ranged between 0.75 to 1.9 (Table 2.4). Rye shoot N uptake varied from 12.5 to 44.6 kg N ha$^{-1}$, and it was observed that the rye shoot N concentration decreased with increasing shoot weight (Table 2.4). The ratio of rye biomass to N uptake (N-use efficiency) was 46 ± 16 for the shoots and almost double for the roots 83 ± 13 kg kg$^{-1}$ N taken up. This difference is due to different N concentrations between shoots and roots (Table 2.4). The C concentration was also different between shoots and roots (39.5 vs. 32.5%; Table 2.4) but was relatively stable across the five years measured.
Table 2.4. Rye cover crop measurements at termination date

<table>
<thead>
<tr>
<th>Year</th>
<th>Biomass</th>
<th>C concentration</th>
<th>N concentration</th>
<th>C:N</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Shoot</td>
<td>Root*</td>
<td>Root:Shoot</td>
<td>Shoot</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Root:Shoot</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>kg ha⁻¹</td>
<td>%</td>
<td>%</td>
</tr>
<tr>
<td>2009</td>
<td>365 (72)†</td>
<td>57 (12)</td>
<td>0.16 (0.01)</td>
<td>39.2 (0.59)</td>
</tr>
<tr>
<td>2010</td>
<td>1180 (81)</td>
<td>1564 (137)</td>
<td>1.33 (0.07)</td>
<td>39.3 (0.14)</td>
</tr>
<tr>
<td>2011</td>
<td>1532 (131)</td>
<td>2093 (311)</td>
<td>1.43 (0.29)</td>
<td>40.9 (0.1)</td>
</tr>
<tr>
<td>2012</td>
<td>2499 (66)</td>
<td>1872 (185)</td>
<td>0.75 (0.08)</td>
<td>39.2 (0.12)</td>
</tr>
<tr>
<td>2013</td>
<td>497 (48)</td>
<td>943 (35)</td>
<td>1.94 (0.15)</td>
<td>38.8 (0.15)</td>
</tr>
<tr>
<td>2014§</td>
<td>120 (7.4)</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

* Samples collected from 0-15 cm depth in 2009 and 0-30 cm the following years
† Values between parenthesis indicate standard error
§ Only shoot biomass was collected in 2014
The rye shoot C:N ranged from 11.3 to 27.1, while the rye root C:N varied from 23.2 to 33.4 and was higher compared to that of shoots. The relationship between rye C:N and biomass is shown in Fig. 2.3, with a non-linear regression fitted to experimental and modeling results along with results from other studies carried out in different locations across the US (supplemental Table S2.1). The analysis showed a strong positive relationship between shoot biomass and C:N (n = 130; RRMSE = 29%), and between C:N of roots and root biomass (n = 16; RRMSE = 35%). The range of the C:N values measured in our study was generally low given that rye was terminated during the vegetative stages. This places rye cover crop residue as a high quality residue in terms of N cycling.

Maize biomass and yield

Statistically significant treatment effects (p < 0.05) were detected for grain yields and biomass in 2012 and 2013 (Table 2.5a). The inclusion of a rye cover crop decreased maize yield by 34% (2.6 Mg ha⁻¹) and biomass by 22% (4.0 Mg ha⁻¹) when compared to CC in 2012. The cover crop yield penalty was less severe in 2013, with reductions of 22% (1.9 Mg ha⁻¹) in grain yield and 14% (2.6 Mg ha⁻¹) in biomass when compared to CC. Both 2012 and 2013 were dry years (Fig. 2.2). No significant treatment effects in maize biomass and grain yields were observed in 2009, 2010, 2011 and 2014. Across the six years, the average yield penalty in the CCW treatment was 6%.

Soil temperature

Soil temperature at different soil depths and time periods was fairly similar between CC and CCW treatments, although the analysis identified a few days with significant differences (22 days in five years; Fig. 2.4). Days with significant differences were clustered in the period before or near to the termination date, tended to record warmer soil temperatures in the CCW treatment in the subsoil (depth > 15 cm), and differences were
small (0.4 °C in 2010 and 1.2 °C in 2013). On these days the top soil layers (5-15 cm) in CCW tended to register cooler temperatures compared to CC (difference of 0.35 °C).

**Soil water content**

The soil water fluctuated greatly during the studied periods following precipitation events (Fig. 2.5). With the exception of 2010 (flood-inducing conditions in mid-summer), the seasonal patterns showed soil water levels near field capacity during the early part of the season (May and June) and a decline in July and August. Most of the statistically significant differences (p < 0.1) were detected in the dry years (2009, 2012 and 2013; Fig. 2.2), at the 0-30 and 0-50 cm soil depths (Fig. 2.5). In general, periods with significant differences revealed lower soil water content for CCW compared to CC. In 2009, the average water deficit for the period with significant differences was 12 and 20 mm in the 0-30 and 0-50 cm depths, respectively. In 2012, significant differences were observed for 14 days prior to N side dress (~V6), but not later in the season. This was probably related to malfunctions in the moisture sensors during that summer (we speculate due to extreme dryness), which decreased the power of the ANOVAs to detect differences during that year. On average, the soil water deficit in 2012 was 12 and 25 mm for the 0-30 and 0-50 cm depths, respectively. In 2013, CCW had significantly lower soil water in 0-50 cm from maize planting to N side dress day (average deficit of 20 mm), but after this period, the trend reversed and the CCW treatment had higher soil water for 45 days (6.6 mm difference) compared to CC (Fig. 2.5).

Interestingly, the differences in soil moisture were not consistent with the differences in maize yields (Fig. 2.5 and Table 2.5a). In 2012, maize yield and soil moisture were both lower in CCW, but in 2013 maize yield was lower and soil moisture was higher in CCW.
Figure 2.3  Relationship between C:N and shoot and root biomass using literature, experimental and simulated values for rye. Dotted lines are the 80% prediction intervals.

Reference:
- COBS - APSIM
- COBS - CCW
- De Bruin et al. (2005)
- Feyerisen et al. (2006)
- Griffin et al. (2000)
- Iqbal et al. (2015)
- Kaspar and Bakker (2015)
- Kaspar et al. (2007)
- Kaspar et al. (2012)
- Krueger et al. (2011)
- Kuo and Jellum (2002)
- Patel et al. (2015)
- Qi et al. (2008)
- Reiter et al. (2008)
- Rich (2008)
- Ruffo and Bollero (2003)
- Singer et al. (2008)
- Strock et al. (2004)
Table 2.5  Treatment effects on soil nitrate (NO$_3$) concentrations in the top 30 cm soil layer at V6, maize grain yield, maize above ground biomass production (a), and annual drainage variables (b) between continuous maize (CC) and continuous maize with rye cover crop (CCW) systems.

### (a) Soil NO$_3$ at V6 (mg N kg$^{-1}$ soil)

<table>
<thead>
<tr>
<th>Year</th>
<th>CC</th>
<th>CCW</th>
<th>p$^\dagger$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2009</td>
<td>15.3 (1.03)</td>
<td>9 (1.22)</td>
<td>&lt;0.001</td>
</tr>
<tr>
<td>2010</td>
<td>21 (3.46)</td>
<td>17.5 (3.93)</td>
<td>ns</td>
</tr>
<tr>
<td>2011</td>
<td>19 (1.73)</td>
<td>10 (1.78)</td>
<td>&lt;0.001</td>
</tr>
<tr>
<td>2012</td>
<td>11.8 (0.48)</td>
<td>10 (0.91)</td>
<td>ns</td>
</tr>
<tr>
<td>2013</td>
<td>13 (3.03)</td>
<td>15.3 (4.48)</td>
<td>ns</td>
</tr>
<tr>
<td>2014$^\dagger$</td>
<td>14.5 (3.29)</td>
<td>16.3 (3.47)</td>
<td>ns</td>
</tr>
</tbody>
</table>

### Maize yield (Mg ha$^{-1}$)

<table>
<thead>
<tr>
<th>Year</th>
<th>CC</th>
<th>CCW</th>
<th>p</th>
</tr>
</thead>
<tbody>
<tr>
<td>2009</td>
<td>10.77 (0.28)</td>
<td>11.64 (0.41)</td>
<td>ns</td>
</tr>
<tr>
<td>2010</td>
<td>8.32 (0.34)</td>
<td>8.66 (0.07)</td>
<td>ns</td>
</tr>
<tr>
<td>2011</td>
<td>8.19 (0.16)</td>
<td>8.61 (0.28)</td>
<td>ns</td>
</tr>
<tr>
<td>2012</td>
<td>7.56 (0.18)</td>
<td>4.96 (0.16)</td>
<td>&lt;0.001</td>
</tr>
<tr>
<td>2013</td>
<td>8.61 (0.33)</td>
<td>6.75 (0.27)</td>
<td>&lt;0.001</td>
</tr>
<tr>
<td>2014$^\dagger$</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

### Maize biomass (Mg ha$^{-1}$)

<table>
<thead>
<tr>
<th>Year</th>
<th>CC</th>
<th>CCW</th>
<th>p</th>
</tr>
</thead>
<tbody>
<tr>
<td>2009</td>
<td>18.67 (0.31)</td>
<td>19.11 (0.48)</td>
<td>ns</td>
</tr>
<tr>
<td>2010</td>
<td>15.31 (0.25)</td>
<td>15.33 (0.5)</td>
<td>ns</td>
</tr>
<tr>
<td>2011</td>
<td>13.99 (0.36)</td>
<td>13.72 (0.36)</td>
<td>ns</td>
</tr>
<tr>
<td>2012</td>
<td>15.33 (0.36)</td>
<td>13.46 (0.4)</td>
<td>&lt;0.001</td>
</tr>
</tbody>
</table>

### (b) Drainage water (mm)

<table>
<thead>
<tr>
<th>Year</th>
<th>CC</th>
<th>CCW</th>
<th>p</th>
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</thead>
<tbody>
<tr>
<td>2009</td>
<td>85 (11.9)</td>
<td>89 (16.4)</td>
<td>ns</td>
</tr>
<tr>
<td>2010</td>
<td>439 (108.8)</td>
<td>353 (66.8)</td>
<td>ns</td>
</tr>
<tr>
<td>2011</td>
<td>164 (36.1)</td>
<td>145 (30.8)</td>
<td>ns</td>
</tr>
<tr>
<td>2012</td>
<td>50 (12.3)</td>
<td>27 (6.8)</td>
<td>ns</td>
</tr>
<tr>
<td>2013</td>
<td>96 (27.5)</td>
<td>84 (12)</td>
<td>ns</td>
</tr>
<tr>
<td>2014$^\dagger$</td>
<td>272 (43.3)</td>
<td>273 (29.5)</td>
<td>ns</td>
</tr>
</tbody>
</table>

### Flow-weighted NO$_3$-N concentration (mg N L$^{-1}$)

<table>
<thead>
<tr>
<th>Year</th>
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<th>CCW</th>
<th>p</th>
</tr>
</thead>
<tbody>
<tr>
<td>2009</td>
<td>8.3 (1.08)</td>
<td>8.0 (0.48)</td>
<td>ns</td>
</tr>
<tr>
<td>2010</td>
<td>7.1 (0.97)</td>
<td>6.8 (1.02)</td>
<td>ns</td>
</tr>
<tr>
<td>2011</td>
<td>7.9 (0.71)</td>
<td>3.6 (0.46)</td>
<td>&lt;0.001</td>
</tr>
<tr>
<td>2012</td>
<td>12 (0.47)</td>
<td>2.6 (0.68)</td>
<td>&lt;0.001</td>
</tr>
<tr>
<td>2013</td>
<td>18.8 (2.18)</td>
<td>17.5 (1.39)</td>
<td>ns</td>
</tr>
<tr>
<td>2014$^\dagger$</td>
<td>12.7 (0.44)</td>
<td>13.6 (2.47)</td>
<td>ns</td>
</tr>
</tbody>
</table>

### NO$_3$-N Losses (kg N ha$^{-1}$)

<table>
<thead>
<tr>
<th>Year</th>
<th>CC</th>
<th>CCW</th>
<th>p</th>
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<tbody>
<tr>
<td>2009</td>
<td>7.3 (1.66)</td>
<td>6.9 (1.0)</td>
<td>ns</td>
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<tr>
<td>2010</td>
<td>31 (8.22)</td>
<td>21.9 (1.82)</td>
<td>ns</td>
</tr>
<tr>
<td>2011</td>
<td>12.6 (2.43)</td>
<td>5.0 (0.78)</td>
<td>&lt;0.004</td>
</tr>
<tr>
<td>2012</td>
<td>5.9 (1.32)</td>
<td>0.6 (0.23)</td>
<td>&lt;0.001</td>
</tr>
<tr>
<td>2013</td>
<td>16.9 (4.62)</td>
<td>14.3 (1.32)</td>
<td>ns</td>
</tr>
<tr>
<td>2014$^\dagger$</td>
<td>14.6 (2.9)</td>
<td>22.9 (4.7)</td>
<td>ns</td>
</tr>
</tbody>
</table>

### Normalized NO$_3$-N Losses (kg loss 100 kg$^{-1}$ N applied)

<table>
<thead>
<tr>
<th>Year</th>
<th>CC</th>
<th>CCW</th>
<th>p</th>
</tr>
</thead>
<tbody>
<tr>
<td>2009</td>
<td>4.3 (0.99)</td>
<td>3.1 (0.46)</td>
<td>ns</td>
</tr>
<tr>
<td>2010</td>
<td>25.2 (6.68)</td>
<td>13 (1.08)</td>
<td>ns</td>
</tr>
<tr>
<td>2011</td>
<td>8.8 (1.7)</td>
<td>2.3 (0.35)</td>
<td>&lt;0.001</td>
</tr>
<tr>
<td>2012</td>
<td>3.0 (0.67)</td>
<td>0.3 (0.11)</td>
<td>&lt;0.001</td>
</tr>
<tr>
<td>2013</td>
<td>8.4 (2.9)</td>
<td>7.9 (0.73)</td>
<td>ns</td>
</tr>
<tr>
<td>2014$^\dagger$</td>
<td>19.1 (2.58)</td>
<td>22.9 (4.7)</td>
<td>ns</td>
</tr>
</tbody>
</table>

$^\dagger$ Values between parenthesis indicate standard error

§ ns indicates non-significant treatment effects ($\alpha=0.05$)

£ Biomass data was not collected in 2014.
Figure 2.4. Average soil temperatures at 5-15 cm, 15-30 cm and 30-50 cm depths for the continuous maize (CC) and the continuous maize with rye cover crop (CCW) treatments. Regions shaded in red (when visible) indicate days where statistically significant differences ($\alpha = 0.05$) between treatments were detected. Dates of rye termination (rT) and maize sixth leaf stage (V6) are included for reference.

**Soil Nitrate**

Analysis of mid-June soil NO$_3$ samples indicated significant treatment effects ($p < 0.05$), as well as a significant treatment$\times$year interaction (Table 2.5a). Rye reduced soil NO$_3$ concentrations only in 2009 and 2011, by about 6.2 and 9.0 mg kg$^{-1}$ respectively. This suggests that rye cover crop had an impact on soil mineral N, but this reduction was most likely negated in this experiment by applying higher N fertilization rates in the CCW treatment (Table 2.2).
Figure 2.5. Seasonal changes in soil profile water content (mm per depth) for the continuous maize (CC) and the continuous maize with rye cover crop (CCW) treatments for the 0-15cm, 0-30cm and 0-50 cm depths. Top panes show the recorded precipitation at the site. Horizontal lines in every soil water pane show field capacity. Regions shaded in red indicate days where statistically significant differences ($\alpha = 0.1$) between treatments were detected. Dates of rye termination (rT), maize planting (P), maize sixth leaf stage (V6) and maize harvest (H) are included for reference.

**Subsurface drainage: water and NO$_3$-N losses**

Over the six-year period, inclusion of rye cover crop reduced measured cumulative drained water and NO$_3$-N losses in subsurface drainage by 12.1% and 20.4%, respectively (Table 2.5b and Fig. 2.6). However, statistically significant treatment differences ($p < 0.05$) were not found in any of the studied years for annual water drainage, and only in 2011 and 2012 for NO$_3$-N losses (Table 2.5b). Likewise, annual flow-weighted NO$_3$-N concentration were significantly different between treatments in 2011 and 2012 (Table 2.5b). When
adjusted for N application rate (Table 2.2) NO₃-N losses were also only significantly reduced in 2011 and 2012 (Table 2.5b), with 31% reduction in the amount of NO₃-N loss per kg of N applied. As expected, the seasonal patterns between drainage water and NO₃-N losses were similar (Fig. 2.6). On average, 67% of the water drainage and NO₃-N losses occurred during the maize-growing season (planting to harvest). The highest NO₃-N loss values were recorded in the wet years for both treatments (2010 and 2014; Fig. 2.2). Regression analysis between cumulative drainage water (Y-dependent variable, Fig. 2.7) and precipitation registered during the drainage period (X-explanatory) showed a strong relationship: \( y = 0.34(x - 162); r^2 = 0.97; n=12, \) where the value of 162 mm denotes the minimum precipitation amount required to initiate soil water flow to subsurface drainage, and the 0.34 slope coefficient denotes the portion of the precipitation water that ends up in subsurface drainage systems. Similarly, the relationship between NO₃-N losses (Y) and precipitation (X) was in the form: \( y = 0.024 x; r^2 = 0.87; n =12, \) where the value of 0.024 is the NO₃-N losses per each mm of precipitation registered during the drainage period.

**Rye transpiration (water use)**

The cumulative treatment difference in soil water profile and subsurface drainage on rye termination day was used to estimate rye transpiration. Results indicated that rye transpiration ranged from 11 to 44 mm over the study period and that a strong relationship exists between transpiration and shoot biomass \( (r^2 = 0.83; \text{Fig. 2.8}) \). The slope of the regression equation indicated that 47 kg ha⁻¹ are produced per mm of water used. APSIM model simulations were of the same magnitude and confirmed the robustness of this approach to estimate transpiration for rye.
Model simulations and scenario analysis

The additional changes made in the rye and maize models (Table 2.3) maintained or improved the overall prediction ability of APSIM compared to the version presented by Dietzel et al. (2016). Noticeable improvements in the simulation process or new tests are presented here (Figs. 6 and 9). For all of the other processes such as soil water, temperature, biomass, soil NO₃, and soil-root CO₂ emissions, we refer to graphs and statistics presented by Dietzel et al. (2016). In general, the model performed well for all system variables and captured satisfactorily the year-to-year variation. Precision was good for yields (RRMSE = 12.3%), grain N concentrations (RRMSE = 14.1%) and annual NO₃-N losses (RRMSE = 28%), although the model tended to under predict years with higher leaching. Simulations were less precise for drainage water and the rye C and N data (RRMSE = 57.9%, 30.3% and 43.4%, respectively), although model predictions were fairly accurate (evidenced by the slope of regression equation of simulated vs. predicted ~1; Fig. 2.9). This means that the long-term simulations were unbiased, and that the average response is reliable.

The range of simulated rye biomass (1.9 ± 1.3 Mg ha⁻¹), C:N (15.5 ± 5.6 and 32.3 ± 7.8 for shoots and roots, respectively), root:shoot (0.65 ± 0.12), water (39 ± 27 mm) and total N use (67 ± 40 kg ha⁻¹) were within the range of values measured in this study (Table 2.4 and Fig. 2.7), with a later termination date associated with greater rye growth (supplemental Table S2.2). The model simulated overall decreases in annual NO₃-N losses (-25.5 ± 26%), though it did not consistently simulate reductions in annual drainage water (-3.9 ± 13%) and maize grain yields (-1.84 ± 6%). Regression analyses of this simulated dataset (n=120; 4 termination dates × 30 yr) showed that increases in rye shoot biomass were not associated with reductions in maize yield and water drainage (p > 0.05; Fig. 2.10). For NO₃-N losses the relationship between rye biomass was significant (p < 0.001), but this was with poor
prediction power, \( (r^2 = 0.23) \). Combined analysis of experimental and literature data yielded similar results to model simulations, although measured values did show a significant relationship for drainage in addition to NO\(_3\)-N losses (Fig. 2.10).

Figure 2.6. Measured (points) and simulated (lines) cumulative drainage water and NO\(_3\)-N losses in subsurface drainage, maize yields, and rye shoot biomass. Shaded area and error bars indicate standard error of measured data.
Figure 2.7. Relationships between cumulative precipitation and drainage water volume to nitrate (NO$_3$)-N losses in subsurface drainage during the drainage season.
Figure 2.8. Rye shoot biomass versus water use (transpiration) as estimated by a water balance difference method using experimental data (●; \( y = 47.414x, r^2 = 0.8279 \)), and by the APSIM model using two sets of transpiration efficiency coefficients (TE) (△; \( y = 60.773x, r^2 = 0.9824 \) and □; \( y = 48.636x, r^2 = 0.9877 \)). Each of the five points reflects a year (2009–2013).

Discussion

In this study, we approached rye cover crop abiotic effects on maize yields and environmental performance from a systems perspective (Fig. 2.1). Initially, we hypothesized that the magnitude of rye effects on maize yields and environmental performance variables such as cumulative drainage water and NO\(_3\)-N losses would be proportionally related to rye biomass production, an easily measurable trait. Experimental, literature and modeling results did not support the hypothesized relationship for yield (Fig. 2.10), meaning that rye biomass at termination date was not a good predictor of cover crop effects on maize yields.
Figure 2.9. Measured versus simulated rye root and shoot C input at termination date (a) and rye root and shoot N uptake at termination date (b), annual drainage (c), annual NO$_3$-N losses (d), maize grain yields (d) and grain N concentration (f) for continuous maize (CC) and continuous maize with rye cover crop (CCW) treatments.
Figure 2.10. Simulated relative treatment differences (see Eq. 1) in maize yield, annual tile drainage and annual NO$_3$-N losses versus rye biomass production (top panes) compared to relative differences from values reported in studies conducted in the US Midwest (bottom panes).

This lack of relationship may be because other factors, such as water and N stresses around flowering and grain filling periods (Çakir, 2004; Ciampitti and Vyn, 2011; Salmerón et al., 2011), may be more important than small changes in soil water and N at maize planting (Fig. 2.1). Additionally, Kaspar and Bakker (2015) found that decreases in maize yield following winter cereal cover crops are sometimes related to lower crop population densities, which seems to suggest that biotic stresses such as allelopathy and increased disease pressure or other factors may also play an important role.

Our experimental results combined with literature values suggest a significant relationship between rye biomass and changes in drainage water volume, but modeling results do not support this hypothesis (Fig. 2.10). The lack of a strong relationship between simulated changes in drained water and rye biomass is probably due to compensatory effects between rye water use and spring precipitation (see discussion on soil water below), or to the
fact that most of the drainage in this site occurs during the maize growing season (67%, Fig. 2.6), or both. For the NO₃ losses, we found a significant proportional relationship for both measured and simulated values (Fig. 2.10), presumably due to a rye N recycling effect, but this relationship was associated with large variability \( (r^2 = 0.23) \), which may be related to the variability in C:N of the rye biomass at termination (Fig. 2.3). Malone et al. (2014) simulated 40 site-climatic conditions in the US using RZWQM model and found a strong relationship between rye N uptake and reduction in NO₃ leaching \((\text{slope} = 40\%, \ r^2 = 0.90)\). Using rye N uptake as a predictor, our modeling results showed a stronger relationship to reduction in NO₃-N losses than biomass \((\text{slope} = 41.8\%, \ r^2 = 0.52)\), but the experimental results did not confirm this relationship (data not shown). Below we synthesize experimental, simulated and literature results to better understand the complex interactions and dynamics in the rye-maize system.

**Soil temperature effects are minor suggesting negligible impacts on maize seedling emergence**

High-resolution, multi-soil profile temperature results that covered five contrasting years (wet, drought, and average years; Fig. 2.2), different rye biomass levels \((0–2.5 \text{ Mg/ha; Table 4})\) and thus shading capacities, showed very minor treatment effects (Fig. 2.4). In the top soil layer, the decrease in soil temperature caused by rye was less than 0.7 °C by the time of rye termination, and none by the time of maize planting (Fig. 2.4), indicating that the temperature effect of rye on maize seedling emergence was minimal. This also means that the putative shading role of rye and its effects on soil water evaporation savings (Fig. 2.1) is probably lower than previously believed in simulation model studies (Basche et al., 2016; Dietzel et al., 2016). If soil water evaporation savings existed, then the additional water in the CCW treatment should have resulted in higher soil moisture levels in the profile or in higher
drainage rates or in higher maize yields in the drought years. None of this was true (Table 5a, and Figs. 5 and 6) providing further evidence that rye shading effect and consequent evaporation savings are much lower than believed. That was the reason for improving parameters in the rye model related to ground cover shade (Table 2.3).

**Soil water stress caused maize yield penalty in drought years via different mechanisms**

Previous research with model simulations has estimated that rye can deplete up to 60 mm of soil water in this region (Basche et al., 2016; Malone et al., 2007). In Iowa, May-June rainfalls are about 260 mm, while the soil water holding capacity is generally above 180 mm, thus combined can minimize the effect of rye transpiration (up to 50 mm; Fig. 2.8). A recent study in a nearby location provided evidence for this, showing that spring precipitation replenished soil moisture of cover crop plots to levels comparable to the no-cover-crop control by the time of corn emergence (Basche et al., 2016b). However, this seems to not be fully true in years with below average precipitation (i.e. dry years: 15 out of 35 cases; Fig. 2.2). In our study, there were two drought years (2012 and 2013; Fig. 2.2) and in those years we observed maize yield penalties (Table 2.5a) and significant treatment differences in soil moisture (Fig. 2.5). However, the drought-induced conditions were different between 2012 and 2013 (see precipitation patterns in Fig. 2.5). Examination of soil water deficits coupled with APSIM model sensitivity analyses (not shown) indicated that a water deficit of 24 mm at rye termination and its subsequent carry-over throughout the season (Fig. 2.5) was probably the main reason for the observed yield penalty in 2012. The deficit most likely impacted photosynthesis, leaf expansion, and kernel number and growth. In the following year (2013), the reason for the yield penalty was either a biotic factor (which is not captured in this analysis) or early season water stress that impacted potential kernel number. The potential kernel number in maize is set before silking (Abendroth et al., 2011), and lowering
this potential at that period has irreversible effects on maize yields. This might be the reason for the 2013 yield penalty (see also water deficit before silking and water surplus after silking in CCW; Fig. 2.5). Many other studies have also noted that lowered maize yields following cover crops are related to early-development stresses (before silking) (Johnson et al., 1998; Krueger et al., 2011; Miguez and Bollero, 2006; Pantoja et al., 2015; Salmerón et al., 2011). A strategy suggested to avoid water-related yield impacts on maize during drought-inducing conditions could be the early termination of rye cover crop (Krueger et al., 2011). Knowing that one Mg ha\(^{-1}\) of rye cover crop growth uses roughly the same amount of water as what is provided by one medium-intensity rainfall event (21.1 mm, see relationship developed in Fig. 2.8) should provide a baseline to decide appropriate termination timing during these conditions.

**Rye roots have greater potential to immobilize N during decomposition than rye shoots**

Another concern regarding inclusion of rye into maize-based systems is possible N immobilization. Experimental results from this study suggest that rye contributes to changes in the way N is cycled through the crop-soil system. Soil NO\(_3\) measurements at V6 (about 40 days after rye termination) showed an average treatment difference (CC vs. CCW) of about 12 kg N ha\(^{-1}\) (2.8 mg kg\(^{-1}\); Table 2.5a), which resulted in the LSNT recommending higher fertilizer application rates for CCW (26 kg N ha\(^{-1}\) on average; Table 2.2). This difference could be related to the fact that not all the N taken up during rye growth may had cycled back into the soil mineral pool by V6. It should be noted, however, that rye took up on average 40 kg N ha\(^{-1}\) in its total biomass by the time of its termination (~60% in shoots and ~40% in roots; Table 2.4), which is about three times greater than the difference observed in soil NO\(_3\) between treatments. This might suggest that at least some portion of rye’s organic N could have been mineralized to plant-available inorganic form by V6, although the exact proportion
mineralized in this experiment is uncertain given that soil NO₃ concentrations were not measured at rye termination. Nonetheless, Pantoja et al. (2016) was able to show in a recent Iowa study that when following maize in a maize-soybean rotation, 64% of rye shoot N was recycled by the end of the growing season.

Net mineralization of N in rye residues is likely because of the low C:N of rye biomass during the vegetative stages (Table 2.4). In general, crop residues with C:N < 25-40 tend to favor N mineralization rather than immobilization during their decomposition (Vigil and Kissel, 1991), and the APSIM residue model simulates these dynamics (Thorburn et al., 2005, 2001). The range of rye C:N values found in this study agrees with what has been measured in other studies in Iowa (Pantoja et al., 2016, 2015; Patel et al., 2015), Minnesota (Feyereisen et al., 2006; Krueger et al., 2011; Strock et al., 2004), Illinois (Miguez and Bollero, 2006; Ruffo and Bollero, 2003) and Washington (Kuo and Jellum, 2002). Most importantly, all these studies together synthesized a robust framework that relates rye biomass quantity to its quality and reveals their relationship (Fig. 2.3). The most important messages from this analysis are: a) decomposition of rye shoot biomass will not tend to immobilize N if it is terminated before 1.57 Mg ha⁻¹ of shoot growth (~ 25 C:N in upper prediction interval in Fig. 2.3.), and b) decomposition of roots is more likely to immobilize N than shoots because of their higher C:N. In this study, however, root C:N was still relatively low (average =27; Table 2.4) and consequently net N immobilization from rye root decomposition was probably minimal.

It should be noted that the shoot C:N is mainly regulated by the N concentration and not by the C concentration, which is fairly stable at about 40 % in shoots (Table 2.4; Brennan et al., 2013; Vigil and Kissel, 1991). The N concentration is a function of rye growth stage
and biomass production as well as soil supply of N and stand density (leaf to stem ratio).

When rye is growing under N limited conditions, the plant will satisfy its minimum requirements (upper confidence intervals in Fig. 2.3). When rye is growing under non-N limited conditions, the plant will uptake N until it satisfies its “luxurious” requirements (lower confidence intervals in Fig. 2.3). This explains the data variability in Fig. 2.3 across literature studies. Another interesting observation from the model analysis is that rye growth in Iowa is not only limited by temperature but also by N availability, and that the amount of the residual soil NO$_3$ at maize harvest will greatly influence its final biomass production. This is because the contribution of soil organic matter to plant available N during winter months is practically zero due to near freezing temperatures. In our study, the APSIM model estimated that total soil mineralization during the period between rye planting and its termination (Table 2.1) was in the range between 12 to 38 kg N ha$^{-1}$, but also that not all of the mineralized N was available for rye uptake because the decomposition of the maize stover (C:N > 70) immobilized some of that N also. In this study, 50% of maize residue was removed at harvest, which probably resulted in different amount of rye growth than if no residue were removed. This also means that rye growth will be maximized in fields with high residual N after crop harvest.

**Carbon inputs are low but of high quality compared to maize**

Rye cover crop terminated during vegetative growth adds a relative small amount of C in the system (160–1800 kg C ha$^{-1}$ yr$^{-1}$; Tables 4 and S2) of high quality (see section 4.3.). This amount of C is approximately 10% the C added by the maize stover. It should be noted, however, that in this study we found exceptionally high root:shoot at termination day in some years (up to 1.9; Table 2.4). This is a topic that we investigated further. On the other hand, APSIM model simulated rye root:shoot from 0.57 to 0.79 at termination day, which is
reasonable given that rye is terminated at early growth stages (see Zadoks stage on Table A2.2; Zadoks et al., 1974).

**Rye decreased NO$_3$-N losses by reducing NO$_3$-N concentration in drainage rather than drainage water volume**

Nitrate-N losses were reduced in two out of the six studied years (2011 and 2012) while no differences were found in drainage water volume in any of the studied years (Table 5b). On the other hand, flow-weighted NO$_3$-N concentrations in drainage water were also reduced during those years (Table 5b) indicating that NO$_3$-N losses were probably lower because rye growth reduced soil mineral N concentrations rather than drainage water volume. This is consistent with our modeling results (Fig. 2.10) and results from other studies in central Iowa (Kaspar et al., 2012, 2007). Over the six experimental years, we observed a 20% reduction in NO$_3$-N losses relative to CC which represented only 4 kg of N ha$^{-1}$ yr$^{-1}$ (Fig. 2.6 and Table 5b), approximately 10% of the amount of N taken up by rye (40 kg N ha$^{-1}$ yr$^{-1}$; Table 4). These reductions are lower than what has been measured in other studies in a nearby location (44% or 20 kg ha$^{-1}$ in Kaspar et al., 2012; 65% or 31 kg ha$^{-1}$ in Kaspar et al., 2007). In this experiment, however, LSNT-based N fertilization resulted in unequal application rates between treatments (higher in CCW from 2009-2012 and lower in 2013-2014; Table 2) which could have influenced the results. When the NO$_3$-N losses are expressed as a percentage of unit of N applied, the benefit of including rye cover crop in this system was 3.3 kg of NO$_3$-N loss reduced per 100 kg$^{-1}$ of N applied yr$^{-1}$, which represents a 31% reduction relative to CC (Table 5b). Finally, it should be noted also that rye cover crop here is evaluated on a continuous maize system (with 50% residue removal), rather than a maize-soybean rotation which is more common in the literature. Thus, differences in residue dynamics (i.e. quantity and quality; e.g. faster decomposition of soybean residue than maize
residue) may partly account for why the reduction in NO3-N losses here are relatively smaller than what has been measured elsewhere.

**Conclusion**

Coupling experimental and literature findings with modeling, we provided a system-level analysis of rye cover crop effects on maize and extrapolated results beyond the study period to obtain a more complete picture of the abiotic effects of the inclusion of a rye cover crop in rain-fed maize-based systems. Modeling scenario analysis showed that in the long term, rye improves environmental performance (26% reduction in NO3-N losses) without consistently reducing maize yields. However, experimental and modeling results did not fully support the hypothesized relationship between rye shoot biomass production (easily measurable trait) and the magnitude of rye abiotic effects on maize yields and environmental performance, which demonstrates the complexity that exists in the rye-maize-soil-atmosphere system (Fig. 2.1). APSIM was able to replicate measurements well and thus it can be used as a tool to identify combinations of practices that can result in win-win scenarios. This study also provided new data on rye water and N use, which are very important in understanding how the rye cover crop affects the system. Most importantly, we showed that: a) rye cover crop soil-temperature effects were negligible; b) rye water use had the potential to affect yield only when spring rains failed to replenish soil moisture (drought-inducing conditions); c) rye terminated during early vegetative stages had little potential to immobilize plant-available N during their decomposition, d) rye residues provided high quality C inputs (low C:N) of low quantity compared to maize, and 5) reduced NO3-N losses were related to lower NO3-N concentrations in drainage. We also developed robust empirical models between water and NO3-N in drainage and precipitation for fast assessments of environmental
performance at this site. Potential trade-offs and risks associated with the use of rye cover crop in maize-based systems will always exist given the complex nature of the system. Thus, further research should advance understanding of biotic and abiotic mechanisms by which rye affects yield and environmental performance of the system, as well as the long-term consequences of including rye cover crops in Midwestern cropping systems.

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Supplemental Figure S2.1 Example of how soil temperature (a) and water content (b) were estimated for soil layers. Solid circles indicate the measurement of the electronic sensors at a given depth position. Small dots and solid lines indicate interpolated values through using fitted splines.
Supplementary Table S2.1 Estimated parameters and error for the non-linear model of C:N and rye biomass for shoots and roots (expressed in Mg ha\(^{-1}\)).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Shoot (( n = 130 ))</th>
<th>Root (( n = 16))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(y = a x^b)</td>
<td>(a)</td>
<td>15.5</td>
</tr>
<tr>
<td></td>
<td>(b)</td>
<td>0.263</td>
</tr>
<tr>
<td>Error</td>
<td>(RRMSE)</td>
<td>0.283</td>
</tr>
<tr>
<td></td>
<td>(r^2)</td>
<td>0.339</td>
</tr>
</tbody>
</table>
Table S2.2 Summary (means and standard deviations) of results from the model scenario analysis of the COBS continuous maize (CC) and continuous maize with rye cover crop (CCW) treatments, assuming four rye termination dates: 13 April, 25 April, 5 May, and 15 May. In each scenario, a total of 35 weather years were simulated, rye was planted on 20 Oct every year, and maize was planted 10 days after rye termination.

<table>
<thead>
<tr>
<th>Variable</th>
<th>13 April</th>
<th>25 April</th>
<th>5 May</th>
<th>15 May</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rye shoot biomass (kg ha$^{-1}$)</td>
<td>908</td>
<td>513</td>
<td>1449</td>
<td>616</td>
</tr>
<tr>
<td>Rye root:shoot (-)</td>
<td>0.783</td>
<td>0.073</td>
<td>0.710</td>
<td>0.064</td>
</tr>
<tr>
<td>Rye Zadoks scale (0-99)</td>
<td>21.9</td>
<td>4.4</td>
<td>24.8</td>
<td>2.3</td>
</tr>
<tr>
<td>Rye total carbon inputs (kg C ha$^{-1}$)</td>
<td>643</td>
<td>330</td>
<td>993</td>
<td>398</td>
</tr>
<tr>
<td>Rye total N uptake (kg N ha$^{-1}$)</td>
<td>47.6</td>
<td>21.7</td>
<td>59.5</td>
<td>26.2</td>
</tr>
<tr>
<td>Rye shoot C:N (-)</td>
<td>10.0</td>
<td>2.5</td>
<td>13.5</td>
<td>3.3</td>
</tr>
<tr>
<td>Rye root C:N (-)</td>
<td>24.8</td>
<td>5.3</td>
<td>31.0</td>
<td>6.4</td>
</tr>
<tr>
<td>Rye water use (transpiration, mm)</td>
<td>18.2</td>
<td>10.3</td>
<td>29.0</td>
<td>12.3</td>
</tr>
<tr>
<td>Maize grain yield in CCW (kg ha$^{-1}$)</td>
<td>9057</td>
<td>2329</td>
<td>8899</td>
<td>1964</td>
</tr>
<tr>
<td>Maize grain yield in CC (kg ha$^{-1}$)</td>
<td>8868</td>
<td>2477</td>
<td>8862</td>
<td>2053</td>
</tr>
</tbody>
</table>
CHAPTER 3. AN IMPROVED ALGORITHM TO PREDICT IN-FIELD DRY-DOWN OF MAIZE AND SOYBEAN GRAINS WITH GENOTYPE-BY-ENVIRONMENT ANALYSIS

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Modified from a manuscript submitted for scientific journal publication

Abstract

A delayed harvest of maize and soybean crops is associated with yield losses, whereas a premature harvest requires additional costs for artificial grain drying. Accurately predicting the ideal harvest date can increase farmers’ profitability, but today’s predictive capacity is low. To fill this gap, we collected and analyzed time-series grain moisture data from field experiments (Iowa, US) with genotype-by-environment treatments to improve, parameterize, and test a mechanistic algorithm for predicting dry-down in the field. The resulting algorithm is driven by air relative humidity as this was found to be the best-performing predictor of field dry-down of maize ($r^2 = 0.75$) and soybean ($r^2 = 0.85$) grains among other factors tested (wind speed, temperature, and their combinations). Evaluation of variance components and treatment effects revealed that genotypes, weather-years, and planting dates had little influence on the post-maturity drying coefficient, but significantly influenced the grain moisture content at physiological maturity. Therefore, estimating the starting moisture content is critical for implementation of the algorithm across environments. Our work provides new insights to understand the post-maturity grain dry-down process and
assist development of robust and scalable predictive tools to forecast grain dry-down and ideal harvest dates across environments.

**Introduction**

As the growing season approaches its end and crops mature, farmers in the United States (US) turn their attention to monitoring grain moisture status in the field to establish appropriate harvest dates, a decision with important economic implications. The natural drying process of maize (*Zea mays* L.) and soybean (*Glycine max* L. [Merr.]) grain crops in the field can take one week to more than a month, as it is influenced by genetics and environmental conditions (Jayas et al., 1991; Yang et al., 2010). The standard moisture content for mechanical harvest and safe storage of grains is from 10 to 15.5%, depending on the type of grain and storage time. Harvesting grains below that threshold causes revenue lost due to grain shrinkage (Sadaka et al., 2016) and due to yield losses due to plant lodging, dropped grains, bird damage, and diseases (Elmore and Roeth, 1999; Kebebe et al., 2014; Philbrook and Oplinger, 1989; Sweeney et al., 1994; Zhang et al., 1996). Harvesting grains above that threshold results in another revenue loss due to buyer’s penalties in selling price or to the additional cost of artificially drying grains prior to marketing. In the northern US Midwest, the cost for artificial grain drying is the second or third largest expense in maize production after fertilizer or seed cost (Plastina, 2017). Every year farmers have to balance these tradeoffs between timing of harvest and drying costs. Development and implementation of data-driven tools that can predict grain dry-down in the field is needed to assist producers in decision-making.

The ability to predict grain dry-down in the field becomes even more important if we consider the increasing weather variability that is already being experienced in many regions.
(Melillo et al., 2014). In the US Midwest as well as in other temperate regions where production of maize and soybean is constrained to the frost-free period, greater weather variability could increase uncertainty in the duration of the growing season (Hatfield et al., 2014; Mueller et al., 2016) and thus in the timing of planting and harvesting operations. Matching the length of the crop growth period to the growing season through choice of cultivars and planting dates is a primary strategy for maximizing crop yields and minimizing operation cost (Jeffrey T Edwards et al., 2005; Jeffrey T. Edwards et al., 2005; Iglesias and Minguez, 1997; Long et al., 2017). While the influence of genotypes and management on crop yields has been thoroughly studied (Andrade et al., 2002; Capristo et al., 2007; Jeffrey T Edwards et al., 2005), the period of grain dry-down remains largely unexplored, with little progress towards selection of genetic traits that promote rapid grain moisture loss (Cross, 1985; Wang et al., 2012; Yang et al., 2010).

The physiological process of grain moisture loss can be divided into two phases. The first phase occurs during the grain filling period and is driven by the displacement of water by assimilates (e.g. starch, protein, oil). As the grain dry matter increases, the grain moisture decreases (Borrás et al., 2004a; Brooking, 1990; Gambín et al., 2007; Sala et al., 2007). Once grains reach their maximum dry matter accumulation, a stage called physiological maturity, transfer of fluids between the plant and seed ceases. At this point, maize kernel moisture normally ranges between 35 and 40% (Daynard, 1972; Sala et al., 2007) while in soybean, seed moisture ranges between 55 and 65% (Borrás et al., 2004b; TeKrony et al., 1979). In the second phase, grain moisture is lost through physical evaporation of water through the grain surface (Kiesselbach and Walker, 1952), a process primarily controlled by endosperm osmotic pressure and pericarp permeability (Crane et al., 1958; Nass and Crane, 1970). Post-
maturity grain dry-down typically follows a negative curvilinear response to days after physiological maturity (Brooking, 1990; Ma and Dwyer, 2012), and continues until grains reach a state of equilibrium with the surrounding air, a point known as the equilibrium moisture content (Henderson, 1952). The equilibrium moisture content depends on grain type and weather conditions. Therefore, the rate of grain dry-down in the field changes on a daily basis, making the scheduling of harvest operations challenging.

Several mathematical models have been developed over time to describe grain drying (Parry, 1985), but the vast majority of these have been used to predict grain moisture loss in controlled environments such as mechanical driers, and only a few have been adapted and tested for field conditions. Most recently, Piggot (Piggott, 2010) and Maiorano et al. (Maiorano et al., 2014) adapted the Henderson and Perry (Henderson and Perry, 1966) equation to develop a mechanistic algorithm that simulates post-maturity changes in maize grain moisture. The algorithm predicts dry-down as a function of days after physiological maturity, and requires inputs such as initial moisture content ($M_0$), a drying rate coefficient ($k$) and the equilibrium moisture content ($M_e$), with the latter computed using daily weather data (see methods for details). However, the scarcity of appropriate field data to parameterize, test, and improve the algorithm has been a main limitation for development and implementation. This gap is clearly reflected by the widespread inability of current crop models such as APSIM (Holzworth et al., 2014), CropSyst (Stockle et al., 2003), Hybrid-Maize (Yang et al., 2004) and others to simulate post-maturity grain moisture loss and harvest day, or the lack of stand-alone decision support tools.

To fill this gap, we collected and analyzed time-series post-maturity grain moisture datasets from field experiments in Iowa, US with various maize ($n=60$) and soybean ($n=36$)
genotype-by-environment treatments (i.e. weather-years and planting dates within each year) to provide insight into the grain drying process, and develop and parameterize scalable algorithms to assist farmers in decision-making. More specifically, our objectives were: i) expand the application of the Henderson-Perry algorithm to soybean dry-down; ii) test various explanatory-weather factors (temperature, relative humidity, wind speed, and their interactions) to improve prediction and explanatory power; iii) validate the improved algorithm; and iv) explore whether genotypes and their interaction with the environment affect model parameters to further inform implementation of the algorithm across environments.

**Methods**

**Grain moisture content data source**

Grain moisture time-series data were collected from maize and soybean field experiments located in central (Ames; 42.01°, -93.74°), northern (Kanawha; 42.93°, -93.79°), and southeast (Crawfordsville; 41.20°, -91.49°), Iowa, US. These sites have deep, fertile soils with fine-loamy texture, and a humid continental climate. Central Iowa data for 2015 and 2016 (n=24) were used to parameterize the dry-down algorithms. Validation of the maize algorithms was done using data from central Iowa in 2014 (n=12), from northern Iowa in 2016 and 2017 (n=12), and southern Iowa in 2016 and 2017 (n=12). Data from central Iowa in 2014 (n=12) were used for validation of the soybean algorithms.

The experimental factors in central Iowa included four different genotypes per crop, three different planting dates per genotype and the experiments were repeated over three years. Within a year, each experimental unit was replicated four times (Table 3.1). Briefly, the experiment was set up in a maize-soybean rotation with both crop phases present in each
year. Maize was planted at 86,450 seeds ha\(^{-1}\) and soybean at 345,800 seeds ha\(^{-1}\) both at a 76 cm row spacing. Three planting dates (i.e. early, mid, and late) were approximately at 25-day intervals beginning in late April (Table 3.1). The maize hybrids represented four relative maturities (104-day, 109-day, 111-day, and 113-day, respectively), and the soybean varieties represented four maturity groups (2.2, 2.5, 2.7, and 3.5, respectively). Soil fertility was managed according to university recommendations (Mallarino et al., 2013; Sawyer et al., 2006). Maize ear and soybean pod samples were collected from late August to final (mechanical) harvest date at one-week intervals. Crop phenological stage was determined according to Abendroth et al. (Abendroth et al., 2011) and Licht and Pedersen (Licht and Pedersen, 2014a) for maize and soybean, respectively. In the field, we collected two maize ears per plot and all the pods from a plant per plot. In the lab, we separated maize kernels from ears and soybean seeds from pods, and weighed subsamples (100 g for maize and 10 g for soybean), and then placed in a forced-air oven at 105 °C until constant weight was achieved. The dry samples were placed in a desiccator with anhydrous calcium chloride for two hours to allow cooling of the sample and removal of the remaining moisture. The dry samples were weighted and percent moisture content was expressed in wet basis (i.e. ratio of water mass in grain to total fresh grain mass).

Table 3.1. Planting dates for the maize and soybean field experiments by year.

<table>
<thead>
<tr>
<th>Year</th>
<th>Maize Early</th>
<th>Mid</th>
<th>Late</th>
<th>Soybean Early</th>
<th>Mid</th>
<th>Late</th>
</tr>
</thead>
<tbody>
<tr>
<td>2014</td>
<td>21-Apr</td>
<td>9-May</td>
<td>3-Jun</td>
<td>6-May</td>
<td>20-May</td>
<td>10-Jun</td>
</tr>
<tr>
<td>2015</td>
<td>15-Apr</td>
<td>13-May</td>
<td>4-Jun</td>
<td>6-May</td>
<td>20-May</td>
<td>10-Jun</td>
</tr>
<tr>
<td>2016</td>
<td>15-Apr</td>
<td>16-May</td>
<td>9-Jun</td>
<td>6-May</td>
<td>19-May</td>
<td>9-Jun</td>
</tr>
</tbody>
</table>
The maize grain moisture validation datasets from northern and southeast Iowa sites have been previously described by Licht et al. (Licht et al., 2017). In short, these datasets included measurements from maize plots with late-April (early) and mid-May (mid) planting dates and genotype (three cultivar relative maturities) treatments collected in 2016 and 2017. Ear samples were collected starting at physiological maturity in one-week intervals and percent grain moisture was determined using AM-5200-A (Perten Instruments, Hägersten, Sweden) and GAC2500 (Dickey-John, Auburn, Ill. US) electronic meters.

**Weather data source**

Weather data at each location were recorded and retrieved from the Iowa Environmental Mesonet database (Iowa Environmental Mesonet, 2018), and included hourly values of precipitation, temperature, relative humidity, and mean wind speed. Hourly data were converted into daily values of cumulative precipitation, minimum and maximum temperatures, mean relative humidity, and mean wind speed.

**Dry-down model**

The Henderson-Perry equation (Henderson and Perry, 1966) states that the change in grain moisture during a time interval is proportional to the difference between the grain moisture content (M; % wet basis) at time x, and the equilibrium moisture content (M_e; %): 

$$\frac{dM}{dx} = -k(M - M_e)$$  (Eq. 1)

where k is a proportionality drying coefficient. The equation is based on diffusion theory (i.e. Fick's second law) which assumes that resistance to diffusion occurs mainly in a thin outer layer. In grains, this layer is often interpreted as the seed coat or pericarp, although the endosperm mass can also limit diffusion (Parry, 1985). Piggott (2010) proposed to adapt this algorithmic to simulate maize grain moisture loss in the field, and used two different k
values for representing grain moisture loss before and after physiological maturity. The post-maturity phase also included an extra term to account for rewetting of the grain due to precipitation and heavy dew. Maiorano et al. (2014) argued that the Henderson-Perry equation was only adequate for the dry-down phase, and proposed an alternative model for the grain-filling phase. Here we only focus on the dry-down phase.

To further improve the model and expand its application to soybean, we modified the Henderson-Perry equation in two ways. First, following Page (1949), we incorporated a power constant \( n \), so the amount of grain moisture loss on a given time-step \( x \) not only depends on the moisture content but also on the time elapsed since physiological maturity:

\[
\frac{dM}{dx} = -k \cdot (M - M_e) \cdot n \cdot x^{n-1}
\]

(Eq. 2)

Note that this expression is equal to the Henderson-Perry equation when \( n = 1 \). The power parameter provides additional flexibility in the model to fit the experimental data. Second, instead of using actual time (i.e. calendar days) as the \( x \)-independent variable, we use the accumulation days scaled by how favorable weather conditions are for grain drying. The concept is similar to growing-degree days (Mcmaster and Wallace, 1997) which are widely used to predict crop development. Finally, the integrated expression is:

\[
M(x) = (M_0 - M_e) \cdot e^{-kx^n} + M_e
\]

(Eq. 3)

where \( M_0 \) is the grain moisture content at physiological maturity, which is R6 for maize (Abendroth et al., 2011) and R6.5 for soybean (Licht and Pedersen, 2014b). The dynamic value for \( M_e \) can be calculated using the following equation (Henderson, 1952):

\[
M_e = \left( \frac{\ln\left(1 - \frac{RH}{100}\right)}{-A(T+B)} \right)^{1/C}
\]

(Eq. 4)
where RH is relative humidity (%), T is daily mean temperature (°C), and A, B and C are constants specific to the drying material. Constants were parametrized as A=0.0001557, B=45.5, and C=2 for maize derived from Thompson et al. (Thompson and Foster, 1968), and as A=0.0000729, B=31.6, and C=1.526 for soybean, according to Yang et al. (2015). These parametrizations produce results on a dry basis (i.e. ratio of water mass in grain to total dry grain mass), so they to be converted to wet basis. Also, because of its dependence on weather, daily values of Me can swing abruptly (see example in suppl. Fig. S3.1) leading to unrealistically fast changes in grain moisture content. This was mitigated by using the 3-day moving average.

**Explanatory weather factors**

In addition to days after physiological maturity, we explored three explanatory weather factors to scale the time-step: a relative humidity factor (h; Eq. 5), a temperature factor (t; Eq. 6) and a wind speed factor (w; Eq. 7):

$$h = \sum_{i=0}^{n} \left( 1 - \frac{RH_i}{100} \right)$$  \hspace{1cm} (Eq. 5)

$$t = \sum_{i=0}^{n} \left( \frac{TMAX_i + TMIN_i}{2} - T_{base} \right) \begin{cases} TMAX_i < T_{base} \rightarrow TMAX_i = T_{base} \\ TMIN_i < T_{base} \rightarrow TMIN_i = T_{base} \end{cases}$$  \hspace{1cm} (Eq. 6)

$$w = \sum_{i=0}^{n} WS_i$$  \hspace{1cm} (Eq. 7)

where for the i\textsuperscript{th} day after physiological maturity, RH is mean relative humidity (%), TMAX and TMIN are maximum and minimum temperatures (°C), and WS is daily mean wind speed (m s\textsuperscript{-1}). The h factor weighs individual days by their drying potential (evaporative demand), with values ranging from 0 to 1. The t factor weighs days by their temperature, equivalent to the second method described by McMaster and Wallace (1997) for calculating growing degree days. After testing various values for base temperature (T\textsubscript{base}), here we used T\textsubscript{base} = 0 (see suppl. Fig. S3). Finally, the w factor weights days by how windy they are, with
possible values ranging from 0 to infinity. Additional factors were computed by multiplying their two-way and three-way combinations (i.e. h×t, h×w, t×w, h×w×t). The default, non-scaled time series was reported as day.

**Model training, testing, and selection**

Selection of the best explanatory weather factor for the dry-down model in the US Midwest was performed in two steps. First, the 2015 and 2016 data from central Iowa was used for model training, that is to estimate the $M_0$, $k$, and $n$ parameters. Non-linear regressions for every weather factor were fitted to the integrated model (Eq. 3), using the non-linear least squares function (nls) of the non-linear and linear mixed effects package (nlme) (Pinheiro et al., 2018) in the R statistical software (R Core Team, 2017) (version 3.4.2). Test of significance for estimated parameters of $M_0$ and $k$ were based on the null hypothesis that the parameter was equal to 0, whereas for $n$ it was based on the null hypothesis that the parameter was equal to 1. Model fit was evaluated using the adjusted coefficient of determination ($\text{Adj. } r^2$), the root mean square error (RMSE), Akaike information criterion (AIC), Bayesian information criterion (BIC), and modeling efficiency ($\text{M}^{\text{Eff}}$). The $r^2$ reflects prediction ability, while $\text{M}^{\text{Eff}}$ is a measure of improvement in model fit with respect to a simple mean, and for both of these the higher the value the better. The AIC and BIC are indices for model selection, while RMSE reflects model error. For the latter three indices, the lower the value the better. Second, the fitted models were then tested by comparing the predicted values with the 2014 data. To do this, we computed the $\text{Adj. } r^2$, RMSE, $\text{M}^{\text{Eff}}$, in addition to the model bias ($\text{M}^{\text{Bias}}$). The latter one is a measure of model accuracy, and the closer the value to zero, the better. In addition, we fitted simple linear regression of measured vs predicted and calculated the slope as another measure of model
accuracy, with a value closer to 1 being better. The equations for all of these metrics can be viewed in Archontoulis and Miguez (Archontoulis and Miguez, 2013).

Validation of the field dry-down model

The prediction accuracy of the parameterized maize dry-down algorithms were further evaluated using the independent datasets from central, northern, and southern Iowa. Simulations were initialized at the first measurement after physiological maturity at the moisture content of the sample (i.e. \( M_0 \)). Model simulation performance was assessed using the aforementioned statistical indices.

Genotype-by-environment analysis

After selecting the most appropriate weather factor to drive the algorithm, we tested treatment effects on the dry-down process. Statistical nls optimizations were performed to every combination of crop, year, planting date, and genotype at the central Iowa site to obtain model parameters for each experimental unit. Only the \( M_0 \) and \( k \) parameters were estimated, whereas \( n \) was hold constant. This is because previous analysis have shown strong correlation between \( k \) and \( n \) parameters, which prevents direct comparison of treatment effects (Jayas et al., 1991). Linear models of the effect of planting date, genotype, weather-year, and their interaction were fitted independently to each dataset of \( M_0 \) and \( k \) parameters for maize and soybean, using the PROC MIXED function in SAS 9.4 software (SAS Institute, 2013). From the resulting type 3 test of significance for fixed effects, the highest-level significant (\( \alpha = 0.05 \)) interactions or main effects were compared using the Tukey-Kramer adjustment. Additionally, variance component analysis was used to estimate the overall variability explained by genotype, weather-year, and planting date with the VARCOMP procedure in SAS using the restricted maximum likelihood method.
Results

Evaluating explanatory weather factors for use in the dry-down algorithm

To find the best predictor of grain dry-down in the field we evaluated cumulative daily measurements (starting at physiological maturity) of relative humidity (h), temperature (t), wind speed (w) as well as their two-way and three-way combinations (i.e. h×t, h×w, t×w, h×w×t). By default, the dry-down algorithm uses cumulative calendar days (day) as the explanatory factor, which was also included in this study. We used two years (2015-2016) of maize and soybean dry-down data from central Iowa to estimate the moisture content at physiological maturity (M₀), the drying rate coefficient (k), and the power constant (n) parameters in the model. Weather conditions during the dry-down period (September and October) tended to be warmer and wetter than the 30-year historical average (Fig. 3.1). Relative humidity generally oscillated around 80% (range: 45-100%, Fig. 3.1a), and wind speed oscillated around 3.8 m s⁻¹ (range: 1-7 m s⁻¹; Fig. 3.1a).

The estimated parameters for M₀ and n were relatively stable within each crop (Fig. 3.2b; and suppl. Table S3.1), while estimates for the k parameter varied between crops. The default model using day explained 86% of the temporal variation in the maize data with an RMSE of 2.9%. Model fit was slightly improved by using h×t and h. All other factors decreased model fit (Fig. 3.2c). Precision of model fit to soybean data was similar to maize, with the default model explaining 88% of the variation, albeit with greater error (RMSE = 7.1%). Performance of the model using h and h×t factors were essentially as good as day, but offered additional explanatory power. All other weather factors decreased model fit (Fig. 3.2c).
To test predictions of all the algorithms, we used the 2014 dry-down datasets from central Iowa (n=12) given that weather conditions during that year were more distinct from the other years (i.e. cooler and wetter than climatic normal; Fig. 3.1). We found that the maize models were able to explain 63 to 75% of the variation in this independent dataset (Fig. 3.3), with a slight tendency to over-predict dry-down by 2.7 to 4.4% moisture. Based on computed statistical indices, the maize models ranked (best to worst): $h \times w \sim w > h > day > > h \times t \times w > h \times t > t \times w > t$ (Fig. 3.3b). Regarding the soybean models, we found that fit to the testing dataset was near to slightly worse than to the training dataset. Most models tend to over-predict moisture content towards the middle of the dry-down period (Fig. 3.3a). The soybean models ranked (best to worst): $h > day > w > h \times w > h \times t > t > t \times w > h \times t \times w$ (Fig. 3.3b).
Figure 3.2. Model development and parameterization using maize and soybean grain moisture data collected in 2015 and 2016. (a) Measured (open circles) and predicted (solid line) moisture content with the x-axis being different weather explanatory variables (h = relative humidity; t = temperature; w = wind speed). (b) Estimated model parameter for each explanatory variable. Asterisks (*) adjacent to the scaling factors indicate that the parameter was significantly different (α = 0.05) than 0 for \( M_0 \) and \( k \) parameters, and different than 1 for \( n \) (see also supplemental Table S3.1 actual values). (c) Evaluation of model fit using the Akaike information criterion (AIC), Bayesian information criterion (BIC), modeling efficiency (M_Eff), adjusted coefficient of determination (r2_adj), and root mean square error (RMSE). Green shading indicates best fit, while orange indicates worst fit.

Based on the performance of the models against the training (years 2015 and 2016) and testing (year 2014) datasets, we selected the \( h \) factor as the preferred explanatory-weather variable for the following reasons: i) it provided good performance that improved prediction compared to the default \( \text{day} \) in both maize and soybean (Fig. 3.3); ii) all estimated model parameters for \( h \) were statistically significant (α = 0.05; Fig. 3.2b and suppl. Table S3.1); iii) relative humidity measurements are more likely to be available (or at least can be
approximated) than wind speed; and iv) use of relative humidity offers a more mechanistic way to scale up results from a specific field to different fields or environments.

**Validation of improved dry-down algorithm**

To validate the simulations of the $h$ dry-down algorithm, we used maize ($n=36$) and soybean ($n=12$) independent datasets from northern, central and southeast Iowa. We also compared the improved approach against the default $day$ algorithm. For maize, the $h$ algorithm satisfactorily simulated grain moisture in 35 out of the 36 validation genotype-by-environment scenarios (Fig. 3.4). Across all combinations of sites, years, and genotypes, the simulation captured a large portion of the variation in post-maturity maize grain moisture (Adj. $r^2 = 0.79$), with good efficiency ($M_{Eff} = 78\%$), small error (RMSE = 2.1 \%) and little bias ($M_{Bias} = 0.22$). Performance of the $h$ algorithm was improved compared to the default $day$ algorithm, which tended to significantly overestimate maize grain moisture towards the end of the drying period. In soybean, we found that dry-down was well characterized by both $h$ and $day$ algorithms, although the $h$ algorithm explained slightly less of the variation (Adj. $r^2 = 0.72$), with less efficiency ($M_{Eff} = 73\%$), greater error (RMSE = 7.1 \%) and some negative bias ($M_{Bias} = -1.94$; Fig. 3.4).

**Dissecting genotype-by-environment effects on dry-down**

Analysis of variance (ANOVA) of the parameters of the $h$ algorithm showed a significant effect ($p < 0.05$) of weather-year on the $M_0$ parameter (grain moisture at physiological maturity) in maize, as well as a significant effect of the interaction of genotype and planting date on the $M_0$ parameter in soybean (Table 4.1). In maize, the $M_0$ was 5.4\% significantly higher in 2016 than in 2014, but not significantly different than in 2015. In soybean, the $M_0$ was 8.6\% significantly higher in one genotype only between early and mid-
season plantings. None of the experimental factors showed a significant effect in the $k$ parameter (drying rate coefficient).

Variance component analysis revealed that the largest share of the variance in $M_0$ and $k$ parameters could be attributed to the experimental error, while the rest could be explained by either genotype, weather-year, planting date, or their interactions (Fig. 3.5). In maize, variance in $M_0$ was largely driven by weather-year (42%), while genotype and weather-year combined played a small role (9%). Very little of the variation (10%) in $k$ parameters could be explained by experimental factors, which is consistent with the ANOVA results. In soybean, the picture was more complex. The interactions of experimental factors explained most of the non-error variance in $M_0$ estimates (28%), while for $k$, genotype, weather-year, planting date, and their interactions together explained roughly equal amounts of the variance in parameter estimates (6-11%). In summary, experimental factors had some influence on values of $M_0$, but not on $k$.

**Discussion**

Due to weather variability and logistic constraints, maize and soybean crops in temperate regions are often harvested at moisture contents above or below the ideal levels required for grain storage, which leads to additional operation costs. Here we improved, parameterized, and tested a grain dry-down scalable algorithm to provide a mechanistic prediction of grain dry-down in the field that was previously missing for the US Midwest. Coupling our algorithms with forecasted weather and economic models could allow decision makers to reliably estimate optimal harvest dates that minimize operational costs and risks. Implementation of these tools has the potential to increase profitability of US Midwest farms.
Figure 3.3. Evaluating performance of different dry-down models using a weather year (2014) that not included in the parameterization dataset (2015-2016). (a) Regression evaluation of measured vs predicted values for each of the weather-scaling explanatory factors (h = relative humidity; t = temperature; w = wind speed). Dotted line indicates y=x line (i.e. perfect fit), while solid colored lines indicate obtained regression. (b) Evaluation of model fit using the Model bias (M_Bias), modeling efficiency (M_Eff), adjusted coefficient of determination (r2_adj), slope of the regression of measured vs predicted (Reg_slope) and root mean square error (RMSE). Green cell fill indicates better fit, while orange indicates worst fit.
Figure 3.4 Simulation of post-maturity maize and soybean grain-dry down for various planting dates and genotypes using independent measurements (symbols) collected at the central Iowa site in 2014, and at northern and southeast, Iowa in 2016 and 2017 (maize only). Solid lines represent simulation with the algorithm using the $h$ factor ($1 - RH/100$) as explanatory variable, whereas dotted line represents simulation with the default algorithm using calendar days. Shaded area represents the 3-day moving average equilibrium moisture content ($Me$). Model fit between these two algorithms are compared using the statistical indices described in the methods section.
Table 3.2. Effect of genotype, weather-year and planting date on initial moisture content ($M_0$) and drying coefficient ($k$) parameters of the relative humidity ($h$) maize and soybean dry down algorithms.

<table>
<thead>
<tr>
<th></th>
<th>Maize</th>
<th>Soybean</th>
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<tbody>
<tr>
<td></td>
<td>$M_0$</td>
<td>$k$</td>
</tr>
<tr>
<td><strong>ANOVA Type-3 test of significance</strong></td>
<td></td>
<td>$(p &gt; F)$</td>
</tr>
<tr>
<td>Genotype (G)</td>
<td>0.346</td>
<td>0.575</td>
</tr>
<tr>
<td>Weather-year (Y)</td>
<td>0.004</td>
<td>0.256</td>
</tr>
<tr>
<td>Planting date (P)</td>
<td>0.115</td>
<td>0.460</td>
</tr>
<tr>
<td>G*Y</td>
<td>0.813</td>
<td>0.636</td>
</tr>
<tr>
<td>G*P</td>
<td>0.503</td>
<td>0.855</td>
</tr>
<tr>
<td>Y*P</td>
<td>0.388</td>
<td>0.521</td>
</tr>
</tbody>
</table>

Effects on $M_0$

<table>
<thead>
<tr>
<th></th>
<th>Maize</th>
<th>Soybean</th>
</tr>
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<tbody>
<tr>
<td></td>
<td>$M_0$ (%)</td>
<td></td>
</tr>
<tr>
<td>Weather-year</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2014</td>
<td>34.3 a</td>
<td>2.2</td>
</tr>
<tr>
<td>2015</td>
<td>35.2 ab</td>
<td>2.5</td>
</tr>
<tr>
<td>2016</td>
<td>39.7 b</td>
<td>2.7</td>
</tr>
</tbody>
</table>

Previous work in maize (Piggott, 2010) has considered the dry-down process to be a function of calendar days after physiological maturity (herein the $day$ algorithm). The default $day$ model was found in this study to capture a large portion of the variation in grain moisture (Figs. 4.2-4.4). However, because $days$ after physiological maturity may not be reliably extrapolated across environments, we explored a suite of different weather variables such as relative humidity, wind speed and temperature and their combinations as dry-down predictors. This analysis expands current knowledge of the dry-down process under field conditions and provides opportunities to mechanistically extrapolate predictions across environments. Somewhat surprising was the fact that the temperature factor (growing degree
days) alone was amongst the worst predictors of grain dry-down. While temperature is related to drying potential of the air, mainly through changes in the vapor pressure deficit (Campbell and Norman, 1998; Murray, 1967), other variables such as air pressure, precipitation, and airflow play an important role (Khatchatourian, 2012; Pfeifer et al., 2010). The wind speed factor appeared to have some importance for predicting dry-down in the maize testing dataset (Fig. 3.3), but the improvement was not consistent in soybean or in the training dataset. In contrast, the relative humidity factor was found to be the best predictor as it performed better in maize and was equally good in soybean as the default day factor in training, testing and validation datasets (Figs. 4.2-4.4).

Air relative humidity is known to have a significant impact on grain moisture loss because it controls the rate of water vapor transport from the grain surface to the surrounding air, and influences the equilibrium moisture content ($Me$) (Jayas et al., 1991; Khatchatourian, 2012). While in grain driers $Me$ is relatively constant, in the field this value is dynamic because of its dependence on air temperature and relative humidity (Maiorano et al., 2014; Piggott, 2010). However, given that $Me$ is calculated based on data from weather stations, which are usually located outside the field, these conditions may be different from the micro-environment that grains experience during drying (i.e. protected by husks or pods). Therefore, a sudden change in weather (e.g. relative humidity) that can cause a large change in $Me$ (suppl. Fig. S3.1), might not translate to such a sudden change in moisture content. Here, we solved this problem by using a 3-day moving average, which helped stabilize $Me$ and improve model fit. Although further smoothing could be achieved by using longer averaging periods (e.g. 5-7 days), this may result in the overestimation of $Me$ in days with high drying potential and hence predict slower drying.
Figure 3.5. Variance components (%) associated with genotype, weather-year, planting date, and their two-way interactions for grain moisture at physiological maturity ($M_0$) and drying constant ($k$) parameters from dry down models fitted to experimental units.

Including a rewetting coefficient in the dry-down algorithm was considered in a previous study to account for the effect of precipitation and heavy dew (Piggott, 2010), but this was at the cost of additional input parameters and data requirements (Maiorano et al., 2014). In the improved algorithm ($h$), the effects of precipitation and dew are already partially captured by the relative humidity because these events essentially occur when air is completely saturated (i.e. relative humidity ~ 100%). High relative humidity leads to an
increase in $Me$, and when $Me$ becomes greater than the grain moisture content, the change is then positive resulting in rewetting of the grain. Furthermore, high relative humidity affects the time step, introducing a feedback on the amount of moisture change during a day. This makes the algorithm more responsive to days with high drying potential, while also mitigating sudden rewetting as the grains approach $Me$ (Fig. 3.4).

By having a dataset (n=36) that captures genotype, weather-years, and planting date effects on model parameters for each crop, we were able to examine the relative importance of each of these factors and their interactions in the dry-down process (Table 3.2 and Fig. 3.5). We found that the studied factors affected grain moisture at physiological maturity ($M_0$) but not the drying coefficient ($k$). This suggests that the $M_0$ parameter should be a user input in future implementations of our algorithm when predicting dry-down across environments. It is known that the $M_0$ is driven by source-sink dynamics during grain filling (Borrás et al., 2004a; Cross, 1995; Gambín et al., 2007; Sala et al., 2007) and in some cases can be affected by genotype (Ma and Dwyer, 2012). Here, we found maize $M_0$ was significantly different among environments but not among genotypes. Planting date in this study essentially meant modification of the environment, but this did not necessarily affect $M_0$ (Table 3.2). The average $M_0$ is about 35% but this value can be higher when stresses occur during grain fill and lead to premature cessation of grain dry matter accumulation (Sala et al., 2007). In contrast, soybean seed dry matter accumulation has been shown to be less sensitive to stresses during grain fill (Borrás et al., 2004a; Egli, 1975; Meckel et al., 1987).

The post-maturity drying coefficient ($k$) is related to atmospheric moisture exchange mechanisms (Cross, 1985). Maize genotypic traits such as husk number, tightness, length and senescence, ear length and angle, and number of grain per rows can influence the drying rate
(Sweeney et al., 1994). However, here we did not find significant effects of genotypes on $k$ (Table 3.2). In contrast, Yang et al. (Yang et al., 2010) detected significant differences among maize hybrids in a breeding program, but in that study grain samples were collected 45 days after silking, irrespective of whether the plants had achieved physiological maturity. As noted earlier, moisture loss before and after maturity are driven by distinct processes, and a failure to distinguish between the two phases may lead to confounding results because the traits controlling grain fill rate are different from those controlling post-maturity moisture loss.

Soybean genotypic traits such as thickness of the pod wall and senescence (Samarah et al., 2009), or seed characteristics (Gely and Giner, 2007; Giner et al., 1994) can influence the drying rate $k$ coefficient. In a laboratory experiment, Giner et al. (Giner et al., 1994) found differences among 25 Argentinian soybean varieties, and showed that drying times were related to seed size, with larger seeds having longer drying times (i.e. lower $k$). In these controlled environment assays, drying of soybean followed a clear exponential-decay trajectory. However, this was not the case with our field data, where drying rates seemed to change as drying progressed (see s-shaped pattern in Fig. 3.2a). Explicitly including the power parameter ($n$) in the soybean algorithm helped to deal with this non-constant drying rate. While it has been previously argued that the $n$ parameter does not have a clear biological interpretation in the drying process (Jayas et al., 1991), in soybean this may possibly be related to processes such as grain de-greening and pod senescence that occur alongside grain dry-down (Miles et al., 1988; Sinnecker et al., 2005; TeKrony et al., 1979). On the other hand, the $n$ parameter in maize was not statistically different than 1 (Fig. 3.2b
and suppl. Table S3.1) meaning that the amount of moisture loss of maize grains is not dependent on time.

In light of these results, important implications arise for developing a robust parameterization of the dry-down algorithm for implementation in existing crop models and for development of stand-alone tools to forecast harvest date and moisture loss across environments. Among the parameters in the dry-down algorithm, we found that $M_0$ is the most sensitive (Table 3.2) meaning that this parameter should be estimated for specific situations. For crop simulation models, this means that the post-maturity dry-down algorithm needs to be coupled to a grain fill moisture algorithm to predict $M_0$, like the one proposed by Maiorano et al. (2014). In stand-alone decision support tools, field-estimated $M_0$ values at a given date could be supplied by farmers, perhaps based on field readings obtained by electronic moisture meters (Yang et al., 2010). The fact that we did not find significant differences in the $k$ coefficient across genotypes, weather-years, and planting dates seems to suggest that a species-specific $k$ value would be adequate to simulate post-maturity grain moisture. This is also supported by Maiorano et al. (2014) who showed that use of a single $k$ value resulted in good model fit to maize grain moisture measurements across 11 genotypes in 9 weather years. All of this supports the theory that post-maturity dry-down is a passive process, mostly driven by atmospheric conditions.

Finally, implementation of the dry-down algorithms may be constrained because relative humidity data are not universally available from weather databases and forecasting systems. In the absence of direct relative humidity measurements, crop models such as APSIM and CropSyst simulate water exchange between the crop canopy and the atmosphere by assuming that the daily average dew point in humid and sub-humid climates is near the
daily minimum temperature (Basso and Ritchie, 2018; Tanner and Sinclair, 1983). Under this assumption, daily relative humidity can be estimated from maximum and minimum air. However, researchers should be aware that this approach may not be applicable in environments where relative humidity and temperature conditions are very different during dry-down (i.e. arid locations). Therefore, data availability constraints, as well as the tradeoffs with predictive ability, need to be taken in consideration when developing, adapting, and implementing these algorithms into modeling platforms and decision support tools.

**Conclusion**

We improved and parameterized scalable post-maturity grain dry-down algorithms for maize and soybean crops to aid harvest date decisions to increase profitability of US Midwest farms. The algorithms are driven by air relative humidity (as opposed to solely by days after physiological maturity), which allows for more mechanistic predictions across environments. Our work advances previous efforts to predict maize dry-down in the field and proposes a new algorithm for predicting soybean dry-down. Analysis of the comprehensive time-series datasets revealed that maize and soybean genotype-by-environment interactions had little influence on the post-maturity drying coefficients, but significantly influenced grain moisture content at physiological maturity. Thus, accurate implementation of the algorithms across environments would require estimating the initial grain moisture content, via modeling approaches or in-field measurements.

**References**


Supplemental Information

Supplemental Table S3.1. Non-linear model parameter estimates (standard error in parenthesis) and test of significance of model fits to the data using days after maturity (day), humidity (h), temperature (t), wind speed (w) and their combinations as explanatory variables. \( M_0 \) = grain moisture content at physiological maturity; \( k \) = drying constant; \( n \) = power constant

<table>
<thead>
<tr>
<th></th>
<th>Mo (%)</th>
<th>K (unitless)</th>
<th>( n^\dagger ) (unitless)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Maize</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>day(^\dagger)</td>
<td>37.4 (0.562)</td>
<td>*** 0.0463 (0.01260)</td>
<td>*** 1.090 (0.0911) ns</td>
</tr>
<tr>
<td>h</td>
<td>37.5 (0.558)</td>
<td>*** 0.2890 (0.03490)</td>
<td>*** 0.951 (0.0766) ns</td>
</tr>
<tr>
<td>t</td>
<td>37.5 (0.612)</td>
<td>*** 0.0017 (0.00102)</td>
<td>Ns 1.120 (0.1010) ns</td>
</tr>
<tr>
<td>w</td>
<td>37.4 (0.615)</td>
<td>*** 0.0211 (0.00775)</td>
<td>** 1.010 (0.0912) ns</td>
</tr>
<tr>
<td>h×t</td>
<td>37.4 (0.547)</td>
<td>*** 0.0118 (0.00435)</td>
<td>** 1.070 (0.0851) ns</td>
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<tr>
<td>h×w</td>
<td>37.5 (0.603)</td>
<td>*** 0.1280 (0.02520)</td>
<td>*** 0.863 (0.0750) ns</td>
</tr>
<tr>
<td>t×w</td>
<td>37.5 (0.665)</td>
<td>*** 0.0012 (0.00080)</td>
<td>Ns 1.000 (0.0970) ns</td>
</tr>
<tr>
<td>h×t×w</td>
<td>37.4 (0.594)</td>
<td>*** 0.0069 (0.00306)</td>
<td>* 0.945 (0.0811) ns</td>
</tr>
<tr>
<td><strong>Soybean</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>day</td>
<td>60.9 (1.27)</td>
<td>*** 0.00404000 (0.0025900)</td>
<td>Ns 2.32 (0.263) ***</td>
</tr>
<tr>
<td>h</td>
<td>61.2 (1.29)</td>
<td>*** 0.18300000 (0.0405000)</td>
<td>*** 2.17 (0.247) ***</td>
</tr>
<tr>
<td>t</td>
<td>60.9 (1.38)</td>
<td>*** 0.00000549 (0.0000079)</td>
<td>Ns 2.29 (0.269) ***</td>
</tr>
<tr>
<td>w</td>
<td>60.0 (1.32)</td>
<td>*** 0.00021000 (0.0002290)</td>
<td>Ns 2.45 (0.310) ***</td>
</tr>
<tr>
<td>h×t</td>
<td>60.8 (1.27)</td>
<td>*** 0.00013500 (0.0001410)</td>
<td>Ns 2.40 (0.278) ***</td>
</tr>
<tr>
<td>h×w</td>
<td>60.3 (1.36)</td>
<td>*** 0.01470000 (0.0085600)</td>
<td>Ns 2.22 (0.295) ***</td>
</tr>
<tr>
<td>t×w</td>
<td>60.1 (1.50)</td>
<td>*** 0.00000063 (0.0000012)</td>
<td>Ns 2.23 (0.290) ***</td>
</tr>
<tr>
<td>h×t×w</td>
<td>60.0 (1.39)</td>
<td>*** 0.00001600 (0.0000231)</td>
<td>Ns 2.26 (0.290) ***</td>
</tr>
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\(^\dagger\)H\(_0\): \( n = 1 \)
\(^\dagger\)Significance codes: ns = (p > 0.05); * = (0.05 > p > 0.01); ** = (0.01 > p > 0.001); *** = (p < 0.001)
Supplemental Figure S3.1. Maize and soybean equilibrium moisture content (Me, %) during the grain dry down period in central Iowa in 2014, 2015, and 2016. Filled circles represent daily values of Me, with color ramp to indicate colder (blue) and warmer (orange) daily mean temperatures. Solid line represents the 3-day moving average of Me. Top and bottom right-most panels show the relationship of maize and soybean daily values of Me as affected by relative humidity (%) and mean temperature (°C).
CHAPTER 4. LINKING CROP- AND SOIL-BASED APPROACHES TO EVALUATE SYSTEM NITROGEN-USE EFFICIENCY AND TRADEOFFS

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Abstract

Increasing nitrogen (N)-use efficiency (NUE) is key to improving crop production while mitigating ecologically-damaging environmental N losses. Traditional approaches to assess N-use efficiency (NUE) are principally focused on evaluating crop responses to N inputs, often consider only what happens during the growing season, and ignore other means to improve system efficiency, such as by tightening the cycling of soil N (e.g. with N scavenging cover crops). As the goals of improving production and environmental quality converge, new metrics that can simultaneously capture multiple aspects of system performance are needed. To fill this gap, we developed a theoretical framework that links both crop- and soil-based approaches to derive a system N-use efficiency (sNUE) index. This easily interpretable metric succinctly characterizes N cycling and facilitates comparison of systems that differ in biophysical controls on N dynamics. We demonstrated the application of this new approach and compared it to traditional NUE metrics using data generated with a process-based model (APSIM), trained and tested with experimental datasets (Iowa, USA). Modeling of maize-soybean rotations indicated that despite their high crop NUE, only 45%
of N losses could be attributed to the inefficient use of N inputs, whereas the rest originated from the release of native soil N into the environment, due to the asynchrony between soil mineralization and crop uptake. Additionally, sNUE produced estimates of system efficiency that were more stable across weather years and less correlated to other metrics across distinct crop sequences and N fertilizer input levels. We also showed how sNUE allows for the examination of tradeoffs between N cycling and production performance, and thus has the potential to aid in the design of systems that better balance production and environmental outcomes.

**Introduction**

Mitigating the environmental impacts of nitrogen (N) use while maintaining or increasing crop production is a major challenge of modern agriculture (Reis et al., 2016). Productivity remains primarily constrained by the availability of N to crops in many soils (Connor et al., 2011; Sinclair and Rufty, 2012). However, only about half of the global N fertilizer inputs to farmland are recovered in harvested yield (Conant et al., 2013; Gardner and Drinkwater, 2009). Unused N fertilizer can be retained in soils, or it can be lost to water bodies and the atmosphere, triggering a cascade of adverse ecosystem effects (Billen et al., 2013; Erisman et al., 2007; Galloway et al., 2003). Nitrate (NO\(_3\)), the dominant source of soil N for many crops, can be leached to ground and surface waters where it contributes to drinking water pollution and aquatic ecosystem eutrophication (Robertson and Vitousek, 2009). Gaseous losses of N through nitrification and denitrification processes produce nitrous oxide (N\(_2\)O) as a byproduct. This greenhouse gas has ~300 times more radiative forcing than CO\(_2\) and also contributes to stratospheric ozone depletion (Davidson and Kanter, 2014; IPCC, 2014). Therefore, increasing agricultural N-use efficiency (NUE) is widely viewed as
the means to concurrently protect environmental quality and improve crop production (Cassman et al., 2002, 2003; Davidson et al., 2015; Foley et al., 2011; Mueller et al., 2017; Robertson and Vitousek, 2009; Zhang et al., 2015).

Agricultural research often focuses on how to modify crop sequences, improve genetics and adjust management practices to increase NUE under a range of conditions. Numerous metrics have been developed to address these questions (see Table 4.1a-b and reviews by Dobermann, 2007; Fixen et al., 2014; Hirel et al., 2011; Ladha et al., 2005) and advance our understanding of how plant physiology, genetics, and management contribute to NUE. However, these metrics often only consider what happens during the growing season and are generally applicable only to crops that receive N fertilizer or manure inputs. Cropping systems typically include sequences of crops that receive fertilizer (e.g. cereals) and crops that do not (e.g. legumes), and many processes that relate to N losses (e.g. mineralization-immobilization, soil water and temperature fluctuations) continue thru fallow periods. Hence, the evaluation of cropping system performance requires approaches that can reflect NUE at the cropping systems scale, irrespective of whether external sources of N are applied or whether crops are growing.

At the cropping system-level, NUE is often evaluated using N budgets (Fig. 4.1). These are accounts of N being added or subtracted from the system (Dobermann, 2007; Meisinger et al., 2008), with different methodologies arising depending on where the system boundaries are drawn (Cherry et al., 2008). In a crop-based N budget, the N balance is calculated by the difference between N inputs to the system and the N removed in crop yield (Oenema et al., 2003). System N inputs often include N fertilizer or manure, atmospheric deposition and legume fixation (Fig. 4.1).
Table 4.1. Review of nitrogen (N) use efficiency metrics traditionally used in agricultural sciences. We classified them according to their scope into: (a) agronomic, (b) regional, and (c) budget-based metrics. Definitions in (a) are based on the review performed by Dobermann (2007), and definitions in (b) are based on the review performed by Hirel et al. (2011). Metrics can also be classified according to type of relationship into: (I) mass or N yield per unit of N input, (II) unit of N output per unit of N input, and (III) mass or N yield per unit of N output.

<table>
<thead>
<tr>
<th>Scope</th>
<th>Type of Relationship</th>
<th>Expressions and formulae</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>I</td>
<td>II</td>
</tr>
<tr>
<td></td>
<td>kg mass or N yield</td>
<td>kg N output kg⁻¹ N input</td>
</tr>
<tr>
<td></td>
<td>kg⁻¹ N input</td>
<td></td>
</tr>
</tbody>
</table>

(a) Agronomic†
Evaluate the crop response to N fertilizer as affected by management. Used mostly with data from short-term plot or field experiments.

Agronomic efficiency (AE)

\[ AE = \frac{\Delta \text{Yield}}{\text{Fertilizer}} \]

Recovery efficiency (RE)

\[ RE = \frac{\Delta \text{Uptake}}{\text{Fertilizer}} \]

Physiologic efficiency (PE)

\[ PE = \frac{\Delta \text{Yield}}{\Delta \text{Uptake}} \]

(b) Regional£
Study physiological, genetic, and management factors that affect crop response to N across environments and evaluate long-term trends. Useful in breeding programs.

Partial factor productivity (PFP)

\[ PFP = \frac{\text{Yield}}{\text{Fertilizer}} \]

Uptake efficiency (UpE)

\[ \text{UpE} = \frac{\text{Uptake}}{\text{Fertilizer}} \]

Utilization efficiency (UtE)

\[ \text{UtE} = \frac{\text{Yield}}{\text{Uptake}} \]

(c) Budget-based‡
Evaluate environmental, management and genetic factors on performance and sustainability of cropping systems. Applied at field, regional and global scales.

Crop N-use efficiency (NUECrop)

\[ \text{NUE}_{\text{Crop}} = \frac{\text{N yield}}{\text{N inputs}} \]

Soil N-use efficiency (NUESoil)

\[ \text{NUE}_{\text{Soil}} = \frac{\text{N outputs}}{\text{N inputs}} \]

System N-use efficiency‡‡

\[ s\text{NUE} = \frac{\text{N yield}}{\text{N outputs}} \]

† \( \Delta \) = change with respect to an unfertilized control

£ Sometimes use aboveground biomass instead of yield, and total plant available N (fertilizer + mineralization) instead of only fertilizer

‡ N inputs include fertilizer or manure, atmospheric deposition, legume fixation; N outputs include N yield and environmental N losses

‡‡ Defined in the present study
Nitrogen-use efficiency in the context of crop-based budgets (NUE\textsubscript{crop}) is then defined by how much N yield is achieved relative to how much N was added to the system (ratio of N yield to N inputs). When N yield is greater than N inputs (i.e. NUE\textsubscript{Crop} > 1), this indicates a cropping system with a net removal of N. If the opposite is true (i.e. NUE\textsubscript{Crop} < 1), then this implies a cropping system with a net surplus of N supply (i.e. either by fixation or applied inputs). The latter is often the case in intensified systems, where N inputs exceed what is removed by N yield over multiple years. Yet, it is unclear whether the surplus N is stored in the soil or lost to the environment (Maaz and Pan, 2017), although it is frequently argued that it is lost over the long-term (Cassman et al., 2002; Robertson et al., 2014; Thorburn and Wilkinson, 2013; Zhang et al., 2015). This crop-based view of NUE works well from an agronomic perspective when maximizing yield and minimizing inputs is prioritized. However, this approach has the potential to mischaracterize environmental impacts given the uncertainties related to the fate of N (Buczko et al., 2010; Cherry et al., 2008; Oenema et al., 2003; Özbek and Leip, 2015).

![Conceptual box diagram of the major N fluxes often used to calculate budgets and efficiency indices. Blue arrows: N inputs; Red arrows: N outputs; Grey arrows: internal crop-soil N cycling. Gaseous losses include ammonia volatilization, and gaseous products of nitrification and denitrification. Hydrological losses include dissolved organic and inorganic N in runoff, drainage, and deep seepage water.](image-url)
In a soil-based N budget, the N balance is calculated by summing N inputs then subtracting all system outputs (Cherry et al., 2008; Sainju, 2017). From this perspective, N outputs include the N removed in crop yield and all other N losses from the system (e.g., leaching of dissolved N to ground or surface waters, gaseous products of nitrification and denitrification, ammonia volatilization, etc.; Fig. 4.1). It is important to note that crop N uptake and mineralization-immobilization from soil organic matter (SOM) and crop residues are considered short-term internal cycling pathways, not long-term inputs or outputs (Norton et al., 2015). Nitrogen-use efficiency in the context of a soil N balance (NUE<sub>soil</sub>) can be then defined by how much N is lost from the system relative to how much was added to the system (ratio of N outputs to N inputs). When N inputs exceed N outputs over the long term (i.e. NUE<sub>Soil</sub> < 1), it can be inferred that the soil is a net sink for N. When the opposite is true (i.e. NUE<sub>Soil</sub> > 1), this indicates that the soil is a net source of N (Cherry et al., 2008). This soil-based view of NUE works well to identify systems where the soil N pool is in decline, threatening the long-term sustainability of soil fertility. However, this interpretation places little emphasis on productivity or N losses, and does not necessarily provide a concise approach to elucidate how tightly N is cycled within systems.

As the goals of improving production, sustaining soil fertility and mitigating environmental pollution converge (Davidson et al., 2015; Tully and Ryals, 2017), cropping system management and design must be evaluated with metrics that can simultaneously capture multiple aspects of system performance (Dietzel et al., 2016; Guilpart et al., 2017; van Ittersum et al., 2013; Karlen et al., 2014). Therefore, developing approaches that concurrently consider NUE from both crop and soil perspectives is needed. In this study, we introduce a new system-level NUE (sNUE), which we define as the ratio of NUE<sub>Crop</sub> to
NUE Soil. This index links both crop- and soil-based approaches into an easily interpretable metric, which succinctly characterizes N cycling and facilitates comparison of systems that differ in biophysical controls on N dynamics (e.g. soil properties, crop sequences, climate, etc.). We demonstrate the integrated application of these metrics by analyzing N cycling of maize (*Zea mays* L.) and soybean (*Glycine max* L. [Merr.]) cropping systems of the Midwestern United States, a hot-spot for N fertilizer use and environmental N losses (David et al., 2010; Sobota et al., 2015). We focused on the following questions: 1) How do crop (NUE Crop), soil (NUE Soil) and system (sNUE) efficiencies differ across crop phases, sequences and weather years? 2) Are there tradeoffs among efficiencies and performance and do these change with N fertilizer input level? 3) How do these NUE indices correlate with each other and with simpler metrics? To answer these questions, we used a well-calibrated model (APSIM; Holzworth et al., 2014; Keating et al., 2003) to simulate long-term, high-resolution, multi-process data on N cycling. The generated data allowed us to dissect the fundamental assumptions of NUE metrics, and discuss their limitations.

**Materials and Methods**

**Sites, weather and experimental datasets**

Experimental data (2008-2016) were collected at two sites in central (Kelley) and northeast (Nashua), Iowa, USA. Both sites are part of the Iowa State University Research and Demonstration Farms network. General information about the sites, soil characteristics, climate and management are provided in Table 4.2, while details can be found in the following studies: Daigh et al. (2014, 2015), Dietzel et al. (2015, 2016, 2017) and Jarchow and Liebman (2012) for Kelley, and Bakhsh et al. (2002), Karlen et al. (1998) and Malone et al. (2007a, 2007b) for Nashua. Meteorological observations (from 1980 to 2016) for both
sites were obtained from the Iowa Environmental Mesonet (2016). Both phases of the maize-soybean rotation were included every year at each site and two types of datasets were used: a) long-term dataset that contained measurements of end-of-season yields and of daily volume water flow and NO$_3$-N concentrations in subsurface drainage tiles (~1.2 m depth; Table 4.2) from March to November for years 2008 to 2016; and b) in-season data for the year 2016 that included soil profile (0-60 cm) water, temperature and NO$_3$-N measurements, and crop biomass, grain dry mass and N uptake. Management records including planting and tillage dates, and fertilization amount and timing were available. These datasets were used for model training and testing.

The APSIM modeling platform

APSIM (Agricultural Production Systems sIMulator) is an open source, daily time-step modeling platform that has been widely used to simulate N cycling processes of cropping systems in the Midwest (Archontoulis et al., 2014; Dietzel et al., 2016; Malone et al., 2007a; Martinez-Feria et al., 2016; Puntel et al., 2016), and elsewhere (Li et al., 2016; Palmer et al., 2017; Probert et al., 1998; Thorburn et al., 2001, 2010). Briefly, the platform includes multiple interconnected process-based models arranged in a modular structure. Input data to the model are daily minimum and maximum temperatures, precipitation and solar radiation. The user also defines a number of parameters to characterize initial conditions, soil characteristics, crop cultivar traits, management and crop sequences. Model outputs include many soil-plant-atmosphere variables, including crop growth processes, soil water, soil temperature, and N and C cycling. For in-depth descriptions of APSIM we refer to Holzworth et al. (2014) and Keating et al. (2003).
Table 4.2. Details on the long-term experimental sites and data.

<table>
<thead>
<tr>
<th>Site</th>
<th>Kelley</th>
<th>Nashua</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>General</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Coordinates</td>
<td>41.92 °N, 93.75 °W</td>
<td>42.93 °N, 92.57 °E</td>
</tr>
<tr>
<td>Experimental design</td>
<td>Spatially balanced complete block (n=4)</td>
<td>Randomized complete block (n=3)</td>
</tr>
<tr>
<td>Plot size (ha)</td>
<td>0.16</td>
<td>0.40</td>
</tr>
<tr>
<td>Soil</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Predominant soil types</td>
<td>Webster silty clay loam (Typic Endoaquoll), Nicollet loam (Aquic Hapludoll)</td>
<td>Kenyon (Typic Hapludoll), Readlyn, (Aquic Hapludoll), Floyd (Aquic Pachic Hapludoll) loams</td>
</tr>
<tr>
<td>SOM (%, 0-30 cm)</td>
<td>5.0</td>
<td>3.5</td>
</tr>
<tr>
<td>Climate (1980-2016)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Average daily temp. (°C)</td>
<td>9.4</td>
<td>8.3</td>
</tr>
<tr>
<td>Annual precipitation (mm)</td>
<td>853</td>
<td>801</td>
</tr>
<tr>
<td>Annual radiation (GJ m⁻²)</td>
<td>5.2</td>
<td>5.0</td>
</tr>
<tr>
<td>Frost-free period (days)</td>
<td>170</td>
<td>161</td>
</tr>
<tr>
<td><strong>Subsurface drainage</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Drain type</td>
<td>Corrugated plastic tubes</td>
<td>Corrugated plastic tubes</td>
</tr>
<tr>
<td>Drain depth (m)</td>
<td>1.1</td>
<td>1.2</td>
</tr>
<tr>
<td>Distance between drains (m)</td>
<td>13.5</td>
<td>28.5</td>
</tr>
<tr>
<td><strong>Management</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Rotation</td>
<td>Maize-soybean</td>
<td>Maize-soybean</td>
</tr>
<tr>
<td>Tillage regime</td>
<td>No-till (since 2008)</td>
<td>Fall chisel plow (~27 cm depth) after maize harvest; spring disking (~15 cm depth) at 1-3 weeks before maize and soybean planting</td>
</tr>
<tr>
<td>Fertilizer management</td>
<td>~168 kg UAN-N ha⁻¹ split application with ~80 kg N ha⁻¹ injected at maize planting, and the balance side-dressed at maize 6th leaf according to a soil nitrate test results</td>
<td>168 kg UAN-N ha⁻¹ injected at maize planting</td>
</tr>
<tr>
<td><strong>Average planting date</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Maize</td>
<td>11-May</td>
<td>28-Apr</td>
</tr>
<tr>
<td>Soybean</td>
<td>11-May</td>
<td>8-May</td>
</tr>
<tr>
<td><strong>Cultivar Maturity</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Maize (relative maturity)</td>
<td>104 – 110</td>
<td>100 – 110</td>
</tr>
<tr>
<td>Soybean (maturity group)</td>
<td>2.3 – 2.5</td>
<td>1.9 – 2.2</td>
</tr>
<tr>
<td><strong>Long-term data (2008-2016)</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Grain yields (Mg dm ha⁻¹)</td>
<td>7.7 – 11.3</td>
<td>8.39 – 11.9</td>
</tr>
<tr>
<td>Maize</td>
<td>2.5 – 3.5</td>
<td>2.93 – 4.02</td>
</tr>
<tr>
<td>Soybean</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tile drainage (March – Nov)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Annual flow (mm)</td>
<td>58 – 537</td>
<td>29 – 269</td>
</tr>
<tr>
<td>Annual NO₃-N load (kg N ha⁻¹)</td>
<td>4.3 – 52.2</td>
<td>4.7 – 62.9</td>
</tr>
<tr>
<td>Annual Flow-weighted average NO₃-N conc. (mg N L⁻¹)</td>
<td>2.8 – 19.4</td>
<td>8.3 – 23.4</td>
</tr>
</tbody>
</table>
APSIM configuration, training and testing

APSIM (version 7.8) was configured to simulate maize-soybean rotations using published information from previous modeling studies at Kelley (Dietzel et al., 2016; Martinez-Feria et al., 2016) and Nashua (Malone et al., 2007a). We used the following modules: *maize*, *soybean*, *surfaceOM* (Probert et al., 1998; Thorburn et al., 2001, 2005), *soilN* (Probert et al., 1998), *SWIM* (Huth et al., 2012) and *manager* (Keating et al., 2003). After configuration, the model was run for a 10-year ‘spin-up’ initialization period to provide initial values for surface and belowground residue mass, soil water and inorganic N content in the soil profile, and soil organic C pool partitioning. All simulations were run in sequential mode, that is, continuous simulation throughout the study period to account for the carryover effects of the previous growing season crop residues, and fluctuations in soil C, N, and moisture. This approach better represents reality as opposed to seasonal re-initialization of soil variables (Basso et al., 2015). Model training largely focused on achieving a satisfactory fit to the long-term measurements of crop yields, annual water volume flows, NO$_3$-N loads and flow-weighted concentrations in subsurface drainage (i.e. annual NO$_3$-N loads normalized by drainage flow), while simulating reasonable annual estimates for denitrification and net mineralization. In-season measurements of crop growth and soil temperature, moisture and NO$_3$-N concentrations were used to test that temporal dynamics (e.g. crop uptake or changes in soil inorganic N pools) were adequately represented.

Soil and management configuration

Soil profile information is provided in Table S4.1. To simulate soil water dynamics, we selected SWIM3 given that this module allows for the simulation of fluctuating shallow groundwater tables and subsurface tile drainage (Huth et al., 2012; Malone et al., 2007). Ground water table depth was initially set at 1.4 m and was allowed to fluctuate dynamically.
throughout the simulation. To initialize surface and belowground (root) residue mass, soil water and inorganic N content in the profile, and SOC pool partitioning, we ran the model for a 10-year ‘spin-up’ initialization period (1998-2007) under a maize-soybean rotation. This time period allowed for the stabilization of the microbial SOC pool (Fbiom; Table S4.2) and avoid confounding effects of microbial SOC buildup or decline on N cycling and dynamics (Dietzel et al., 2016; Puntel et al., 2016).

Management information for the experimental period (2008-2016), including planting and tillage operations, as well as fertilizer application timing, rate, and source, was configured in APSIM to match available records (see Table 4.2). In the long-term modeling scenarios (1982-2016), planting dates were held constant for all years, using the experimental average planting dates for maize and soybean at each site (see Table 4.2). Rye plantings were simulated on 15 Oct, while termination was 10 days before main crop planting. Tillage operations for Nashua were simulated on 15 Nov for chisel plow after maize (no chisel plow tillage in maize-soybean with rye) and 10 days before planting for spring disking.

**Calibration of crop cultivar parameters**

Cultivar-specific parameters for the crops used in the experiments were derived from a previous calibration at the Kelly site (Dietzel et al., 2016), with the changes described below. In maize, we lowered the critical N concentration in grains (n_conc_crit_grain) from 1.5% to 1.2% given evidence that N concentration in grains has been decreasing in new-era hybrids (Ciampitti and Vyn, 2012), and also based on our in-season measurements. This change has been seen to improve simulation of NO₃-N leaching (Martinez-Feria et al., 2016). Maximum and minimum N concentrations in grains were also lowered as well from 2.0% to 1.75% and from 1.0 to 0.75%, respectively. To reflect the shorter relative maturity of the hybrids used at Nashua (see Table 4.2), we reduced thermal time from flowering to
physiological maturity (tt_flower_to_maturity) from 770 to 750 °C-d and increased the grain growth rate (grain_gth_rate) from 8.17 to 9.17 mg g⁻¹ day⁻¹.

The differences in maturity group and yield potential of soybean at Nashua was reflected by reducing the thermal time from start to end of grain filling (y_tt_start_grain_fill) by 4%, and changing the node senescence rate (node_sen_rate) from 60 to 95 °C-d node⁻¹. To improve simulation of N dynamics, we reduced the critical N concentration of different plant tissues at physiological maturity, following the calibrated values reported in a simulation study in a nearby site (Puntel et al., 2016). Additionally, the grain N critical concentration (n_conc_crit_grain) was reduced from 6.5 to 5.8% to better match the in-season measurements. This reduced simulated values for soybean N uptake, the percent of aboveground N uptake derived from fixation, and the C:N of residues at harvest, but all of these were well within the ranges reported in the literature (Salvagiotti et al., 2008). Finally, to simulate rye cover crop in the model scenarios, we used the APSIM-wheat module using the crop cultivar parameters reported in a previous study at the Kelley site (Martinez-Feria et al., 2016).

**Calibration of nitrogen cycling processes**

Daily atmospheric N deposition was simulated with the implementation of a manager module script that estimated N deposition by multiplying daily precipitation (mm) by a factor of 0.01 (Holland et al., 2005). On average N deposition added ~8 kg N ha⁻¹ yr⁻¹, which is well within the range for this region (Zhang et al., 2012). The initial APSIM soil and management configuration satisfactorily simulated crop yields and water drainage flow through subsurface tiles. However, it significantly under estimated tile NO₃-N loads and average annual flow-weighted concentrations. To improve the simulation of soil N dynamics we made two changes to the soil N module. First, similar to a previous study at the Kelly site
(Dietzel et al., 2016), we decreased the soil temperature above which temperature does not limit N mineralization (opt_temp) from 32 to 30°C, which increased the annual net N mineralization and the amount of inorganic N in soils available for leaching. Secondly, the soil layer structures here defined were up to 2.4 m (Table S4.1) to allow for water table fluctuation (Singh et al., 2006). This triggered exceptional high denitrification rates from the deep soil layers (1.5 to 2.4 m depth). The problem was caused by the formulation of active carbon in the denitrification equation in the soilN module (Thorburn et al., 2010):

\[
\text{Active carbon} = 24.5 + 0.0031 \cdot (\text{hum}_c + \text{fom}_c)
\]

where hum_c and fom_c are the amount of C in humic and fresh organic matter pools in each layer (in mg C kg⁻¹ soil), respectively. Because this equation has an intercept this means that denitrification continues even when actively cycling soil organic C is zero (e.g. in the deep soil layers) if the other three factors of the denitrification equation (NO₃, soil water and temperature) are at sufficient levels to trigger denitrification. Given the simulation of shallow water tables, which meant seasonally and or permanently saturated (oxygen-deficient) conditions below 1 m depth, this resulted in unrealistically large estimates for denitrification. To address this problem, we introduced a denitrification depth threshold parameter (depth_inhibit) in the soilN module to cease denitrification below a certain depth. Furthermore, we incorporated a factor (dul_fac_dnit) that determines the start of the denitrification as a function of soil water. By default, denitrification is triggered at field capacity in APSIM, while recent studies have shown that N₂O emissions (one component of denitrification) are more accurately predicted when the denitrification routine starts at moisture levels above field capacity (Mielenz et al., 2016).
Model calibration indicated that both additions were valuable and together improved the simulation of NO3-N loads and average annual flow-weighted concentrations across nine years of data (see calibrated model simulations in Fig. S4.1). The calibrated parameters were depth_inhibit = 1.0 m (i.e. no denitrification below 1 m depth) and dul_fac_dnit = 1.1 (i.e. denitrification is triggered at 10% above field capacity) at both sites. Similar approaches have been taken to improve simulation of NO3-N leaching in other studies. For instance, in modeling studies at a nearby site using the Root-Zone Water Quality Model (RZWQM), better fit to NO3-N losses data was achieved by increasing the rate coefficient of soil N mineralization and decreasing the rate coefficient of soil denitrification (Fang et al., 2012; Malone et al., 2014; Thorp et al., 2007).

Model performance

Model training was deemed complete when satisfactory balance between measured and simulated data was achieved for the following variables: end of season yields, annual water volume flows, NO3-N loads and flow-weighted concentrations in subsurface drainage (i.e. annual NO3-N loads normalized by drainage flow), and 2016 seasonal crop growth variables and soil temperature, moisture and NO3-N concentrations. Three statistical tests were used to judge model performance: i) mean bias error (MBE), ii) root mean-square error (RMSE) and iii) relative mean-square error (RRMSE). The equations for these indices can be viewed in Archontoulis and Miguez (2015). The RMSE and RRMSE reflect simulation error, and are indicators of model precision (i.e. prediction ability). The MBE is a measure of model accuracy (i.e. to assess the systematic bias of the prediction). For these statistical indices, the closer the value to 0, the better.

Overall, the calibrated APSIM model satisfactorily reproduced long term yields, subsurface drainage, and N leaching dynamics (Fig. S4.1a-d and Table S4.2) as well as in-
season crop growth, and soil water, temperature, and NO$_3$ data (Fig. S4.2a-b and Table S4.3). Grain yields across both CS and SC at both sites were simulated with a RRMSE < 15% (Fig. S4.1a and Table S4.2). Across the eight years, two sites and four cropping systems, the model simulated subsurface drainage water flow with an MBE of 17 mm yr$^{-1}$ (9.7%), and NO$_3$-N loads by 0.3 kg N ha$^{-1}$ yr$^{-1}$ (0.8%). Most importantly, the APSIM model captured the up and downward trends observed in flow-weighted NO$_3$-N concentrations (Fig. S4.1b), although it was slightly under-predicted across both sites (-1.8 mg N L$^{-1}$; Table S4.2). The model simulated most crop growth and biomass accumulation during the 2016 season with a RRMSE < 20% (Fig. S4.2a and Table S4.2). APSIM also captured the general patterns of soil water fluctuations (peaks and valleys) and temperature dynamics at both sites, and statistics showed good agreement with measured data (Fig. S4.2b and Table S4.3). Finally, the model captured in-season soil NO$_3$-N temporal dynamics, but with less accuracy compared to other data (Fig. S4.2b and Table S4.3).

**Modeling scenarios**

The calibrated model was used to simulate the following N dynamics: atmospheric deposition, mineralization, immobilization, crop uptake, soybean fixation, fertilizer applications, leaching, denitrification and N content in harvested grains. APSIM does not simulate fertilizer ammonia volatilization losses (Probert et al., 1998), but these were assumed to be negligible given that liquid fertilizer was injected at planting (Christianson et al., 2012; Table 4.2), and therefore were not included in the N budget. Three long-term crop sequences were simulated for 35 sequential years of historical weather records (1982-2016): i) continuous maize (CC), ii) maize-soybean rotation (CS), and iii) maize-soybean with rye (Secale cereale L.) cover crop grown between main crops (CRSR). Each of these rotations was simulated across a gradient of N fertilizer rates applied at maize planting: 0, 40, 80, 120,
168, 200, 240, 280 and 320 kg N ha\(^{-1}\). The 168 kg N ha\(^{-1}\) is the recommended ‘standard’ rate for maize in CS in this region (Sawyer et al., 2006). No fertilizer N was applied to soybean. The combination of three crop sequences, nine fertilization rates and 35 years resulted in 945 individual simulation-years.

**Analysis of simulated data**

All processing and analysis of simulated data was conducted using the R statistical software (version 3.2.2; R Core Team, 2016). Simulated values were averaged across both sites, and aggregated at daily, annual and long-term (35 years) temporal scales.

**Nitrogen budgets**

Data from the modeling scenarios were used to calculate N budget components (in kg N ha\(^{-1}\) yr\(^{-1}\)). Nitrogen budget inputs included N fertilizer, deposition, and soybean N fixation. Nitrogen budget outputs included the gaseous products of denitrification, NO\(_3\)-N leaching to surface drainage and groundwater (defined as leaching below 2.0 m depth), and grain N removal during mechanical harvest. To explain seasonal patterns and trends, we used additional simulated variables such as net mineralization, crop uptake and dry matter yield.

**System nitrogen-use efficiency**

To analyze and compare data from the modeling scenarios, we evaluated cropping system efficiency using crop and soil-based balances and NUE indices. The crop N balance was calculated as:

\[
\text{N Balance}_{\text{Crop}} = (N_{\text{Fertilizer}} + N_{\text{Depositon}} + N_{\text{Fixation}}) - N_{\text{Yield}}
\]

therefore,

\[
\text{NUE}_{\text{Crop}} = \frac{N_{\text{Yield}}}{N_{\text{Fertilizer}} + N_{\text{Depositon}} + N_{\text{Fixation}}}
\]
Values for $\text{NUE}_\text{Crop}$ range from 0 to $\infty$, and characterize cropping systems with net removal ($\text{NUE}_\text{Crop} > 1$) or net surplus ($\text{NUE}_\text{Crop} < 1$) of N. The soil N balance was calculated as:

$$\text{N Balance}_{\text{Soil}} = (N_{\text{Fertilizer}} + N_{\text{Depositon}} + N_{\text{Fixation}}) - (N_{\text{Yield}} + N_{\text{Loss}})$$

therefore,

$$\text{NUE}_{\text{Soil}} = \frac{N_{\text{Yield}} + N_{\text{Loss}}}{N_{\text{Fertilizer}} + N_{\text{Depositon}} + N_{\text{Fixation}}}$$

Values for $\text{NUE}_{\text{Soil}}$ range from 0 to $\infty$, and indicate whether the soil is a net sink ($\text{NUE}_{\text{Soil}} < 1$) or net source ($\text{NUE}_{\text{Soil}} > 1$) of N. When $\text{NUE}_{\text{Soil}}$ approaches unity, then the soil pool can be thought as in equilibrium. System N-use efficiency ($\text{sNUE}$) was defined as the ratio of $\text{NUE}_\text{Crop}$ to $\text{NUE}_{\text{Soil}}$.

$$\text{sNUE} = \frac{\text{NUE}_\text{Crop}}{\text{NUE}_{\text{Soil}}} = \frac{N_{\text{Yield}}}{N_{\text{Yield}} + N_{\text{Loss}}} = \frac{1}{1 + \frac{N_{\text{Loss}}}{N_{\text{Yield}}}}$$

$s\text{NUE}$ ranges from 0 to 1, and higher values indicate a system with tighter N cycling. Simplifying the equation shows that $\text{sNUE}$ can also be more specifically interpreted as the fraction of system N outputs that are captured as N yield rather than lost to the environment. $\text{sNUE}$ is inversely related to yield-scaled N losses (here shown as the ratio of N losses to N yield), a metric commonly used in sustainable intensification assessments (e.g. Linquist et al., 2012; Zhao et al., 2016; Zhou and Butterbach-Bahl, 2014).

Under this framework, the ideal is a cropping system with net neutral N supply-removal (i.e. $\text{NUE}_\text{Crop} \sim 1$) and a soil N pool in equilibrium (i.e. $\text{NUE}_{\text{Soil}} \sim 1$), thus a tight N cycling (i.e. $\text{sNUE} \sim 1$). These indices are expressed as dimensionless ratios (kg N kg$^{-1}$ N). A summary of the interpretation of these budget-based NUE indices is shown in Table 4.3.
Table 4.4. Interpretation of the budget-based NUE indices as defined in the present study.

<table>
<thead>
<tr>
<th>Condition</th>
<th>Interpretation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$NUE_{Crop} &gt; 1$</td>
<td>Cropping system with net removal of N (i.e. removal greater than input)</td>
</tr>
<tr>
<td>$NUE_{Crop} &lt; 1$</td>
<td>Cropping system with net surplus of N (i.e. removal less than input)</td>
</tr>
<tr>
<td>$NUE_{Crop} = 1$</td>
<td>Cropping system with net neutral N (i.e. removal equals input)</td>
</tr>
<tr>
<td>$NUE_{Soil} &gt; 1$</td>
<td>Soil pool is a net source of N (i.e. soil N declining)</td>
</tr>
<tr>
<td>$NUE_{Soil} &lt; 1$</td>
<td>Soil pool is a net sink of N (i.e. soil N increasing)</td>
</tr>
<tr>
<td>$NUE_{Soil} = 1$</td>
<td>Soil N pool is in equilibrium</td>
</tr>
<tr>
<td>$sNUE \rightarrow 1$</td>
<td>System tightly cycles N (i.e. greater recycling)</td>
</tr>
<tr>
<td>$sNUE \rightarrow 0$</td>
<td>System releases N to the environment (i.e. greater leaking)</td>
</tr>
</tbody>
</table>

**Response to weather and fertilizer inputs**

To assess the year-to-year variation of the budget-based NUE indices in response to weather for each of the cropping systems studied, we: 1) calculated the coefficient of variation (CV; standard deviation divided by the mean), and 2) regressed the annual values of the indices against cumulative annual precipitation.

To characterize efficiency tradeoffs as influenced by N fertilizer inputs, we computed the long-term 35-year cumulative for all the N budget variables of each cropping system at the simulated level of N fertilizer rate applied to maize. Then these responses were interpolated across the N fertilizer continuum by using the spline smoothing function in R, and these data were used to calculate NUE indices. Likewise, grain dry matter yields for each cropping system were also integrated as a 35-year cumulative, interpolated, and then expressed as relative to maximum yield. To characterize tradeoffs between efficiency and productivity, we computed the product of relative yield and sNUE:

$$f(x) = \text{Relative yield} \times sNUE$$
In this tradeoff function, sNUE acts as a ‘weighting factor’ that proportionally decreases system performance with increasing N losses relative to total system N outputs.

**Comparison among metrics**

The budget-based indices (Table 4.1c) were compared with each other and with the following NUE metrics (see definitions in Table 4.1a-b): agronomic efficiency (AE), recovery efficiency (RE), physiological efficiency (PE), partial factor productivity (PFP), uptake efficiency (UpE) and utilization efficiency (UtE). To facilitate comparison, NUE metrics were standardized by subtracting the mean and dividing by the standard deviation. Then, correlation matrices across all indices and crop yields were computed using the standardized values at each combination of site, year, crop phase and N fertilizer level.

**Results**

How do crop (NUE\textsubscript{Crop}), soil (NUE\textsubscript{Soil}) and system (sNUE) efficiencies differ across crop phases, sequences and weather years?

Nitrogen budgets and associated NUE indices varied considerably among crop phases, cropping systems (Fig. 4.2 and Table 4.4) and weather years (Fig. 4.3). Averaged across both sites and 35 weather years at the standard N fertilizer rate applied to maize (168 kg\(N\) ha\(^{-1}\); Sawyer et al., 2006), N inputs to the CC cropping system were 176 kg N ha\(^{-1}\) yr\(^{-1}\) (Table 4.4), with 96% originating from fertilizer and only 4% from deposition. In the CS and CRSR systems, N inputs were very similar and averaged 170 kg ha\(^{-1}\) yr\(^{-1}\), with 50% originating from fertilizer (note that fertilizer was applied in maize phase only), 4% from atmospheric deposition and 46% from legume fixation. In all rotations, N removed in grains was the main output. Across systems, maize grains removed on average 118 kg N ha\(^{-1}\) yr\(^{-1}\) (NUE\textsubscript{Crop} = 0.67; net N surplus) while soybean grains removed 174 kg N ha\(^{-1}\) yr\(^{-1}\) (NUE\textsubscript{Crop} =
1.08; net N removal). On average, the CS and CRSR systems removed about 87% of N inputs, resulting in an average crop-based N balance of 21 kg N ha yr\(^{-1}\) (Table 4.4).

Compared to N in grains, annual environmental N losses (leaching + denitrification) were a smaller part of the N budget (ranging from 32 to 64 kg N ha\(^{-1}\) yr\(^{-1}\); Table 4.4), although distinct patterns across crop sequences were evident. Mean annual N losses were 40% higher in CC and 21% lower in CRSR compared to CS (Table 4.4). Of these losses, about 63% occurred in CS and CRSR fallow periods and 49% in CC fallow periods (Fig. 4.2). Furthermore, N losses were substantial in the (unfertilized) soybean phase: 53% in the CS and 44% in the CRSR. Across years, average maize and soybean grain yields, crop N uptake and N yield changed very little among crop sequences.

![Figure 4.2. Long-term average daily N fluxes for three crop sequences receiving 168 kg fertilizer N ha\(^{-1}\) at maize planting. Shaded area under the curve represents average simulated value across sites and 35 weather years (1982-2016). Average annual values for the budget-based NUE indices (units: kg N kg\(^{-1}\) N) are included above each pane, represented by the horizontal bars and their respective adjacent values.](image-url)
Table 4.4. Nitrogen balances and efficiency indices calculated with simulated data for continuous maize, maize-soybean and maize-soybean with rye cover crop cropping systems averaged across 35 years (1982-2016) and two sites (Kelley and Nashua). N balances are presented for each maize and soybean crop phases, and in the case of the two-year systems, also for the rotation (i.e. the average of the two crop phases).

<table>
<thead>
<tr>
<th></th>
<th>N Inputs</th>
<th>N output</th>
<th>Efficiency indices</th>
</tr>
</thead>
</table>
|                | Fertilizer | Fixation | Deposition | Yield | Losses | N balance | NUE
|                | kg N ha⁻¹ yr⁻¹ | kg N ha⁻¹ yr⁻¹ | kg N ha⁻¹ yr⁻¹ | kg N ha⁻¹ yr⁻¹ | kg N ha⁻¹ yr⁻¹ | kg N ha⁻¹ yr⁻¹ |
| **Cont. Maize**|           |          |            |        |        |           | NUEₘₙₑₜ
| Maize          | 168       | 0        | 7.5        | 116    | 64     | 60 -5     | 0.66 1.03 0.64 |
| Soybean        |           |          |            |        |        |           | NUEₘₙₑₜ NUEₙₑₜ sNUE
| **Maize-Soybean**|          |          |            |        |        |           | NUEₘₙₑₜ NUEₙₑₜ sNUE
| Maize          | 168       | 0        | 7.5        | 119    | 43     | 57 14     | 0.68 0.92 0.74 |
| Soybean        | 0         | 150      | 7.5        | 173    | 49     | -15 -64   | 1.09 1.41 0.78 |
| Rotation       | 84        | 75       | 7.5        | 146    | 46     | 21 -25    | 0.87 1.15 0.76 |
| **Maize-Soybean + Rye** |          |          |            |        |        |           | NUEₘₙₑₜ NUEₙₑₜ sNUE
| Maize          | 168       | 0        | 7.5        | 120    | 41     | 56 15     | 0.68 0.92 0.75 |
| Soybean        | 0         | 156      | 7.5        | 175    | 32     | -12 -44   | 1.07 1.27 0.85 |
| Rotation       | 84        | 78       | 7.5        | 147    | 37     | 22 -15    | 0.87 1.09 0.80 |

Despite rye mitigation of N losses (Fig. 4.2 and Table 4.4), the crop N balance was equal across CS and CRSR (NUEₘₙₑₜ = 0.87). In contrast, inclusion of a rye cover crop enhanced the soil’s sink capacity, increasing the soil N balance by 10 kg ha⁻¹ yr⁻¹ with respect to CS (NUEₙₑₜ decreased from 1.15 to 1.09; Table 4.4). This ultimately was reflected as tighter N cycling in CRSR (sNUE = 0.80) than CS (sNUE = 0.76). In the three systems, the soil was a net source of N (NUEₙₑₜ > 1) except that CC was very close to equilibrium (Table 4.4).

At the standard N fertilizer rate and across crop sequences, annual values of NUEₙₑₜ were a little less variable (CV = 27%) than NUEₘₙₑₜ (CV = 29%), while sNUE exhibited a relatively more stable behavior (CV = 15%). The annual variability of NUEₘₙₑₜ and NUEₙₑₜ was higher for the CS (CV = 28% and 29%, respectively) and CRSR (CV = 28% and 25%,
respectively) that for CC (CV = 16% and 22%, respectively). On the other hand, variation of sNUE was higher for CC (CV = 17%) than CS (CV = 13%) and CRSR (CV = 12%). A portion of this variation in NUE\textsubscript{Crop} and NUE\textsubscript{Soil} seemed to be explained by crop phase and its response to weather (Fig. 4.3). In maize, highly significant (p < 0.01) positive relationships were found between cumulative annual precipitation and annual values of NUE\textsubscript{Crop} and NUE\textsubscript{Soil} for all three systems, whereas the relationships (p < 0.001) were negative for sNUE (Fig. 4.3). The latter were a reflection of the higher N losses with increased precipitation relative to maize yield gains. In soybean, no significant relationships of cumulative annual precipitation to NUE\textsubscript{Crop} and NUE\textsubscript{Soil} were found (p > 0.1, Fig. 4.3). This was mainly related to the fact that, although soybean N fixation was suppressed in wet years due to increased N mineralization, higher N yields ultimately compensated N balances, rendering them relatively insensitive to variation in weather. Soybean sNUE was negatively related to precipitation in CS and CRSR, although these relationships were marginal (0.05 < p < 0.1; Fig. 4.3).

Integrating CS and CRSR across a two-year rotation cycle showed that NUE\textsubscript{Crop} and NUE\textsubscript{Soil} were positively related to precipitation (p < 0.05), but not significantly related to sNUE (p > 0.1; Fig. 4.3).

**Are there tradeoffs among efficiencies and performance and do these change with N fertilizer input level?**

Simulated long-term maize yields across all crop sequences responded positively to N fertilizer application, with average yields ranging from 3.9 with no N fertilizer applied up to 9.7 Mg dm\textsuperscript{-1} with 320 kg N ha\textsuperscript{-1}. Soybean yields (average of 3.2 Mg dm\textsuperscript{-1}) did not change across residual levels of the N fertilizer applied to maize. As expected, higher NUE\textsubscript{Crop} (greater response to N inputs) was always achieved at lower levels of N fertilizer, but importantly, the shapes of the response curves generally differed among crop sequences.
For instance, at low N rates, higher NUE\textsubscript{Crop} was achieved in CC compared to CS and CRSR. The reverse was true at higher N rates. The reason for this was a lack of response of soybean to N fertilizer applied to maize, from both N yield and the amount of N fixed (although fixation did decrease slightly at high fertilizer rates). This rendered more gradual response curves in CS and CRSR (Fig. 4.4a).

Figure 4.3 Year-to-year variation of NUE\textsubscript{Crop}, NUE\textsubscript{Soil} and sNUE (see interpretations on Table 3) for three crop sequences receiving 168 kg fertilizer N ha\textsuperscript{-1} at maize planting, as affected by annual cumulative precipitation. Points represent the annual NUE index value for each maize (yellow circles) and soybean (green squares) crop phases. For the two-year systems (i.e. maize-soybean and maize-soybean with rye cover crop), the points for rotation (gray diamonds) are also included, in which case they represent the aggregate of two consecutive crop phases (i.e. maize + soybean). Linear regressions were fitted independently to each set of data, and report the estimate of the slope (s), test of significance (ns = non-significant; * = p < 0.1, ** = p < 0.05; *** = p <0.01), and coefficient of determination (r\textsuperscript{2}).
Figure 4.4. Response of (a) NUE$_{Crop}$, (b) NUE$_{Soil}$, and (c) sNUE to N fertilizer inputs to maize for three crop sequences. Lines represent index values calculated from simulated data of the cumulative (35 years) N fluxes, averaged across two sites. See Table 3 for interpretation of the indices.
Although cropping systems shifted from net removal to net surplus with increasing N fertilizer (Fig. 4.4a), the soil remained a net source of N (Fig. 4.4b) even at very high N input levels. This was related to the fact that environmental N losses also increased with fertilizer inputs (ranging from 5 to 121 kg N ha$^{-1}$ yr$^{-1}$) but the increased losses were proportionally greater than yield gains, and this was captured by sNUE (Fig. 4.4c). At levels where additional N fertilizer did not further increase maize yields, the N oversupply was lost from the soil over the long-term.

The tradeoffs between N cycling and production performance of each of the cropping systems studied across a continuum of N fertilizer input level was characterized by the product of relative yield and sNUE (Fig. 4.5). In all systems, overall performance increased as N fertilizer applied increased and maize yield became less N limited. At the same time, increases in N inputs led to more environmental losses, resulting in a decrease in sNUE (see Fig. 4.4c). The peak of the tradeoff function, where high yields and tight N cycling was achieved, was 69 kg N ha$^{-1}$ in CS (96% relative yield), 75 kg N ha$^{-1}$ in CRSR (96% relative yield) and 117 kg N ha$^{-1}$ CC (93% relative yield). These levels were about 65% of those where additional N fertilizer did not further increase yield (Fig. 4.5).

**How do these NUE indices correlate with each other and with simpler metrics?**

Nitrogen-use efficiency metrics (Table 4.1) were compared by inspecting whether they vary together over time. An example is presented in Fig. 4.6a for the continuous maize system receiving 168 kg fertilizer N ha$^{-1}$ yr$^{-1}$, where standardized values of the metrics (i.e. by subtracting the mean and dividing by the standard deviation) were compared. As shown in this example, NUE is characterized differently depending on the metric used, but most seemed to vary more or less consistently with each other. This was evident because most metrics were correlated to crop yields: lower yields generally resulted in lower efficiency,
while efficiency was high with higher yields (Fig. 4.6a-b). Notably, sNUE seemed to vary more independently from other metrics, and from crop yields, as indicated by poor correlations (Fig. 4.6b). sNUE was only moderately negatively correlated to NUE\textsubscript{Soil} in the maize phase, and poorly correlated to every other metric. On the other hand, NUE\textsubscript{Crop} and NUE\textsubscript{Soil} were better correlated to each other. NUE\textsubscript{Crop} was almost perfectly correlated to PFP and UpE (>0.9) in maize. This is because the variables in the numerator of these indices (i.e. dry matter yield, uptake, and N yield) are highly correlated (not shown). Correlation was much lower to the agronomic indices (Table 4.1a), although RE was moderately correlated to NUE\textsubscript{Crop} and NUE\textsubscript{Soil}. It should be noted that indices with fertilizer in the denominator (i.e. AE, RE, PFP and UpE) could not be calculated for soybean because it received no fertilizer, which highlights a major weakness of these indices.

**Discussion**

Measurable improvements in crop N-use efficiency (NUE\textsubscript{Crop}) have been documented in some regions (Conant et al., 2013; Lassaletta et al., 2014; Zhang et al., 2015). In the case of the Midwestern United States, NUE\textsubscript{Crop} has increased from 57% in the mid 1970s to close to 70% in 2010 (Zhang et al., 2015). Rising efficiency is often attributed to increasing yields under stable levels of N inputs, mainly through advancements in crop genetics and management (Sinclair and Rufty, 2012). For instance, evidence suggests that breeding in maize has led to an increased capacity to produce more grain mass per unit of N taken up, which has led to lower N concentrations in grain (Ciampitti and Vyn, 2012; Duvick and Cassman, 1999). Modern maize hybrids have an average UtE of 47.6 kg dm kg\textsuperscript{-1} N taken up (Ciampitti and Vyn, 2012), which is similar to the average value simulated in this study (49.7 kg dm kg\textsuperscript{-1} N taken up).
Figure 4.5. Visualization of the tradeoff between production and N cycling performance across a fertilizer N input continuum in three crop sequences. The solid line represents the production performance, which is characterized by relative yield \( f(x) = \text{Relative yield} \). The dash line indicates the tradeoff function, which is the product of relative yield and sNUE \( f(x) = \text{Relative yield} \times \text{sNUE} \). Both of these functions are expressed as dimensionless ratios (ranging from 0 to 1). Shaded area between the two curves represents the sNUE gap, which here is evaluated at the rate where additional fertilizer does not further increase crop yield (as indicated by the double arrows).
Figure 4.6. Comparison of sNUE with traditional NUE metrics. (a) shows as an example the simulated continuous maize system receiving 168 kg fertilizer N ha\(^{-1}\) yr\(^{-1}\) (averaged across two sites), and how all the metrics vary across time (see Table 1 for definitions). Metrics were standardized by subtracting the mean and dividing by the standard deviation. Colors and symbols are coded according to their scope (agronomic, regional, budget-based) and type or relationship (I, II, and III) as outlined on Table 1. Annual variation in maize yields (top pane) are included for reference. (b) presents the correlations among the standardized value of all these metrics and crop yields, calculated with simulated data that includes years, locations and N fertilizer input levels, for each maize (yellow) and soybean (green) crop phase. The correlation between two metrics is shown in the intersecting squares (e.g. between NUE\(_{\text{Crop}}\) and NUE\(_{\text{Soil}}\) for maize is 0.72), which is represented graphically by the size of the circle and its color (direct correlations are shown in black, and inverse correlations are shown in white). For the soybean phase, “n/a” indicates that the index could not be calculated because no N fertilizer was applied.

Despite these improvements, environmental impacts on water and atmospheric quality remain high (David et al., 2010; Davidson and Kanter, 2014; Hatfield et al., 2009; Linquist et al., 2012). Some have argued that this might be related to legacies from a history of N fertilizer use (Van Meter et al., 2016; Sebilo et al., 2013), but this interpretation is inconsistent with the dramatic reductions in N losses following conversion from annual to perennial systems or by inclusions of N-scavenging cover crops (Castellano and David,
2014; Tully and Ryals, 2017). Other research has pointed to the low recovery efficiency of applied fertilizer in crop biomass (RE), which is often less than 40% (Cassman et al., 2002; Gardner and Drinkwater, 2009; Ladha et al., 2016), suggesting that increasing crop N uptake response to applied N should be targeted as the primary mechanism for mitigating N losses (Cassman et al., 2002; Hirel et al., 2011; Ladha et al., 2005; Sinclair and Rufty, 2012). Although this may be generally true for systems in which the state variables are relatively stable, this view neglects complex feedbacks of residual fertilizer N on other system processes, such as the amount of legume fixation N (Salvagiotti et al., 2008) or soil N turnover in microbial, root and residue pools (Dietzel et al., 2017; Gardner and Drinkwater, 2009). These processes can render residual N available to subsequent crops in the rotation or vulnerable to losses (Maaz and Pan, 2017; Sebilo et al., 2013).

Our analysis of Midwestern maize-soybean systems clearly showed that these dynamics have meaningful impacts on cropping system efficiency and environmental performance. In this context, traditional NUE metrics (Table 4.1a-b), while helpful for comparing crop performance across management treatments or cultivars (Hirel et al., 2011; Ladha et al., 2005), do not offer a straightforward way to evaluate the contributions of soil N cycling processes to system NUE. In contrast, accounting for major fluxes and balances at the system level is a powerful approach that provides the means for evaluation within and across systems (Dobermann, 2007). Below we synthesized our results to show how linking crop- and soil-based N budget approaches with the new sNUE reveals insights into system N cycling dynamics, and the tradeoffs with production performance. We also addressed the limitations posed by lack of data and uncertainty, and proposed potential solutions.
N losses are related to poor N retention as much as to inefficient use of N inputs

Crop-based N balances characterized the maize-soybean system (CS) to be highly efficient from the crop perspective (NUE_{Crop} = 0.87), which led to relatively low crop N balances (21 kg N ha\(^{-1}\) yr\(^{-1}\); Table 4.4). It is generally assumed that this surplus of N is lost to the environment over the long-term, thus it is widely accepted to be a good proxy for environmental N losses (Cassman et al., 2002; Oenema, 2015; Thorburn and Wilkinson, 2013; Zhang et al., 2015). However, here the magnitude of simulated N losses in CS (46 kg N ha\(^{-1}\) yr\(^{-1}\)) was ~2.2 times greater than what was predicted by the crop N balance (Table 4.4). The hydrological N losses exceeded the United States federal threshold for NO\(_3\) concentration in drinking water (10 mg N L\(^{-1}\); USEPA) in 74% of the simulated crop-years. These losses aggregated across the ~36 million hectares of maize and soybean in the Midwest are the leading contributors to hypoxia in the Gulf of Mexico (David et al., 2010).

To adequately reflect environmental losses, crop-based N balances assume that the soil N pool is in equilibrium, i.e. that the soil is neither a net sink nor net source of N (Oenema et al., 2003). Although useful for regional scale assessments (Thorburn and Wilkinson, 2013), this assumption has the potential to over- or underestimate the magnitude of environmental N losses if this condition is not met (Cherry et al., 2008; Oenema et al., 2003, 2005; Özbek and Leip, 2015). Evidence suggests that this may be the case for the rainfed maize-soybean systems of the Midwest. Indeed, a recent meta-analysis found no relationship between NO\(_3\)-N loads in subsurface drainage and the crop-based N balance across 31 studies (Zhao et al., 2016), which is consistent with negative soil N balances shown in regional N budgets (Christianson et al., 2012) and long-term N fertilizer rate trials in Iowa (Jaynes et al., 2001; Poffenbarger et al., 2017; Puntel et al., 2016). In this study, the soil-based N balance indicated that the soil N pool in CS was declining by 25 kg N ha\(^{-1}\) yr\(^{-1}\).
(NUE_{Soil} = 1.15) both due to N removed in grains and high environmental losses. Considering that soils in this region contain about 17 Mg ha\(^{-1}\) of total N in the top 1.0 m (Van Meter et al., 2016), such a decline in the soil N pool represents a turnover rate of only 0.15 % y\(^{-1}\) (mean residence time = 680 yr). Yet, this small turnover rate is sufficient to render a crop N balance inadequate for estimating the amount of N losses. Linking both crop- and soil-based approaches indicated that only 45% of the N losses (i.e. the ratio of the crop-N balance to actual N losses; Table 4.4) can be attributed to the inefficient use of N inputs in the maize-soybean system. The rest originates from the release of native soil N into the environment due to the asynchrony between soil mineralization and crop uptake (Fig. 4.2).

The crop-based approach also cannot capture improvements associated with increasing soil N retention (Buczko et al., 2010; Cherry et al., 2008; Oenema et al., 2003, 2005). This was evident in our rye cover crop example where the NUE\(_{Crop}\) did not increase, regardless of the reductions in environmental N losses (Table 4.4 and Fig. 4.2 and 3.4a). Consistent with literature, here the rye cover crop did not affect the long-term productivity of the maize-soybean system but decreased N losses (Basche et al., 2016; Malone et al., 2017; Marcillo and Miguez, 2017; Martinez-Feria et al., 2016; Tonitto et al., 2006) by enhancing the soil’s capacity to act as a net sink of N with the addition of C inputs. Similarly, a recent field study found that N\(_2\)O-N losses from maize were strongly related to the crop N balance, but the use of denitrification inhibitors had no effect on this metric, despite a significant reduction in N\(_2\)O-N losses (Omonode et al., 2017). Therefore, researchers should be aware that efforts that rely solely on crop N balances are at risk of drawing inaccurate conclusions about environmental impacts. Field-level NUE\(_{Crop}\) should be used to capture crop response to
N inputs, and interpretations on N losses can only be made after the soil N retention is characterized.

**The need for a system-level approach to NUE**

Efforts to increase sNUE should focus on designing cropping systems that function well from both crop and soil perspectives. In the context of the intensified cropping systems of the Midwest, increasing the crop response to N inputs (increasing NUE\textsubscript{Crop}) has the potential to mitigate the environmental losses by diminishing surpluses of applied N fertilizer. At the same time, making the soil a stronger sink for N (decreasing NUE\textsubscript{Soil}) will promote tighter cycling and the long-term sustainability of soil fertility. The latter is fostered by practices that recouple C and N cycling (Gardner and Drinkwater, 2009) such as improved residue management (Poffenbarger et al., 2017; Thorburn et al., 2005), cover crops (Chatterjee et al., 2016; Tully and Ryals, 2017), manure applications (Ross et al., 2008; Zhou et al., 2016), reduced tillage (Lafond et al., 2011), addition of legume forages to rotations (Iannetta et al., 2016; Korsaeth and Eltun, 2000; Ross et al., 2008) or agroforestry (Tully and Ryals, 2017).

sNUE also provides the means to compare systems that differ in biophysical controls on N dynamics, accounting for potential tradeoffs between efficiency in crop N use and soil N retention. For instance, in our example more N is retained in CC than CS. This is related in part to the greater amounts of N that are cycled back into the soil through crop residues in continuous maize, and in part because immobilization during maize residue decomposition acts as a temporary N sink during fallow periods (Poffenbarger et al., 2017). Greater immobilization, however, also renders the system reliant on more N fertilizer inputs to produce same amount of N yield in CC, which results in lower NUE\textsubscript{Crop} (Fig. 4.4a) and thus lower sNUE (Fig. 4.4c). On the other hand, including a rye cover crop in the maize-soybean
rotation (CRSR) does not change NUE\textsubscript{Crop} and improves NUE\textsubscript{Soil}, increasing sNUE (Fig. 4.4). In addition, sNUE is more stable (lower variation) than either NUE\textsubscript{Crop} and NUE\textsubscript{Soil}, and it is less correlated to these and other metrics (Fig. 4.6b). This suggests that sNUE produces more stable estimates of system efficiency across weather years (Fig. 4.3), and that provides distinct information from other known metrics (Fig. 4.6).

sNUE also has practical applications for characterizing tradeoffs between N cycling and production performance, and thus has the potential to aid in the design of systems that better balance production and environmental outcomes. In our example, we showed how performance tradeoffs changed in response to N fertilizer inputs (Fig. 4.5). The product of relative yield and sNUE was highest at about 60-65% of the N fertilizer level needed to maximize yield (i.e. agronomic optimum N rate), but this resulted on an average yield penalty of 5-7%. This means that to achieve maximum yield in these systems we sacrificed environmental performance (represented by the size of the sNUE gap in Fig. 4.5). This tradeoff between productivity and regulating functions of annualized cropping systems is well documented in literature (e.g. Davis et al., 2012; Robertson et al., 2014; Ross et al., 2008). This approach, however, does not necessarily provide a basis for optimal N fertilizer recommendations, given that other dimensions of system performance (e.g. economic return, risk) must be also taken into consideration. Nevertheless, the approach should be useful if applied in the context of efficiency frontiers (Keating et al., 2010) when tracking improvements and exploring management scenarios. The goal would be then to close the sNUE gap at N input levels where other aspects of system performance are optimized (e.g. agronomic optimum N rate). Such was achieved in our example with the use of a rye cover crop (e.g. see reduction of the sNUE gap with CRSR compared to CS in Fig. 4.5).
The proposed approach may be limited by lack of data and uncertainty

Accounting for all major system N fluxes (Fig. 4.1) offers a detailed understanding of the fate of N, which can provide insights on system processes that can be exploited to tighten N cycling and reduce losses. However, budgets and related efficiencies can be relatively variable from year-to-year, which in part is related to variation in weather (Fig. 4.3). Therefore, robust evaluations need multiple years of data, which are not always available (Buczko et al., 2010). Additionally, the difficulty of measuring or estimating N losses makes such data seldom available, limiting the application of the approach. For this reason, we compared budget-based indices to traditional NUE metrics by computing correlations (Fig. 4.6b). High correlation does not imply that two metrics are equivalent, given that each metric has a distinct conceptual basis and interpretation. Rather, correlation indicates whether two metrics are directionally related. For example, the high correlation of PFP and UpE with NUE_{Crop} in maize suggests that increases in PFP and UpE almost always resulted in increases in NUE_{Crop}. This means that these simpler metrics could be used as proxies when data is limited, although these are only applicable to crops that received N fertilizer.

Modeling approaches have often been used to fill gaps in data availability (Basso et al., 2016; Dietzel et al., 2016; Malone et al., 2007a; Martinez-Feria et al., 2016; Qi et al., 2012; Wang et al., 2015), though they require additional data to drive simulations and test predictions. Here, model fit was tested using data on long-term yields and NO₃-N loads in subsurface tile drains, and in-season crop biomass and uptake, soil moisture, temperature and NO₃ concentrations, with overall good agreement between measured and simulated data. Data for additional N cycling processes, such as mineralization-immobilization, legume fixation, denitrification, and NO₃-N leaching into groundwater were not available, and so we also used literature comparisons and expert judgment to guide model calibration. Yet, even
small changes in some of the major N fluxes could alter conclusions about N balances, thus these could be considered to have a high degree of uncertainty (Wallach and Thorburn, 2014). Nonetheless, a recent simulation study of maize-soybean rotations in Iowa showed that APSIM simulated the long-term change in SOM with the same amount of error before and after calibration (Puntel et al., 2016). This was attributed to the fact that the cumulative C input (i.e. residue) is the most important determinant to changes in SOM (Poffenbarger et al., 2017), so annual over- and under-prediction of C and N fluxes are compensated over time so-long the long-term crop removal and residue inputs are well characterized.

An alternative approach to overcome lack of data for N losses can be circumvented by experimentally characterizing the long-term change in SOM and therefore soil N pool ($\Delta N_{\text{Soil}}$; Sainju, 2013, 2017). In this case, N losses could be estimated as the ‘unaccounted’ N:

$$N_{\text{Loss}} = N_{\text{Input}} - N_{\text{Yield}} - \Delta N_{\text{Soil}}$$

In theory, this approach provides an avenue for constructing complete N budgets and calculating sNUE when N losses are not known. However, detecting management-driven changes in soil pools is difficult, even when using long-term data. This is because of the intrinsic variability of soil measurements (Cambardella et al., 1994; Kravchenko and Robertson, 2011), especially in SOM-rich soils such as those in the Midwest (Brown et al., 2014; Osterholz et al., 2016). Moreover, hard-to-measure pathways of N inputs, such as legume fixation, dry ammonia deposition, dissolved N in lateral water flow and erosion sediment deposition, can introduce uncertainty in calculations (Oenema et al., 2003; Sainju, 2017). Legume fixation is especially critical given that can be a large contributor to N budgets (Iannetta et al., 2016; Korsaeth and Eltun, 2000; Ross et al., 2008; Table 4.4).
Measuring legume fixation is time-consuming and expensive, and estimates vary widely with growing conditions (Liu et al., 2011; Salvagiotti et al., 2008). While some empirical approaches can assist in this task (e.g. Korsaeth and Eltun, 2000), they are often too general to be implemented for site-specific situations (Liu et al., 2011). Better estimates will likely come from wider application of robust process-based models and their improvement (Liu et al., 2011).

Researchers whose aim is to characterize environmental impacts of cropping system N use should consider using sNUE, even if data for all major environmental N losses are not available. In this case, a partial sNUE could still be computed using data for some N losses (Fig. 4.7), which can be either derived from field measurements or estimated using empirical relationships developed for specific locations and management. While a partial sNUE will almost always overestimate the true sNUE, it would still be useful for comparing relative differences between management options or tracking progress made towards environmental stewardship. The above highlights the need for research investment toward better characterizing the sensitivity of specific budget components on N balances, as well as on improving our ability to estimate hard-to-measure fluxes across a number of environments.

**Conclusion**

The choice of metrics used in a study greatly affects the conclusions about NUE and performance of a cropping system or crop. Here we connect and compare various metrics to better understand how to increase cropping system NUE and mitigate environmental losses across a range of environments, crop sequences, and management scenarios. We showed that higher efficiency and lower losses can be achieved by increasing the crop yield response to N inputs, improving soil N retention, or most likely by optimizing both. Linking both crop- and
soil-based N budget efficiency metrics into one system-level index provides a framework to quantify, interpret and communicate the efficiency associated with increasing crop productivity (NUE<sub>Crop</sub>), maintaining soil fertility (NUE<sub>Soil</sub>) and improving cycling (sNUE), which can facilitate the characterization of performance tradeoffs. Progress toward meeting the goals of productivity, sustainability and environmental quality can be achieved by using integrative, long-term views that deepen our understanding of complex processes of N cycling. Therefore, research should adopt more comprehensive frameworks that capture multiple dimensions of agroecosystem function and performance.

Figure 4.7. Example of system N-use efficiency (sNUE) calculated with simulated data for three crop sequences, using two sets of data for N losses: i) leaching and denitrification, and ii) only leaching. While a partial sNUE will almost always over-estimate sNUE, it is still useful for comparing relative differences among cropping systems and management options.
References


Supplemental Information

Supplemental Table S4.1 Soil profile parameters used in APSIM simulations. BD, bulk density; AirDry, air-dried soil water content, LL, lower limit; DUL, drained upper limit; SAT, saturated volumetric water content; OC, soil organic carbon; Finert, fraction of inert of soil organic C (not decomposing); Fbiom, fraction of microbial soil organic (fast decomposing).

<table>
<thead>
<tr>
<th>Depth (cm)</th>
<th>BD (g/cm³)</th>
<th>AirDry (mm mm⁻¹)</th>
<th>LL (mm mm⁻¹)</th>
<th>DUL (mm mm⁻¹)</th>
<th>SAT (%)</th>
<th>OC (0-1)</th>
<th>Fbiom (0-1)</th>
<th>Finert</th>
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<td></td>
<td></td>
<td></td>
<td></td>
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</tr>
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<td>0.120</td>
<td>0.140</td>
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<td>0.435</td>
<td>3.02</td>
<td>0.080</td>
<td>0.319</td>
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<td>0.110</td>
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<td>0.386</td>
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<td>0.110</td>
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<td>0.446</td>
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<td>0.452</td>
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<td>0.125</td>
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<td>0.132</td>
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<td>0.138</td>
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<td>0.144</td>
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<td>0.010</td>
<td>0.990</td>
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<tr>
<td><strong>Nashua</strong></td>
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<td></td>
<td></td>
<td></td>
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<td></td>
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<td>0.102</td>
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<td>0.144</td>
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<td>0.10</td>
<td>0.027</td>
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</table>
### Supplemental Table S4.2 Overview of APSIM model fit to long-term (2008-2016) end-of-season experimental data

<table>
<thead>
<tr>
<th>Variable</th>
<th>Kelley MBE</th>
<th>Kelley RMSE</th>
<th>Kelley RRMSE</th>
<th>Nashua MBE</th>
<th>Nashua RMSE</th>
<th>Nashua RRMSE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maize yield (kg ha(^{-1}))</td>
<td>780</td>
<td>1160</td>
<td>11.9%</td>
<td>-280</td>
<td>770</td>
<td>7.20%</td>
</tr>
<tr>
<td>Soybean yield (kg ha(^{-1}))</td>
<td>180</td>
<td>390</td>
<td>13.1%</td>
<td>-20</td>
<td>290</td>
<td>8.40%</td>
</tr>
<tr>
<td>Subsurface tile drainage (mm)</td>
<td>22.9</td>
<td>94.4</td>
<td>41.1%</td>
<td>11.3</td>
<td>70.9</td>
<td>58.2%</td>
</tr>
<tr>
<td>NO(_3)-N load (kg N ha(^{-1}))</td>
<td>1.7</td>
<td>15.4</td>
<td>84.6%</td>
<td>-1.2</td>
<td>10.1</td>
<td>59.2%</td>
</tr>
<tr>
<td>Flow weighted NO(_3)-N conc.(mg L(^{-1}))</td>
<td>-0.4</td>
<td>4.5</td>
<td>53.7%</td>
<td>-3</td>
<td>4</td>
<td>29.2%</td>
</tr>
</tbody>
</table>

MBE = Mean bias error; RMSE = root mean-squared error; RRMSE = relative root mean squared error.

### Supplemental Table S4.3 Overview of APSIM model fit to the 2016 in-season field data

<table>
<thead>
<tr>
<th>Variable</th>
<th>Crop</th>
<th>Kelley MBE</th>
<th>Kelley RMSE</th>
<th>Kelley RRMSE</th>
<th>Nashua MBE</th>
<th>Nashua RMSE</th>
<th>Nashua RRMSE</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Biomass (kg ha(^{-1}))</strong></td>
<td>Maize</td>
<td>424.3</td>
<td>987.9</td>
<td>7.5%</td>
<td>557.3</td>
<td>1155.3</td>
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</tr>
<tr>
<td></td>
<td>Soybean</td>
<td>-302.3</td>
<td>1271.4</td>
<td>25.2%</td>
<td>893.1</td>
<td>1208.1</td>
<td>23.1%</td>
</tr>
<tr>
<td><strong>Uptake (kg N ha(^{-1}))</strong></td>
<td>Maize</td>
<td>-2.2</td>
<td>3.8</td>
<td>18.4%</td>
<td>1</td>
<td>2.5</td>
<td>16.5%</td>
</tr>
<tr>
<td></td>
<td>Soybean</td>
<td>1.5</td>
<td>2</td>
<td>16.2%</td>
<td>-0.9</td>
<td>1.5</td>
<td>10.2%</td>
</tr>
<tr>
<td><strong>Grain mass (kg ha(^{-1}))</strong></td>
<td>Maize</td>
<td>-419.4</td>
<td>445.1</td>
<td>4.6%</td>
<td>-225</td>
<td>477</td>
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<td></td>
<td>Soybean</td>
<td>204.8</td>
<td>246.9</td>
<td>7.7%</td>
<td>-149.1</td>
<td>628.8</td>
<td>15.6%</td>
</tr>
<tr>
<td><strong>Soil NO(_3)-N(kg N ha(^{-1}))</strong></td>
<td>Maize</td>
<td>31.7</td>
<td>31.8</td>
<td>102%</td>
<td>16.7</td>
<td>34.3</td>
<td>100.7%</td>
</tr>
<tr>
<td></td>
<td>Soybean</td>
<td>-7.3</td>
<td>17.4</td>
<td>62.6%</td>
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<td>8.6</td>
<td>39.3%</td>
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<tr>
<td><strong>Soil temperature (°C)</strong></td>
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<td>1.3</td>
<td>6.6%</td>
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<td>1</td>
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<td>-1.9</td>
<td>1.2</td>
<td>6.3%</td>
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<tr>
<td><strong>Soil water (mm)</strong></td>
<td>Maize</td>
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<td>11.9</td>
<td>8.6%</td>
<td>6.3</td>
<td>12</td>
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<td>11.2%</td>
<td>11.5</td>
<td>11.5</td>
<td>6.9%</td>
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MBE = Mean bias error; RMSE = root mean-squared error; RRMSE = relative root mean squared error.
Supplemental Figure S4.1 APSIM model fit to (a) the long-term experimental crop yields, (b) flow-weighted NO$_3$-N concentrations in drainage tiles, (c) cumulative subsurface tile drainage and (d) NO$_3$-N loads in tiles for maize-soybean (CS) and soybean-maize (SC) systems at Kelley and Nashua sites. Blue bars and points represent measured data, with associated error bars or shaded area showing standard deviation in the measurements. Pink points and solid lines show model predictions; MBE = mean bias error; RRMSE = relative root mean-square error.
Supplemental Figure S4.2 APSIM model fit to the 2016 in-season experimental data on (a) crop growth variables and (b) soil variables for maize-soybean (CS) and soybean-maize (SC) systems at the Kelley and Nashua sites. Blue points represent measured data, with associated error bars or shaded area showing standard deviation in the measurements. Pink solid lines show model predictions; RRMSE = relative root mean-square error.
CHAPTER 5.  MULTI-PRACTICE MANAGEMENT STRATEGIES FOR REDUCING DRAINAGE NITRATE LOSS FROM MIDWESTERN CROPLAND

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Modified from a manuscript prepared for submission to a scientific journal

Abstract

Developing and implementing effective and scalable strategies to mitigate agricultural nitrate (NO$_3$)-nitrogen (N) losses to surface waters is crucial for the long-term sustainability of the Midwestern United States. Evaluation of the effectiveness of crop management practices has so far relied on experimental approaches, the outcomes of which are highly variable in time and space. We used a cropping systems model (APSIM) to simulate management-by-environment scenarios (n > 2.9 million) and their effect on crop yield, drainage NO$_3$ loads and flow-weighted concentrations, and residual soil NO$_3$ at harvest in maize and soybean cropping systems across a soil-climate gradient. Analysis of the simulated scenarios sought to: 1) quantify sensitivity of NO$_3$ losses to various practices and environmental factors, 2) understand their link to local soil-climate characteristics, and 3) rank the effectiveness of simultaneously implementing multiple management practices. We found a dominant role of carryover soil N and weather-year for determining annual NO$_3$ loads, and of management for curbing the amount of residual soil NO$_3$ after harvest. The analysis also shows that soil-climate influences on NO$_3$ loss responses to weather-year, soil state, and management can broadly dictate whether practices optimizing N supply or soil N retention should be the focus of strategies. Adopting well-designed multi-practice packages can improve yield-scaled NO$_3$ reduction effectiveness compared to a baseline of current
practices (up to 70 and 33% reduction in maize and soybean respectively), but found small synergistic advantages among the individual practices. These results can guide future research and implementation to tailor strategies to specific sets of environmental conditions, farmers’ objectives, and policy goals.

**Introduction**

The loss of nitrate (NO$_3$) from maize (*Zea mays* L.) and soybean (*Glicyne max* L [Merr.]) cropland into surface waters is one of the most widespread environmental impacts of agriculture in the United States Midwest. It is a major causal factor for the development of seasonal marine hypoxia in the Gulf of Mexico (David *et al* 2010), and NO$_3$ pollution of drinking water supplies poses risks to human health (Robertson and Vitousek 2009).

Historically, losses of NO$_3$ have been attributed to the overuse or mismanagement of fertilizer nitrogen (N), leading to a focus on improving fertilizer N-use efficiency (NUE) (Cassman *et al* 2002, Zhang *et al* 2015). However, in the maize-soybean systems of the Midwest, the release of native soil N contributes to losses as much or more than the inefficient use of N inputs (Bowles *et al* 2018, Martinez-Feria *et al* 2018). Without a strong sink (e.g. plant growth) available to retain N during the extensive fallow periods (October to May), NO$_3$ from fertilizer or mineralization sources builds up in soils and is flushed into subsurface drainage systems during heavy rains (Randall and Mulla 2001, Iqbal *et al* 2017). Given the rainfed, weather-driven nature of crop production and the ubiquity of subsurface drainage networks in the region (Blann *et al* 2009) (Fig. 5.1), the development and implementation of effective and scalable management strategies has remained elusive.

Practices aimed at reducing NO$_3$ losses can be grouped into two categories. The first includes those aimed to optimize the supply of N inputs to crops, such as i) adjusting N
fertilizer application rates to the maximum return to N rate (MRTN) (Sawyer et al 2006), ii) applying fertilizer at planting in the spring or during the growing season rather than the previous fall (Randall and Sawyer 2008, Eagle et al 2017), enhanced-efficiency fertilizers (Li et al 2018, Eagle et al 2017) or iv) selecting genotypes that more efficiently utilize N taken up (Cassman et al 2002, Gardner and Drinkwater 2009). The second category includes practices that improve the retention of actively cycling soil N such as i) crop rotation (Randall et al 1997, Zhao et al 2016), ii) cover crops (Tonitto et al 2006), and in some cases iii) crop residue management and no-tillage (Zhao et al 2016). Outcomes from implementing these practices often are highly variable across time and space (Zhou and Butterbach-Bahl 2014, Christianson and Harmel 2015a, 2015b) and little is known about how soil-climate characteristics render localities more or less responsive to specific sets of practices and environmental factors.

Figure 5.1. Geographic location of the long-term experimental sites used for modeling. These sites fall within a gradient of soil and climatic characteristics, as shown in the insert plots (top). Choropleth shading indicates county-level estimates for the share of cropland under subsurface drainage tiles (Data source: USDA-NASS, 2012 Census of Agriculture). PAWC = soil plant-available water holding capacity (mm; 0-1 m depth). SOC = soil organic carbon content (%; 0-1 m depth).
Implementing multiple practices simultaneously could improve overall NO\textsubscript{3} reduction effectiveness compared to single-practice implementation (Christianson \textit{et al} 2017). However, the effectiveness of multi-practice packages for reducing NO\textsubscript{3} losses is largely unknown, and potential synergistic advantages among practices remain unexplored. Importantly, because implementation protocols remain based on voluntary farmer adoption, the mitigation effectiveness of practices should be evaluated within the context of potential crop productivity tradeoffs, so as not to undercut the incentives for adoption (Zhou and Butterbach-Bahl 2014, Zhao \textit{et al} 2016, van Groenigen \textit{et al} 2010, Zhao \textit{et al} 2017).

An inherent limitation to studying the effectiveness of combined practices is that field studies are often constrained by time and resources, such that only a few experimental factors can be examined simultaneously. Statistical techniques for analysis of literature studies (e.g. meta-analysis) generally lack sufficient power or are unsuited to detect interactive treatment effects given the often large variation among studies and unbalanced nature of these types of data (Philibert \textit{et al} 2012). On the other hand, process-based simulation models explicitly account for the underlying mechanisms that drive N losses and crop yields, so that the contributions to the response from a range of interactive factors (e.g. weather, soil characteristics, carry-over effects and management) can be assessed to provide insights to better understand the behavior of the system (Jones \textit{et al} 2017, Holzworth \textit{et al} 2014). This can ultimately aid in the design of more resilient cropping systems. To this end, simulation models are routinely used to evaluate interactive effects of management, environment and genetics on crop yields (Puntel \textit{et al} 2016, Grassini \textit{et al} 2009, Teixeira \textit{et al} 2014b, Casadebaig \textit{et al} 2016), but they have been less used to investigate NO\textsubscript{3} loss mitigation strategies.
Here we used a cropping system model to simulate simultaneous implementation of management practices and their effect on crop yield, NO₃ losses, and residual soil NO₃ at harvest in maize and soybean cropping systems across different soils and weather-years. Analysis of the simulated management-by-environment scenarios (n > 2.9 million) sought to: 1) quantify sensitivity of NO₃ losses to various practices and environmental factors, 2) understand their link to local soil-climate characteristics, and 3) identify combinations of management practices that most effectively reduce NO₃ loss and residual soil NO₃, while minimizing tradeoffs with crop yields. This study aims to highlight which practices and combinations thereof merit more research.

**Methods**

**Soil and weather data**

We obtained soil and weather data from seven long-term experimental field sites located across the Midwest. These data were used to drive, configure, and test the simulation model. The KELLEY and NASHUA sites have been described in detail in previous studies (Martinez-Feria *et al* 2018, Dietzel *et al* 2016), while the remaining sites (DPAC, HICKS.B, GLIMORE, SERF and STJOHNS) were extracted from the Sustainable Corn CAP Research Database (Abendroth *et al* 2017). The sites fall within gradients of soil and climate characteristics, including: soil organic carbon (SOC; range 1.0-2.7 % averaged over 1 m depth), soil plant-available water holding capacity (PAWC; range 70-132 mm integrated to 1 m depth), mean annual precipitation (range 711-1050 mm) and mean annual temperature (range 7.6-10.6 °C; Fig. 5.1). Soil information for each site was obtained from the SSURGO database (Soil Survey Staff n.d.). In general, soils in these sites are deep, fertile, and artificially drained using subsurface drain tubes (Table 4.1). Daily weather (1987-2016) for
all sites was retrieved from the Daymet dataset (Thornton et al 2018) using the single pixel extraction tool (downscaled to 1 km×1 km resolution). Further details about the sites are included in the supplemental information (Table S5.1).

**Simulation modeling**

We used the Agricultural Production Systems sIMulator (APSIM; version 7.8) to conduct simulation experiments. APSIM is an open source cropping systems platform that is conformed of interconnected, crop, hydrological, and N cycling process-based models. Using daily weather and user-defined soil and management information, the model calculates many soil-plant-atmosphere variables, including crop growth processes, soil water, soil temperature, and N and C cycling. For in-depth descriptions of APSIM see references (Holzworth et al 2014, Keating et al 2003).

Prior to performing simulation experiments, we configured APSIM using the obtained soil, weather and management information to replicate the long-term experiments at the sites (Fig. 5.1). We compared these simulations against crop yield and NO₃ losses measured at the sites to assess of the robustness of the model outputs. Experimental treatments at the sites encompassed one or more crop rotation sequences of maize, soybean, wheat and rye cover crop. Management records (planting date and rate, tillage type and timing, and N fertilizer amount and timing), cultivar relative maturity, and drainage system characteristics (depth and spacing) were available (Table S5.1). Measured data included end-of-season maize and soybean yields, daily water flow in subsurface drainage tiles and NO₃ concentrations in drainage, spanning at least five weather years (Table S5.1). The latter two were used to calculate cumulative annual NO₃ loads (kg N ha⁻¹) and flow-weighted NO₃ concentrations in subsurface drainage (mg N L⁻¹). These observations were used to test the robustness of the model predictions.
As a first step, we used the management, soil information and weather data available for each crop rotation treatment at the seven experimental sites (Table S5.1) to configure APSIM (version 7.8) to replicate the experimental data. All simulations were set up using the following modules: maize, soybean, and wheat (to simulate rye cover crop), SWIM (soil hydrology; Huth et al 2012), soilN (soil C and N cycling), surfaceom (residue model; Probert et al 1998; Thorburn et al 2005, 2001) and manager (Keating et al 2003).

**Maize, Soybean and Wheat**

The maize and soybean cultivars used at the experimental sites were represented in the model with generic APISM cultivars. For maize these corresponded to the “A” cultivars (Archontoulis et al 2014b), while for soybean these corresponded to the “MG” cultivars (Archontoulis et al 2014a). These have been previously calibrated to broadly characterize locally adapted commercial genotypes in the region. We selected maturity groups appropriate for each site based on the management records available. Changes made to the crop cultivar parameters included lowering the critical N concentration in grains (n_conc_crit_grain) from 1.5 to 1.2% in maize and 6.5 to 6% in soybean. This follows experimental evidence of declining grain N concentrations in new-era maize hybrids (Ciampitti and Vyn 2012) and soybean cultivar (Tamagno et al 2017). These changes have been seen to improve simulation of soil NO₃ (Puntel et al 2016) and NO₃ leaching (Martinez-Feria et al 2016a). The wheat module was used to simulate rye cover crop at the KELLEY and GILMORE sites, employing the calibrated wheat version developed by Dietzel et al (2016) and improved by Martinez-Feria et al (2016).

**SWIM, SoilN and surfaceom**

Soil hydrological and organic matter parameters were derived from the SSURGO database (Soil Survey Staff n.d.) This was done by conducting database queries using the
fields’ geospatial coordinates with the FedData (Bocinsky et al 2018) package in R (R Core Team 2017). Then, we extracted the tabular data of the major components for each of the map units present at the field sites. Given that the soil layer structure for SSURGO components differ across map units, we standardized the soil layers (breaks = 0, 5, 10, 15, 20, 30, 45, 60, 80, 100, 130, 160, 200, 240, and 280 cm) across all sites using linear interpolation. To represent the whole field site, data were aggregated across all map units, using the average weighted with the percent of area occupied by each map unit. Data extracted included estimates for APSIM parameters such as drainage upper limit (DUL, mm mm\(^{-1}\)), drainage lower limit (LL15, mm mm\(^{-1}\)), saturation point (SAT, mm mm\(^{-1}\)) and saturated hydraulic conductivity (Ksat, mm mm\(^{-1}\)), bulk density (BD g cm\(^{-3}\)), and soil organic carbon (SOC; %). The crop lower limit (CLL, mm mm\(^{-1}\)) for maize, soybean, and wheat was assumed equal to LL15, while the soil/root water extraction coefficient (KL, d\(^{-1}\)) was set to 0.08 in the top soil and decreased exponentially to values of 0.03 at 180 cm soil depth (Hammer et al 2009). The root penetration parameter (XF, 0–1) was set to 1 for all sites. Subsurface drainage was set up according to site specifications (Table S5.1), with lateral saturated soil water conductivity (klat) at 2800 mm d\(^{-1}\) (Dietzel et al 2016). We induced the “water table” option in SWIM to represent water table fluctuation (Singh et al 2006), initialized at the depth of the subsurface drains. The R code used to download, process and write soil files with the APSIM format has been made available through the APssurgo repository (Martinez-Feria and Archontoulis 2018)

Daily atmospheric N deposition was simulated with the implementation of a manager module script that estimates N deposition by multiplying daily precipitation (mm) by a factor of 0.01 (Holland et al 2005). This approach adds on average ~8 kg N ha\(^{-1}\) yr\(^{-1}\) to soils in this
region, which is well within measured ranges (Zhang et al 2012). To mitigate exceptionally high denitrification in the deep soil layers (> 1m) we used the change to the soilN module which has been described in detail in Martinez-Feria et al (2018). We used depth_inhibit = 1.0 m (i.e. no denitrification below 1 m depth) and dul_fac_dni = 1.1 (i.e. denitrification is triggered at 10% above field capacity) at all sites.

To remove the confounding effects of buildup or decline in soil organic carbon humic (Hum) or microbial pools (Biom), we ran the model for a “spin-up” period (Dietzel et al 2016, Puntel et al 2016), during which a maize-soybean rotation with fertilizer applied at the MRTN (Table S5.1) was continuously simulated for 15 years at each site. Initial values for soil NO$_3$ and moisture, and above and below-ground residue amount and C:N were also derived from this step. To avoid introducing bias from a given set of conditions experienced during the last year of the spin-up, we used the average value of these variables at harvesting for the last five simulated years for each crop. The values derived from this step, which were used as the initial conditions in model test runs and scenario experiments are shown on Figure S5.1.

**Model performance**

Having configured APSIM, the goal of this next step was to use the observed crop yields, drainage NO$_3$ loads and flow-weighted NO$_3$ concentrations to test the robustness of the predictions. Model fit was evaluated visually by means of plotting the observed vs. simulated values, and statistically by computing root mean squared error (RMSE), relative root mean squared error (RRMSE) and the mean bias error (MBE). The RMSE and RRMSE are measures of model error and the smaller the value the better. The MBE is a measure of model accuracy, and the closer the value to zero the better. The equations for these indices can be viewed in Archontoulis and Miguez (2013).
Considering that configuration and calibration of the simulations were largely based on limited (i.e. publicly available) data and literature values, the APSIM model was able to satisfactorily reproduce the measured crop yields and subsurface drainage NO$_3$ losses (Fig. S5.2). Grain yields across all sites and crop rotation treatments were simulated with a RMSE of 1.27 and 0.38 Mg ha$^{-1}$ yr$^{-1}$, for maize and soybean respectively. This represented a RRMSE of around 13% in both crops. Across all sites and cropping systems, the model simulated subsurface drainage NO$_3$ loads with a MBE of -3 kg N ha$^{-1}$ yr$^{-1}$, although the model slightly under predicted NO$_3$ loads in the GILMORE and STJOHNS sites. The observed flow-weighted NO$_3$ concentrations were similarly under-predicted across those two sites, which seems to indicate this may be due to an underestimation of drainage water flow. At the rest of the sites, drainage NO$_3$ loads and concentrations were simulated with good precision; except for drainage NO$_3$ concentrations at HICKS.B, where the model over-predicted the measured data (Fig. S5.2).

**Simulation experiments**

The simulation experiments were designed to quantify the impact of various environmental and management factors on four variables: end-of-season crop yields (Mg dm ha$^{-1}$), cumulative annual (harvest-to-harvest) NO$_3$ loads (kg N ha$^{-1}$) and flow-weighted concentration in subsurface drains (mg N L$^{-1}$), and residual soil NO$_3$ at crop harvest (kg N ha$^{-1}$; 0-1.3 m). These model outputs represent productivity and N cycling variables relevant to water quality impact assessments. The factorial combinations (Fig. 5.2) aimed to characterize the influence of soil state variables (previous crop, carryover N from previous crop and water table depth), crop management (planting date and cultivar), soil management (cover crop and residue removal), and N fertilizer management (rate and timing). Note that previous crop and N management factors were simulated for maize only, given that soybean in this region is
grown after maize and receives no N fertilizer. With the exception of previous crop in maize, each simulation factor had three levels. The crop, soil and N management factors were designed to represent levels of practice implementation. The combination of 2 crops, 26 total factor levels, 7 sites, and 30 years, resulted in more than 2.9 million scenarios (Fig. 5.2).

Figure 5.2. Diagram of the factors investigated in the simulation experiments at the seven experimental sites and 30-weather years (1987-2016). Average levels for soil state variables were derived from the average of the last 5 years under previous crop during the spin-up initialization (see suppl. Information S1). Early planting time was determined based on when 10-day moving average of soil temperatures at the surface was > 10°C. In maize, the Nitrogen-use efficient (NUE) cultivar trait means 10% lower critical grain N concentration, while radiation-use efficient (RUE) trait means 10% greater RUE than the normal cultivar. In soybean MG indicates maturity group, as adapted to local conditions. For cover crops, winter kill meant termination on 1-Jan, whereas overwinter meant termination 7 days before main crop planting. Residue removal was simulated 5 days after harvesting of previous crop. MRTN rate is based on university recommendations for the Corn Belt (Sawyer et al., 2006). Numbers within parenthesis indicates the implementation level of the management factors: poor (0), medium (1), and advanced (3). Asterisk (*) indicate the levels used to define the baseline scenario for the yield-scale effectiveness assessment.
Every model run corresponded to an instance of a full factorial design, so that all possible scenarios were simulated. Each scenario was ran with 30 weather years (1987-2016). To decouple the effect of weather-year from soil state variables, the initial conditions (i.e. soil moisture and N levels) were reset every year on 20-Oct, which were derived from values from spin-up initializations (see supplemental information). Simulation started 20-Oct and ended on 19-Oct of the next year.

**Analysis of simulated data**

To rank the importance of the simulated factors on the model outputs, we employed a variance-based sensitivity analysis approach (Santer *et al* 2003). This technique measures the sensitivity of model outputs to each input factor and interactions by approximating the proportion of factor or interaction sums of squares in relation to the total sums of squares. For full-factorial designs, factor variances are decomposed into orthogonal variance terms for main effects, two-way interactions, and so on, which are added to calculate the total variance. This is analogous to the classic analysis of variance (ANOVA) decomposition (Iooss and Lemaître 2015, Teixeira *et al* 2014a). We computed first-order (i.e. main effect) and second-order (i.e. two-way interactions) sensitivity indices and attributed the residual variance to higher order interactions. A total sensitivity index was then calculated as the sum of all sensitivity indices involving the given factor. These sensitivity indices were computed for all simulation factors (Fig. 5.2), within each combination of crop and site. Changes in total sensitivity of model outputs to simulation factors across gradients in soil-climate characteristics were explored by computing correlations and performing simple regression analyses ($\alpha = 0.05$) with those variables that were strongly correlated and overall sensitive in APSIM model outputs.
To assess the potential of implementing multiple management practices on their combined NO$_3$ reduction effectiveness and crop yields, we calculated a new response variable using the following expression:

\[
y = \left( \frac{\text{NO}_3 \text{ Load} + \text{Residual Soil NO}_3}{\text{Yield}} \right)
\]

where \( y \) (expressed as kg N Mg$^{-1}$) is the sum of annual NO$_3$ loads in subsurface drains and the residual NO$_3$ leftover in the soil at harvest (0-1.3 m depth), scaled by the end-of season crop yields. We defined a baseline scenario \((y_B)\) to reflect current practice implementation levels across the region. For maize, this corresponded to a normal cultivar, with average planting timing, no residue removal, no cover crop, and N fertilizer at the university recommended rate (i.e. MRTN) (Sawyer et al. 2006) applied at planting. The baseline for soybean corresponded to medium maturity cultivar, with average planting timing, no cover crop and no residue removal (see Fig. 5.2 for details). The changes relative to the baseline at every combination of site, carryover N and water table depth level were calculated using the following equation:

\[
\text{Yield-scaled NO}_3 \text{ reduction effectiveness (\%)} = 100 \times \left( \frac{y_B - y}{y_B} \right)
\]

where \( y_B \) is the yield-scaled NO$_3$ loss in the baseline scenario. A negative value indicates the combination of practices are less effective than the baseline \((y_B)\), while a positive value represents improved effectiveness relative to the baseline. Because management was the focus of this part of the analysis, we averaged these data across the 30 weather-years.

We explored how different configurations of management affect yield-scaled effectiveness with the conditional inference regression tree algorithm \((ctree)\) from the
Toolkit for Recursive Partitioning (*partykit*) package (Hothorn and Zeileis 2015) in R version 3.5.0 (R Core Team 2018). This algorithm fits non-parametric statistical regression tree models based on binary splits (i.e. grouping) of the predictor variables. These splits are performed recursively if the global null hypothesis of independence between any of the input variables and the response cannot be rejected ($\alpha = 0.05$). At each iteration, the algorithm seeks the predictor with the strongest association to the response, as measured by the p-value of the test for the partial null hypothesis of a single predictor and the response (Hothorn *et al* 2006). Regression trees were fitted separately for the simulated maize and soybean, with the yield-scaled NO$_3$ reduction effectiveness as the response variable, and crop, soil and N management factors (Fig. 5.2) as predictors. We restricted the maximum depth (*maxdepth*) of the tree to 4 splits in a branch, and the minimum number of observations in a leaf (*minbucket*) to 5% of the total number of observations in each dataset. All data munging, analyses and visualizations were performed in R using the *tidyverse* family of packages (Wickham and Grolemund 2017).

**Results and Discussion**

**Sensitivity to weather, soil state, and management factors**

Simulation of drainage NO$_3$ loads and concentrations, as well as residual soil NO$_3$ were highly variable across all scenarios (coefficient of variation (CV) = 55-133%), whereas the variation of simulated yields was much lower (CV = 16-18%; Table 4.1). Maize yields were strongly sensitive to weather-year, which accounted for 40-82% of the variation, depending on the site (Fig. 5.3). By comparison, simulated soybean yields were less sensitive to weather year (24-58% of the variation). These estimates are consistent with findings from a recent study, in which weather accounted for > 60% of the variability in maize yields and
~36% in soybean yields in the Midwest (Ray et al. 2015). Simulated soybean yields were sensitive to cultivar, planting timing, and their interactions, although the response was not consistent across sites (Fig. 5.3). This is indicative of the important role that management factors play in determining soybean yields (Egli and Cornelius 2009).

Nitrate loads in both maize and soybean were also sensitive to weather-year, although less so in the eastern sites where water table depth had a large effect (Fig. 5.3). Weather-year influences NO₃ loads mainly through the amount and distribution of precipitation, and therefore by changes in water drainage flows (Randall and Mulla 2001, Bowles et al. 2018, Randall and Goss 2008). Such a large influence on weather year renders NO₃ loads much less responsive to management than drainage NO₃ concentrations (Fig. 5.3). These were mainly driven by carryover soil NO₃ content, previous crop in maize, and cover crop in soybean, which reflect the soil NO₃ levels at the beginning of the simulation and conceptually represent the residual soil NO₃ from the preceding crop year. Previous crop also can affect soil NO₃ concentrations at harvest by changes in soil NO₃ immobilization-mineralization through differences in the quality and quantity of residues (Thorburn et al. 2005, Poffenbarger et al. 2018). Meanwhile, cover crops reduce drainage NO₃ concentrations through the uptake of soil NO₃ (Martinez-Feria et al. 2016b). The amount of residual soil NO₃ after maize harvest was very sensitive to N rate, and moderately to carryover N and previous crop. Residual soil NO₃ after soybean harvest was driven by many interactive factors, though the response was highly site-specific (Fig. 5.3).

This analysis indicates that if high residual NO₃ remains in soils after harvest, there is little management can do to decrease NO₃ loads in the following spring. Only cover crop had a minor influence through the reduction of drainage NO₃ concentrations (Fig. 5.3).
Table 5.2. Means, ranges and coefficient of variation (CV) for the output variables in the simulation experiments at the long-term sites.

<table>
<thead>
<tr>
<th>Site</th>
<th>Crop</th>
<th>Yield (Mg dm ha(^{-1}))</th>
<th>Drainage NO(_3) load (kg N ha(^{-1}))</th>
<th>Drainage NO(_3) concentration (mg N L ha(^{-1}))</th>
<th>Residual soil NO(_3) (kg N ha(^{-1}) (0-1.3m))</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Mean</td>
<td>CV</td>
<td>Mean</td>
<td>CV</td>
</tr>
<tr>
<td>HICKS.B</td>
<td>Maize</td>
<td>7.9</td>
<td>28.3%</td>
<td>11</td>
<td>139%</td>
</tr>
<tr>
<td></td>
<td>Soybean</td>
<td>2.09</td>
<td>22.8%</td>
<td>16.4</td>
<td>115%</td>
</tr>
<tr>
<td>NASHUA</td>
<td>Maize</td>
<td>9.95</td>
<td>19.7%</td>
<td>9.3</td>
<td>131%</td>
</tr>
<tr>
<td></td>
<td>Soybean</td>
<td>2.4</td>
<td>20.2%</td>
<td>12.4</td>
<td>101%</td>
</tr>
<tr>
<td>GILMORE</td>
<td>Maize</td>
<td>9.37</td>
<td>18.9%</td>
<td>11.9</td>
<td>129%</td>
</tr>
<tr>
<td></td>
<td>Soybean</td>
<td>2.39</td>
<td>19.5%</td>
<td>16.2</td>
<td>100%</td>
</tr>
<tr>
<td>KELLEY</td>
<td>Maize</td>
<td>9.86</td>
<td>15.4%</td>
<td>16.8</td>
<td>133%</td>
</tr>
<tr>
<td></td>
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<td>19.8%</td>
<td>20</td>
<td>97.10%</td>
</tr>
<tr>
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<td>23.5%</td>
<td>16.6</td>
<td>138%</td>
</tr>
<tr>
<td></td>
<td>Soybean</td>
<td>2.35</td>
<td>23.6%</td>
<td>19.6</td>
<td>102%</td>
</tr>
<tr>
<td>STJOHNS</td>
<td>Maize</td>
<td>11</td>
<td>16.2%</td>
<td>18</td>
<td>130%</td>
</tr>
<tr>
<td></td>
<td>Soybean</td>
<td>2.3</td>
<td>25.7%</td>
<td>11.6</td>
<td>129%</td>
</tr>
<tr>
<td>DPAC</td>
<td>Maize</td>
<td>11</td>
<td>19.3%</td>
<td>17.4</td>
<td>135%</td>
</tr>
<tr>
<td></td>
<td>Soybean</td>
<td>2.55</td>
<td>21.3%</td>
<td>11.9</td>
<td>130%</td>
</tr>
<tr>
<td>All sites</td>
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<td>22.4%</td>
<td>14.4</td>
<td>139%</td>
</tr>
<tr>
<td></td>
<td>Soybean</td>
<td>2.36</td>
<td>22.6%</td>
<td>15.4</td>
<td>112%</td>
</tr>
</tbody>
</table>

Rather, crop and N management appears to have a larger influence in the potential NO\(_3\) loads for the next year, here characterized by levels of the residual soil NO\(_3\). This may provide some basis for the often observed temporal lags between management implementation and NO\(_3\) loads responses in annual cropping systems (Sebilo et al. 2013, Castellano and David 2014). It may also suggest that measurements of deep-profile residual soil NO\(_3\) after harvest may be a better indicator of the performance of N management practices on an annual scale. Thus, these types of data could prove useful in the development and validation of predictive tools for use in adaptive management (Qin et al. 2018, Puntel et al. 2018, Banger et al. 2017).
Influence of soil-climate characteristics

Further analysis of the sensitivity of model outputs to simulation factors revealed trends in how the response in NO$_3$ losses changes with hydrological properties and fertility of soils. Total sensitivities (i.e. the sum of all sensitivity indices involving a factor) were strongly correlated to PAWC for NO$_3$ loads and drainage concentrations, and to SOC for residual NO$_3$. No clear pattern was discerned for crop yields (supplemental Table S5.2).

Implementing practices that improve soil N retention (e.g. cover crops) becomes more important with increasing soil productivity (i.e. higher soil water holding capacity and fertility), whereas optimizing N supply becomes less crucial (Fig. 5.4). Specifically, PAWC is an important soil characteristic influencing the overall responsiveness of drainage NO$_3$ loads and concentrations to both environmental and management factors (Fig. 5.4(a-d)). For instance, NO$_3$ loads had high sensitivity to water table depth at low PAWC, but this sensitivity decreased significantly as PAWC increased (Fig. 5.4(a)). Interestingly, sensitivity
of NO₃ loads to the weather-year had the opposite trend: as PAWC increased, NO₃ loads became more sensitive to the weather-year (Fig. 5.4(b)). This could be explained in part by the soils reduced capacity to buffer the influence of water table in the sites where soil water holding capacity is low, which here had an overwhelming effect and suppressed the relative influence of all other factors including weather-year (Fig. 5.3). Likewise, the sensitivity of drainage NO₃ concentrations to the previous crop in maize, and to cover crop in soybean, was significantly related to PAWC (Fig. 5.4(c-d)). The lower sensitivity of NO₃ losses to these simulation factors in sites with low water-holding capacity is consistent with their overall lower drainage NO₃ concentrations but comparable NO₃ load (i.e. greater drain water discharge; Table 4.1). Similarly, a recent study found that PAWC and other hydrological parameters are critical for predicting site-year changes in the maize yield response to fertilizer N (Qin et al 2018).

Figure 5.4. Total sensitivity of (a-b) subsurface drainage NO₃-N load, (c-d) flow-weighted NO₃ concentration, and (e-h) residual NO₃ in the soil profile (0-1.3m) to selected factors across a gradient of soil characteristics (0-1 m). For example, panel (a) shows the change in sensitivity of NO₃ load to water table, as influenced by soil water holding capacity.
As SOC increased, residual soil NO$_3$ became significantly more sensitive to carryover N, with a greater impact in soybean than maize (Fig. 5.4(f)). In maize, residual NO$_3$ was less sensitive to N rate as SOC increased (Fig. 5.4(f)), but more sensitive to the previous crop (Fig. 5.4(h)). This is most likely related to changes in the magnitude and variation of soil N mineralization rates. It is important to note, however, that the SOC from the sites here examined were significantly related to mean annual precipitation (p = 0.001, $r^2 = 0.9$) and marginally to temperature (p = 0.052, $r^2 = 0.56$). Both variables are known to control plant litter and soil organic matter decomposition rates (Zhang et al. 2008). Given this collinearity, we cannot attribute changes in residual NO$_3$ sensitivities directly to SOC. These soil characteristics should be instead considered within the regional climate context to more meaningfully inform decision-making.

**Effectiveness of multi-practice packages**

Simultaneous implementation of improved practices can enhance the overall yield-scaled NO$_3$ reduction effectiveness of management strategies. Generally, we found that adopting improved practices led to greater effectiveness compared to the baseline (Fig. 5.5). In maize, fertilizer N rate was the factor most strongly related to the response, and the effectiveness progressively increased as applied N decreased. This follows a well-established relationship, where yield-scaled losses increase exponentially as fertilizer N supply exceeds crop requirements (i.e. surplus N) (Zhao et al. 2017, 2016). Here, scenarios with high N rate applications (i.e. 30% more N fertilizer than the MRTN; supplemental Table S5.1) were generally less effective than the baseline (Fig. 5.5(a)). Fertilizer application timing instead provided few advantages, consistent with experimental findings (Christianson and Harmel 2015a, Jaynes 2013, Pittelkow et al. 2017).
The choice of cultivar was also an important consideration when assembling effective multi-practice packages. In maize, a cultivar with high radiation use efficiency (RUE) and N-use efficiency only seem to provide advantages under high N rates. In other cases, the NUE trait alone actually reduced effectiveness (Fig. 5.5(a)). In fact, paring high fertilizer rates with the NUE trait was among the worst-performing scenarios. Nitrogen-use efficient hybrids produce greater yield per unit of N taken up (Cassman et al 2002, Ciampitti and Vyn 2012), which means that their N requirements are lower, and fertilizer N rates need to be adjusted accordingly to fully realize this advantage. In soybean, cultivar selection was the strongest driving factor to yield-scaled effectiveness, with progressive improvements from short- to long-maturing cultivars (Fig. 5.5(b)). Short-maturing cultivars generally did worse than the baseline, and paring them with late planting was among the worst scenarios. With medium- and long-maturing cultivars, effectiveness was slightly improved by timely planting. In other words, the longer the growth cycle of a soybean crop, the better in terms of environmental benefits.

Within N fertilizer level and cultivar selection, we found that including overwintering cover crops can either lessen the detrimental or enhance the positive effects of these decisions on yield-scaled NO₃ losses. Even though all best performing scenarios included overwintering cover crops, they generally produced smaller changes than those driven by N rate or cultivar (Fig. 5.5(a-b)), suggesting that appropriately choosing these is a pre-requisite for cover crop to be most effective. This point has been largely overlooked in the literature, where often the effects of cover crops are evaluated in cropping systems with already improved N and crop management. This information should be considered in policy and implementation to better target adoption incentives (Roesch-McNally et al 2018).
Figure 5.5. Configurations of practices and their average yield-scaled NO$_3$ reduction effectiveness relative to a baseline scenario of current practices within a range of soil conditions (see Fig. 2). Negative values indicate that the combination of practices did worse than the baseline. Nodes (shaded boxes) represent individual practices, followed by the most significant ($\alpha = 0.05$) binary split among implementation levels (elbow arrows). Factor importance decreases with node depth (from left to right). Terminal nodes show the mean value (red symbol) of the management configuration along with their $10^{th}$ and $90^{th}$ percentiles (error bars). $r^2$ = coefficient of determination; MAE = mean absolute error; RMSE = root mean squared error.
The most effective scenarios for maize were those that included low N rates, normal or NUE+RUE cultivars, and with overwintering cover crop (Fig. 5.5(a)). In soybean, this was achieved with long-maturing cultivars, early or average planting, and overwintering cover crop (Fig. 5.5(b)). These multi-practice packages not only bested all other practice configurations, but also were much more effective than adopting each of the practices individually (Fig. 5.6). It is worth mentioning that the combined effectiveness of management cannot be appropriately determined by simply adding the effectiveness of individual practices (Christianson et al. 2017). Instead, the multiplicative approach proposed by Christianson et al. (see suppl. Table S5.3 for details) seems to provide reasonable estimates of combined effects, although these were slightly less than the average simulated value (67 vs 70% and 27 vs 33%, for maize and soybean, respectively). Given that this approach does not account for interactions, this could point to synergisms among the implemented practices, albeit these seem to be small.

Figure 5.6. Example of individual and combined adoption of improved practices and their effect on average yield-scaled NO\textsubscript{3} reduction effectiveness with respected to a baseline scenario. Red symbols indicate mean value of the management configuration, and error bars indicate their 10\textsuperscript{th} and 90\textsuperscript{th} percentiles.
Methodology scope and limitations

A 59% reduction in riverine NO₃ loads from current levels is needed to achieve regional hypoxia policy goals (Scavia et al 2017). While our analysis may suggest that certain configurations of practices could achieve reductions above this mark (Fig. 5.5), the measure of effectiveness used in this study cannot be interpreted directly within this context. This is because our approach also accounts for reductions in residual soil NO₃ as well as yield tradeoffs. This is important if we consider that some practices impact crop yields or residual soil NO₃ more than NO₃ loads directly (Fig. 5.3). The main reason for this choice of metric is that evaluation of practices cannot be realistically achieved by only including the amount of NO₃ loss during the year, given the important influence of residual soil NO₃ on the next year’s losses (i.e. carryover N in Fig. 5.3). Additionally, yield-scaled metrics are widely used in evaluations to capture both environmental and food security dimensions of agricultural systems (Zhao et al 2016). Nonetheless, adopting well-designed packages of practices, as shown in this analysis, will likely produce substantial water quality improvements, compared to adopting each of the practices individually (Fig. 5.6).

To date, many different management practices have been experimentally evaluated in different locations by considering one or two factors in isolation, and conclusions about effectiveness are often made on limited data and without knowledge of the potential synergistic or antagonistic feedbacks. Findings from these studies provide the basis for recommendations in the various regional science-based assessments, which are the backbone of current policy and implementation efforts (Christianson et al 2017). While necessary to refine our understanding of the biophysical controls on yield and NO₃ losses, experimental approaches are often limited to a descriptive capacity (i.e. hindsight) so that extrapolating across weather, soils and management conditions becomes challenging. By leveraging data
from long-term experiments with process-based simulation modeling we provided the first evaluation of multi-practice management in Midwestern cropping systems. With this we aimed to explore more predictive (i.e. insight) and prescriptive (i.e. foresight) levels of understanding (National Academy of Sciences 2018). However, this approach could be limited by simulation uncertainty, not only due to how hydrological and N cycling processes are characterized in models (Tao et al 2018, Wallach and Thorburn 2014), but also due to uncertainties in the soil and weather data sources available to guide model configuration. Therefore, assessing model performance using field data (suppl. Fig. S5.4) remains a necessary step in simulation-based water quality assessments (Baffaut et al 2017).

**Conclusion**

The simulation approach used in this study allowed us to evaluate and rank the importance of various environmental, soil state and management factors in driving NO$_3$ losses from cropland in the US Midwest. The analysis pointed to the dominant role of carryover soil N and weather-year for determining annual NO$_3$ loads, and of management for curving the amount of residual soil NO$_3$ after harvest (i.e. potential NO$_3$ losses for the next year). We also found soil-climate influences on the response of NO$_3$ losses to weather-year, soil state, and management factors, and showed that these characteristics can broadly dictate whether practices optimizing N supply or soil N retention should be the focus of management strategies. Adopting well-designed packages of practices was able to improve yield-scaled NO$_3$ reduction effectiveness, not only compared to a baseline of current practices (up to 70 and 33% reduction in maize and soybean respectively), but also to adopting each of the practices individually. However, the synergistic advantages among the individual practices were small. While no specific combination of practices is likely to perform best across all
locations, weather-years, and soil conditions, this study provides key information to guide future research and implementation toward tailoring recommendations to specific environmental conditions, farmers’ objectives and policy goals.

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Supplemental Information

Supplemental Table S5.1. Summary of the experimental datasets used to configure and test the APSIM model. CC = Continuous Maize; CS = Maize-Soybean; SWC = Soybean-Wheat-Maize; MRTN = Maximum Return to N rate

<table>
<thead>
<tr>
<th>Site Name</th>
<th>Location</th>
<th>Soil Classification</th>
<th>Subsurface drain specifications</th>
<th>Cropping System(s)</th>
<th>MRTN$^4$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Depth</td>
<td>Spacing</td>
<td>CC (2011-2015)</td>
</tr>
<tr>
<td>HICKS.B$^1$</td>
<td>Walnut Grove, MN (44.351, -95.537)</td>
<td>Havelock clay loam, Du Page silt loam, Hawick sandy loam</td>
<td>120</td>
<td>15</td>
<td>178</td>
</tr>
<tr>
<td>NASHUA$^2$</td>
<td>Nashua, IA (42.931, -92.572)</td>
<td>Clyde silty clay loam, Floyd loam, Kenyon loam, Readlyn loam</td>
<td>120</td>
<td>28.5</td>
<td>CS* (2007-2015)</td>
</tr>
<tr>
<td>GILMORE$^1$</td>
<td>Gilmore City, IA (42.748, -94.495)</td>
<td>Canisteo clay loam, Nicollet loam, Webster silty clay loam</td>
<td>110</td>
<td>7.6</td>
<td>CS* with and without tillage (2011-2015), CS* with rye cover crop no tillage (2011-2015)</td>
</tr>
<tr>
<td>SERF$^1$</td>
<td>Crawfordsville, IA (41.193, -91.483)</td>
<td>Kalona silty clay loam, Taintor silty clay loam</td>
<td>122</td>
<td>18.3</td>
<td>CC (2012-2015), CS* (2011-2015)</td>
</tr>
<tr>
<td>DPAC$^1$</td>
<td>Albany, IN (40.267, -85.161)</td>
<td>Blount silt loam, Pewamo clay loam, Glynwood silt loam</td>
<td>91</td>
<td>15.2</td>
<td>CS (2011-2015)</td>
</tr>
<tr>
<td>STJOHNS$^1$</td>
<td>St. Johns, OH (40.518, -84.085)</td>
<td>Minster silty clay loam, Blount silt loam</td>
<td>91</td>
<td>12.2</td>
<td>SWC (2011-2015)</td>
</tr>
</tbody>
</table>

$^*$ Includes both phases of the rotation every year
$^1$ Abendroth et al (2017)
$^2$ Martinez-Feria et al (2018)
$^3$ Dietzel et al (2016)
$^4$ Sawyer et al (2006)
Supplemental Figure S5.1. Soil organic carbon pools (a), inorganic N concentrations (b) and hydrological parameters (c) used for model simulation at the seven experimental sites. Values from (a) and (b) were derived from a 15 year spin-up model run, during which a maize-soybean rotation was simulated. Horizontal line in (c) indicates depth of the subsurface drainage tube (tile). FBiom = microbial carbon pool; FHum = humic carbon pool; FInert = inert carbon pool. DUL = Drainage upper limit (0.3 bar); LL = Lower limit (15 bar); SAT = Saturation point.
Supplemental Figure S5.2. Testing the robustness of the parameterization of the APSIM model at the seven long-term experimental sites. Symbols represent the average for every treatment across years at every site. Solid line represent the 1:1 relationship (i.e., perfect fit), while dotted lines the ±20% error range for maize and soybean yield and ±40% for drainage NO₃ loads and concentrations. RMSE = root mean squared error; RRMSE = relative root mean squared error; MBE = mean bias error.
Supplemental Table S5.2. Correlation and absolute range (within parentheses) of total sensitivity of model outputs to simulation factors as related to various pedo-climatic characteristics. Cells highlighted in yellow denote the relationships that were further explored with simple linear relationships in the main text. PAWC = Soil plant-available water holding capacity; SOC = Soil organic carbon; MAP = mean annual precipitation; MAT = mean annual daily temperature.

<table>
<thead>
<tr>
<th>Model Output</th>
<th>Simulation Factor</th>
<th>PAWC</th>
<th>SOC</th>
<th>MAP</th>
<th>MAT</th>
</tr>
</thead>
<tbody>
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<td><strong>Crop yields</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cultivar</td>
<td>-0.35 (0.06)</td>
<td>-0.64 (0.06)</td>
<td>0.71 (0.06)</td>
<td>0.55 (0.06)</td>
<td></td>
</tr>
<tr>
<td>Planting time</td>
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<td>0.11 (0.17)</td>
<td>-0.33 (0.17)</td>
<td></td>
</tr>
<tr>
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<td>-0.34 (0.04)</td>
<td>0.34 (0.04)</td>
<td>0.33 (0.04)</td>
<td></td>
</tr>
<tr>
<td>Residue removal</td>
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<td>-0.6 (0.01)</td>
<td>0.58 (0.01)</td>
<td>0.48 (0.01)</td>
<td></td>
</tr>
<tr>
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<td>-0.63 (0.09)</td>
<td>0.64 (0.09)</td>
<td>0.57 (0.09)</td>
<td></td>
</tr>
<tr>
<td>N time</td>
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<td>-0.65 (0.07)</td>
<td>0.68 (0.07)</td>
<td>0.64 (0.07)</td>
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</tr>
<tr>
<td>Carryover N</td>
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<td>-0.65 (0.02)</td>
<td>0.66 (0.02)</td>
<td>0.51 (0.02)</td>
<td></td>
</tr>
<tr>
<td>Water table</td>
<td>-0.65 (0.01)</td>
<td>-0.55 (0.01)</td>
<td>0.52 (0.01)</td>
<td>0.53 (0.01)</td>
<td></td>
</tr>
<tr>
<td>Previous crop</td>
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<td>-0.63 (0.03)</td>
<td>0.63 (0.03)</td>
<td>0.55 (0.03)</td>
<td></td>
</tr>
<tr>
<td>Weather-year</td>
<td>0.2 (0.27)</td>
<td>0.56 (0.27)</td>
<td>-0.51 (0.27)</td>
<td>-0.2 (0.27)</td>
<td></td>
</tr>
<tr>
<td><strong>NO₃ load in drainage</strong></td>
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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cultivar</td>
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<td>0.24 (0)</td>
<td>-0.43 (0)</td>
<td>-0.35 (0)</td>
<td></td>
</tr>
<tr>
<td>Planting time</td>
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<td>0.35 (0)</td>
<td>-0.58 (0)</td>
<td>-0.57 (0)</td>
<td></td>
</tr>
<tr>
<td>Cover crop</td>
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<td>-0.38 (0.01)</td>
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<td>Residue removal</td>
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<td>0.53 (0.03)</td>
<td>-0.7 (0.03)</td>
<td>-0.88 (0.03)</td>
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</tr>
<tr>
<td>N rate</td>
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<td>-0.71 (0.05)</td>
<td>0.79 (0.05)</td>
<td>0.86 (0.05)</td>
<td></td>
</tr>
<tr>
<td>N time</td>
<td>-0.72 (0.1)</td>
<td>-0.8 (0.1)</td>
<td>0.74 (0.1)</td>
<td>0.68 (0.1)</td>
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<tr>
<td>Carryover N</td>
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<td>-0.7 (0.05)</td>
<td>-0.93 (0.05)</td>
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</tr>
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<td>Water table</td>
<td><strong>-0.87 (0.63)</strong></td>
<td>-0.67 (0.63)</td>
<td>0.61 (0.63)</td>
<td>0.63 (0.63)</td>
<td></td>
</tr>
<tr>
<td>Previous crop</td>
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<td>0.56 (0.34)</td>
<td>-0.6 (0.34)</td>
<td>-0.79 (0.34)</td>
<td></td>
</tr>
<tr>
<td>Weather-year</td>
<td><strong>0.76 (0.57)</strong></td>
<td>0.7 (0.57)</td>
<td>-0.59 (0.57)</td>
<td>-0.49 (0.57)</td>
<td></td>
</tr>
<tr>
<td><strong>Flow-weighted NO₃ concentration in drainage</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cultivar</td>
<td>-0.79 (0.01)</td>
<td>-0.68 (0.01)</td>
<td>0.65 (0.01)</td>
<td>0.69 (0.01)</td>
<td></td>
</tr>
<tr>
<td>Planting time</td>
<td>-0.74 (0.02)</td>
<td>-0.63 (0.02)</td>
<td>0.57 (0.02)</td>
<td>0.63 (0.02)</td>
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</tr>
<tr>
<td>Cover crop</td>
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<td>-0.08 (0.04)</td>
<td>0.3 (0.04)</td>
<td>0.21 (0.04)</td>
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</tr>
<tr>
<td>Residue removal</td>
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<td>-0.58 (0.01)</td>
<td>0.53 (0.01)</td>
<td>0.59 (0.01)</td>
<td></td>
</tr>
<tr>
<td>N rate</td>
<td>-0.81 (0.1)</td>
<td>-0.72 (0.1)</td>
<td>0.71 (0.1)</td>
<td>0.73 (0.1)</td>
<td></td>
</tr>
<tr>
<td>N time</td>
<td>-0.59 (0.16)</td>
<td>-0.84 (0.16)</td>
<td>0.81 (0.16)</td>
<td>0.75 (0.16)</td>
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</tr>
<tr>
<td>Carryover N</td>
<td>0.57 (0.24)</td>
<td>0.72 (0.24)</td>
<td>-0.72 (0.24)</td>
<td>-0.59 (0.24)</td>
<td></td>
</tr>
<tr>
<td>Water table</td>
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<td>-0.65 (0.3)</td>
<td>0.63 (0.3)</td>
<td>0.66 (0.3)</td>
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</tr>
<tr>
<td>Previous crop</td>
<td><strong>0.9 (0.49)</strong></td>
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<td>-0.61 (0.49)</td>
<td>-0.72 (0.49)</td>
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<tr>
<td>Weather-year</td>
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<td>-0.52 (0.2)</td>
<td>0.5 (0.2)</td>
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<tr>
<td><strong>Residual Soil NO₃</strong></td>
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<td></td>
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<tr>
<td>Cultivar</td>
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<td>-0.81 (0.06)</td>
<td>0.79 (0.06)</td>
<td>0.55 (0.06)</td>
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<tr>
<td>Planting time</td>
<td>-0.19 (0.04)</td>
<td>0.07 (0.04)</td>
<td>-0.08 (0.04)</td>
<td>0.23 (0.04)</td>
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<tr>
<td>Cover crop</td>
<td>0.58 (0.04)</td>
<td>0.47 (0.04)</td>
<td>-0.28 (0.04)</td>
<td>-0.11 (0.04)</td>
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<td>Residue removal</td>
<td>0.68 (0.01)</td>
<td>-0.37 (0.01)</td>
<td>0.36 (0.01)</td>
<td>-0.05 (0.01)</td>
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<tr>
<td>N rate</td>
<td>-0.33 (0.39)</td>
<td><strong>-0.92 (0.39)</strong></td>
<td>0.89 (0.39)</td>
<td>0.62 (0.39)</td>
<td></td>
</tr>
<tr>
<td>N time</td>
<td>-0.71 (0.09)</td>
<td>-0.74 (0.09)</td>
<td>0.71 (0.09)</td>
<td>0.71 (0.09)</td>
<td></td>
</tr>
<tr>
<td>Carryover N</td>
<td>0.1 (0.26)</td>
<td><strong>0.9 (0.26)</strong></td>
<td>-0.93 (0.26)</td>
<td>-0.68 (0.26)</td>
<td></td>
</tr>
<tr>
<td>Water table</td>
<td>-0.83 (0.06)</td>
<td>-0.59 (0.06)</td>
<td>0.59 (0.06)</td>
<td>0.61 (0.06)</td>
<td></td>
</tr>
<tr>
<td>Previous crop</td>
<td>0.58 (0.27)</td>
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<td>-0.91 (0.27)</td>
<td>-0.78 (0.27)</td>
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</tr>
<tr>
<td>Weather-year</td>
<td>0.64 (0.11)</td>
<td>-0.04 (0.11)</td>
<td>0.15 (0.11)</td>
<td>0.15 (0.11)</td>
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</table>
Supplemental Table S5.2 (cont).

<table>
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<tr>
<th>Model Output</th>
<th>Simulation Factor</th>
<th>Soybean</th>
<th>PAWC</th>
<th>SOC</th>
<th>MAP</th>
<th>MAT</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Crop yields</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cultivar</td>
<td>-0.08 (0.32)</td>
<td>-0.21 (0.32)</td>
<td>0.46 (0.32)</td>
<td>0.64 (0.32)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Planting time</td>
<td>0.5 (0.27)</td>
<td>0.33 (0.27)</td>
<td>-0.32 (0.27)</td>
<td>-0.46 (0.27)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cover crop</td>
<td>-0.75 (0.03)</td>
<td>-0.69 (0.03)</td>
<td>0.67 (0.03)</td>
<td>0.63 (0.03)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Residue removal</td>
<td>-0.81 (0.06)</td>
<td>-0.71 (0.06)</td>
<td>0.66 (0.06)</td>
<td>0.63 (0.06)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>N rate</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>N time</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>Carryover N</td>
<td>-0.77 (0.03)</td>
<td>-0.76 (0.03)</td>
<td>0.7 (0.03)</td>
<td>0.62 (0.03)</td>
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</tr>
<tr>
<td>Water table</td>
<td>-0.78 (0.01)</td>
<td>-0.67 (0.01)</td>
<td>0.67 (0.01)</td>
<td>0.67 (0.01)</td>
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<td></td>
</tr>
<tr>
<td>Previous crop</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
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</tr>
<tr>
<td>Weather-year</td>
<td>-0.01 (0.28)</td>
<td>0.27 (0.28)</td>
<td>-0.54 (0.28)</td>
<td>-0.61 (0.28)</td>
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<td></td>
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<tr>
<td><strong>NO₃ load in drainage</strong></td>
<td></td>
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<td></td>
</tr>
<tr>
<td>Cultivar</td>
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<td>-0.91 (0.01)</td>
<td>-0.68 (0.01)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Planting time</td>
<td>0.51 (0.01)</td>
<td>0.85 (0.01)</td>
<td>-0.73 (0.01)</td>
<td>-0.56 (0.01)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cover crop</td>
<td>0.86 (0.08)</td>
<td>0.52 (0.08)</td>
<td>-0.35 (0.08)</td>
<td>-0.38 (0.08)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Residue removal</td>
<td>0.88 (0.04)</td>
<td>0.55 (0.04)</td>
<td>-0.58 (0.04)</td>
<td>-0.75 (0.04)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>N rate</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>N time</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>Carryover N</td>
<td>-0.24 (0.04)</td>
<td>-0.87 (0.04)</td>
<td>0.82 (0.04)</td>
<td>0.54 (0.04)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water table</td>
<td><strong>-0.86 (0.62)</strong></td>
<td>-0.68 (0.62)</td>
<td>0.62 (0.62)</td>
<td>0.63 (0.62)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Previous crop</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>Weather-year</td>
<td><strong>0.81 (0.59)</strong></td>
<td>0.73 (0.59)</td>
<td>-0.67 (0.59)</td>
<td>-0.65 (0.59)</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Residual Soil NO₃</strong></td>
<td></td>
<td></td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cultivar</td>
<td>0.64 (0.19)</td>
<td>-0.28 (0.19)</td>
<td>0.46 (0.19)</td>
<td>0.31 (0.19)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Planting time</td>
<td>-0.77 (0.23)</td>
<td>-0.74 (0.23)</td>
<td>0.77 (0.23)</td>
<td>0.83 (0.23)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cover crop</td>
<td>0.5 (0.2)</td>
<td><strong>0.95 (0.2)</strong></td>
<td>-0.9 (0.2)</td>
<td>-0.7 (0.2)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Residue removal</td>
<td>0.87 (0.05)</td>
<td>0.11 (0.05)</td>
<td>0 (0.05)</td>
<td>-0.19 (0.05)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>N rate</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>N time</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>Carryover N</td>
<td>0.35 (0.55)</td>
<td><strong>0.97 (0.55)</strong></td>
<td>-0.94 (0.55)</td>
<td>-0.71 (0.55)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water table</td>
<td>-0.49 (0.04)</td>
<td>-0.72 (0.04)</td>
<td>0.7 (0.04)</td>
<td>0.67 (0.04)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Previous crop</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>Weather-year</td>
<td>-0.35 (0.56)</td>
<td>-0.95 (0.56)</td>
<td>0.86 (0.56)</td>
<td>0.57 (0.56)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Supplemental Table S5.3. Example of a multiplicative approach to estimate combined effectiveness of practices compared to the average simulated value.

<table>
<thead>
<tr>
<th>Practice configuration</th>
<th>Mean yield-scaled NO₃ reduction</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Maize</strong></td>
<td></td>
</tr>
<tr>
<td>Baseline* + N rate₄₅</td>
<td>47%</td>
</tr>
<tr>
<td>Baseline + Cover crop₄₅</td>
<td>22%</td>
</tr>
<tr>
<td>Baseline + Cultivar₄₅</td>
<td>20%</td>
</tr>
<tr>
<td>Baseline + N rate₄₅ + Cultivar₄₅ + Cover crop₄₅</td>
<td>70%</td>
</tr>
<tr>
<td>Simulated</td>
<td>Multiplicative**</td>
</tr>
<tr>
<td></td>
<td>67%</td>
</tr>
<tr>
<td><strong>Soybean</strong></td>
<td></td>
</tr>
<tr>
<td>Baseline + Cultivar₄₅</td>
<td>15%</td>
</tr>
<tr>
<td>Baseline + Cover crop₄₅</td>
<td>12%</td>
</tr>
<tr>
<td>Baseline + Planting time₄₅</td>
<td>2%</td>
</tr>
<tr>
<td>Baseline + Planting time₄₅ + Cultivar₄₅ + Cover crop₄₅</td>
<td>33%</td>
</tr>
<tr>
<td>Simulated</td>
<td>Multiplicative</td>
</tr>
<tr>
<td></td>
<td>27%</td>
</tr>
</tbody>
</table>

* See Fig. 2 in main text for details.

** This is calculated following Christianson et al (2017). For example:

Combined effectiveness = 100% - (100% - 47%)*(100% - 22%)*(100% - 20%) = 67%
CHAPTER 6. GENERAL DISCUSSION AND CONCLUSIONS

The goal of the work presented in this dissertation was to examine and quantify the impact of various genetic, environmental and management drivers of yield and N-loss tradeoffs in the maize and soybean cropping systems of the US Midwest. Research also sought to identify potential management strategies to lessen these tradeoffs (Fig. 1.2). To offer feasible and scalable pathways for improvement, we evaluated scenarios within the socio-ecological context in which current production systems operate (i.e. annual cycle, rainfed, intensive input use, commodity grain production). To this end, a system analysis framework was employed (Fig. 1.1), which used field data from small plots, long-term experiments, publicly available databases, and process-based modeling to fully examine the soil-plant-atmosphere continuum and extrapolate the behavior of systems across a wide range of weather, soil, and management.

Chapters 2 and 3 aimed to fill knowledge gaps and increase understanding of the mechanisms underlying: i) rye cover crop effects on maize yields and nitrate (NO₃) losses in subsurface drainage (Chapter 2), and ii) grain dry down in the field and hence timing of harvesting and crop residue additions (Chapter 3). Findings from these studies allowed us to better calibrate process-based models within APSIM, and apply this tool to i) evaluate the contributions of the efficiency of N input use and soil N retention to environmental N losses (Chapter 4), and ii) explore drivers of yield and N-loss tradeoffs and potential solutions (Chapter 5). Below I briefly summarize the findings of each of the studies and discuss their implications to guide future research and implementation efforts.
Summary of Findings

Rye cover crop biomass accumulation is related to NO$_3$ loss reductions but not to maize yield penalties.

Previous research has reported overall neutral effects of grass cover crops on maize yields and reductions in NO$_3$ loss, but wide variation exists within and among studies (Marcillo and Miguez, 2017). This suggests that rye effects on the maize system depend on specific combinations of management choices and environmental conditions, but few studies have explored the mechanisms by which rye affects these systems. In Chapter 2, we hypothesized that the amount of rye biomass accumulated by termination could explain the magnitude of maize yield and NO$_3$ loss effects, and tested this hypothesis with long-term, high-resolution, multi-process observations collected at a field study in central Iowa.

Experimentally, rye cover crop reduced drainage by 12% and NO$_3$ losses by 20% (or 31% per unit of N applied), and maize yields by 6%. Minimal effects were found on soil temperature, and rye water use, which we estimated to be 21 mm Mg$^{-1}$ biomass, reduced yields only during drought years. Importantly, we found that rye lowers NO$_3$ loads mainly by decreasing NO$_3$ concentrations in drainage water, but that most of the N taken up by rye was likely mineralized and made available for the maize crop. Extrapolating field data with the APSIM model indicated that rye cover crop decreases NO$_3$ loads ($-26\pm26\%$) but does not always reduce drainage flow ($-4\pm13\%$) or grain yields ($-2\pm6\%$). This is consistent with experimental and literature results (Fig. 2.10). Therefore, we concluded that there is evidence to support the hypothesized relationship for NO$_3$ loss, but not for yields and drainage water.

Grain dry down depends largely on atmospheric conditions and less on genotype or management

In Chapter 3, we analyzed time-series maize and soybean grain moisture data collected from various genotype-by-environment treatments. Results indicated that air
relative humidity was the best predictor of field dry down of maize ($r^2 = 0.75$) and soybean
($r^2 = 0.85$) grains among other explanatory weather factors tested (wind speed, temperature,
and their combinations). The analysis also examined the relative importance of genotype,
weather-years, planting date, and their interactions on the dry-down process (Fig. 3.5). We
found the studied factors affected grain moisture at physiological maturity ($M_0$), but not the
drying coefficient ($k$).

This means the $M_0$ should be estimated for specific situations. The fact that we did
not find significant differences in the $k$ across genotypes, weather-years, and planting dates
seems to suggest that a species-specific $k$ would be adequate to simulate post-maturity grain
moisture. Based on these findings, we concluded that grain dry down of maize and soybeans
in the field can be reasonably predicted using data available from most weather stations, if
grain moisture at or shortly after physiological maturity is known.

**Poor soil nitrogen retention can contribute as much or more to nitrogen losses than inefficient use of nitrogen inputs.**

A fundamental assumption of most environmental impact assessments is that lower N
losses from cropland can be achieved by reducing the net surplus of applied fertilizer N
(Zhang et al., 2015). However, this assumption largely ignores potential long-term changes in
soil N stocks, and thus contributions from the release of native soil N into the environment.
In Chapter 5, we examined N cycling dynamics of various rotations that included maize,
soybean, and rye cover crops in the Midwest, and showed that this crop-based view generally
underestimates N losses, and that it is insensitive to improvements in soil N cycling (e.g.,
with cover crops). We also laid out a conceptual framework to link the soil and crop
components of N-use efficiency at the system level.
The application of the framework to the studied systems indicated that the majority (55%) of N losses in maize-soybean systems actually originate from the release of native soil N into the environment because of the asynchrony between soil mineralization and crop uptake. The fertilizer N rate to maize that minimized the tradeoff between N losses and crop yields was ~65% of those where additional N fertilizer did not further increase yields (i.e. agronomic optimum N rate), but this resulted in an average yield penalty of 5–7%. This means that to achieve maximum yield in these systems, we sacrificed environmental performance. Based on these findings, we concluded that overall improvement in system efficiency will likely come from both optimizing the crop yield response to N inputs (e.g. fertilizer management) while enhancing soil N retention (e.g. cover crops).

**Soil and climate influences on how NO$_3$ loss responds to management can help prioritize N supply or soil N retention strategies**

In Chapter 5, we used simulated data from seven long-term experimental sites across the Midwest to rank the importance of various environmental, soil state and management factors in driving NO$_3$ losses in drainage. The analysis highlighted the dominant role of carryover soil N and weather-year for determining annual NO$_3$ loads, and of management for curbing the amount of residual soil NO$_3$ after harvest (i.e. potential NO$_3$ losses for the next year). Soil plant-available water content and soil organic carbon seem to be important characteristics influencing the overall responsiveness of drainage NO$_3$ loads and concentrations of both environmental and management factors. In general, we found that implementing practices that improve soil N retention (e.g. cover crops) becomes more important with increasing soil productivity (i.e. higher soil water holding capacity and fertility), whereas optimizing N supply becomes less crucial.
Across sites and weather years, reducing N rate to maize, and choosing full-season soybean varieties seem to be the practices with the most potential to improve yield-scaled NO\textsubscript{3} reduction effectiveness of multi-practice management strategies, when compared to a baseline of current practices. In maize, genotypes with high NUE (greater yield per unit of N taken up) actually decreased effectiveness compared to the baseline, if this was not paired with lowering fertilizer N rates. Even though the best performing scenarios often included overwintering cover crops, they generally produced smaller changes than those driven by N rate in maize or cultivar in soybean, suggesting that appropriately choosing these is a prerequisite for assembling effective strategies.

Simultaneous implementation of multiple management practices improved yield-scaled NO\textsubscript{3} reduction effectiveness up to 70 and 33% compared to the baseline in maize and soybean respectively, but also compared to adopting each of the practices individually. However, the synergistic advantages among the individual practices were small. Therefore, we conclude that substantial improvement in NO\textsubscript{3} reduction can be achieved by designing multi-practice management strategically without substantially decreasing yields.

**Recommendations and Future Work**

**Improving simulation tools**

Process-based simulation models are useful tools that can help fill data gaps and aid our understanding of how cropping systems might react to changes in weather and management. They are especially useful when addressing questions that are too costly or impractical for field research (e.g. Chapters 4 and 5). Yet, application of simulation models is limited by many uncertainties in various crop-soil processes that directly or indirectly affect the overall representation of water and N cycling. Some of these processes are not currently
accounted for within the APSIM platform, or have not been sufficiently evaluated against measured data for application in the Midwest. This dissertation included efforts to improve modeling of rye cover crop, maize and soybean yields, nitrate (NO\textsubscript{3}) losses in subsurface drainage (Chapter 2), and grain dry down in the field (Chapter 3).

In Chapter 2, we show that simulations of rye cover crop in APSIM can be improved by making the wheat model more N demanding, increasing its ability to extract water and nutrients from deeper soil layers, decreasing the transpiration efficiency constant, and modifying parameters that affect the soil water evaporation after rye termination. Additionally, underestimation of NO\textsubscript{3}-N losses can be fixed by better matching maize grain N concentration to reflect measurements in modern maize hybrids (Ciampitti and Vyn, 2012). The speed and extent of maize root growth were found to be important, but field observations are rare and deserve further research investment (Ordóñez et al., 2018). Finally, it is important to note that cropping systems models have flexibility to fit experimental observations via different pathways. Therefore, improvements to models must make use of a wealth of data to evaluate various crop-soil processes simultaneously.

Accurately predicting the timing of grain dry down in the field would be valuable to inform the scheduling of harvest operations, and has the potential to help farmers minimize additional costs of artificial grain drying (Chapter 3). In the context of this dissertation, realistically estimating harvest timing for maize and soybeans was necessary to improve representation of residue decomposition in long-term crop rotation evaluations (e.g. Chapter 4). Like most of the available crop models, the APSIM maize and soybean models currently contain routines to harvest at physiological maturity (~35% moisture). In the Midwest, this is
usually around early September. In reality, however, farmers wait until grain reaches 22-15% moisture which can take between 1 to 4 weeks, depending on the year.

Misrepresenting harvest timing also means that crop residues are added to soil earlier in the model than would occur in the field, which leads to an overestimation of the decomposition of residues during the fall. Hence, cropping system modeling platforms would benefit from representing this process, especially in temperate climates where seasonal temperature changes are a major constraint. Chapter 3 is one of the few studies dedicated to this subject, thus more research is needed to test the developed algorithm on a wider range of environments and management. Because the starting moisture content ($M_0$) varies with environmental conditions, there is a need to estimate this value, perhaps by coupling the developed algorithm with a grain fill model or other approaches.

**Managing maize and soybean cropping systems for high yields and low nitrogen loss**

Assessment of environmental impacts and crop productivity tradeoffs can paint very distinct pictures, depending on what components of the system are taken into consideration. This in turn can lead to different conclusions about potential solutions. The assumption that the soil N pool is in long-term equilibrium (i.e. that it is not increasing or decreasing) obscures the very important contributions of soil N mineralization to environmental N losses (Chapter 4), and it is insensitive to the contributions of improving soil N retention, such as with cover crops. Lack of uniformity among literature studies on the use of concepts like N-use efficiency (NUE) is the source of much confusion, and it can create unrealistic expectations about the potential of N management for reducing environmental impacts.

It is possible that this is mainly a problem only in the well-managed maize-soybean rotations in the fertile soils of the Midwest, and that much progress can be still realized by targeting those areas where N surplus is very large. However, Midwestern producers on the
aggregate seem to already be applying fertilizer at near-optimum levels. For instance, the average N fertilizer rate to maize-following soybean in Iowa is about 169 kg ha\(^{-1}\) (IDALS, 2016), which is only 8% greater than the current university-recommended maximum return to N rate (MRNT; Sawyer et al., 2006). Thus reducing N fertilizer rate to maize-following soybeans does not seem to be a feasible alternative, unless farmers are willing to accept yield penalties. Besides, even if all N fertilizer-related losses are mitigated, losses might not be reduced beyond the “background” level, that is, those that cannot be directly attributed to a surplus of applied N (~25 kg total N ha\(^{-1}\) loss or ~15 kg NO\(_3\)-N ha\(^{-1}\) in drainage tiles; Table 4.4).

On the contrary, more opportunities for N management improvements appear to be available in continuous maize systems, where about 93% of the losses are related to inefficient use of N inputs. It is important to note that continuous maize systems receive fertilizer annually as opposed to biannually. Hence, the risk of losing N derived from fertilizer into the environment is higher than in maize-soybean. Meanwhile, the greater amount and higher C:N of maize residues provide a stronger sink for N during decomposition (i.e. immobilization) and mulching effects (i.e. lower soil temperature) suppress soil N mineralization during the fall and spring. As discussed in Chapter 2, this might be one of the reasons why rye cover crops (i.e. soil N retention practice) had such a small absolute effect in our field experiment (4 kg NO\(_3\)-N ha\(^{-1}\) yr\(^{-1}\) loss reduction).

Undoubtedly, overwintering cover crops have the potential to improve soil N retention and hence reduce NO\(_3\) loads, while potential yield tradeoffs seem to be an issue only in dry years (Chapter 2). However, they more consistently reduce NO\(_3\) concentrations in drainage (Chapters 2 and 5). This is because NO\(_3\) loads depend more on precipitation and
drainage water flow, which are uncontrollable factors (Randall and Goss, 2008) and widely change from year to year. Hence, focus on measuring drainage NO₃ concentrations rather than loads might be a more effective strategy for monitoring progress of the benefits of cover crop implementation. Cover crops seem to have the greatest advantage to decrease losses in sites with highly productive soils (Fig. 5.4), especially when established following the maize phase of the maize-soybean rotation (Fig. 5.3).

In conclusion, this dissertation provides evidence that crop yields and N-loss tradeoffs can be minimized with careful design of management strategies. These invariably seem to benefit from inclusion of cover crops, but they also require simultaneously choosing appropriate genotypes, optimal planting dates, and optimizing N inputs to better match crop requirements (Fig. 5.5). Because water and N cycling dynamics, and thus tradeoffs, are largely driven by environmental conditions (i.e. weather, soil state and characteristics; Fig. 5.3 and 5.4), the ‘optimal’ management is different from year-to-year and between sites. The latter makes the case for investing research efforts in developing more adaptive management approaches (Banger et al., 2017; Puntel et al., 2018; Qin et al., 2018; Chapter 5) that can be informed by more active monitoring of crop and soil dynamics through a combination of advanced sensors, geospatial technologies, and quantitative methods. This would transform agronomic data into more relevant knowledge to improve the economic and environmental sustainability of crop production systems of the Midwest.

References


IDALS, IDNR, ISU, 2016. Iowa nutrient reduction strategy: A science and technology-based framework to assess and reduce nutrients to Iowa waters and the Gulf of Mexico.


