



Balancing indicators for sustainable intensification of crop production at field and river basin levels

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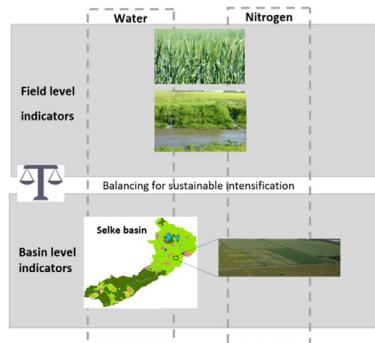
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HIGHLIGHTS

- Sustainable intensification (SI) is assessed at the field and basin levels.
- Interdependencies between water and nitrogen indicators are key for SI evaluation.
- The SI framework links crop production, resource use and environmental indicators.
- Climatic factors dominantly influence water quantity and quality in the study area.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:

Received 12 July 2019

Received in revised form 17 November 2019

Accepted 2 December 2019

Available online 5 December 2019

Editor: Ouyang Wei

Keywords:

Selke Basin

Crop production

Water-use efficiency

Nitrogen-use efficiency

Sustainable intensification

Water quality and quantity indicators

ABSTRACT

Adequate tools for evaluating sustainable intensification (SI) of crop production for agro-hydrological system are not readily available. Building on existing concepts, we propose a framework for evaluating SI at the field and river basin levels. The framework serves as a means to assess and visualise SI indicator values, including yield, water-use efficiency and nitrogen-use efficiency (NUE), alongside water and nitrogen surpluses and their effects on water quantity and quality. To demonstrate the SI assessment framework, we used empirical data for both the field level (the Static Fertilization Experiment at Bad Lauchstädt) and the river basin level (the Selke basin, 463 km²) in central Germany. Crop yield and resource use efficiency varied considerably from 1980 to 2014, but without clear trends. NUE frequently fell below the desirable range (<50%), exposing the environment to a large N surplus (>80 kg N ha⁻¹). For the catchment as a whole, the average nitrate-N concentration (3.6 mg L⁻¹) was slightly higher than the threshold of 2.5 mg L⁻¹ nitrate-N in surface water. However, weather and climate-related patterns, due to their effects on transport capacity and dilution, influenced water quantity and quality indicators more than agronomic practices. To achieve SI of crop production in the Selke basin, irrigation and soil moisture management are required to reduce yield variability and reduce N surpluses at field level.

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In addition, optimum application of fertiliser and manure could help to reduce the nitrate-N concentration below the set water quality standards in the Selke basin. In this way, there is scope for increase in yields and resource use efficiencies, and thus potential reduction of environmental impacts at basin level. We conclude that the framework is useful for assessing sustainable production, by simultaneously considering objectives related to crop production, resource-use efficiency and environmental quality, at both field and river basin levels.

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1. Introduction

Increased crop production is needed to meet growing demands for food, feed and fibre (Koning and Van Ittersum, 2009; Tilman et al., 2011). To unlock production potential, both abiotic and biotic stresses have to be managed (Van Ittersum and Rabbinge, 1997). One way to achieve this is to relieve abiotic stresses by intensifying the use of yield-enhancing resources such as nitrogen (De Wit, 1992; Zhang et al., 2015), phosphorus (Steen, 1998) and water (Godfray et al., 2010). However, increased crop production can deplete phosphorus, which is a non-renewable resource (Cordell et al., 2009). Moreover, higher production can contribute to water scarcity by increasing water consumption (Mekonnen and Hoekstra, 2016), and excessive fertiliser use in agriculture causes pollution, degrading water quality and reducing the availability of water resources of good quality (van Vliet et al., 2017; Carpenter et al., 1998).

In high-input cropping systems such as those in northwestern Europe, there are tendencies to focus on improving resource use efficiencies (RUEs) and protecting environmental quality. Thus, a local balancing of crop production, RUEs and environmental effects is considered the best way to safeguard a food-secure and sustainable future. This sustainable intensification (SI) (Tilman et al., 2011) or ecological intensification (Cassman, 1999) is a function of resource input, crop uptake and the interaction between hydrological processes and nutrient dynamics at both the field and river basin levels.

Previous studies, for example, Pittelkow et al. (2016) and Musumba et al. (2017), have evaluated the SI of crop production using indicators such as productivity, water- and N-use efficiencies, as well as environmental impacts. Pittelkow et al. (2016) and Musumba et al. (2017) assessed the relative performance of these indicators at country (Uruguay) and community (Golomoti in Malawi) levels and applied 'spider plots' and 'radar charts' respectively. In the agro-hydrological systems, however, we lack a reliable approach for evaluating the SI of crop production and thus a framework to assess how agricultural practices in relation to water and nutrients at field level influence water quantity and quality indicators at the river basin.

River basins link agricultural practices at field and landscape levels, together with other point-source activities, with their effects on water resources within a well-defined spatial boundary (Vörösmarty and Moore, 1991; Burt and Pinay, 2005). This means that both the agricultural field and the river basin represent informative spaces for analysing the interaction and transfer of water and nitrogen within agro-hydrological systems. Although socio-economic factors at the farm level may be overlooked when focusing on these two levels (Giller et al., 2006; Meuwissen et al., 2019), the field and river basin levels are relevant to assess productivity and RUE indicators, as well as to evaluate biophysical and environmental thresholds for SI within the context of particular production and water resource objectives. The river basin is furthermore recognised as an important unit for environmental quality assessment. Such an assessment requires testing the efficiency of different nutrient emission mitigation measures (Klauer et al., 2012) and compared with environmental guidelines, such as those in the EU Water Framework Directive (EC, 2000). It also requires a long-term perspective rather than a short-term perspective and a clear understanding of how biophysical conditions may favour or restrict environmental impacts in particular years.

The purpose of the current study is to propose an SI assessment framework at field and river basin levels. Our study builds on various existing concepts, including biophysical yield ceilings (De Wit, 1992), crop growth explaining factors (Van Ittersum et al., 2013; Silva et al., 2017) and desirable threshold ranges for N (De Vries et al., 2013; Oenema et al., 2015). In addition, the interdependence of water quantity and quality is assessed (van Vliet et al., 2017) in conjunction with standards set by the EU Nitrates Directive (Monteny, 2001), the EU Water Framework Directive and the German Environment Agency (UBA, 2017).

This study hypothesizes that the combination of detailed field and river basin data with a multi-decade analysis (1980–2014) provides relevant insights for SI implementation. We present a framework that builds on existing concepts to evaluate the SI of crop production at the field and river basin levels, considering objectives related to crop production and water quantity and quality indicators. The framework's aim is to allow investigating how crop production, RUEs and environmental quality can be balanced at the field and river basin levels. The presented framework serves as a means to assess and visualise SI indicator values, including crop yield, water-use efficiency (WUE) and N-use efficiency (NUE), alongside water and N surpluses in crop production and their effects on water quantity and quality. We demonstrate our framework using empirical data from the Selke basin (463 km²) in central Germany. Long-term field experimental data, modelling and observed stream water quantity and quality data are available in this area and were used in this study.

2. Theory, methods and data

2.1. SI assessment framework

Fig. 1 shows the relationships between water and N inputs for crop production at the field level, and the effect on water quantity and quality at the river basin level.

The SI assessment framework applies the mass balance of resources to relate the use of water and N for crop production to environmental effects. The mass balance at a specific boundary links resource input to output (Oenema et al., 2015). At the field level, water input for crop production typically includes plant-available soil moisture from precipitation (green water) and possibly capillary rise and irrigation (blue water) (Chukalla et al., 2015). Sources of N input for crop production generally include mineralisation, seed, irrigation, fertiliser and atmospheric N deposition. N output, as defined by Oenema et al. (2015), is the share of the N input that is embedded in harvested or marketable yield (assuming crop residues are left on the field). Drawing a parallel with N, the equivalent concept for water is crop transpiration (T).

Resource input minus resource output is the surplus that is returned (or emitted) to the environment (i.e., to the soil, surface water, groundwater and air). Water surplus is input minus output where the input is precipitation and irrigation, and the output is transpiration. Water surplus consists of (i) surface runoff and groundwater recharge, which join the water sources; (ii) evaporation that escapes to the air, and (iii) soil moisture increment in the soil. N input is the natural and artificial addition to a field, and N output is the N harvested with the crop yield. N surplus, in forms such as ammonia (NH₃), dinitrogen (N₂), nitrous oxide (N₂O) and nitrogen oxide (NO), escapes to the air. N fluxes,

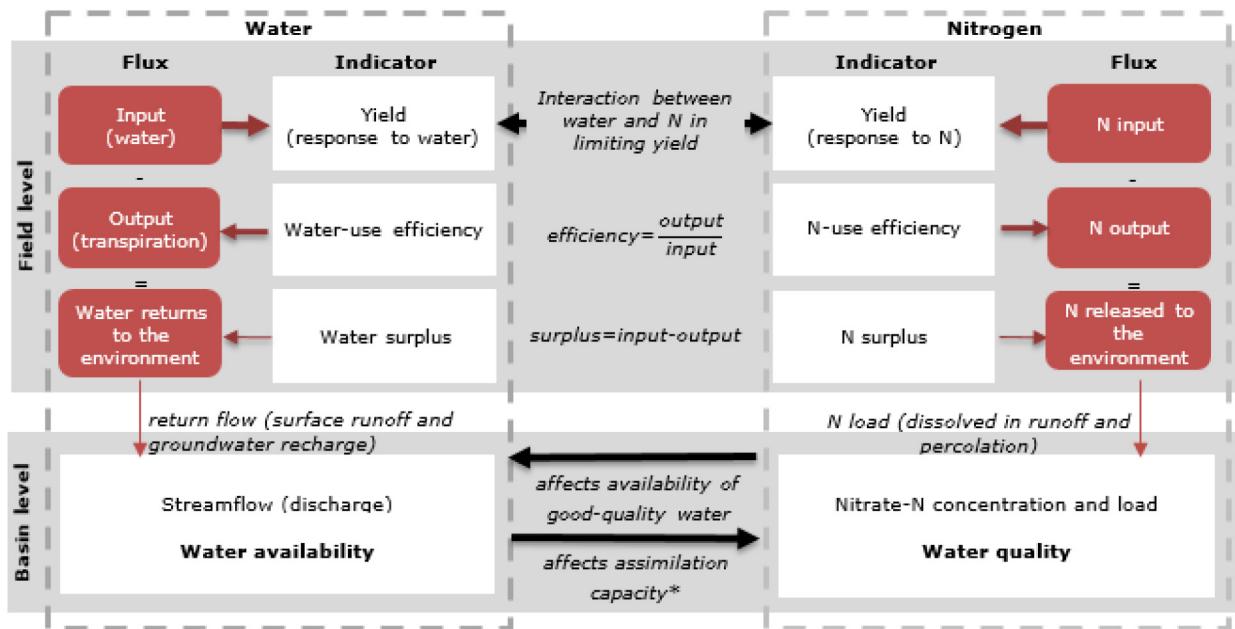


Fig. 1. Schematic representation of the SI assessment framework. Water and nitrogen-related fluxes in the crop production system at the field level and their implications for indicators of production, resource-use efficiency, field-level resource surpluses and basin-level water availability and water quality. Out of all water and N surpluses returned (or emitted) to the environment, only the portion affecting water quantity and quality are shown. *Assimilation capacity is the capacity of groundwater and surface water to receive pollution (Hoekstra, 2014).

such as N leaching from the soil profile and N transported from land to water via runoff, enter the aquatic environment, influencing water quantity and quality at the basin level. The remaining N surplus increases the soil N.

2.1.1. Field-level indicators for water and N inputs

The SI assessment framework links agronomic practices to water resources and presents indicators at both the field level (crop yield, RUE and resource surplus) and the river basin level (discharge, nitrate-N concentration and load in a river). Fig. 2 presents the SI assessment framework for the field level. It contains six connected conceptual panels exhibited in three pairs. Each pair consists of panels pertaining to water (left) and nitrogen (right).

There is a clear dependence between water and N inputs; that is, the effect of N on crop yield depends on the availability of water, and vice versa (Ehlers and Goss, 2016; De Wit, 1992). Adequate moisture in the plant root zone is vital for N availability, movement and uptake by crops (Aulakh and Malhi, 2005). Adequate nitrogen availability is equally important to stimulate crop growth, particularly roots and leaves (Brouwer and De Wit, 1968). Maintaining adequate resource availability throughout the season is, however, challenging. Soil moisture and N availability at the field level are influenced by the amount and timing of supply. Limited availability induces stress, which compromises crop development and yield. In such cases, crop yield responds positively to the supply of the most limiting input (De Wit, 1992). Excessive availability of water or N may also undermine yield. Excessive water reduces N availability through N leaching and runoff (Schepers et al., 1995), which may result in lower yield. Over supply of N causes excessive vegetative growth and may result in a relative reduction of crop yield as well (Kong et al., 2017).

Fig. 2 depicts the relationship between water and N as input factors, both facilitating and limiting crop growth (De Wit, 1992). Panels A1 and A2 show yield levels within the biophysical limits. The relative importance of growth-defining, -limiting and -reducing factors explains the actual yield (Y_a), which is the yield achieved in farmers' fields (Van Ittersum and Rabbinge, 1997). Y_a can be increased to the technical efficient yield level (Y_{TE}) by improving RUEs at a given input level. This can

be done through improvements in the timing, placing and form of the inputs applied. Crop yield can be increased further to the highest farmer's yield (Y_{HF}) by adding the most limiting resources (water, nutrients) up to the levels used by the highest yielding farmers. Further yield increases to the potential yield (Y_p) for irrigated crops, or the water-limited yield (Y_w) for rainfed crops, require the adoption of precision agriculture practices and/or improved varieties. Y_p is the maximum crop yield as defined by climatic factors such as CO_2 , radiation and temperature and crop genetics (Van Ittersum et al., 2013). These yield levels provide the basis for calculating the efficiency yield gap ($Y_{TE} - Y_a$), the resource yield gap ($Y_{HF} - Y_{TE}$) and the technology yield gap ($Y_p - Y_{HF}$) (Silva et al., 2017).

Panels B1 and B2 in Fig. 2 indicate the associated water-use efficiency (WUE) and nitrogen-use efficiency (NUE), respectively. The WUE and NUE are defined as the ratio of, respectively, transpiration and N uptake during the growing season over water and N input per year. The panels show desirable ranges of WUE (B1) and NUE (B2). For NUE, the desirable range was established by the EU Nitrogen Expert Panel (Oenema et al., 2015). The Expert Panel provided four thresholds to delineate the desirable range of NUE (Oenema et al., 2015), using average EU level performance as a basis. First, a maximum NUE of 90% is suggested to help protect soil against N mining. Second, a minimum NUE of 50% is suggested to help maintain the current average NUE level in the EU. Third, a minimum level of N harvested of $80 \text{ kg N ha}^{-1} \text{ year}^{-1}$ is proposed to maintain a minimum of crop production. Fourth, an N surplus of $80 \text{ kg N ha}^{-1} \text{ year}^{-1}$ is proposed to limit N load in the environment (pollution), which is equal to the mean N surplus of agriculture in the EU-27 (including animal production). We adopt these thresholds here, but note that based on empirical assessments, these thresholds should be adapted to local conditions.

For WUE, we propose a similar approach as for NUE, and the desirable range for rainfed agriculture can be defined by three thresholds. First, a WUE of 80% can be considered as maximum to control salt build-up (Darzi-Naftchali and Ritzema, 2018; Letey et al., 2011), and land subsidence (Querner et al., 2012). This allows 20% for leaching requirements, as suggested in the literature (Letey et al., 2011). If the salt build-up is not a concern, the leaching fraction can be zero, and thus a

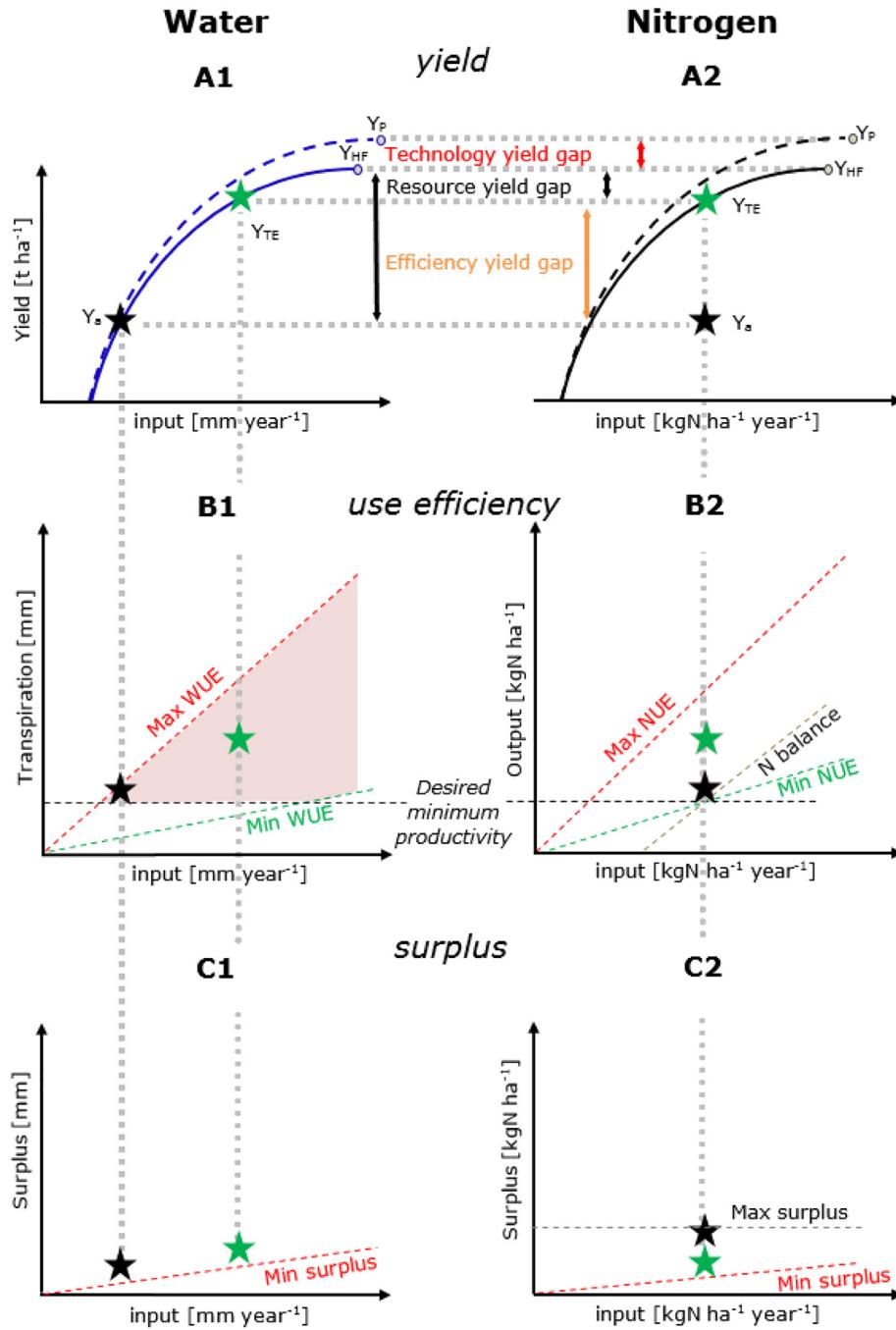


Fig. 2. SI assessment framework at the field level relating yield (A1 and A2), resource-use efficiency (B1 and B2) and resource surplus (C1 and C2) within the biophysical and environmental thresholds for water (left column) and nitrogen (right column) as production factors. The dashed and solid production curves represent simulated yields for an improved production scenario and actual frontier yields, respectively. The two graphs in the middle present the actual and desirable range of resource-use efficiencies for water (B1) and nitrogen (B2). The yield increase from the dark star to the green star and resource-use efficiency and resource surplus are shown for a hypothetical production case in which the efficiency, resource and technology yield gaps are marked by orange, dark and red arrows, respectively.

maximum WUE of 100% is acceptable. Second, the minimum WUE is the level required to maintain a wheat productivity of 80 kg N ha^{-1} . For rainfed agriculture, the minimum WUE is calculated by drawing a parallel with the minimum NUE proposed by the EU Nitrogen Expert Panel (Oenema et al., 2015), calculated by dividing the minimum water output (productive water use represented by transpiration) by the water input (precipitation). At the EU level, a minimum WUE of 17% is suggested for wheat (the dominant crop in the EU), considering EU values for transpiration and water input ($T = 111 \text{ mm}$ and water input =

650 mm). The transpiration of 111 mm corresponds to an N output (N uptake) of $80 \text{ kg N ha}^{-1} \text{ year}^{-1}$ (see Oenema et al. (2015)). T is estimated based on the established linear relationship between T and N uptake [g m^{-2}] = $0.0644 * T [\text{mm}] + 0.8354$, $R^2 = 0.96$. Note, this transpiration and N uptake relate to a yield of 3.4 t ha^{-1} , which is low for many European regions - see e.g., average winter wheat yield in EU is estimated at 4.6 t ha^{-1} (Schils et al., 2018). The minimum N uptake, T and derived minimum crop yield should be economically viable for a

farmer (Smith and McDonald, 1998). For rainfed wheat production, an average water input of 650 mm per unit area is assumed, estimated using average precipitation values reported at the EU level (i.e., 621 mm by Cerdan et al. (2010), and 677 mm by Abbaspour et al. (2015)). Yearly, and not growing season, precipitation is considered as water input, as this influences the surplus and consequently discharge at basin level.

Resource surpluses indicate how field-level processes affect the environment, particularly groundwater and surface water in the direct vicinity (Fig. 2, panels C1 and C2). The water and nitrogen surpluses at the field level represent the amount that resource inputs exceed resource outputs. Runoff and excess N from agricultural fields can potentially influence the quantity and quality of surface waters (stream discharge). Excess water can be used for services downstream. However, water surplus (i.e., return flows in the form of runoff and percolation) may pose risks to the environment as well, for example, if the waters have a high N concentration due to elevated N surplus. Water surplus comprises unproductive outflows in the form of evaporation and return flows in the form of runoff to the aquatic environment and recharge to the groundwater. As noted, a minimum water surplus of ~20% is required for leaching to avoid salt build-up in soil (Letey et al., 2011). The N surplus may escape to the atmosphere, it may be washed out into groundwater or surface water, or accumulate in the plant root zone. A minimum N surplus of 10% has been suggested to reduce the risk of N mining; this is calculated by drawing a parallel to the maximum NUE of 90% (Oenema et al., 2015). Falling below the minimum N surplus threshold, particularly in a low N input production system, suggests overexploitation of N from the soil.

Fig. 2 shows for a hypothetical crop production case the mutual dependence between water and N applied in crop production and the relationship between production, RUE and resource surplus. Here Y_a is limited by water input (i.e., the N input is larger than crop N requirements). This example assumes that all essential nutrients are sufficiently available and biotic stresses are fully controlled. Thus Y_a , denoted by the dark star, is on the biophysical production-limiting curve of water (A1) but below the production-limiting curve of N (A2). In this situation, first water and then N limitations should be addressed to reduce the yield gap ($Y_p - Y_a$). This requires a stepwise process of reducing the efficiency yield gap (by improving the timing, space and form of resources applied), the resource yield gap (by applying the growth-limiting resource) and the technology yield gap (e.g., by use of precision agriculture practices or improved varieties). Increasing Y_a to Y_{TE} , denoted by the green star, requires a simultaneous increase of water input (reducing the resource yield gap of water) and NUE (closing the efficiency yield gap of N). To increase the yield further to the level of the highest yielding farmers (Y_{HF}) requires the addition of both water and N (closing the resource gap). As yield increases along the production curve, for example, from Y_{TE} to Y_{HF} , both WUE and NUE decrease. This is particularly the case at high input levels, due to the law of diminishing returns (De Wit, 1992). However, introducing precision agriculture practices (e.g., in crop nutrition and crop protection) and improved crop varieties can help to raise the yield from Y_{HF} to Y_p , which implies closing the technology yield gap ($Y_p - Y_{HF}$). Such interventions are expected to improve RUEs and reduce N surplus to the environment. At Y_{TE} (the green star), production is in the desirable range of WUE and NUE. Further increases in crop yield and RUEs, while still meeting environmental objectives, are relevant for sustainable intensification (SI) of crop production.

2.1.2. Implications of surpluses for water quantity and quality in a river basin

Water and N surpluses may vary across an area and time due to differences in crops (e.g. crop rotations), soils, climate and management at the field and basin level, but also land use across the area. Hydrological processes link practices on farmlands with other landscapes in a river basin (Vörösmarty and Moore, 1991; Burt and

Pinay, 2005). Water or N surpluses that are transferred to groundwater or surface water influence basin water quantity and quality and overall water scarcity. A large part of the N surplus from the land flows into surface water, mostly in soluble form, though also in particulate form, such as in eroded soil.

At the river basin level, the SI assessment framework (Fig. 1) is used to indicate the status of water quantity and quality in relation to sustainable thresholds for water withdrawal, consumption and pollution. Relevant indicators for evaluating water quantity and quality at the river basin level are 1) river discharge (Damkjaer and Taylor, 2017; Vanham et al., 2018), 2) nitrate-N concentration (Sánchez et al., 2007) and 3) nitrate-N load. The EU Nitrates Directive sets a limit of 50 mg L⁻¹ nitrate-N in groundwater (or 11.3 mg N L⁻¹) (Monteny, 2001); while the German Environment Agency has set a limit of 2.5 mg L⁻¹ nitrate-N for surface water (UBA, 2017). No thresholds are currently available for nitrate-N load, which is expressed in g s⁻¹. These thresholds are thought to be consistent with sustainable water use in terms of quality. There are, however, no clearly agreed-upon threshold values for sustainable water use in terms of quantity.

2.2. Demonstration of the SI assessment framework at field and river basin levels

We demonstrate the SI assessment framework using observed data at the field level and river basin level. Field-level data was obtained from the Static Fertilization Experiment at Bad Lauchstädt (latitude 51.40, longitude 11.88), while the basin-level data was obtained from the Selke basin outlet at Hausneindorf (latitude 51.84, longitude 11.26, Fig. 3). Crop production was rainfed in both the experimental field and the Selke basin.

2.2.1. Demonstration at field level

2.2.1.1. Description of the study area. The Static Fertilization Experiment at Bad Lauchstädt (Fig. 3) is located in the loess belt area of the federal state of Saxony-Anhalt in central Germany. The average yearly temperature is 8.9 °C and annual precipitation averages 486 mm. A description of the Haplic Chernozem soil in Bad Lauchstädt is given in Altermann et al. (2005). The Static Fertilization Experiment started in 1902 with the crop rotation sugar beet – spring barley – potato – winter wheat, in eight strips covering 4 ha (description in Körscamps (1994)). There were two treatment factors: (a) application of organic manure, with (a₁) 30 ton per ha farmyard manure every second year, (a₂) 20 ton per ha farmyard manure every second year and (a₃) no farmyard manure; and (b) application of mineral fertilisation, with (b₁) NPK, (b₂) NP, (b₃) NK, (b₄) N, (b₅) PK and (b₆) without NPK. For our investigations the treatments with 20 ton per ha farmyard manure every second year and NPK for winter wheat were selected to mimic average farm practices for this crop in the Selke basin. In the 20 ton per ha manure + NPK treatment, the N applied with mineral fertilisers ranged between 30 and 100 kg N ha⁻¹ (average of 60 kg N ha⁻¹) and neither P nor K were applied with mineral fertilisers over the period of the experiment analysed in this manuscript.

The crop management used in the selected treatment of the Static Fertilization Experiment at Bad Lauchstädt is assumed to represent average farm practices in the agricultural fields of the Selke basin, which are located in the lower part of the basin. Even though the distance between the Static Fertilization Experiment at Bad Lauchstädt and Selke basin is about 60 km (Fig. 3), biophysical conditions in Bad Lauchstädt are similar to those in the lower part of the Selke regarding elevation (is about 100 m amsl), climate conditions (rainfall and mean temperature are 450 mm and 9.0 °C, and 487 mm and 8.7 °C, for the lower Selke and for Bad Lauchstädt, respectively) and soil type (Haptic Chernozem is the dominant soil type in both).

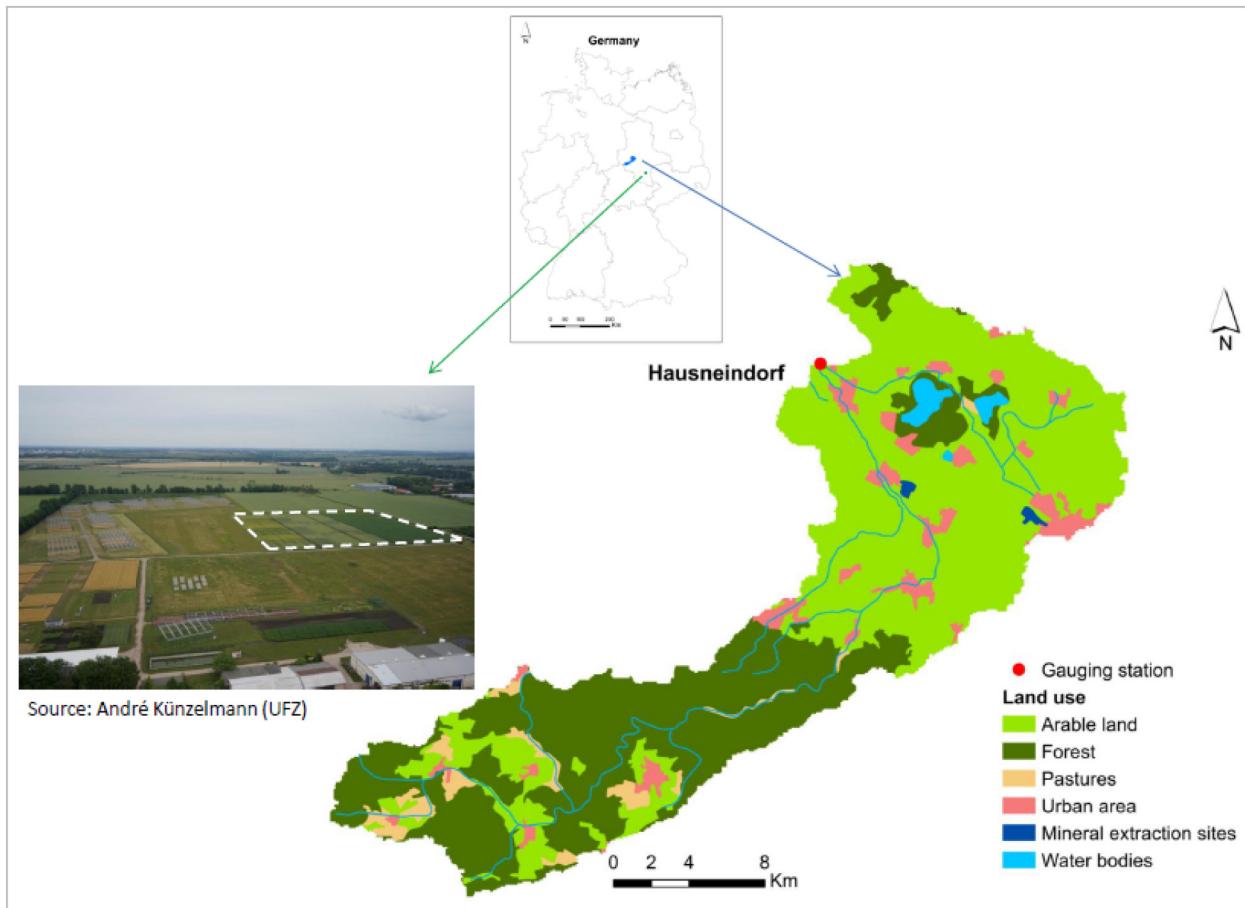


Fig. 3. Geographical location of Bad Lauchstädt and the Selke catchment in central Germany and its dominant land use classes.

2.2.1.2. Methods and data. For the SI assessment at field level, long-term experimental data (1980–2014) were used from the Static Fertilization Experiment at Bad Lauchstädt. The resource balance was analysed for winter wheat under rainfed conditions, as this crop covered about half of all the cropland area in the Selke basin (Fig. A1). The water and N balance for a rainfed winter wheat field were calculated as described in Sections 2.1.1 and 2.1.2. Results of the analyses were assumed to be representative of the conditions of the dominant crop production in the lower Selke basin.

The N balance calculation included crop data (yield and above-ground biomass), N balance data (N manure, N fertiliser, N uptake, N biomass and N yield) and climatic data (Blair et al., 2006). The N input for the winter wheat field was calculated as the sum of N soil, N seed, N mineral, N manure and N deposition. N organic from the manure applied to the root crop and from the stubble in the previous season were assumed as N soil. An amount of N in seed of $3.5 \text{ kg N ha}^{-1} \text{ year}^{-1}$ was assumed based on a seeding rate of 150 kg per ha (Iqbal et al., 2012) and an N content of 2.33% in the wheat grain (Van Duivenbooden et al., 1995). N mineral refers to mineral N applied in the form of mineral fertiliser and that in manure. An N deposition of $58.5 \text{ kg N ha}^{-1} \text{ year}^{-1}$ was assumed; this value being the average N deposition reported over 19 years of the experiment (1978–1996) (Weigel et al., 2000). Updating N deposition for the period between 1996 and 2014 is expected to improve the N balance calculation.

The water balance of the winter wheat crop during 1980–2014 was simulated with the crop model WOFOST (De Wit et al., 2019). WOFOST is a semi-deterministic crop growth model that simulates crop growth and development under potential and water-limited conditions. In the latter case, a soil water balance based on a 'tipping bucket' approach is also simulated with a daily time step. Further details about the crop

soil water routines and assumptions underlying WOFOST are provided by De Wit et al. (2019).

WOFOST simulations of water-limited potential yields, and associated water balance were conducted using daily weather data on solar radiation, minimum and maximum temperature and precipitation. These were obtained from an automated weather station located next to the Static Fertilization Experiment. Simulations were conducted for rainfed winter wheat assuming initial soil moisture at field capacity and no nutrient or biotic stresses and, considering the year-specific sowing and harvesting dates as per the experiment. In general, the model reproduced crop development well, but tended to underestimate maximum yields observed in the experiment (Fig. A2).

Water balance components from WOFOST such as actual evapotranspiration (ET), runoff, percolation and soil moisture change were assumed to reflect the actual water balance components at the experimental site. However, the simulated transpiration and thus evaporation fluxes were thought to be different from that at the experiment site, as the yields differed. Water fluxes may differ due to non-water related constraints, such as nutrient stress and soil-borne diseases, in turn affecting transpiration and harvest-index, as explained by Edreira et al. (2018). Thus, while assuming the simulated and actual ET to be equal, transpiration (T) at the experimental site was adjusted to reflect the observed yield at the site (using Eq. (A1) in the Appendix), thus the adjusted evaporation becomes ET - T. This adjustment considers the conservative transpiration efficiency (TE), which is defined as the ratio of aboveground biomass (AGBM) over transpiration (Passioura, 1977). We took the simulated and actual TE in a particular year to be equal, which assumes that the nutrient and total water availability in a production system are neither too low or too high (De Wit, 1958).

2.2.2. Demonstration at river basin level

2.2.2.1. Description of the study area. The Selke is a tributary of the Bode River in south-west Saxony-Anhalt (Fig. 3). The Selke originates from Harz Mountain (605 m), flowing from there to the outlet gauging station at Hausneindorf (53 m). The basin-level data used in this study were collected at this gauging station. The upper part of the Selke basin is dominated by broad-leaved, coniferous and mixed forest. The lower part is dominated by arable land. Main crops in the catchment are winter wheat, rapeseed, winter barley, sugar beet and corn (Fig. A1 in the Appendix shows the area share of each crop). The Selke basin has different soil types, though Cambisols predominate in the mountain area and Chernozems are more common in the lowlands (Jiang et al., 2014). Average annual precipitation across the whole catchment is about 660 mm, though rainfall amounts range from 792 mm in the mountain areas to 450 mm in the lowlands. The mean temperature is 9.0 °C, with monthly averages varying between −1.8 °C in January and 15.5 °C in July.

2.2.2.2. Method and data. To assess SI at the river basin level, we used a long-term time series of observed daily discharge and biweekly nitrate-N data (Fig. A3 in the Appendix) at Hausneindorf in the Selke basin (Rode et al., 2016). The average discharge and nitrate-N concentration for the period 1993–2014 were $1.67 \text{ m}^3 \text{ s}^{-1}$ and 3.6 mg L^{-1} , respectively.

Two sets of consecutive wet, intermediate and dry years were identified from 1993 to 2014 using the observed discharge and precipitation data. These years were selected to examine the relationship between agronomic practices at field level and water quantity and quality (nitrate-N) at the basin level. The dry and wet years in the current study is defined at 12-month standardised precipitation index (SPI) and 12-month standardised streamflow index (SSI); streamflow here meaning discharge. To estimate the SPI and SSI, a tool from the website of the National Drought Mitigation Center was used (McKee et al., 1993). Fig. A4 in the Appendix presents the indices from 1993 to 2014. A year was defined as dry when both the 12-month SSI and 12-month SPI were less than zero, and a year was considered to be wet if these indices were greater than zero. An intermediate year was defined as one between the dry and wet years. Thus, 2001, 2002 and 2003 is one set and 2006, 2007 and 2008 is another set of dry, intermediate and wet years, respectively.

The observed nitrate-N concentration at Hausneindorf was compared to the thresholds set by the German Environment Agency for surface water (2.5 mg L^{-1} ; UBA, 2017).

3. Results

3.1. Field-level assessment

There was no clear relationship between winter wheat yields, water or N input across different years (Figs. 4, A1 and A2). Winter wheat yields stabilized in the high water or N input ranges. This is because the winter wheat yield, in the high water or N input ranges, had reached its biophysical limit (which was estimated to be ca. $7\text{--}11 \text{ t ha}^{-1}$, Fig. A2). Variation in winter wheat yields at the same input levels could be due to abiotic stresses caused by differences in the timing and intensity of precipitation events, which could also affect N availability. It might also be due to cultivar differences, inefficient nutrient application and pests and diseases.

In Fig. 4, B1 and B2, the WUE and NUE panels show the relationship between resource input and resource output for water and N, respectively. The productive resource output (T or N) at harvest did not respond to increased water and N inputs in different years. In most years, winter wheat treatments at the experiment site showed WUE within the desirable range (17%–100%) and NUE within the desirable range (50% to 90%). However, most of the time, the N surplus was

outside the desirable range, exposing the environment to a large N surplus. The water and N surpluses, in general, increased with increasing water and N inputs, as is evident in the water and N surplus panels (Fig. 4C).

3.2. Basin-level assessment

Fig. 4D shows the discharge, nitrate-N concentration and N load in the Selke basin for consecutive years that were dry (2006), intermediate (2007) and wet (2008). The discharge increases from the relatively dry year (2006) to the intermediate (2007) and wet year (2008) (Fig. 4D). This is in line with increasing water input (in the form of soil moisture and precipitation) and water surplus at the field level from 2006 to 2008 (see Fig. 4, C1). The water input and surplus at the field level was greater during the intermediate year (2007) than in the wet year (2008), though discharge to the river was higher in that year (2008) than in 2007. This is because not all water surpluses at the field level in 2007 became runoff. Some of the water surplus evaporated or replenished soil moisture, after the preceding relatively dry year (2006). Both runoff and groundwater recharge at the field level increased from dry to wet years; that is, from 2001 to 2003 and from 2006 to 2008 (Fig. A4). This was accompanied by increasing basin-level discharge (see Fig. A4 for 2001 to 2003 and Fig. 4D, blue box plots, for 2006 to 2008).

The water quality indicators (Fig. 4D), including nitrate-N concentration (grey box plots) and nitrate-N load (orange box plots), can be explained by water surplus at the field level throughout the basin, leading to increased basin-level discharge. Water surplus at the field level was greater in relatively wet years (2003 and 2008), compared to relatively dry years (2001 and 2006). As a result, the nitrate-N load was higher in wet years than in dry years. The nitrate-N concentration was, however, higher in dry years than in wet years, due to the limited dilution in the streams. The average nitrate-N concentration (3.6 mg L^{-1}) in the Selke basin was slightly higher than the threshold set by the German Environment Agency, which is 2.5 mg L^{-1} nitrate-N in surface water (UBA, 2017). In dry years, such as 2006, the nitrate-N concentration was 4 mg L^{-1} , and it significantly exceeded the threshold set for surface water (see Fig. 4D). Results at river basin level thus confirm that exceeding the threshold of $80 \text{ kg N ha}^{-1} \text{ year}^{-1}$ at field level leads to environmental impacts. In our assessment, variability in water quality is mainly explained by weather patterns.

Each cropping or hydrological year was distinct with regard to yield, RUE and resource surplus at the field level, as well as discharge and nitrate-N concentration and nitrate-N load at the basin level. The uniqueness of the years could be due to differences in the amount or distribution of precipitation, and differences in agronomic practices, such as sowing dates, crop varieties and fertilisation schedules. However, interrelated patterns were found between precipitation, discharge and nitrate-N load and concentration. Nitrate-N concentration was relatively high when the discharge was low, and vice versa. This pattern at the basin level seems to be generic for all years from 1993 to 2014 (Fig. A3 in the Appendix).

4. Discussion

4.1. Framework

The SI assessment framework introduced in this paper considers three field-level indicators for water and N use: crop production, RUE and resource surplus. At the river basin level, three indicators were also examined: discharge, nitrate-N concentration and N load. We quantified these and explored sustainable thresholds building on previous studies related to yield response to water and N input (De Wit, 1992); findings of the EU Nitrogen Expert Panel (Oenema et al., 2015); and water quality standards set by the EU Nitrates Directive (Monteny, 2001), the EU Water Framework Directive and the German

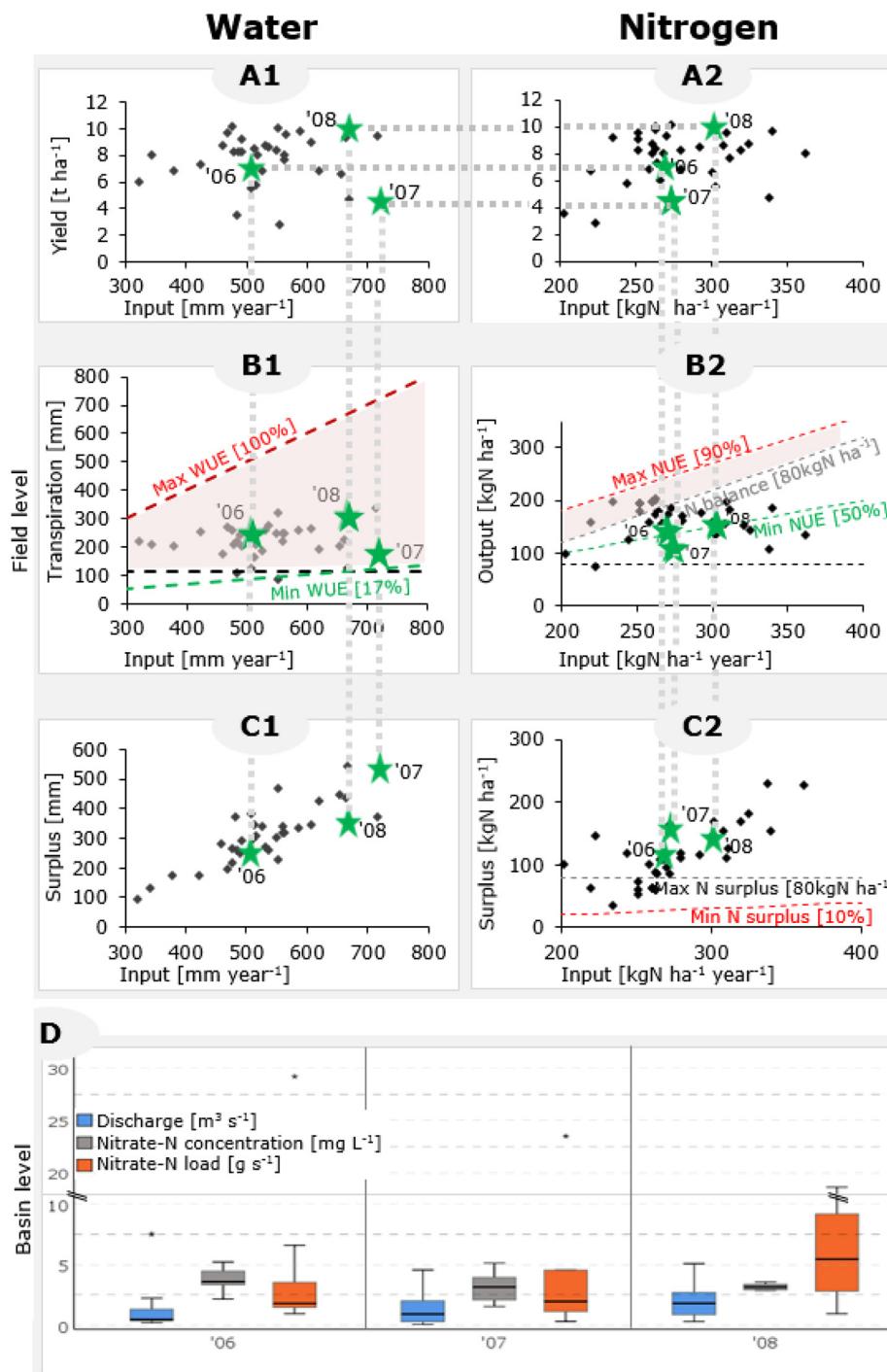


Fig. 4. Observed data from 35 years (1980–2014) depicting the relationship between crop production and water and N input (A1 and A2, respectively), use efficiency of water and N (B1 and B2, respectively), and surplus of water and N (C1 and C2, respectively) for winter wheat production at the field level (Static Fertilization Experiment at Bad Lauchstädt). The minimum water surplus is zero for this case, as salt build-up is not a problem. The box plots (D) show the variation in discharge (blue box plot), nitrate-N concentration (grey box plot) and nitrate-N load (orange box plot); discharge was measured daily and nitrate-N was measured biweekly at Hausneindorf, for the years 2006 (dry year), 2007 (intermediate year) and 2008 (wet year) in the Selke basin. The lower boundary of the box indicates the 25th percentile, a line within the box marks the median, and the upper boundary of the box indicates the 75th percentile. Whiskers above and below the box indicate the 10th and 90th percentiles. The asterisks denote extreme values. (For interpretation of the references to colour in this figure, the reader is referred to the web version of this article.)

Environment Agency (UBA, 2017). No standards have yet been set for water quantity and nitrate-N load in a streamflow, which calls for action by policymakers.

We must be cautious in applying the reported threshold values to local assessments. The threshold values are approximate for rainfed winter wheat production and consider practices, policies and experiences in the EU. Even within the EU, the indicators and framework

require tailoring to the context under study, notably the local environmental setting and conditions. The threshold values for grain yield, N output and transpiration were derived from the lower N output value assumed by the EU N-expert panel (Oenema et al., 2015). Obviously the latter (80 kg N output ha⁻¹) is an arbitrary value and way lower than current production levels in Germany (Weiser et al., 2018) and other parts of NW Europe (Schils et al., 2018), which for wheat are

above 7 t ha⁻¹. Clearly, economic criteria will be important to establish acceptable lower limits of grain productivity, and thus N output and transpiration values. The upper threshold of NUE of 90% was proposed by the EU N-expert panel to avoid the risk of soil mining. This may, however, not be immediately relevant in regions with high soil nutrient availability due to long-term fertiliser application or high natural soil fertility (Janssen, 2017). In such cases, an NUE of >90% would not lead directly to soil N mining.

In addition, the maximum WUE and minimum water surplus (leaching fraction) depend on soil salinity, crop salt tolerance and the amount of precipitation (Hanson et al., 1999). In areas where salt build-up is not a threat or where percolation in the off-season naturally controls salt build-up, the threshold values for the maximum WUE and the minimum water surplus (leaching fraction) should be adjusted. In that case, the threshold value for the maximum WUE can be 100%, and the required water surplus (i.e., percolation fraction) can be zero. A WUE of 100% will however be difficult to reach, as crops are only cultivated during the growing season and some soil evaporation is unavoidable also during the growing season.

For simplicity, the SI assessment framework focuses on N and water but does not cover P. In developing P related thresholds, one should consider the unique nature of P compared to N. For the P balance computation, the legacy of soil P is very important. P recovery (the fraction of the applied P harvested with yield) in a particular year is generally low, often around 10–15% (Roberts and Johnston, 2015), which could suggest an enormous P surplus and potential for environmental degradation. However, much of this P accumulates in the soil and becomes available for crop uptake in later years (Syers et al., 2008; Sattari et al., 2012). Studies show that, after continuous fertilisation, the ratio of P harvested to P applied can exceed 90% (Johnston and Syers, 2009; Roberts and Johnston, 2015). Thresholds for P use need to account for N:P ratios in the crop and for the historical use of P. For the latter the average P balance of agricultural lands in EU states, reported in EUROSTAT (2018), could be used.

4.2. Sustainable intensification in the Selke basin

Sustainable intensification of crop production requires balancing indicators at field and river basin levels. Average nitrate-N concentration at the Hausneindorf outlet of the Selke basin was 3.6 mg L⁻¹. This is greater than the target maximum of 2.5 mg L⁻¹ nitrate-N set by the German Environment Agency to ensure the ecological health of surface water (UBA, 2017). The results of our case study suggest that excess N at the field level translates into high nitrate levels at the outlet of the river basin (Fig. 4B2, C2 and D). Yet, considering the high N surplus at the field level, a higher nitrate-N concentration in the stream was expected. The divergence may be explained by N being retained in the soil and groundwater, and taken up by natural vegetation, or emitted to the atmosphere before it could enter the stream (Klein, 2008). Alternatively, dilution in the total amount of runoff entering the stream may also have occurred. Determining the cause of this divergence with any certainty would require a more detailed exploration of the fate of field N surplus, such as N pollution of surface water and groundwater, and the emission of N₂O (a greenhouse gas) and NH₃ (depositing N in nature areas).

The current assessment at the basin level was simplified as it focused on a single crop with an average crop management practice. We acknowledge that analysing SI at basin level requires going beyond improvements in crop management at the field level. For instance, the choice of crops, crop rotations and farming practices, and their interplay at landscape level, have also been shown useful to reduce stream N loads in other catchments in Germany (e.g., Jomaa et al. (2016)). This makes it very difficult to evaluate the exact impact of crop management practices on water quality for individual years and hence, to infer possible environmental impacts of single year interventions. As such, weather patterns may be a better proxy for environmental impacts at

basin level than average crop management practices used at the field level and options to mitigate such externalities need to consider past history in addition to present situation. Future modelling studies can help clarifying the efficacy of different field and landscape level interventions in reducing stream N loads at catchment scale in both the short- and the long-term.

In the Selke catchment, the scope for intensification of winter wheat is limited as the crop yield in the high input ranges has approached its biophysical potential, but there is scope for increased stability and sustainability. Several water and fertiliser management measures can be considered at the field level. In the Selke basin, improved soil moisture management and supplementary irrigation might help to control the water stress caused by unevenly distributed precipitation, which may limit nutrient uptake and cause high N surplus. Future precision agriculture should seek to match the application and availability of water (irrigation) and fertiliser vis-à-vis the crop demand in time and space. For instance, improving water management, particularly in dry years, also promotes N uptake by crops and NUE, while reducing N surplus. Managing the amount, timing, location and form of inputs (e.g., through variable rate application and slow-release fertiliser) and residue management could improve the N recovery fraction and NUE (Hirel et al., 2011), and thus reduce the N surplus to surface water and groundwater (Chukalla et al., 2018). Other ways to potentially improve NUE are better management of biological stresses, such as weeds, pests and diseases; enhanced crop management, for example, by optimising crop rotations, planting dates, planting densities and crop varieties; and application of conservation tillage. Co-identifying agricultural measures in close collaboration with the agricultural agencies and farmers can help to consider site-specific conditions and have a high chance of implementation (Rode et al., 2009). In addition to these field measures, the N joining water sources could be reduced at the river basin level by implementing cover crops and crop rotations (Hashemi et al., 2018), and other land use changes (Jomaa et al., 2016).

Further research is recommended to identify the fate of field N surplus and the effectiveness of combinations of the measures listed at both the field and basin levels in improving NUE and reducing N surplus in the Selke basin. In this regard, the availability of long-term data at the field and basin levels and the coordination of expertise in agronomy, hydrology, water management and environmental protection will remain valuable for the study of SI and its environmental impacts but will also complicate future SI assessments in other catchments where long-term data are not collected or not readily available. Therefore, alternative methods and approaches based on e.g. remote sensing could prove useful to help upscaling resource use efficiencies and environmental impacts from the field to the catchment scale (Bastiaanssen et al., 2000).

5. Conclusion

This paper introduced an SI assessment framework that can help decision-makers in agricultural land and water management to evaluate whether SI indicators, particularly crop production, resource-use efficiency and environmental (water) quality are balanced in a river basin.

The framework was demonstrated using time-series data (1980–2014) for winter wheat production from the Static Fertilization Experiment at Bad Lauchstädt and observed discharge and nitrate-N data (1993–2014) in the Selke basin. Field and river data were collected over a long period of time for agricultural and environmental indicators separately. The main interaction between the field and river basin levels was in runoff and groundwater recharge at the field level, which directly impacted discharge and nitrate-N concentration at the river basin level. At the field level, WUE fell within the assumed desirable range in all of the years, meaning that water use in crop production was efficient. However, NUE indicators, particularly N surplus, fell outside the desirable range in most years. This resulted in exceedance of the target value for nitrate-N concentration at the basin level, although weather

also strongly impacted nitrate-N values. In dry years, nitrate-N load was smaller compared to wet years, but nitrate-N concentrations in surface water were higher. Reducing N surplus at the field level would be required for the environmental objectives to be achieved, specifically in dry years. From this result, we can conclude that stakeholders wishing to introduce environmental improvement measures first need to understand the environmental setting and conditions and be clear on the main aim pursued. To achieve SI of crop production in Selke basin, soil moisture management and irrigation are required to stabilize high yields, and reduce N surpluses at field level. However, irrigation comes with costs and its economic viability must be considered. In addition, optimum use of chemical fertiliser and manure help to reduce the N concentration below the set water quality standards in the Selke basin.

The proposed SI assessment framework constitutes a crucial first step in the development of a practical tool to inform decision-makers in agricultural land and water management on alternative pathways to sustainable intensification of crop production and the effects of different options on the environment (particularly on water resources).

The framework integrates scientific insights with experiences from practice in the fields of agronomy, hydrology, and agricultural and water resources management. As such, the framework can serve as a starting point for SI assessment at a specific production site or in a wider region, within or beyond the EU. Stakeholders aiming to increase

production while maintaining environmental integrity can apply the SI assessment framework for multiple purposes: (i) for benchmarking a crop production system or comparing SI indicators such as productivity, RUE and resource surplus at different production sites and over time; and (ii) for comparing the impact and potential of different agricultural measures and strategies in terms of SI outcomes. For more comprehensive SI assessments, the framework should be extended through adding socio-economic and equity aspects and widening the environmental scope beyond a river basin.

Declaration of competing interest

There is no conflict of interest.

Acknowledgements

This research was conducted as part of the investment theme Resource Use Efficiency (RUE) funded by Wageningen University and Research. The authors gratefully acknowledge the WaterFARMING project (grant agreement 689271) for the data.

$$T_{\text{Experimental site}} = AGBM_{\text{Experimental site}} * \frac{T_{\text{WOFOST}}}{AGBM_{\text{WOFOST}}} \quad (\text{A1})$$

Appendix A

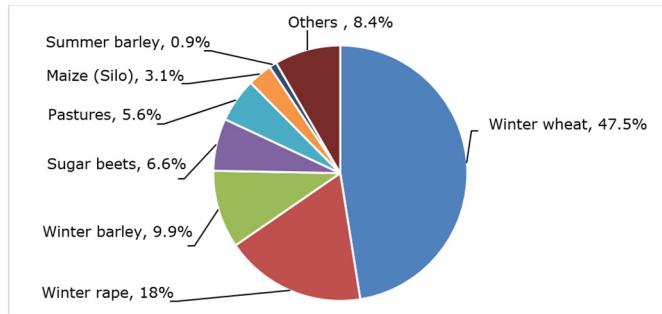


Fig. A1. Typical distribution of crops grown in Selke basin (average over the years).

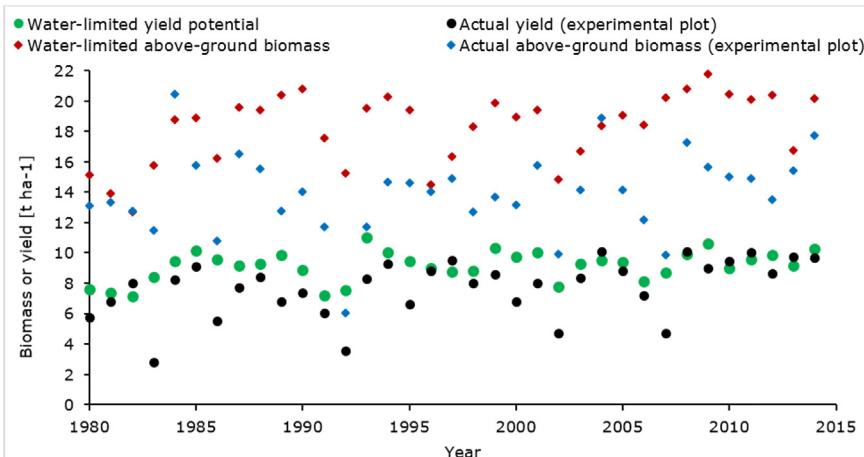


Fig. A2. Wheat yield and above-ground biomass of WOFOST simulated and experimental data (from different plots) at the extended Static Fertilization Experiment, Bad Lauchstädt, Germany, 1980–2014.

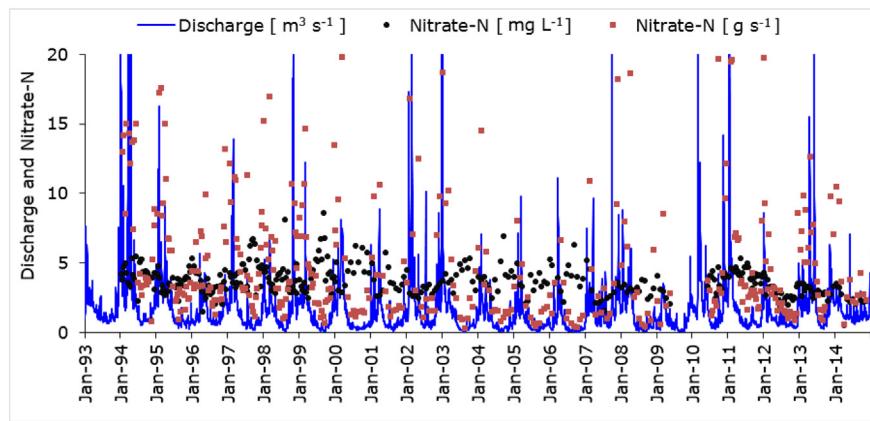


Fig. A3. Discharge, nitrate-N concentration and nitrate-N load at Hausneindorf, Selke basin, 1993–2014.

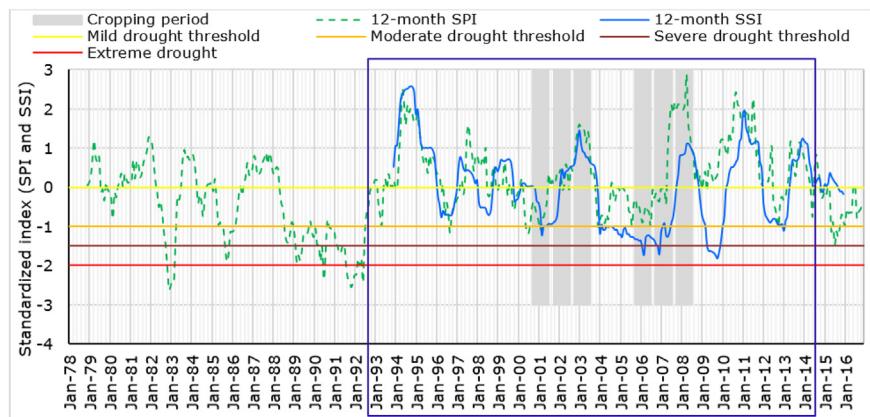


Fig. A4. The cropping periods of two consecutive dry, intermediate and wet years (2001–2003 and 2006–2008) in Selke basin. The SPI and SSI are the standard precipitation and stream indices. SPI and SSI were estimated using a tool from the website of the National Drought Mitigation Center.

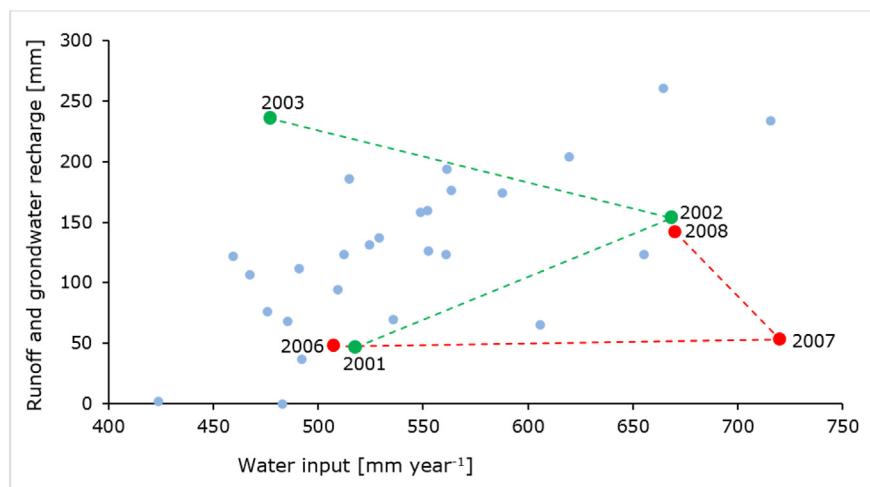


Fig. A5. Water input versus runoff and groundwater recharge for two sets of consecutive years (2001–2003 and 2006–2008) with relatively increasing water inputs at the extended Static Fertilization Experiment, Bad Lauchstädt, Germany.

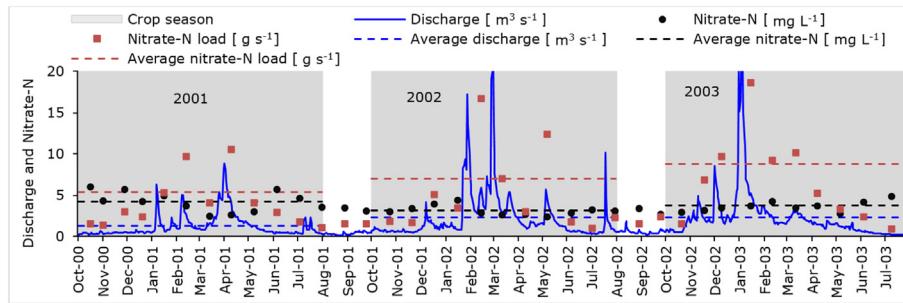


Fig. A6. Discharge, nitrate-N concentration and nitrate-N load for consecutive dry, intermediate and wet years (2001, 2002 and 2003) in Selke basin. Average discharge, average nitrate-N concentration and N load are represented by the blue, dark and orange dashed lines, respectively.

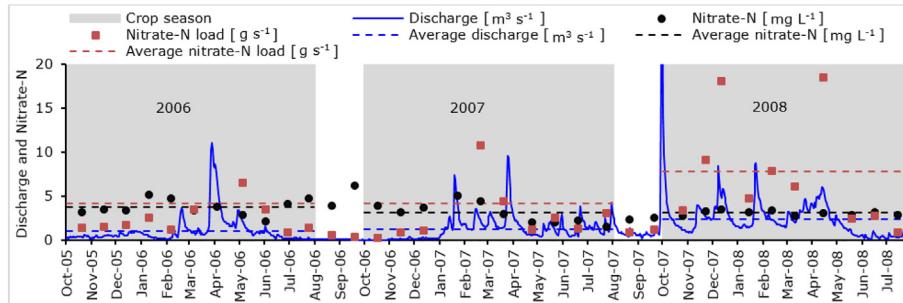


Fig. A7. Discharge, nitrate-N concentration and N load for consecutive dry, intermediate and wet years (2006, 2007 and 2008) in Selke basin. Average discharge, average nitrate-N concentration and N load are represented by the blue, dark and orange dashed lines, respectively.

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