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### Key Points:

- Parsimonious crop responses to Nitrogen fertilizer are derived from agricultural experimental data and upscaled by catchment N modeling
- Integrating agricultural budgets and catchment modeling reveals spatio-temporally different agri-environmental behaviors across scales
- The integrated analysis provides implications for targeted mitigation measures under varying climatic conditions and fertilizer inputs

### Supporting Information:

Supporting Information may be found in the online version of this article.

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## Functional Multi-Scale Integration of Agricultural Nitrogen-Budgets Into Catchment Water Quality Modeling

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**Abstract** Diffuse Nitrogen pollution from agriculture maintains high pressures on groundwater and aquatic ecosystems. Further mitigation requires targeted measures that reconcile agricultural interests in environmental protection. However, the agriculture-related processes of catchment N modeling remain poorly defined due to discipline-specific data and knowledge gaps. Using field-experimental data, crop N uptake responses to fertilizer management were parsimoniously conceptualized and integrated into a catchment diffuse-N model. The improved catchment modeling further facilitated integration with agricultural budget-based assessments. The integrated analysis in a mesoscale catchment disentangled contrasting agri-environment functional mechanisms in typically flashy chemodynamic and transport-limited chemostatic export regimes. Moreover, the former was actively responsive to interannual climatic variability and agricultural practices; the latter exhibited drought-induced enhancement of N enrichment, which could likely be mitigated through reduced fertilization. This interdisciplinary integration of data and methods provided an insightful evidence base for multi-sector targeted measures, especially under cumulative impacts of changing climate and fertilizer-use intensities.

**Plain Language Summary** Due to intensive nitrogen fertilizer use in agriculture over recent decades, excessive nitrogen has largely accumulated in soil and groundwater systems and is gradually being released to surface waters, polluting aquatic environments. Considering the changing climate and growing food demand, future environmental mitigation should pursue actions that specifically target high-risk areas and periods in order to better reconcile agricultural demand and environmental protection needs. This study integrated long-term agricultural data sets into catchment nonpoint N pollution modeling, in ways that are methodologically complementary and provide interdisciplinary benefits. The integrated analysis advances scientific understanding of important catchment agri-environmental processes that are coupled both spatially and temporally. The enhanced knowledge base can further support decision-making for sustainable solutions between the needs of agriculture and the water environment.

## 1. Introduction

Agricultural nitrogen (N) pollution has become the major pressure on inland and coastal aquatic ecosystems (Reusch et al., 2018; Van Meter et al., 2018). Meanwhile, agricultural intensification remains one of the main strategies to satisfy increasing global food demand (Chukalla et al., 2020; Schils et al., 2018). Overarching policies for sustainable development are increasingly calling for better reconciliation of agricultural interests with environment protection needs and further development of cost-effective and targeted measures, especially under changing climatic conditions (EEA, 2020a, 2020b; Reusch et al., 2018).

In agricultural research, budget methods are commonly used to assess nitrogen use efficiencies and potential environmental impact (Cassman et al., 2002). The latter is often indicated by N surplus (input minus output) and assessed based on readily available data from the farm gate to national scales (Eurostat, 2013). The budgeting methods provide a clear evidence base of complex relationships between agricultural activities and environmental responses and therefore are particularly favorable for communicating to policy makers (Cherry et al., 2008; Zhang et al., 2020). However, in addition to potential uncertainty embedded in data acquisition (Oenema et al., 2003), it is well recognized that budget calculations only provide estimates of potential N losses, and their credibility

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is largely restricted to site-specific assessment stages, potentially lacking transferability across spatio-temporal scales (Cherry et al., 2008; Zhang et al., 2020).

Catchment science provides complementary information on N dynamics and actual N loss pathways in catchment systems. Many process-based catchment water quality models have been proposed with continuously improved representations of multi-scale processes and their spatio-temporal variability (Rode et al., 2010; Wellen et al., 2015; Yang et al., 2018). Moreover, spatially differentiated catchment N responses to climatic variability and agricultural management practices can be further investigated. However, due to poorly understood mechanisms of crop/plant N-uptake (Fatichi et al., 2016), catchment models typically employ highly simplified approaches in conceptualizing the potential N-uptake (e.g., using the logistic growth function (Lindström et al., 2010), or relating to biomass calculations according to optimal N contents (Arnold et al., 1998)). The parameterization is often generically determined as a static boundary condition and excluded from further modeling evaluations (Rode et al., 2010). Specifically for N-fertilization, its effects are often taken as relaxing soil N constraints, while overlooking the enhanced effects on crop growth rates and agronomic yields that are evidenced from experimental data (Gastal & Lemaire, 2002; Merbach & Schulz, 2013). As such, catchment water quality modeling is generally weak in capturing crop growth and yield variations in correspondence to different fertilization practices. This further hinders its integration with budget-based assessments.

Here, we argue that agricultural advances should be better integrated into catchment modeling and that bridging N-budget assessment and water quality modeling is increasingly necessary for evaluating targeted measures at larger scales. In this study, we parsimoniously extracted crop N-uptake information using agricultural fertilization experimental data and further integrated this into a catchment diffuse-N model (the mHM-Nitrate model (Yang et al., 2018)). With the improved modeling, we implemented an integrated analysis of N-budgets and N-modeling in the highly heterogeneous Selke catchment (456 km<sup>2</sup>, central Germany). The objectives of this study were as follows: (a) to upscale the experiment-data informed approach to the catchment scale and to validate its performance based on available survey data; (b) to illustrate dominant agri-environmental processes and their spatio-temporal dynamics at scales from arable fields to the whole catchment; and (c) to estimate agricultural N-budgets and catchment responses under varying climate, landscape and management conditions. The interdisciplinary integration of data and methods could provide insights into catchment agri-environmental functioning and management implications for further targeted measures with associated impacts of the changing climate.

## 2. Materials and Methods

### 2.1. The mHM-Nitrate Model and Crop N-Uptake Process Descriptions

The grid-based catchment hydrological and nitrate model (Yang et al., 2018; Yang & Rode, 2020) is developed based on the hydrological platform mHM — the mesoscale hydrological model (Kumar et al., 2013; Samaniego et al., 2010). Nitrate process descriptions are mainly introduced from the widely used HYPE (Lindström et al., 2010) and INCA models (Wade et al., 2002), with specific implementations for spatial distributions of crop rotation. Advanced process descriptions and the flexible multi-scale structure ensure the model representations of spatial heterogeneity that are induced by natural conditions and anthropogenic activities (Yang et al., 2018, Yang, Jomaa, Bütter, & Rode, 2019). The model structure and parameters are briefly described in Supporting Information (Text S1 and Table S1 in Supporting Information S1).

Following the SOILN method implemented in the HYPE model (Lindström et al., 2010), a three-parameter logistic function is used to estimate the accumulation of potential N-uptake  $\bar{P}_{uptk}$ ,  $kgN ha^{-1} yr^{-1}$  during the growing season:

$$\bar{P}_{uptk} = \int_{DOS}^{DOH} p_{uptk} dD \quad (1)$$

$$p_{uptk} = up1 \cdot up2 \cdot up3 \cdot \frac{help}{(up2 + help)^2} \cdot UT$$

$$help = (up1 - up2) \cdot e^{-up3 \cdot DAS}$$

where  $p_{uptk}$  denotes the daily potential uptake between the date of sowing (DOS) and the date of harvest (DOH);  $up1$ ,  $up2$  and  $up3$  denote the logistic-function parameters; DAS denotes the number of days after sowing. With the unit transform constant ( $UT = 10$ ), parameter  $up1$  is equivalent to  $\bar{P}_{uptk}$ . The actual daily crop uptake ( $a_{uptk}$ ) for each soil layer is further limited by the soil water factor ( $f_{sm}$ ) and Nitrate-N pool ( $IN_{pool}$ ):

$$a_{uptk} = \min(p_{uptk}, f_{sm} \cdot IN_{pool}) \quad (2)$$

where  $f_{sm} = \begin{cases} (sm - wp)/sm, & sm > wp \\ 0, & sm \leq wp \end{cases}$  represents soil water constraint, depending on actual soil moisture ( $sm$ ) and the wilting point ( $wp$ ).

## 2.2. Potential N-Uptake Responses to Fertilization

The most crucial challenge is to determine  $\bar{P}_{uptk}$  under specific fertilizer applications. Empirical curve-style methods are commonly used to extract crop physio-agronomic characteristics based on agricultural fertilization experiments (Cerrato & Blackmer, 1990; Reid, 2002). Likewise, we propose a parsimonious method of estimating  $\bar{P}_{uptk}$  as the sum of the potential uptake under zero fertilizer ( $\bar{P}_{0uptk}$ ) and the increase of potential uptake ( $\Delta P$ ) under different fertilizer levels ( $N_{fert}$ ):

$$\bar{P}_{uptk} = \bar{P}_{0uptk} + \Delta P(N_{fert}) = \bar{P}_{0uptk} + a + b \cdot \ln(N_{fert}) \quad (3)$$

where  $a$  and  $b$  denote parameters of the natural logarithm response curve, to be fitted through data from fertilization experiments. We introduced two assumptions: (a)  $\bar{P}_{0uptk}$  is equivalent to 95% quantile of measured actual N-uptake under zero fertilizer application, and (b)  $\Delta P$  is equivalent to that of measured actual N-uptake ( $\Delta uptk$ ) under different fertilizer levels.

## 2.3. Agricultural N Budget and Surplus Calculations

Different budget methods with varying degrees of complexity are suggested according to assessment system boundaries and scales (Eurostat, 2013). Here, we adopted the soil surface budget definition, where N input consists of fertilizer/manure application and atmospheric deposition, and N output is the crop N-uptake in the harvested yield (Oenema et al., 2003; Poisvert et al., 2017). The soil surface budget provides a simple method that is sensitive to agricultural N sources and can be applied to various scales (Cherry et al., 2008). The resulting surplus is therefore available for soil biogeochemical processes (e.g., denitrification and transformation into soil biomass) and hydrological transport (e.g., leaching to groundwater and exporting to surface waters).

## 3. Study Sites and Data

### 3.1. The Selke Catchment and Data Collection

The mesoscale Selke catchment (456 km<sup>2</sup>, central Germany; Text S2 and Figure S1 in Supporting Information S1) exhibits marked hydro-climatic and physiographic gradients from upper mountainous areas to lowland arable areas. Elevation decreases from ca. 600 to 100 m, with annual precipitation decreasing from 790 to 450 mm. Drainage from the heterogeneous landscape is captured by three nested gauging stations, from the uppermost arable forest mixed (station Silberhütte), to the middle forest-dominant (station Meisdorf), and to the lower intensive arable-dominant lands (the outlet Hausneindorf; Figure S1 in Supporting Information S1). The upland areas are predominated by shallow schist and wacke, with overlying Cambisols; the lowland areas are part of the loess region with overlying Chernozems and small patches of highly sandy soils near the outlet (the German soil map, BGR (2013)). We reclassified three types of representative arable lands, that is, loamy-loess lowlands, sandy-loess lowlands, and uplands, and selected grid cells (1 km<sup>2</sup>) with arable areal share >0.9 (Figure S1 in Supporting Information S1).

Agricultural activities have long been conducted in both upland and lowland arable areas. Major crops were winter wheat, winter rapeseed and sugar beet (only in the lowland region) as reported in a detailed survey from the local authority in 2009 (Table S2 in Supporting Information S1). Detailed fertilizer application rates and

measured actual N-uptake for each major crop were also uniquely available in the upland and lowland regions (Table S2 in Supporting Information S1).

We set up daily simulations for 2010–2018 (with a spin-up period of 2005–2009) at  $1 \times 1$  km spatial resolution. Meteorological forcing (from the German Weather Service) and geographic model inputs were collected and prepared for the mHM-Nitrate model (Table S3 in Supporting Information S1). Following the Dynamically Dimensioned Search method used by Yang et al. (2018), daily discharge and nitrate-N ( $\text{NO}_3^-$ -N) concentration data at the three gauging stations were used for the multi-criteria model calibration (Text S3 in Supporting Information S1). Additionally, seasonal soil mineral N measurements were available at Siptenfeld ( $51^\circ 39'$  N,  $11^\circ 03'$  E). Due to the lack of detailed information on crop distributions in specific years, we used unique crop type per year, following rotation sequences of winter wheat — sugar beet — winter rapeseed in the lowlands, and winter wheat — winter rapeseed in the uplands. Then, the model simulations were repeated with different starting crops. As such, each crop was simulated under weather conditions from 2010 to 2018.

### 3.2. Fertilization Experimental Sites and Data Collection

Field experimental data of winter wheat and sugar beet were collected from the UFZ-Research Station Bad Lauchstädt ( $51^\circ 23'$  N,  $11^\circ 52'$  E; 118 m a.s.l.), located in the same lowland region as the Selke catchment (75 km southeast, Figure S1 in Supporting Information S1). In 1978, the Extended Static Fertilization Experiment was set up, with the crop rotation of winter wheat, sugar beet, spring barley and potato (Merbach & Schulz, 2013). We collected the N-uptake data over 1980–2016, including 10-year's winter wheat and 9-year's sugar beet data. Parallel N fertilizer treatments were 0, 40, 80, 120 and 160  $\text{kgNha}^{-1}$  for winter wheat, and 0, 60, 120, 180 and 240  $\text{kgNha}^{-1}$  for sugar beet (Yang, 2022).

Rapeseed data were retrieved from Rathke et al. (2005). The experiment was conducted at a nearby station (Leipzig-Seehausen, ca. 50 km west of Bad Lauchstädt) during 1995–2000. Crop N-uptake was calculated based on the values of seed yield and N content provided in Rathke et al. (2005). Parallel rates of 0, 80, 160, and 240  $\text{kgNha}^{-1}$  were applied from mineral and organic fertilizer trials (100% and 60% eligible, respectively; Rathke et al. (2005)). Details of all experimental data and preprocessing were provided in Text S2 in Supporting Information S1.

## 4. Results

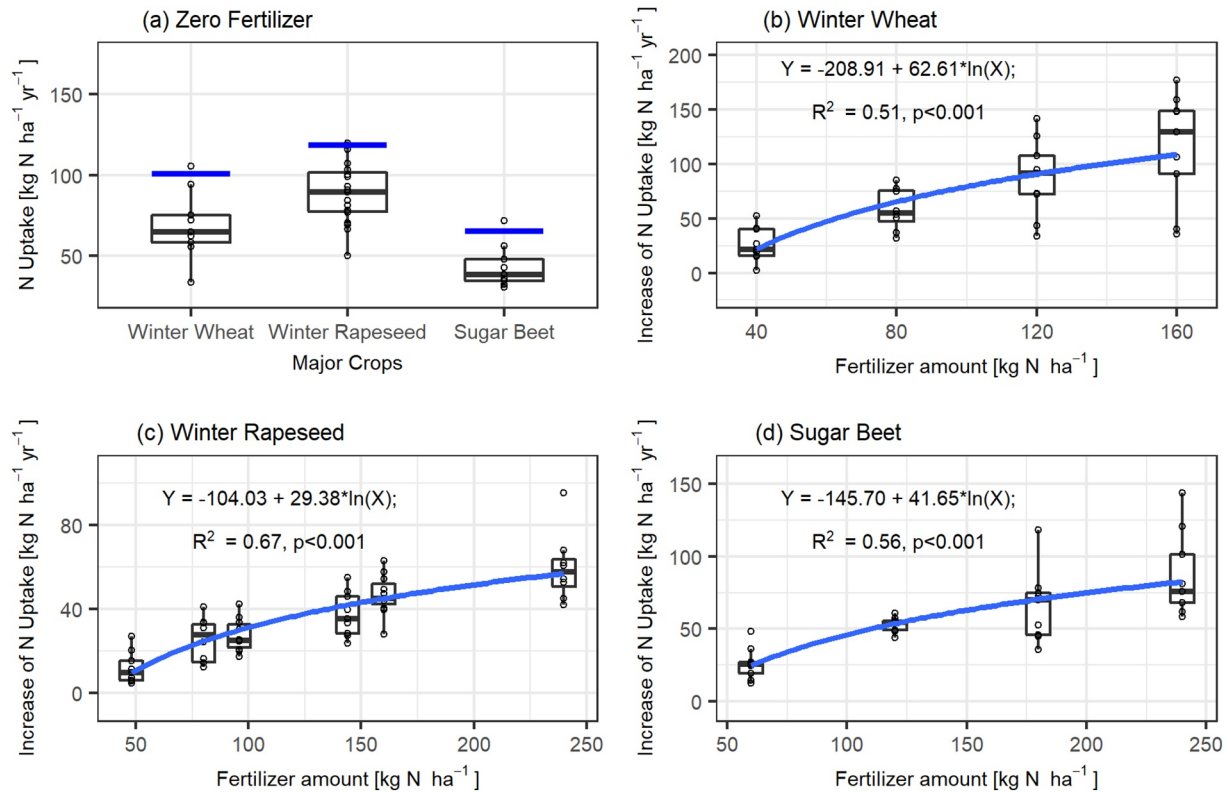
### 4.1. Potential N-Uptake Under Different Fertilizer Levels and Catchment Upscaling

Measured crop N-uptake showed large interannual variations for all parallel treatments (Figure 1). The potential uptake  $\bar{P}_{0uptk}$  (95% quantile under zero fertilizer) were 100.9, 118.4, and 65.4  $\text{kgNha}^{-1} \text{yr}^{-1}$  for wheat, rapeseed and sugar beet, respectively (Figure 1a). The uptake increases  $\Delta uptk$  under specific fertilizer levels also varied, with deviations likely enlarged for higher fertilizer treatments (Figures 1b–1d). The fitted empirical functions reasonably predicted the  $\Delta uptk$  response to different fertilizer applications (i.e.,  $R^2 = 0.51, 0.67$  and  $0.56$ , respectively).

The field experiment-derived  $\bar{P}_{uptk}$  was upscaled and used to determine parameter  $up1$  of logistical growth functions for each crop according to fertilizer rates in the current situation and the 10% and 20% less fertilizer scenarios (Table S4 in Supporting Information S1). Note that  $\bar{P}_{0uptk}$  in the uplands was arbitrarily taken as 90% of that in the lowlands, due to the less-fertile soils (Altermann et al., 2005). Multicriteria calibration of the mHM-Nitrate model showed good performance for both discharge (NSE ranged 0.78–0.84) and  $\text{NO}_3^-$ -N concentrations at gauging stations (NSE ranged 0.50–0.79, Figure S2 in Supporting Information S1). The seasonal soil mineral N measurements confirmed reasonable simulations at the measuring site (Figure S3 in Supporting Information S1). Particularly, the modeled actual N uptake values were in line with the available survey measurements (e.g.,  $177.5 \pm 9.3$  vs.  $178 \text{ kgNha}^{-1} \text{yr}^{-1}$  for the lowland wheat, Table S4 in Supporting Information S1).

### 4.2. Spatiotemporal Variability of Catchment N Functioning Across Scales

The temporal pattern of flow dynamics was similar throughout the catchment, reflecting the high runoff proportions from the upper mountains especially during high flow periods (Yang, Jomaa, & Rode, 2019). However, the highly complex dynamics of riverine  $\text{NO}_3^-$ -N concentrations were evident at the outlet, presumably due to time-varying mixing of low-N upland discharge and high-N lowland diffuse sources from intensive agricultural



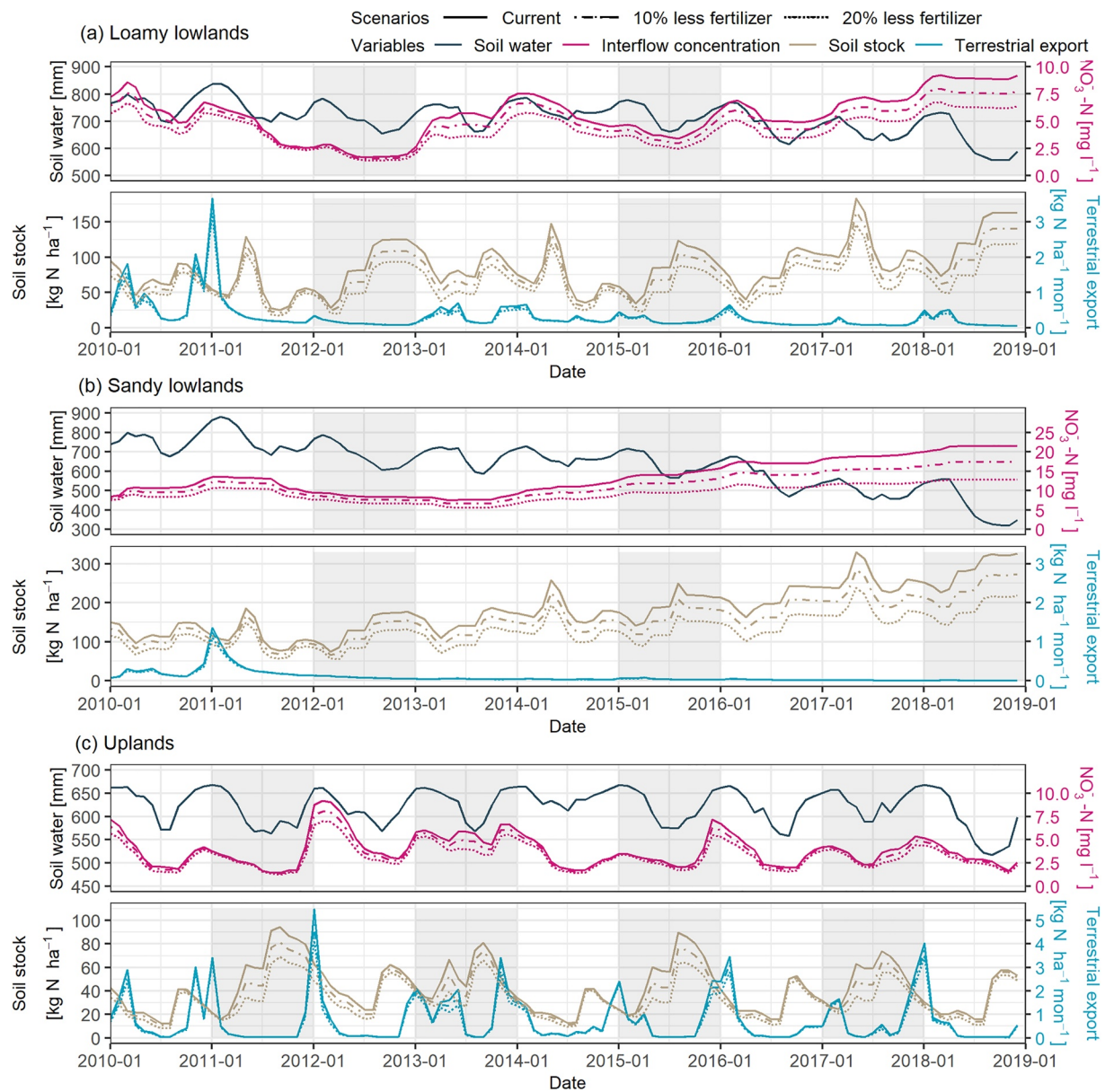
**Figure 1.** (a) Measured N-uptake under zero fertilizer treatment, and the uptake increases under different fertilizer treatments for (b) winter wheat, (c) winter rapeseed and (d) sugar beet. The blue lines in (a) represent the 95% quantile.

areas (Figure S2 in Supporting Information S1). Moreover, riverine concentrations were responsive to different fertilizer scenarios during high-flow periods, whereas almost identical during summer-autumn low-flow periods. This led to 9.5% and 10.1% reductions of annual N-load under the 20% less scenario at Silberhütte and Hausneindorf, respectively (Figure S2 in Supporting Information S1).

The distinct temporal patterns of modeled soil water and N dynamics were further explored at three types of arable lands (Figure 2). Seasonal patterns of soil  $\text{NO}_3^-$ -N stock depended largely on crop growth uptake and fertilizer inputs, of which the amount and timing varied between crops. The stock was generally higher in high-surplus cropping years (rapeseed > wheat and sugar beet years after harvesting) and spatially much higher in the lowlands than in the uplands. Terrestrial export loads from the lowlands were generally very low ( $2.64$  and  $0.41 \text{ kgNha}^{-1} \text{ yr}^{-1}$  in the loamy and sandy lowlands, respectively), except for the extraordinary high exports in 2010–2011, which presumably further caused the high summer riverine  $\text{NO}_3^-$ -N concentrations at Hausneindorf (Figures 2a and 2b; Figure S2 in Supporting Information S1). In contrast, the exports from the uplands were much higher ( $9.17 \text{ kgNha}^{-1} \text{ yr}^{-1}$ ) and exhibited strong seasonal variations (Figure 2c). In addition, the export-associated  $\text{NO}_3^-$ -N concentration, as reflected by that of the dominant interflow pathway, exhibited contrasting levels and dynamic patterns, that is, significantly elevated and damped patterns in the lowlands, whereas strong seasonal variations in the uplands (Figure 2a vs 2c, red lines).

The three types of arable lands also showed contrasting responses to changing conditions. During the prolonged droughts since 2016, soil water storage has significantly reduced in the lowlands, indicating limited terrestrial hydrological connectivity and reduced N-removal by soil denitrification.

Consequently, increasing trends of soil stock and interflow  $\text{NO}_3^-$ -N concentration were simulated (Figures 2a and 2b). Under the lower fertilizer scenarios, higher degrees of soil stock reduction occurred in the high-surplus cropping years (e.g., rapeseed years > wheat years in the uplands, Figure 2c) as well as in locations/periods with already high stocks; similarly, the decreases of interflow  $\text{NO}_3^-$ -N concentration were more obvious during high-value periods (e.g.,  $>5.0 \text{ mgNl}^{-1}$ ). Notably, with the reduced fertilizer, terrestrial N-load exports were more



**Figure 2.** Modeled soil water, interflow  $\text{NO}_3^-$ -N concentration, soil stock and terrestrial export loads to the streams at arable areas of (a) loamy loess lowlands, (b) sandy loess lowlands and (c) loamy uplands. The dashed and dotted lines represent corresponding simulations under 10% and 20% less fertilizer scenarios, respectively. The shaded periods indicate the rapeseed cropping years.

responsive in the uplands than in the lowlands, especially during high-export wet months; while the simulated increases of soil stock and interflow  $\text{NO}_3^-$ -N concentration in the lowlands were significantly prevented during recent prolonged droughts.

#### 4.3. Integrated Analysis of Agricultural Budget and Catchment Responses Under Varying Conditions

The differentiated modeling of temporal N dynamics revealed that the catchment functioning was spatially and temporally (inter-annually) complex due to the combined variability of climate conditions (wetter vs. dryer years), landscape characteristics (uplands vs. lowlands with different soil properties) and cropping management practices (different crop types and fertilizer levels). We integrated responses of N-budgets (crop uptake and surplus) and N redistribution pathways (soil stock changes, denitrification and exporting to surface water system) under the contrasting environmental conditions (Figure 3).



**Figure 3.** Integrated annual agri-environmental responses of agricultural N budgets (actual crop uptake and surplus) and environmental redistribution (annual mean soil stock, soil denitrification and terrestrial export) for the low-surplus winter wheat (left) and the high-surplus rapeseed (right). The values at the current situation are shown as bar plot, and those under 10% and 20% less fertilizer scenarios as solid and dotted whiskers, respectively.

Under current management practices, the actual N-uptake showed variations between years, primarily related to the weather conditions and catchment wetness during the crop growing periods; and the variations were relatively larger for wheat than for rapeseed (Figures 3a and 3b). For example, due to the low soil water and N availability during May-July 2011 (Figure 2), the lowland wheat and rapeseed uptake decreased by 11.4% and 6.7%, respectively. The surplus for wheat was generally low and even negative (i.e., N deficit) in some years (Figure 3c), while for rapeseed, it reached up to  $43.02 \pm 6.27 \text{ kgNha}^{-1} \text{ yr}^{-1}$  (Figure 3d). Soil denitrification varied significantly under different soil wetness and nitrate availability conditions ( $43.46 \pm 24.36 \text{ kgNha}^{-1} \text{ yr}^{-1}$ , Figure 3e and 3f). Denitrification removal was significantly higher for rapeseed than for wheat in the uplands, while similar for both crops in the lowlands; extremely low removal occurred in the sandy lowlands during the drought periods. Annual mean soil  $\text{NO}_3^-$ -N stock in the uplands was stable and low across years and significantly higher for rapeseed than for wheat; while in the lowlands, the stock was high and further increased during the drought years, especially for the sandy lowlands (Figures 3g and 3h). The terrestrial export load was primarily driven by hydro-climatic variations across locations and years, and impacts of crop types were marginal, except for the slightly higher values after rapeseed cropping years in the uplands (Figures 3i and 3j).

The modeled catchment system showed varied responses under 10% and 20% less fertilizer scenarios (Figure 3). The actual N-uptake of rapeseed decreased by 2.4% and 5.2%, compared to that of wheat by 7.5% and 14.6% across fields. This resulted in a larger decrease in surplus for rapeseed (reduced to  $28.25 \pm 6.26$  and  $13.80 \pm 6.45$   $kgNha^{-1} yr^{-1}$ , respectively; Figure 3c). Soil denitrification decreased similarly for different crops in the lowlands, whereas much more for rapeseed than for wheat in the uplands (e.g., by 30% and 17%, respectively, under the 20% less scenario). Additionally, denitrification is generally more responsive in high removal years (Figures 3e and 3f). Similar spatial response patterns were found for soil stock; given the dramatic increases in the sandy lowlands, it is noteworthy that a reduction of ca.  $100 kgNha^{-1}$  stock could be achieved under the 20% less scenario (Figures 3g and 3h). Terrestrial export was generally more responsive in the uplands than in the lowlands, both in terms of degree of decrease (means of 13.5% and 10.2%, respectively, under the 20% less scenario) and absolute load reduction ( $1.24$  and  $0.46 kgNha^{-1} yr^{-1}$ , respectively).

## 5. Discussion

### 5.1. The Dynamic Agricultural Boundary of Catchment N Modeling Informed by Experimental Field Data

The adopted logistic growth functions provided parsimonious estimates of crop N-uptake characteristics under prevailing climatic and alternative management regimes (Lindström et al., 2010; Yang et al., 2018), without involving complicated mechanisms of crop physiological growth and agronomic characteristics (Reid, 2002). The key parameter  $\bar{P}_{uptk}$  is not directly linked to catchment dynamics since the actual uptake is further constrained by the dynamics of soil water and N availability (Equation 2). Therefore, conventional catchment model calibration is unlikely to be able to constrain  $\bar{P}_{uptk}$  uncertainty, nor to reflect its changes under different management practices. We made use of extensively available local fertilization experimental data in agricultural research (Grosse et al., 2020; Körschens et al., 2013). The measured actual uptake exhibited interannual variations (Figure 1), presumably due to climatic variability, crop variety changes, and specific differences of management practices and pest controls during the long-term experiments. Our approach utilized the uptake increases ( $\Delta uptk$ ) under different fertilizer treatment trials, such that fertilizer is the only varying factor in the same year. This justifies the assumption that the fertilization effect on measured actual uptake increase (i.e.,  $\Delta uptk(N_{fert})$  in Figures 1b–1d) is equivalent to that of potential uptake  $\Delta P(N_{fert})$ . In addition, potential impacts of accumulative factors (e.g., soil fertility changes) were marginal because no significant trend was observed in all treatments (Merbach & Schulz, 2013). Therefore, the fertilizer response  $\Delta P(N_{fert})$  could be reasonably added to  $\bar{P}_{uptk}$  in obtaining estimates of  $\bar{P}_{uptk}$  under different fertilizer rates.

Catchment water quality modeling studies increasingly utilize agricultural information (Bauwe et al., 2019; Ilampooranan et al., 2021; Nair et al., 2011). However, most studies used roughly reported crop yield information in improving model parameterization. The potential for such interdisciplinary integration has not been explored in depth yet. The reasons are two-fold: (a) current simplified process descriptions suffice for the purpose of providing generic agricultural boundaries for catchment dynamics; (b) existing knowledge and data gap between agricultural and water quality disciplines. The latter has inhibited integration, particularly at larger scales, due to the scaling challenges of process conceptualization and data assimilation (Siad et al., 2019). Moreover, integrating mechanistic crop growth models often further complicates constraining catchment modeling uncertainty. Using agricultural experimental data, the proposed parsimonious approach improved model description of crop N-uptake and extended model capability under dynamic fertilizer conditions. We note that transferring the approach to different agricultural regions needs further local experimental data, which have become increasingly available in agricultural research.

### 5.2. The Integrated Agri-Environmental Functioning and Differentiated Responses to Varying Conditions

The contrasting temporal variations in N dynamics from the field to catchment scales revealed spatially differentiated agri-environmental functioning under different conditions in the study catchment. Characterized as semiarid with a flashy hydro-climatic regime (Dupas et al., 2017), the uplands were unfavorable for accumulating surplus N, and the interflow  $NO_3^- - N$  concentration increased significantly during high-flow seasons (Figure 2c). Meanwhile, the environmental N-redistribution pathways (denitrification removal and terrestrial export) were more



responsive to annual climate variations, crop types and fertilizer conditions (Figure 3). In contrast, the lowlands exhibit a relatively arid climate, and flat topography with deep loess soils, all favoring high accumulation of agricultural N surplus. After decades of intensive management, the lowland soil nitrate profile has been homogeneously enriched (Dupas et al., 2016). This has resulted in a transport-limited, more chemostatic export behavior, with a reduced seasonal  $NO_3^- - N$  amplitude in the subsurface flow. The contrasting functional features are highly representative of intensively managed catchments (Rode et al., 2009; Basu et al., 2010), and our modeling reliably captured such catchment functional heterogeneity.

Moreover, based on agricultural experimental data, the refined modeling further enabled compatible integration with N-budget assessments, thereby obtaining agri-environmental responses under different weather and crop/fertilizer management conditions. The actual N-uptake of high-surplus rapeseed was less responsive to fertilizer variations both at experimental trials (Figure 1) and catchment levels (Figure 3), compared to that of the low-surplus wheat. This is primarily because rapeseed is physiologically characterized by high N-demand although with low agronomic seed yield and N-efficiency (Rathke et al., 2006). Moreover, our simulations showed marginal responses of rapeseed N-uptake to weather variability, compared to that of wheat (Figures 3a and 3b). This indicates that the high soil N stock, as a result of high surplus, likely ensures crop physiological development, which further provides greater tolerance to soil water constraints (Postma et al., 2014; Wu et al., 2018). N removal by soil denitrification was similarly higher in higher surplus cropping years and also generally higher in the wetter, although less N-enriched, uplands (Figures 3e–3h). This is in line with the findings of the sensitivity analysis by Yang, Jomaa, and Rode (2019) that wetter soil condition favors the denitrification process, and denitrification in agricultural catchments is more sensitive to soil wetness than to soil N availability. Overall, the integrated budget modeling analysis unraveled the spatially distributed agri-environmental functioning, providing an insightful evidence base for targeted agri-environmental management.

### 5.3. Implications for Targeted Management and Further Perspectives

The presented interdisciplinary integration overcomes the data constraint of budget assessments (being farm-specific or nation-wide low-resolution; Cherry et al., 2008); meanwhile, spatio-temporally differentiated, model-aided budgeting responses to varying weather and crop/fertilizer conditions can be concisely communicated to multi-sector stakeholders, in terms of increasing their acceptance of management implications and better reconciling agricultural interests in water environment protection. We particularly demonstrated the joint agri-environmental responses and management implications in the contrasting arable lands of the Selke catchment.

Compared to that of the low-surplus wheat, the actual N-uptake (indicating yield) of high-surplus rapeseed was largely maintained under reduced fertilizer rates. Meanwhile, multiple environmental benefits were anticipated, that is, reduced denitrification and gaseous emission (by 15.0% and 29.5%, respectively, under the 10% and 20% less fertilizer scenarios) as well as slightly reduced export to surface water systems. This strongly implies that the source mitigation measures targeted especially at high-surplus crops could be highly beneficial across sectors.

Our spatially differentiated analysis further showed that the source-related measures had greater multi-sector benefits in the hydrologically flashier and more chemodynamic upland fields. Meanwhile, these export regimes are plausibly cost-effective candidates for implementing transport-related measures, which pursue an increased catchment retention by restoring natural system functioning (e.g., the guides from EU NWRM (2015)) or constructing artificial wetlands/buffer zones (Hoffmann et al., 2020). However, remediating the agricultural N legacy in transport-limited regions (e.g., the lowland Selke fields) remains a long-term challenge (Van Meter et al., 2018), which requires science-based, systemic actions from multi-sector stakeholders (BMU/UBA, 2018; EEA, 2020a). The changing climate has introduced overarching and coupled uncertainty for water environment mitigation (Reusch et al., 2018). Regions such as the Selke are likely to be very sensitive to the expected increasing frequency of prolonged droughts, showing substantial N accumulation in soils and increasing risks of high  $NO_3^- - N$  concentration in exports once the hydrological connectivity is reestablished (Figures 2 and 3). Importantly, our fertilizer scenarios demonstrated that the lower fertilizer inputs had strong mitigation effects under drought conditions and largely prevented such dramatically increased pressures.

This study presented in-depth agri-environmental integration from both data-driven and modeling perspectives, focusing specifically on spatio-temporally differentiated agri-environmental functioning and multi-scale model-aided assessments under varying conditions. The integrated analysis is based on easily accessible data

and open-sourced modeling tools, and therefore, is highly transferable to other regions for providing an insightful scientific evidence base for agri-environmental management. There are good opportunities for further developments, for example, implementing management modules for detailed assessments of specific agricultural practices (e.g., Rode et al. (2009)) and further improving process descriptions from ecohydrology and crop modeling communities (Fatichi et al., 2016; Siad et al., 2019).

## Data Availability Statement

The data used are available at <https://doi.org/10.48758/ufz.12211>. The mHM-Nitrate model code is available at <https://doi.org/10.5281/zenodo.3891629>.

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## References

- Altermann, M., Rinklebe, J., Merbach, I., Körschens, M., Langer, U., & Hofmann, B. (2005). Chernozem—soil of the year 2005. *Journal of Plant Nutrition and Soil Science*, 168(6), 725–740. <https://doi.org/10.1002/jpln.200521814>
- Arnold, J. G., Srinivasan, R., Muttiah, R. S., & Williams, J. R. (1998). Large area hydrologic modeling and assessment Part I: Model development I. *JAWRA Journal of the American Water Resources Association*, 34(1), 73–89. <https://doi.org/10.1111/j.1752-1688.1998.tb05961.x>
- Basu, N. B., Destouni, G., Jawitz, J. W., Thompson, S. E., Loukina, N. V., Darracq, A., et al. (2010). Nutrient loads exported from managed catchments reveal emergent biogeochemical stationarity. *Geophysical Research Letters*, 37(23), L23404. <https://doi.org/10.1029/2010GL045168>
- Bauwe, A., Kahle, P., & Lennartz, B. (2019). Evaluating the SWAT model to predict streamflow, nitrate loadings and crop yields in a small agricultural catchment. *Advances in Geosciences*, 48, 1–9. <https://doi.org/10.5194/adgeo-48-1-2019>
- BGR. (2013). Soil map of the Federal Republic of Germany 1: 1 000 000 (BÜK1000DE), Bundesanstalt für Geowissenschaften und Rohstoffe.
- BMU/UBA. (2018). *Water resource management in Germany. Fundamentals, pressures, measures*. Dessau-Roßlau. Retrieved from <https://www.umweltbundesamt.de/en/publikationen/water-resource-management-in-germany>.
- Cassman, K. G., Dobermann, A., & Walters, D. T. (2002). Agroecosystems, nitrogen-use efficiency, and nitrogen management. *AMBIO: A Journal of the Human Environment*, 31(2), 132–140. <https://doi.org/10.1579/0044-7447-31-2-132>
- Cerrato, M. E., & Blackmer, A. M. (1990). Comparison of models for describing: corn yield response to nitrogen fertilizer. *Agronomy Journal*, 82(1), 138–143. <https://doi.org/10.2134/agronj1990.00021962008200010030x>
- Cherry, K. A., Shepherd, M., Withers, P. J. A., & Mooney, S. J. (2008). Assessing the effectiveness of actions to mitigate nutrient loss from agriculture: A review of methods. *The Science of the Total Environment*, 406(1), 1–23. <https://doi.org/10.1016/j.scitotenv.2008.07.015>
- Chukalla, A. D., Reidsma, P., van Vliet, M. T. H., Silva, J. V., van Ittersum, M. K., Jomaa, S., et al. (2020). Balancing indicators for sustainable intensification of crop production at field and river basin levels. *The Science of the Total Environment*, 705, 135925. <https://doi.org/10.1016/j.scitotenv.2019.135925>
- Dupas, R., Jomaa, S., Musolff, A., Borchardt, D., & Rode, M. (2016). Disentangling the influence of hydroclimatic patterns and agricultural management on river nitrate dynamics from sub-hourly to decadal time scales. *The Science of the Total Environment*, 571, 791–800. <https://doi.org/10.1016/j.scitotenv.2016.07.053>
- Dupas, R., Musolff, A., Jawitz, J. W., Rao, P. S. C., Jäger, C. G., Fleckenstein, J. H., et al. (2017). Carbon and nutrient export regimes from headwater catchments to downstream reaches. *Biogeosciences*, 14(18), 4391–4407. <https://doi.org/10.5194/bg-14-4391-2017>
- EEA. (2020a). *Water and Agriculture: Towards Sustainable Solutions (17/2020)*. European Environment Agency. <https://doi.org/10.2800/73735>. Forestry Report.
- EEA. (2020b). *Nutrients in freshwater in Europe (CSI 020, WAT 003)*. European Environment Agency. fc81e2396ae1406489a96c000941cfb6.
- Eurostat. (2013). *Nutrient budgets - methodology and handbook*. Eurostat and OECD.
- Fatichi, S., Pappas, C., & Ivanov, V. Y. (2016). Modeling plant–water interactions: An ecohydrological overview from the cell to the global scale. *WIREs Water*, 3(3), 327–368. <https://doi.org/10.1002/wat2.1125>
- Gastal, F., & Lemaire, G. (2002). N uptake and distribution in crops: An agronomical and ecophysiological perspective. *Journal of Experimental Botany*, 53(370), 789–799. <https://doi.org/10.1093/jexbot/53.370.789>
- Grosse, M., Hierold, W., Ahlborn, M. C., Piepho, H. P., & Helming, K. (2020). Long-term field experiments in Germany: Classification and spatial representation. *SOIL*, 6(2), 579–596. <https://doi.org/10.5194/soil-6-579-2020>
- Hoffmann, C. C., Zak, D., Kronvang, B., Kjaergaard, C., Carstensen, M. V., & Audet, J. (2020). An overview of nutrient transport mitigation measures for improvement of water quality in Denmark. *Ecological Engineering*, 155, 105863. <https://doi.org/10.1016/j.ecoleng.2020.105863>
- Ilampooranan, I., Schnoor, J. L., & Basu, N. B. (2021). Crops as sensors: Using crop yield data to increase the robustness of hydrologic and biogeochemical models. *Journal of Hydrology*, 592, 125599. <https://doi.org/10.1016/j.jhydrol.2020.125599>
- Körschens, M., Albert, E., Armbruster, M., Barkusky, D., Baumecker, M., Behle-Schalk, L., et al. (2013). Effect of mineral and organic fertilization on crop yield, nitrogen uptake, carbon and nitrogen balances, as well as soil organic carbon content and dynamics: Results from 20 European long-term field experiments of the twenty-first century. *Archives of Agronomy and Soil Science*, 59(8), 1017–1040. <https://doi.org/10.1080/03650340.2012.704548>
- Kumar, R., Samaniego, L., & Attinger, S. (2013). Implications of distributed hydrologic model parameterization on water fluxes at multiple scales and locations. *Water Resources Research*, 49(1), 360–379. <https://doi.org/10.1029/2012WR012195>
- Lindström, G., Pers, C., Rosberg, J., Strömquist, J., & Arheimer, B. (2010). Development and testing of the HYPE (Hydrological Predictions for the Environment) water quality model for different spatial scales. *Hydrology Research*, 41(3–4), 295–319. <https://doi.org/10.2166/nh.2010.007>
- Merbach, I., & Schulz, E. (2013). Long-term fertilization effects on crop yields, soil fertility and sustainability in the Static Fertilization Experiment Bad Lauchstädt under climatic conditions 2001–2010. *Archives of Agronomy and Soil Science*, 59(8), 1041–1057. <https://doi.org/10.1080/03650340.2012.702895>
- Nair, S. S., King, K. W., Witter, J. D., Sohngen, B. L., & Fausey, N. R. (2011). Importance of crop yield in calibrating watershed water quality simulation Tools I. *JAWRA Journal of the American Water Resources Association*, 47(6), 1285–1297. <https://doi.org/10.1111/j.1752-1688.2011.00570.x>
- NWRM. (2015). Final report: Pilot project -atmospheric precipitation -protection and efficient use of fresh water:integration of natural water RetentionMeasures in river basin management - 2015. <https://doi.org/10.2779/619247>

- Oenema, O., Kros, H., & de Vries, W. (2003). Approaches and uncertainties in nutrient budgets: Implications for nutrient management and environmental policies. *European Journal of Agronomy*, *20*(1), 3–16. [https://doi.org/10.1016/S1161-0301\(03\)00067-4](https://doi.org/10.1016/S1161-0301(03)00067-4)
- Poisvert, C., Curie, F., & Moatar, F. (2017). Annual agricultural N surplus in France over a 70-year period. *Nutrient Cycling in Agroecosystems*, *107*(1), 63–78. <https://doi.org/10.1007/s10705-016-9814-x>
- Postma, J. A., Schurr, U., & Fiorani, F. (2014). Dynamic root growth and architecture responses to limiting nutrient availability: Linking physiological models and experimentation. *Biotechnology Advances*, *32*(1), 53–65. <https://doi.org/10.1016/j.biotechadv.2013.08.019>
- Rathke, G. W., Behrens, T., & Diepenbrock, W. (2006). Integrated nitrogen management strategies to improve seed yield, oil content and nitrogen efficiency of winter oilseed rape (*Brassica napus* L.): A review. *Agriculture, Ecosystems & Environment*, *117*(2), 80–108. <https://doi.org/10.1016/j.agee.2006.04.006>
- Rathke, G. W., Christen, O., & Diepenbrock, W. (2005). Effects of nitrogen source and rate on productivity and quality of winter oilseed rape (*Brassica napus* L.) grown in different crop rotations. *Field Crops Research*, *94*(2), 103–113. <https://doi.org/10.1016/j.fcr.2004.11.010>
- Reid, J. B. (2002). Yield response to nutrient supply across a wide range of conditions: 1. Model derivation. *Field Crops Research*, *77*(2), 161–171. [https://doi.org/10.1016/S0378-4290\(02\)00088-6](https://doi.org/10.1016/S0378-4290(02)00088-6)
- Reusch, T. B. H., Dierking, J., Andersson, H. C., Bonsdorff, E., Carstensen, J., Casini, M., et al. (2018). The Baltic Sea as a time machine for the future coastal ocean. *Science Advances*, *4*(5), eaar8195. <https://doi.org/10.1126/sciadv.aar8195>
- Rode, M., Arhonditsis, G., Balin, D., Kebede, T., Krysanova, V., van Griensven, A., & van der Zee, S. E. A. T. M. (2010). New challenges in integrated water quality modelling. *Hydrological Processes*, *24*(24), 3447–3461. <https://doi.org/10.1002/hyp.7766>
- Rode, M., Thiel, E., Franko, U., Wenk, G., & Hesser, F. (2009). Impact of selected agricultural management options on the reduction of nitrogen loads in three representative meso scale catchments in Central Germany. *The Science of the Total Environment*, *407*(11), 3459–3472. <https://doi.org/10.1016/j.scitotenv.2009.01.053>
- Samaniego, L., Kumar, R., & Attinger, S. (2010). Multiscale parameter regionalization of a grid-based hydrologic model at the mesoscale. *Water Resources Research*, *46*(5), W05523. <https://doi.org/10.1029/2008WR007327>
- Schils, R., Olesen, J. E., Kersebaum, K.-C., Rijk, B., Oberforster, M., Kalyada, V., et al. (2018). Cereal yield gaps across Europe. *European Journal of Agronomy*, *101*, 109–120. <https://doi.org/10.1016/j.eja.2018.09.003>
- Siad, S. M., Iacobellis, V., Zdruli, P., Gioia, A., Stavi, I., & Hoogenboom, G. (2019). A review of coupled hydrologic and crop growth models. *Agricultural Water Management*, *224*, 105746. <https://doi.org/10.1016/j.agwat.2019.105746>
- Van Meter, K. J., Van Cappellen, P., & Basu, N. B. (2018). Legacy nitrogen may prevent achievement of water quality goals in the Gulf of Mexico. *Science*, *360*(6387), 427–430. <https://doi.org/10.1126/science.aar4462>
- Wade, A. J., Durand, P., Beaujouan, V., Wessel, W. W., Raat, K. J., Whitehead, P. G., et al. (2002). A nitrogen model for European catchments: INCA, new model structure and equations. *Hydrology and Earth System Sciences*, *6*(3), 559–582. <https://doi.org/10.5194/hess-6-559-2002>
- Wellen, C., Kamran-Disfani, A.-R., & Arhonditsis, G. B. (2015). Evaluation of the current state of distributed watershed nutrient water quality modeling. *Environmental Science and Technology*, *49*(6), 3278–3290. <https://doi.org/10.1021/es5049557>
- Wu, W., Ma, B. L., & Whalen, J. K. (2018). Chapter three - enhancing rapeseed tolerance to heat and drought stresses in a changing climate: Perspectives for stress adaptation from root system Architecture. In D. L. Sparks (Ed.), *Advances in agronomy* (p. 87–157). Academic Press. <https://doi.org/10.1016/bs.agron.2018.05.002>
- Yang, X. (2022). *Crop N-uptake responses to fertilization and its upscaling for catchment water quality modeling*. Helmholtz-Centre for Environmental Research. <https://doi.org/10.48758/UFZ.12211>
- Yang, X., Jomaa, S., Büttner, O., & Rode, M. (2019). Autotrophic nitrate uptake in river networks: A modeling approach using continuous high-frequency data. *Water Research*, *157*, 258–268. <https://doi.org/10.1016/j.watres.2019.02.059>
- Yang, X., Jomaa, S., & Rode, M. (2019). Sensitivity analysis of fully distributed parameterization reveals insights into heterogeneous catchment responses for water quality modeling. *Water Resources Research*, *55*(12), 10935–10953. <https://doi.org/10.1029/2019WR025575>
- Yang, X., Jomaa, S., Zink, M., Fleckenstein, J. H., Borchardt, D., & Rode, M. (2018). A new fully distributed model of nitrate transport and removal at catchment scale. *Water Resources Research*, *54*(8), 5856–5877. <https://doi.org/10.1029/2017WR022380>
- Yang, X., & Rode, M. (2020). A Fully Distributed Catchment Nitrate Model - mHM-Nitrate v2.0 [Computer software]. Zenodo. <https://doi.org/10.5281/ZENODO.3891629>
- Zhang, X., Davidson, E. A., Zou, T., Lassaletta, L., Quan, Z., Li, T., & Zhang, W. (2020). Quantifying nutrient budgets for sustainable nutrient management. *Global Biogeochemical Cycles*, *34*(3), e2018GB006060. <https://doi.org/10.1029/2018GB006060>