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Aggregation of activity data on crop management can induce large uncertainties in estimates of regional nitrogen budgets

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A complete understanding of the nexus between productivity and sustainability of agricultural production systems calls for a comprehensive assessment of the nitrogen budget (NB). In our study, data from the well-monitored Danish Agricultural Watershed Monitoring Program (LOOP-program; 2013–2019) is used for a quantitative inter-comparison of three different approaches to drive the process-based model LandscapeDNDC on the regional scale. The aim is to assess how assumptions and simplifications about farm management activities at a regional scale induce previously unquantified uncertainties in the simulation of yields and the NB of cropping systems. Our findings reveal that the approach based on detailed field-level management data (A) performs the best in simulation of yield ($r^2 = 0.93$). In contrast, the other two different data aggregation approaches (B: Sequential mono-cropping of six major crops with simulation results averaged according to proportional area, and C: simulation of 20 most frequent crop rotations) have lower correlations to the observed yields ($r^2 = 0.92$ and 0.77 , respectively) but are still statistically significant at $p < 0.05$ level. Notable differences arise between detailed and more aggregated crop system simulations concerning the NB, particularly concerning N losses to the environment. Compared to the detailed approach (A) (gaseous N fluxes: $24.3 \text{ kg-N ha}^{-1} \text{ year}^{-1}$; nitrate leaching: $14.7 \text{ kg-N ha}^{-1} \text{ year}^{-1}$), the aggregation approach B leads to a 31.4% over-estimation in total gaseous N fluxes ($+7.6 \text{ kg-N ha}^{-1} \text{ year}^{-1}$), while nitrate leaching shows a similar average with a distinct pattern. Conversely, employing aggregation approach C leads to a 17.6% over-estimation in total gaseous fluxes ($+4.3 \text{ kg-N ha}^{-1} \text{ year}^{-1}$) and a 204.9% over-estimation in nitrate leaching ($+30.2 \text{ kg-N ha}^{-1} \text{ year}^{-1}$). These findings suggest that management representation should be chosen carefully because it can induce large uncertainties, especially when simulating large-scale NBs or assessing the environmental impact of cropping management. This may compromise the accuracy of national and international nutrient budgets, and preclude comparisons among different sources when the approaches for management representation differ.

The global agricultural sector is the main source of non- CO_2 anthropogenic greenhouse gases (GHGs)¹. Croplands are a significant source of the potent GHG nitrous oxide (N_2O)^{2–4}, contributing approximately 78.6% to N_2O emissions worldwide⁵. Nitrous oxide emissions from cropping systems have

increased at national and regional levels, primarily due to changes in management practices, such as a substantial increase in the use of synthetic nitrogen (N) fertilizers^{5,6}. The Intergovernmental Panel on Climate Change reports that alternative cropland nutrient management strategies can

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significantly reduce GHG emissions by 2050, potentially cutting emissions by 0.03–0.7 GtCO₂e per year for N₂O, accounting for 0.17–4.1% of the total land-based measures to mitigate climate change⁷. As one of the most intensively farmed regions in the world⁸, Denmark provides an example of how to balance concerns for agricultural production with environmental protection goals. With more than 60% of its land used for agriculture and food exports exceeding twice its national consumption⁹, Denmark has one of the most developed environmental regulatory systems in the world¹⁰, and has made significant progress in reducing the consumption of synthetic fertilizers since the mid-1990s^{11,12}. The country has set an ambitious national target, which includes the agricultural sector, to reduce emissions by 70% from 1990 levels by 2030 and achieve net-zero GHG emissions by 2050 at the latest¹³. The fact that 89% of Denmark’s total N₂O emissions originate from agriculture, according to the Danish Emission Inventories for Agriculture from 1985 to 2018¹⁴, underscores the urgency of implementing interventions to reduce emissions. However, to identify feasible N₂O mitigation options and the yield impact of improved management practices, detailed modeling approaches of the carbon (C) and N balances of croplands are critical.

In practice, the performance of existing agroecosystem models remains a question. Process-based models that simulate various biogeochemical cycles, including C, N, and phosphorus (P), offer a cost-effective framework to assess the effectiveness of different management practices quantitatively¹⁵ by estimating GHG emissions sources and sinks. However, these models are often developed at a scale that does not align with the spatial extent and resolution required by policymakers¹⁶. In addition, due to data limitations, various assumptions are needed to aggregate field-scale information (e.g., management, soil, and climate variables) to a coarser resolution, raising concerns about how aggregating detailed information on crop rotations, field management, or soil properties may affect the uncertainty of simulation results (e.g., yields and nitrogen budget (NB)).

Previous studies have examined the effect of aggregating soil and climate input data using various methods to minimize the errors associated with this aggregation^{17–21}. These studies revealed that the aggregation effect is variable and strongly influenced by region, crop type, and agro-climatic conditions. Especially in water-scarce regions, the aggregation of

precipitation and soil data resulted in significant deviations of simulated biomass production and nitrate leaching losses from observed data (e.g., refs. 22–24). However, little is known about how spatial aggregation of field-activity data, such as crop rotations and fertilization can affect simulated NBs at the regional level. Two recent studies have provided some insight into the importance of detailed activity data for deriving realistic yield and GHG simulations: Constantin et al.²⁵ highlighted the value of management inputs for simulating winter wheat and maize, including yield, evapotranspiration, and drainage, while using different management scenarios and input resolutions in Germany. Similarly, Butterbach-Bahl et al.²⁶ emphasized the significance of activity data in identifying hotspot regions of CH₄ and N₂O emissions from rice systems in Vietnam.

Since 1989, Denmark has implemented a unique monitoring program to quantify the effects of agricultural policies on nutrient leaching and transport, called the LOOP-program (in Danish: Landovervågningsprogrammet). These catchments are average and are not specifically representative, but they cover a wide range of soil types, climatic conditions, and agricultural practices observed in Denmark. The collected datasets include comprehensive information collected through annual farmer surveys, covering agricultural practices such as crop types, cropping calendars, the timing, type, and amount of synthetic and organic fertilizer applications at field scale, and provide estimates of the catchment NB using a semi-empirical approach^{27,28}. Our investigation aims to evaluate the results of two common aggregation approaches using the LandscapeDNDC (LDNDC) model: (1) the mono-cropping approach (Fig. 1—Approach B) (e.g., refs. 29,30) and (2) the simulation of dominating crop rotations only (Fig. 1—Approach C) (e.g., refs. 31,32), in comparison to the detailed, actual field management-driven approach of data from individual fields (Fig. 1—Approach A). Our comprehensive assessment uses reported crop yields and N balances from six well-monitored catchments in the Denmark’s National Program for Monitoring Aquatic Environment and Nature (NOVANA; ref. 33) from 2013 to 2019.

Results

Sub-field scale simulations (Approach A)

We used detailed field-level management data and sub-field soil information to simulate realistic crop rotations for the 20 crops within the 6 studied

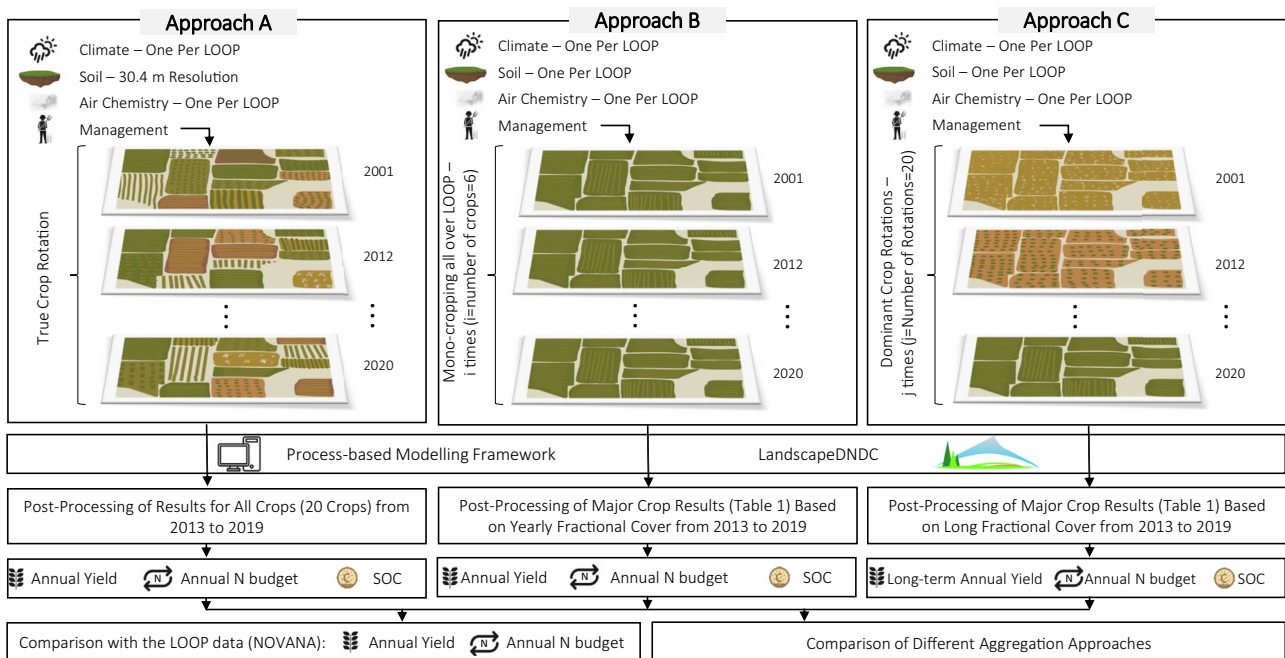


Fig. 1 | Overview of the different aggregation approaches tested. Schematic representation of the modeling process using different approaches. Approach A utilizes detailed field-level management data. Approach B involves sequential mono-

cropping of six major crops, with simulation results averaged based on proportional area. Approach C simulates the 20 most dominant crop rotations in Denmark.

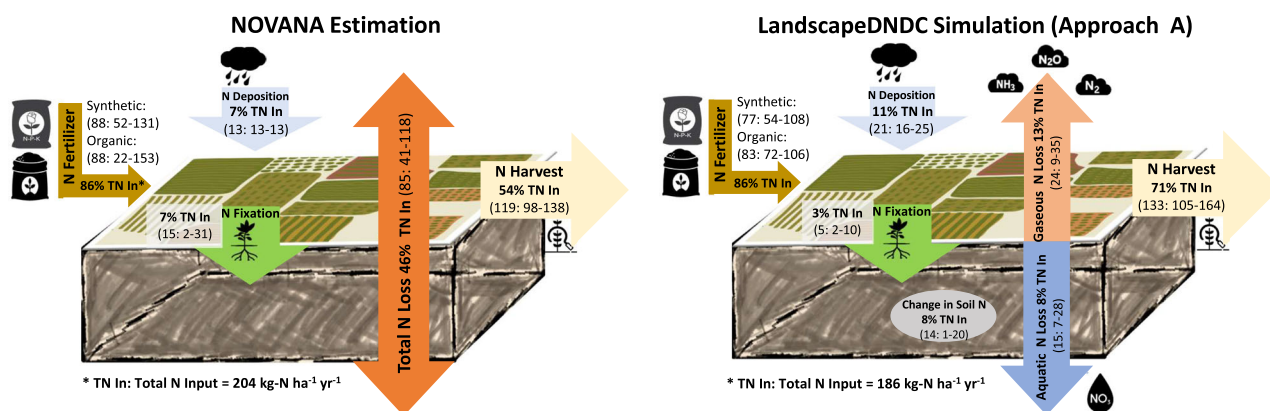


Fig. 2 | Differences in reported (LOOP) and simulated (approach A) NB parameters. The numbers in brackets represent the average of reported (NOVANA) and simulated (LDNDC model) values for each component, along with their ranges for

the six LOOP catchments, in kg-N ha⁻¹ year⁻¹. TN In indicates the share of each component from the total N input.

catchments (LOOPS). These simulations (Approach A) comprehensively represent agricultural practices and their effects on yield and NB over the simulation period. The simulation results of LDNDC using approach A are compared to the NOVANA reported values in Fig. 2. The underestimation of total N inputs could be due to the inclusion of all areas in this approach, which includes marginal lands simulated as extensive grassland (not subject to organic fertilization) in our calculations but excluded in the NOVANA estimates. Therefore, our mean applied organic fertilization is consistently lower than the reported values in all catchments (17.7 kg-N ha⁻¹ year⁻¹). The harvest of N is also 14 kg-N ha⁻¹ year⁻¹ higher in the DNDC simulations than in the NOVANA estimations, which may lead to differences in overall mean N-use efficiency at the LOOP level (71% compared to 54%). Furthermore, the input dataset we utilized for the N deposition differs from the one used for the NOVANA estimations (see “Model input data”). However, the primary advantage of the simulated NB over the reported one lies in the information it provides about N-loss, where NOVANA’s estimates do not distinguish between gaseous and aquatic N loss. Furthermore, NOVANA does not account for legacy effects and always set the annual N balance to zero, i.e., no accumulation or depletion of ecosystem N pools can occur. LDNDC simulations may provide a more detailed view of catchment and ecosystem N balances and losses, as the simulations account for changes in soil N and biomass N of permanent crops and provide estimates of compound-specific N-losses along gaseous or aquatic pathways.

Model simulations provide spatio-temporal variations of various NB components at the sub-field level. This information is valuable for determining the contribution of each field to the overall NB, identifying hotspots of N loss, and targeting mitigation options. The net N flux of the NB assessment, N-use efficiency, and total N loss at the sub-field level (30.4 m) using the detailed approach (A), covering the period 2013–2019 for all six studied catchments, is illustrated in Fig. 3. As shown, even at the sub-field level, differences in NB components are evident, mainly due to different soil characteristics. These differences provide valuable insights for targeting site-specific mitigation strategies, e.g., by introducing precision agriculture approaches. Among the studied catchments, LOOP6 showed the highest N loss, while LOOP2 showed the highest N-use efficiency during the study period from 2013 to 2019. Regarding the total area covered by different classes shown in Fig. 3, across all catchments, ~30% of the total area (ranging from 9% of the LOOP4 to 58% of the LOOP2) shows indication for N depletion conditions as net N budget values were negative. Furthermore, ~43% of the entire area has a N-use efficiency ranging from 60% to 80%.

Comparing two alternative aggregation approaches

Yield. The results of comparing the two aggregation approaches with detailed management simulations for yield are presented in Fig. 4, covering all LOOPS and major crops during the period 2013–2019 (to match

with the reported yield data observations). We present the coefficient of determination (r^2) values in two forms to allow meaningful comparisons (long-term simulation: LTS, and annual simulation: YS), as approach C does not provide annual results (see section “Comparison of aggregation approaches”). The approach based on detailed field-level management data (A) outperforms the others, with a superior LTS- r^2 value of 0.93, followed by approaches B and C with LTS- r^2 values of 0.92 and 0.77, respectively. Notably, when considering YS- r^2 , approach A still maintains superiority over approach B. All correlations were statistically significant at the $p < 0.05$ level.

For simulations at the catchment scale using the detailed approach (A), LOOP1 is the most accurate in yield simulation (YS- $r^2 = 0.77$). On a crop basis, the highest accuracy is achieved in the winter barley (WBAR) simulations (YS- $r^2 = 0.78$), while potato (POTA) yields show the lowest accuracy (YS- $r^2 = 0.41$). These discrepancies could be attributed to several factors, including the relatively limited number of site measurements used for the region-specific crop parameterization. However, it is important to note that some of these uncertainties may be due to the calibration process of the crop parameters (i.e., not accounting for all the differences between different cultivars) and, in part, to an overestimation of recorded yields, as discussed by Blicher-Mathiesen et al.³³. In addition, conversion factors used to establish comparability between simulated and reported yields—such as conversion from fresh weight to dry weight and carbon content to dry weight—may contribute to the observed deviations between observations and simulations.

N budget components. The simulated gaseous fluxes from approach A, averaged over all LOOPS, consisted of N₂O emissions estimated at 1.5 kg-N ha⁻¹ year⁻¹ (0.9–2.9), which is in the range of values previously reported from field measurements at four representative agricultural sites in Denmark (Foulum, Taastrup, Askov, and Vejle)³⁴. Nitric oxide (NO) emissions were estimated to be 0.6 kg-N ha⁻¹ year⁻¹ (0.3–1.0), dinitrogen (N₂) emissions were estimated to be 16.6 kg-N ha⁻¹ year⁻¹ (3.6–23.9), and ammonia (NH₃) emissions were estimated to be 5.6 kg-N ha⁻¹ year⁻¹ (4.6–7.7). Of these, gaseous N losses as N₂ accounted for the largest proportion (68.3%), followed by NH₃ volatilization (23.1%), N₂O (6.3%), and NO (2.3%). The mean estimate for NO₃ leaching was 14.7 kg-N ha⁻¹ year⁻¹ (6.9–27.9). This amount is lower than field measurements for the LOOP catchments, 31, 77, 47, 45, and 100 kg-N ha⁻¹ year⁻¹ for LOOP 1, 2, 3, 4, and 6^{35,36}. This discrepancy could be due to several factors, including uncertainties in the timing and amount of irrigation in our simulations and the reported values resulting from the upscaling of point measurements to regional scales using empirical models. Since the objective of our study is to compare different field management aggregations, the uncertainties are consistent across all three approaches.

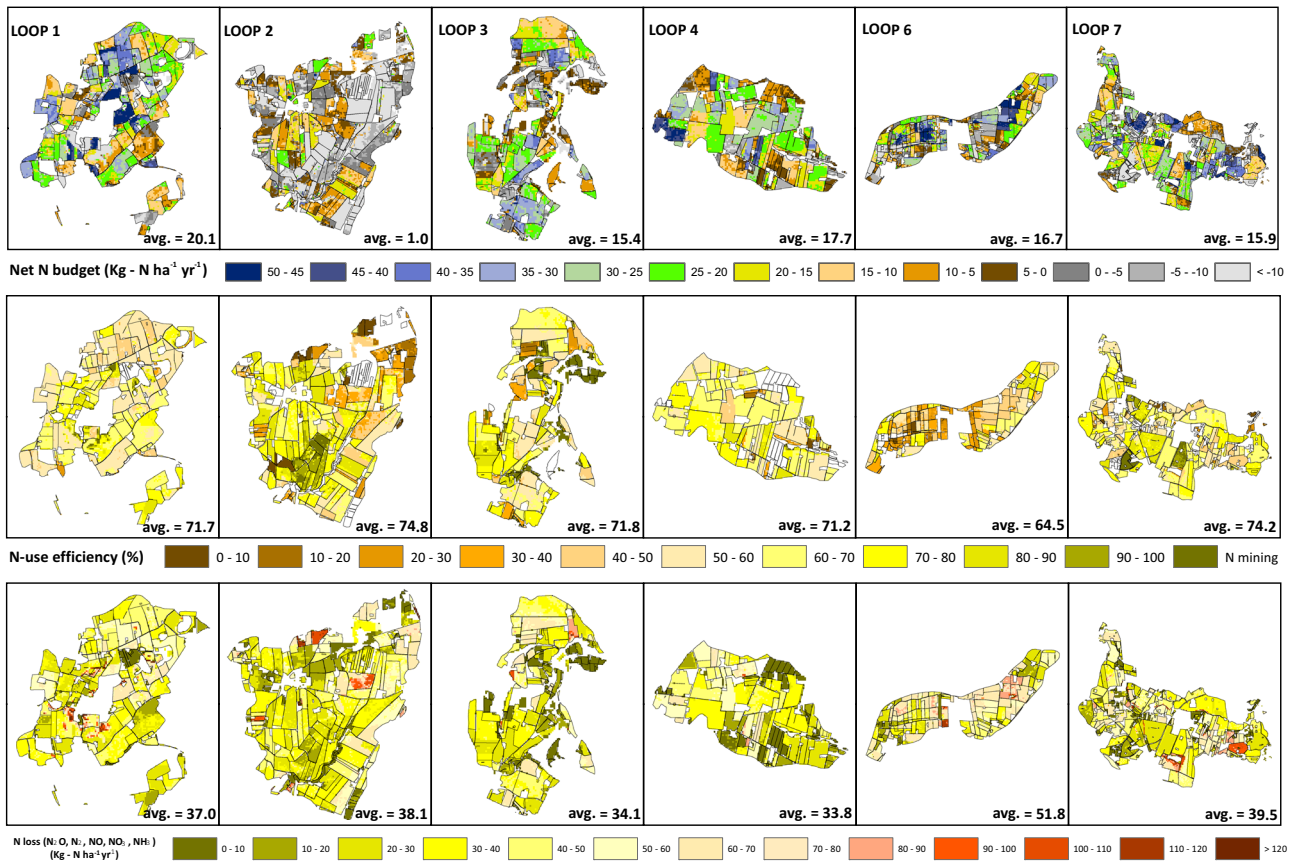


Fig. 3 | The net N flux of the NB assessment, N-use efficiency, and total N loss at sub-field level using the detailed, actual field management-driven approach (A) (2013–2019 average, all 6 studied catchments). Positive net N budget values indicate increase in soil N storage over time.

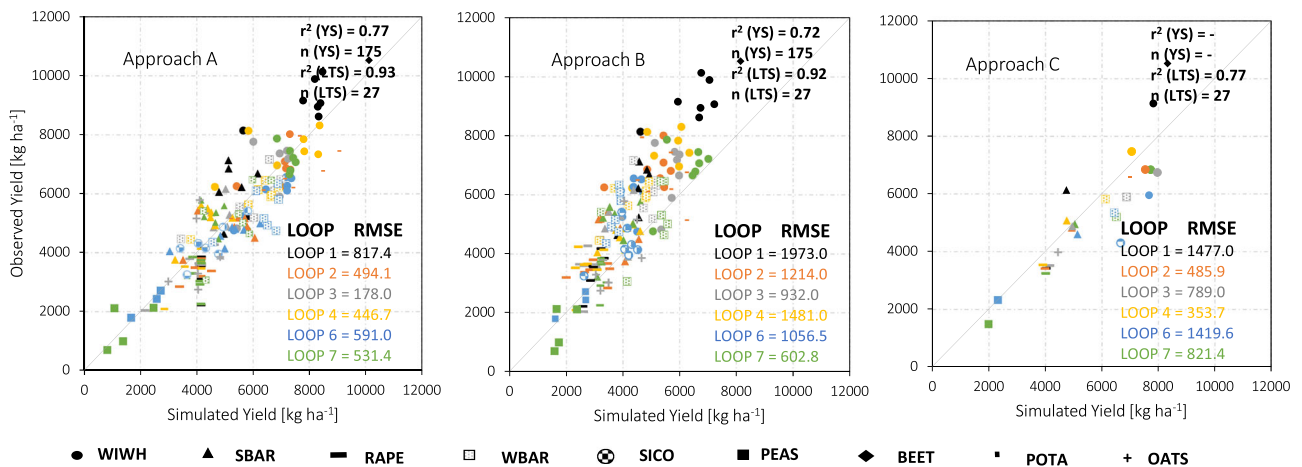


Fig. 4 | Observed and model-simulated yields of major crops across the studied catchments (2013–2019) using three different approaches. WIWH winter wheat, SBAR spring barley, RAPE rapeseed, WBAR winter barley, SICO silage corn, PEAS

peas, BEET sugar beet, POT potato, OATS oats. LTS denotes outcomes corresponding to long-term simulations (averaged over the 2013–2019 period), while YS signifies results pertaining to individual years.

Total N yield and N biomass export (straw and grass cut) reached 132.8 kg-N ha⁻¹ year⁻¹, with uncertainty ranging from 115.9 to 159.1 kg-N ha⁻¹ year⁻¹.

Figure S.1 illustrates the NB through a diagram, showing the cumulative flux contributions across all LOOPS and approaches. This diagram offers an overview of the overall N balance, representing N accumulation in the soil as the difference between all out-fluxes and all in-fluxes. Among all the LOOPS, LOOP6 and LOOP7 show the highest

average (2013–2019) gaseous fluxes of 31.3 kg-N ha⁻¹ year⁻¹, followed by LOOP1 (30.0 kg-N ha⁻¹ year⁻¹), which can be attributed to higher N inputs compared to other LOOPS (Fig. S.1). However, other approaches (B and C) result in a different pattern, with LOOP1 having the highest gaseous N flux (LOOP1-approach B: 47.7 kg-N ha⁻¹ year⁻¹; LOOP1-approach C: 43.0 kg-N ha⁻¹ year⁻¹). The peak of absolute gaseous fluxes occurred in 2018 for LOOP7 (41.7 kg-N ha⁻¹ year⁻¹), while the lowest absolute gaseous fluxes were observed in 2014 for

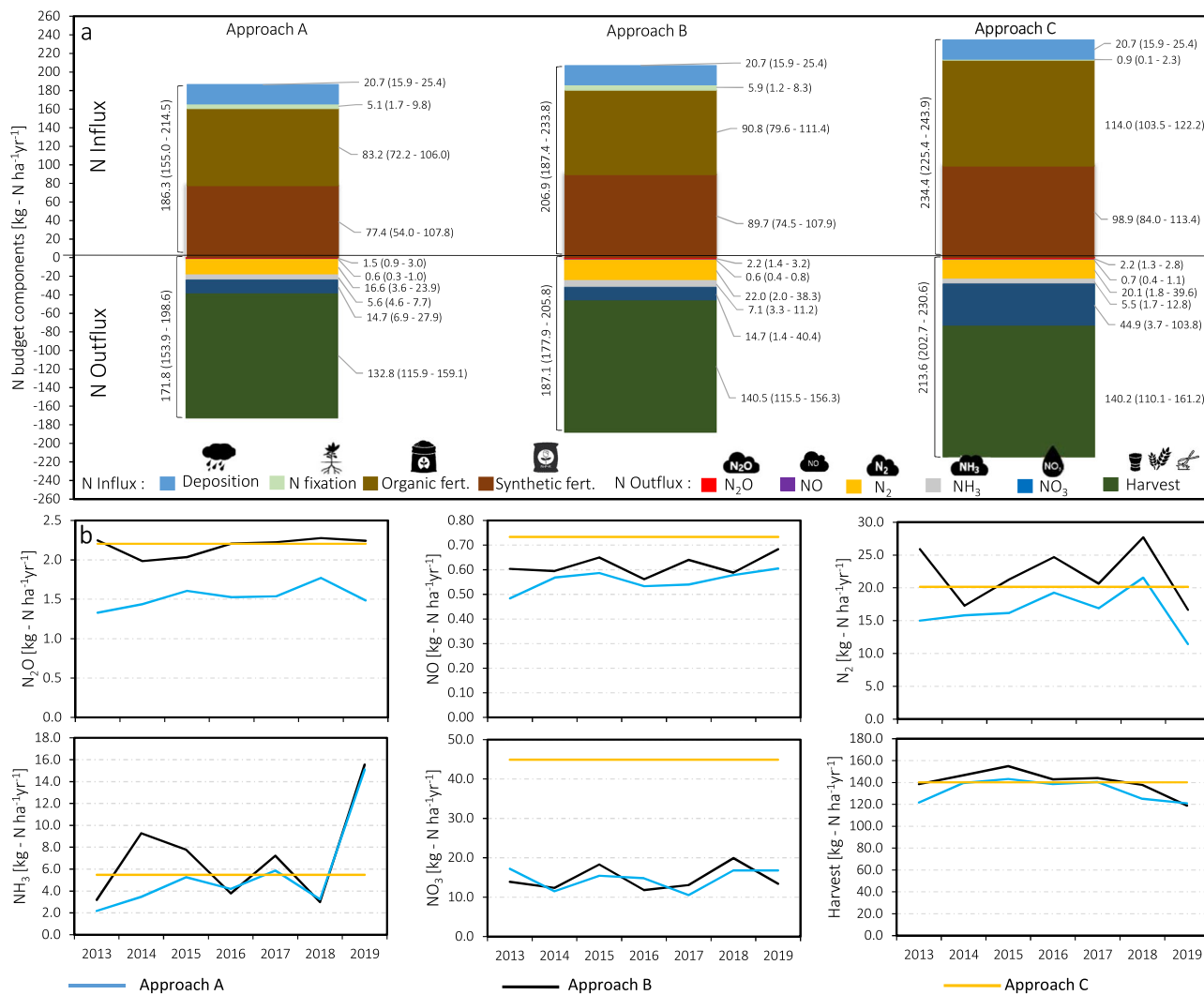


Fig. 5 | Comparative assessment of the three approaches in simulating N in- and out-fluxes versus the detailed, actual field management-driven, approach (A). a N fluxes for approaches A–C, averaged throughout 2013–2019; **b** the temporal variation of NB components simulated by different approaches. All numbers are

expressed in kg-N ha⁻¹ year⁻¹, with each value representing the contribution of a specific component from the total NB simulated by each of the three approaches. The values between brackets represent the minimum and maximum across the studied catchments.

LOOP2 (6.3 kg-N ha⁻¹ year⁻¹). Regional differences in mean NO₃ leaching among the five LOOP catchments indicate that LOOP2 has the highest NO₃ leaching (27.9 kg-N ha⁻¹ year⁻¹), while LOOP1 has the lowest (6.9 kg-N ha⁻¹ year⁻¹). The highest absolute NO₃ leaching was recorded in 2016 for LOOP2 (35.6 kg-N ha⁻¹ year⁻¹).

Regarding total yield and biomass (straw and cut grass), LOOP7 and LOOP1 have the highest average values, with 159.1 and 144.1 kg-N ha⁻¹ year⁻¹, respectively. The highest absolute value was observed in 2015 for LOOP7 (184.5 kg-N ha⁻¹ year⁻¹). The lowest was attributed to drought and low yields in 2018 for LOOP4 (91.7 kg-N ha⁻¹ year⁻¹).

All approaches in the LOOPS consistently agree to the overall N balance and simulate, on average, a pattern of N-accumulation in the soil for 2013–2019. However, the magnitude differs: approach C consistently yields the highest N accumulation (20.8 kg-N ha⁻¹ year⁻¹), followed by approach B (19.9 kg-N ha⁻¹ year⁻¹) and it should be noted that the annual base N balance differs in magnitude and does not always accumulate. Using approach A, the maximum N accumulation was observed in 2013 for LOOP4 (46.6 kg-N ha⁻¹ year⁻¹), while, LOOP7 in 2015 showed the most significant depletion (−23.6 kg-N ha⁻¹ year⁻¹). Analyzing the variations in the overall N balance, the annual trends observed in the organic C and N pools in the topsoil (30 cm) over the evaluation period are consistent, showing an average annual carbon sequestration of 261.7 kg-C ha⁻¹ year⁻¹

(150.0–449.3) across all catchments. However, some years exhibit carbon loss, which could be attributed to local climate or management practices.

Figure 5a illustrates the N fluxes comprising the nitrogen balance (NB) simulated by approaches B and C compared to approach A, considering the mean value for each component.

Our findings reveal that, using approach B, about 1.2% of the total system N outflux is due to N₂O emissions. However, compared to approach A, total gaseous N losses are, on average 31.4% (+7.6 kg-N ha⁻¹ year⁻¹) higher. Similarly, approach C overestimates gaseous N losses by an average of 17.6% (+4.3 kg-N ha⁻¹ year⁻¹).

Regarding total yield and biomass, there are no notable differences between approaches A–C, with approaches B and C both yielding a ~5.7% higher estimate (~7.5 kg-N ha⁻¹ year⁻¹). For NO₃ leaching, a remarkable discrepancy is observed when applying approaches B and C compared to approach A. Specifically, approach C tends to overestimate the contribution of leached N by twice as much (44.9 kg-N ha⁻¹ year⁻¹ as compared to 14.7). For approach B, the averages across all catchments remain the same, but the pattern differs. This discrepancy is particularly noteworthy in countries such as Denmark, where NO₃ leaching is important due to the predominance of sandy soils. These results provide valuable insights into the quantitative assessment of the uncertainty introduced by each approach when aggregating management activities for modeling NBs.

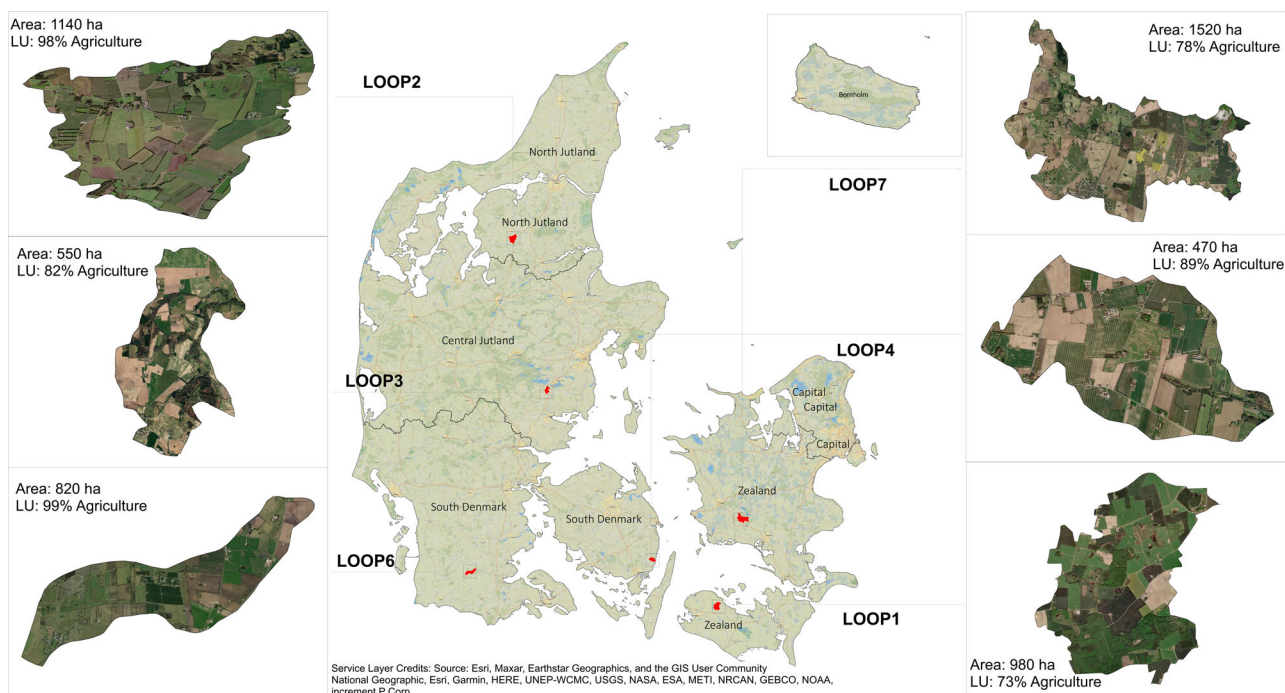


Fig. 6 | Location and characteristics of the agricultural monitoring catchments (LOOP1–4, 6, and 7). DMI represents the Climate ID of the Danish Meteorological Institute (DMI). LU land use.

The temporal variation of NB components simulated by different approaches from 2013 to 2019 is shown in Fig. 5b. As can be seen, approach B effectively captures NB component anomalies. However, it systematically overestimates gaseous N fluxes and underestimates other components. This is mainly because approach B cannot account for carbon and N sequestration in the soil, leading to these discrepancies.

Discussion

When upscaling field activity data from individual fields to larger areas, understanding the variability and uncertainties arising from input aggregation becomes critical. An optimal resolution should balance providing sufficient fine-scale detail to capture accurate spatial variability relevant to the study objectives while conserving computational resources and simplifying data compilation and model execution.

Our study systematically evaluated two dominant management simplification approaches and compared them with simulations involving field-scale management in six catchments in Denmark. The evaluations were carried out for both yield and NB simulations. The results underline that although all three approaches show varying degrees of effectiveness in yield simulation and overall NB estimation, significant differences emerge in the simulation of individual NB components.

The insights gained from this study can serve as a guideline for modelers tasked with selecting the appropriate spatial resolution for regional process-based modeling and GHG inventory assessments. This insight allows for understanding the trade-offs in advantages and disadvantages associated with choosing one of the two approaches, thus helping to make informed decisions to achieve the desired modeling results.

Methods

Case studies and NOVANA data overview

The case studies in this research comprise six Danish catchments from the National Monitoring Program for Water Environment and Nature, NOVANA (LOOP-program; In Danish: Landovervågningsprogrammet). These catchments represent the variation in predominant soil types, climate conditions, and agricultural practices observed within Denmark.

The monitoring program provides comprehensive information about catchment-specific agricultural practices. This includes details about crop types, the presence or absence of catch crops, cropping calendars and the timing, type, and amount of synthetic and organic fertilizer applications. Additionally, estimations for the NB for the entire cultivated area using a semi-empirical approach, including fallow land, are also provided^{27,28}.

In this dataset, N removal is based on reported crop yields provided by farmers and corresponding standards for N content in the yields. The N content for oats, winter and spring wheat, and barley is derived from measured annual averages (e.g., ref. 37), while for other crops, it is based on standards outlined by the National Committee for Cattle (e.g., ref. 38). For this reason, there is uncertainty in calculating field N surplus due to farmers' variability in accurately reporting field yields and applying standardized N content levels. For example, a comparison of reported field yields and measured values from sold crops during 2000–2003 showed an r^2 value ranging from 0.82 to 0.93 for winter wheat, spring barley, beets, and grass³⁹.

The same calculation scheme was applied for applying mineral and manure fertilizer. These interviews employ relevant norms for livestock manure production and nutrient content, as outlined in the “harmony rule” (<https://lbst.dk/landbrug/goedning/vejledning-om-goedsknings-og-harmoniregler>). In NOVANA, N fixation was computed by considering dry matter, N content in the yield, and the proportion of fixed N in both harvest yield and stubble/roots⁴⁰. For fields with non-fixing crops, a background fixation of 2 kg-N ha⁻¹ was assumed. Permanent grasslands with a high biodiversity of N-fixing plant species used a default value of 5 kg-N ha⁻¹ for N fixation.

Agriculture dominates the land use in all six catchments, accounting for 73–99% of the LOOP's total areas. Figure 6 and Table 1 provide an overview of the characteristics of the six catchments and the major crops grown in 2020. The average management (timing, fertilizing, and manuring) for each catchment is provided in Fig. S.2.

Model input data

To feed the model for the catchment scale LOOPs and to assess the impact of different aggregation approaches (see section “Comparing two alternative

Table 1 | Fractional cover (%) of major crops (2011–2020), catchment elevations, climate (2013–2019), and soil information

Catchment	Fractional cover (%)											Elevation (m)	Climate (2013–2019)		Soil	
	Crop	2011	2012	2013	2014	2015	2016	2017	2018	2019	2020		Prec.	Temp.	Type	Organic C (0–30 cm) g kg ⁻¹
		(mm)	(°C)													
LOOP1 Højvads Rende	BEET	27.4	24.2	29.5	15.7	19.2	14.1	23.6	25.0	12.2	31.6	3.3	650.3	9.8	80% Sandy loam 14% Clay	2.1 (0–22.2)
	RAPE	2.2	4.9	1.9	2.1	1.4	6.0	7.2	9.9	0.1	1.9					
	SBAR	26.9	33.5	27.8	34.0	35.0	37.5	23.6	31.7	30.9	30.2					
	SICO	0.2	0.2	0.2	0.2	0.3	0.3	0.3	0.2	0.2	0.0					
	WIWH	35.6	28.0	32.6	44.6	37.2	34.7	39.1	28.2	51.4	28.0					
	GRASS	5.0	5.0	2.8	1.3	5.9	6.6	3.5	3.4	2.9	5.6					
LOOP2 Odder Bæk	POTA	2.4	1.2	3.7	3.6	2.5	4.7	5.7	5.8	7.6	3.3	12.6	849.2	8.7	72% Coarse sand 17% Fine sand	3.3 (0–33.2)
	RAPE	1.1	2.6	8.0	3.3	7.6	4.5	9.4	6.2	3.4	6.6					
	SBAR	19.7	21.3	14.6	16.5	29.1	28.5	19.0	25.6	19.1	22.8					
	SICO	20.7	21.2	18.3	18.2	17.6	0.0	14.5	8.1	15.6	27.7					
	WIWH	17.5	13.2	14.5	18.5	11.1	17.3	13.8	23.2	23.9	10.3					
	GRASS	31.2	32.0	33.3	30.5	23.3	34.5	22.2	21.4	18.7	19.5					
LOOP3 Horndrup Bæk	OATS	3.7	1.7	0.9	0.0	2.6	4.8	1.8	17.2	6.2	9.1	39.8	806.1	9	70% Sand-mixed clay 24% Clay- mixed sand	1.7 (0–22.6)
	RAPE	7.9	0.0	13.7	6.8	18.3	1.1	3.6	3.1	2.1	0.0					
	SBAR	12.3	15.9	42.1	17.1	18.9	31.6	25.8	24.0	12.4	27.0					
	WBAR	7.7	17.2	8.7	30.9	12.8	7.3	8.3	5.6	2.8	16.1					
	WIWH	45.6	39.5	13.4	27.4	13.6	27.9	29.5	22.7	32.7	17.2					
	GRASS	12.9	17.8	15.9	14.3	18.2	18.6	19.1	25.3	25.5	18.7					
LOOP4 Lille Bæk	RAPE	11.1	7.9	18.7	9.1	20.2	6.8	3.4	10.3	4.9	17.7	7.4	804.9	9.7	86% Sand-mixed clay 4% Clay- mixed sand	1.3 (0.8–10.1)
	SBAR	15.0	24.7	21.0	19.8	23.0	33.7	33.1	25.7	17.1	20.5					
	SICO	8.1	8.1	7.8	5.9	0.0	0.0	0.0	0.0	3.5	12.9					
	WBAR	6.8	8.2	12.8	13.5	6.9	1.4	5.7	1.4	5.5	1.6					
	WIWH	22.0	20.7	21.7	31.5	26.9	32.4	21.7	14.5	22.5	17.8					
	GRASS	18.9	12.6	6.4	7.3	5.0	14.1	16.6	23.7	24.9	11.2					
LOOP6 Bolbro Bæk	PEAS	3.8	1.7	2.1	1.6	0.7	3.6	3.9	6.9	5.0	1.1	23.4	1003.5	9.2	67% Coarse sand 18% Clay-mixed sand 14% Humus	4.0 (1–20.6)
	SBAR	21.2	25.8	27.6	21.7	15.9	17.3	16.1	26.1	21.1	18.2					
	SICO	13.4	19.5	30.0	31.8	34.5	31.2	34.4	25.3	23.8	26.9					
	WBAR	7.2	1.4	3.2	3.6	2.8	3.7	5.9	0.0	0.0	0.7					
	WIWH	15.2	14.5	7.9	12.2	8.1	8.9	7.3	6.0	9.0	12.2					
	GRASS	25.1	28.1	21.5	23.4	25.2	24.9	21.5	18.2	29.8	26.5					
LOOP7 Hule Bæk	PEAS	6.0	8.7	0.0	0.0	3.6	1.8	6.6	4.9	3.3	7.4	38.5	682.9	9.3	76% Sandy clay 20% Clay	1.8 (0–28.4)
	RAPE	5.1	1.3	16.6	13.7	19.6	7.6	9.5	12.3	6.5	8.4					
	SBAR	26.2	43.2	30.6	24.7	24.4	33.1	26.3	31.6	19.0	26.0					
	WBAR	2.6	1.2	8.5	5.8	5.9	1.4	5.2	1.7	1.1	4.2					
	WIWH	38.4	28.6	27.0	38.2	30.6	35.1	35.0	11.5	35.5	24.7					
	GRASS	12.3	13.4	9.3	9.5	12.0	13.1	11.8	21.2	22.9	11.9					

aggregation approaches”) on yield estimates and NB, different sets of input data have been prepared from the field level to the catchment level. The main sources and methods to prepare such inputs are summarized below.

Information about crop types in agricultural areas and cropland boundaries was obtained from the General Farm Register (GLR in Danish), covering the period from 2011 to 2020 at the field scale. For the agricultural practices, the monitoring data of the LOOP-program for each catchment encompasses a collection of detailed information on crop types, tillage and plowing time, catch crop, irrigation, and time/amount/application method of mineral and organic fertilizer at field level. Furthermore, this dataset provides data on atmospheric N deposition, N deposited by grazing livestock, and total NB at the catchment scale, which were used in our

simulations and analysis³³. The catchment-level inputs for the management were prepared by averaging over year and crop type in each LOOP catchment.

Soil characteristics including soil texture (Adhikari et al.⁴¹), soil organic carbon (SOC), and bulk density (BD)⁴² at five standard soil depths of 0–5, 5–15, 15–30, 30–60, and 60–100 cm were taken as geographic raster datasets with a 30.4 m resolution. Furthermore, the soil pH for the same depths and at 100 m resolution was obtained from Adhikari et al.⁴³. The saturated hydraulic conductivity estimations (KS) was calculated using a pedotransfer function using relevant soil properties^{44,45}. For the catchment-level soil input, the dominant soil type within each catchment was employed to characterize the soil properties (see Table 1). It is, however, important to

mention that the high-resolution soil inputs used in this study can also be subject to uncertainty, as already addressed in previous studies (e.g., refs. 41,46), which can affect the simulation accuracy. It is, however, important to mention that the high-resolution soil inputs used in this study can also be subject to uncertainty, as already addressed in previous studies (e.g., refs. 41,46), which can affect the simulation accuracy.

The estimates from the regional-scale simulation of the atmospheric chemical transport model, The Danish Eulerian Hemispheric Model, were utilized as input for N deposition in our model^{47,48}.

The climate data (10 × 10 km grid) included daily mean air temperature, global radiation, and precipitation. Data were taken from interpolated daily climate information provided by the Danish Meteorological Institute⁴⁹.

LDNDC model and simulations set up

LDNDC is a process-based modeling framework that can simulate C, N, and water processes in cropland, grassland, and forest ecosystems⁵⁰. In this framework, a set of different modules are used to simulate plant growth and other processes: plant physiology (PlaMox)^{51,52}, micro-climate (CanopyECM)⁵³, water balance (WatercycleDNDC)^{54,55}, air chemistry (airchemistryDNDC), and soil biogeochemistry (MeTrx)⁵⁶. The model has been parameterized, calibrated, and validated using measurements gathered from a wide range of ecosystems, including temperate regions⁵⁷, tropical areas⁵⁶, and African savannahs⁵⁸. It has been used for different purposes, such as estimating yield gaps⁵⁹, grassland productivity¹², water balance⁶⁰, GHG emissions⁶¹, residue management³², and nitrate leaching⁶². The model has also been previously calibrated, validated, and used, for example, to simulate SOC⁶³, crop productivity, and soil GHG emissions⁶⁴ in Denmark.

The simulations were driven by 1-m depth soil physical, chemical, and hydrological properties, crop growth and development parameters, climate variables, and, most importantly, management events (i.e., tilling, planting, fertilization, harvest, and Irrigation) data from 2011 to 2020. To ensure stability in C-N pools after soil initialization, the simulations were started 10 years earlier (model spin-up) with model input data copied and extrapolated from 2011–2020 to the spin-up period 2001–2010. Result data analysis was performed for the period 2013–2019. For irrigated crops, irrigation was assumed to prevent water stress, with an application rate of 30 mm triggered by low soil moisture periods (four events, with an annual water dose of 1200 m³ ha⁻¹). Assumptions about the physicochemical characteristics of pig and cattle slurry used as organic fertilizer are based on information provided by Hamelin et al.⁶⁵.

Comparison of aggregation approaches

Approach A. In this approach, we used all available high-resolution information without aggregating any data, such that the soil database (~30.4 m spatial resolution) determined the simulation resolution. Therefore, the model was deployed at the sub-field level (aligning with the resolution of the soil database), incorporating available management data at field scale, such as fertilizer type, amount, and management dates, along with accurate crop rotation information for 20 main crops (SBAR Spring barley, WIWH Winter wheat, VEGETABLE Vegetable, SICO Silage corn, GRASS Grass, RAPE Rapeseed, PERG Perennial grass, SPRINGRYE Spring rye, WBAR Winter barley, PEAS Pea, POTAT Potato, OATS Oats, LOPE Ryegrass, WINTERRYE Winter Rye, BEET Sugar beet, FABA Faba bean, SPWH Spring wheat, FOCO Food corn, TRSE Triticale, FLOWER Flower). Subsequently, after applying the model throughout the entire study period, the outcomes for the 2013–2019 timeframe were subjected to post-processing for comparison with other approaches. It is worth noting that all the approaches utilize the same crop and soil process parameterizations.

Approach B. In this approach, we aimed to reduce the complexity of the catchments to six different mono-cropping systems occurring on a representative soil for each catchment (i.e., running six mono-cropping simulations in parallel and subsequently merging the results based on area shares). Catchment-level management data (see section “Model

input data”) was utilized to condense the actual crop rotations to six main crops and derive average management (timing, fertilizing, manuring, etc.) for each catchment individually throughout the simulation period. Subsequently, leveraging the fractional cover information of each major crop in each year, the results were aggregated to their proportion during post-processing and prepared for comparison.

Approach C. This approach is built upon representative major crop rotations for Danish agriculture, as outlined by Rashid et al.⁶⁶, deployed on the representative soil for each catchment as in Approach B. These 20 crop rotations include various combinations of all major crops within the six LOOPs and feature diverse arrangements of cereals, industrial crops (POTA, BEET, RAPE), legumes (PEAS), forage crops (SICO), GRASS, and PERG. The crop rotations have been extrapolated to cover the simulation period, and the catchment-level input data (see section “Model input data”) has been used to define the management (timing, fertilizing, manuring, etc.) for each rotation. The annual simulation results were subsequently averaged for the main crops across all rotations and from 2013 to 2019 to provide average results. Further, the averaged results were then post-processed based on the long-term average fractional cover of each major crop in each LOOP. It is important to note that this approach does not provide yearly results as the rotation data lacks temporal information. To facilitate meaningful comparisons with other approaches, we aggregated and organized the data from these other approaches into the same format.

The annual average amounts of synthetic and organic fertilizers used for simulation by each approach are provided in Fig. S.1.

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Author contributions

J.R., E.H., and K.B.B. conceived and designed the study. J.R. and E.H. prepared model input data and performed the simulations, data processing, and analysis. J.R. wrote the first draft, while other co-authors (E.H., D.G., D.A., M.O.A., C.S., G.B.-M., and K.B.B.) have contributed in improving the manuscript.

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