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RESEARCH ARTICLE

A model-based estimate of nitrate leaching in Germany for GHG reporting

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Abstract

Background: Conversion of leached and runoff nitrate (NO_3^-) from agricultural land into emissions of the greenhouse gas (GHG) nitrous oxide (N_2O) by denitrification in water bodies has to be reported in national GHG inventories. The global IPCC default methodology for estimating these indirect N_2O emissions assumes that a fixed fraction of nitrogen (N) inputs ($Frac_{LEACH}$) is lost through leaching and runoff. However, this method does not consider all relevant country-specific conditions that may influence NO_3^- leaching.

Aims: The aim of this study was to apply a model-based approach for estimating indirect N_2O emissions through NO_3^- leaching and runoff from agricultural soils for use in Germany's national GHG inventory.

Methods: High-resolution spatial data and a comprehensive model system (RAUMIS-mGROWA-DENUZ) were used to derive regionally differentiated and temporarily dynamic $Frac_{LEACH}$ values from N surplus and hydrogeological conditions. These were then used to estimate indirect N_2O emissions in accordance with the IPCC methodology.

Results: The nationwide average of the new implied $Frac_{LEACH}$ values was 0.099 kg N (kg N input)$^{-1}$ in 2019. The new estimate of indirect N_2O emissions was 10.4 Gg N_2O in 1990 and 5.7 Gg N_2O in 2019, which are 27 and 52% less than the calculation based on the 2006 IPCC Tier 1 methodology.

Conclusions: The model-based method for estimating $Frac_{LEACH}$ incorporates relevant factors that influence NO_3^- leaching and runoff and considers site-specific, spatially varying conditions and differences in the agrarian structure. The use of N surplus as the model driver allows annual changes in cropping conditions and the effects of N-regulating policies and mitigation measures to be represented.

KEYWORDS
emission inventory, indirect N_2O emissions, nitrate leaching model, nitrogen surplus

1 | INTRODUCTION

Nitrogen (N) is an essential input to crop production. Since the invention of the Haber-Bosch process, there has been an overabundant supply of N. N flows are considered to exceed the safe operating space for the planet (Steffen et al., 2015). Modern intensive agriculture is the major source of reactive N losses to the environment (Galloway et al., 2003), presenting a wide range of challenges for ecosystems and human health (Brink et al., 2011). Reactive N is lost via different pathways, for example, through nitrate (NO_3^-) leaching (N leaching), gaseous ammonia (NH_3) losses or nitrous oxide (N_2O), nitric oxide (NO), and dinitrogen (N_2) emissions from denitrification processes.

N leaching is a hydrological pathway from topsoil into groundwater, through which mineral N is dissolved and transported in seepage water. Leaching occurs when precipitation and/or irrigation exceeds field capacity and evapotranspiration, and soil NO_3^- has accumulated because N inputs have exceeded current crop needs. N leaching has numerous environmental impacts and potential implications for human health. These include negative effects on surface water and groundwater quality, eutrophication of ecosystems, acidification, and reduced biodiversity (Di & Cameron, 2002; Galloway et al., 2003; Hashemi et al., 2018; Molina-Navarro et al., 2014; Wang et al., 2019; Zhang & Yu, 2020).

The natural process of N conversion via nitrification and denitrification that occur in soil and in groundwater and surface water bodies can contribute to indirect emissions of the long-lived greenhouse gas (GHG) N_2O, a contributor to global warming and ozone depletion (IPCC, 2014; Ravishankara et al., 2009). Its 100-year global warming potential is 265 times greater than that of an equal mass of carbon dioxide (Butterbach-Bahl et al., 2013; IPCC, 2014). The increasing use of N to fertilize agricultural crops has altered the natural N cycle, and it is estimated that 22% of current global N_2O emissions result from N inputs in agriculture (Tian et al., 2020).

Progress in meeting the GHG reduction goals set in the Kyoto Protocol and subsequent agreements within the United Nations Framework Convention of Climate Change (UNFCCC) is evaluated based on national GNG inventory reports, which have to be compiled annually by countries listed in its Annex I. The Intergovernmental Panel on Climate Change (IPCC) provides internationally agreed guidelines for the estimation of GHG emissions for national GNG inventories (IPCC, 2006, 2019). The guidelines distinguish between two pathways that lead to N_2O emissions from N inputs in agriculture. In the direct pathway, N_2O is emitted directly from the soil, where N is added through fertilization, harvest residues, or mineralization of soil organic matter. A smaller but still important source are two indirect pathways: (1) volatilization of NH_3 and oxides of N (NO_x) and their subsequent redeposition and (2) N_2O emissions originating from N losses from agricultural land through leaching and runoff ($N_2O_{(L)}$). Both pathways result in N_2O emissions in other locations. In the IPCC Tier 1 approach, total $N_2O_{(L)}$ emissions are calculated using the fraction of N that is lost through leaching and runoff ($Frac_{LEACH}$), all N inputs to managed soils in regions where leaching and runoff occur, and an emissions factor (EF) (IPCC, 2019, Equation 11.10):

$$N_2O_{(L)} - N = N_{input} * Frac_{LEACH} * EF_5. \quad (1)$$

These total N_2O emissions are the sum of emissions that “may take place in the groundwater below the land to which the N was applied, or in riparian zones receiving drain or runoff water, or in the ditches, streams, rivers and estuaries (and their sediments) into which the land drainage water eventually flows” (IPCC, 2019, p. 11.21). EF_5 functions as a combined EF for these locations (IPCC, 1996, 2006, 2019). Distinct EFs for each location are not available in the IPCC methodology (IPCC, 2019) and therefore only the combined emission of N_2O from denitrification and other processes at these locations can be estimated.

Germany’s National Greenhouse Gas Inventory currently calculates indirect N_2O emissions from N leaching and surface runoff with this methodology using the default values for $Frac_{LEACH}$ (0.3 kg N [kg N input]$^{-1}$) and EF_5 (0.0075 N_2O-N [kg N leaching/runoff]$^{-1}$), as stated in the 2006 IPCC guidelines (Federal Environment Agency, 2021; IPCC, 2006; Rösemann et al., 2021). The IPCC has recently updated estimates of $Frac_{LEACH}$ to a value of 0.24 kg N (kg N input)$^{-1}$ and EF_5 to a value of 0.011 N_2O-N (kg N leaching/runoff)$^{-1}$ for wet climates (IPCC, 2019). However, this global estimate of $Frac_{LEACH}$ remains very uncertain, with a confidence interval of between 0.1 and 0.8 kg N (kg N input)$^{-1}$ (IPCC, 2019). This updated $Frac_{LEACH}$ value was derived from a global meta-analysis and does not consider different soil properties and varying hydrological conditions (Wang et al., 2019). As N leaching is dependent on soil properties, different climatic factors, agricultural management practices, and agricultural N surplus (Blicher-Mathiesen et al., 2014; Di & Cameron, 2002; De Notaris et al., 2018; Wang et al., 2019), a global default value may not be a true reflection of respective national conditions (Zhou & Butterbach-Bahl, 2014). N_2O emissions from agricultural soils are a key category in Germany’s GHG inventory (Federal Environment Agency, 2021), for which IPCC guidelines require the use of a Tier 2 (country-specific) or Tier 3 (modeling) method, which should consider regional information and thereby reduce uncertainty and improve accuracy.

To facilitate fulfillment of this requirement, the aim of this study was to estimate regional and dynamic $Frac_{LEACH}$ values utilizing a model system. It considered high-resolution data on animal and crop production together with site-specific climate and hydrological factors and soil properties to reflect the heterogeneity of climatic and hydrogeological conditions, as well as farm types and agricultural production structures in Germany.

Western Germany is influenced by an oceanic climate with moderate temperatures and high precipitation, whereas in the east of the country, a more continental climate with particularly low precipitation rates in the north-east is prevalent. Due to intensive animal production, N surpluses are highest in north-west Germany, and even though some soils display high denitrification potentials (Ackermann et al., 2015), N leaching rates are generally high in this region. The north-east is dominated by intensive arable farming. N surpluses are lower, but NO_3^- concentrations in the leachate are elevated due to predominantly sandy soils and low precipitation (Kunkel et al., 2017). In the southern part of Germany, dairy farming on grassland is widespread, especially in the Alpine foothills. The heterogeneous natural conditions and agricultural structure necessitate a spatially differentiated modeling approach to derive a new estimate of $Frac_{LEACH}$ values for use in Germany's GHG inventory.

In addition to including detailed spatial characterization of soil properties in the model, a particular focus was put on agricultural N surpluses as a driver of N leaching (Di & Cameron, 2002; Wang et al., 2019). The agricultural N surplus of an area is defined as the difference between N application and removal through crop harvest products. Studies have found a positive correlation between N surplus and N leaching (Blicher-Mathiesen et al., 2014; Huang et al., 2017; Zhou & Butterbach-Bahl, 2014), and a greater influence of N surplus than N input on N leaching (De Notaris et al., 2018).

Simulation models have been used for more than 30 years to calculate NO_3^- concentrations in the leachate (Groenendijk et al., 2014). Each of these models has been developed against the backdrop of both a specific research question and a certain spatial scale of application. Physically based models, such as HYDRUS-1D (Šimůnek et al., 2008) and the Daisy model (Manevski et al., 2016), may be suitable for simulating site-specific pore water fluxes of NO_3^- at field scale (Colombani et al., 2020). However, their applicability on the scale of larger regions or entire countries is limited due to the fact that numerous input data are not available on this scale (Kunkel et al., 2017). For application at the spatial resolution of German federal states, models such as SWAT (Arnold et al., 1998), HYPE (Arheimer et al., 2012), and MONERIS (Fuchs et al., 2010) are more suitable. However, their maximum spatial resolution is limited to the level of subcatchment areas. Thus, the identification of site-specific hotspot areas of N leaching below this level is impeded. The model system RAUMIS-mGROWA-DENUZ (Heidecke et al., 2015; Herrmann et al., 2015; Kunkel et al., 2017; Wendland et al., 2009) is not only suitable for applications on a state scale, but also allows the NO_3^- concentration in the leachate to be determined with high spatial resolution (i.e., on a 100 × 100 m grid).

The model system has been applied at regional scales, for instance, in the Weser catchment (Heidecke et al., 2015; Hirt et al., 2012; Kreins et al., 2011; Kuhn et al., 2016; Wendland et al., 2009, 2010) and in the federal state of Lower Saxony (Ackermann et al., 2015; Heidecke et al., 2016). The models have also been applied to several other German states (Kuhr et al., 2014; Kunkel et al., 2017; Tetzlaff et al., 2009, 2017, 2021; Wendland et al., 2014, 2015, 2021). Most recently, the model system has been deployed nationwide in the AGRUM-DE project (Schmidt et al., 2020). Model results from this project have been used as a basis of information to help German authorities identify nitrate polluted areas, in accordance with the German Fertilizer Ordinance (Fertilizer Ordinance, 2020), and prepare river basin management plans (2021–2027) under the EU Water Framework Directive (The European Parliament and The Council of the European Union, 2000).

The model system has been proven to be a capable instrument for evaluating N-related issues at a high spatial resolution. The main aim of this study was to apply the RAUMIS-mGROWA-DENUZ model system to derive regionally differentiated $Frac_{LEACH}$ values thereby enabling quantification of indirect agricultural N_2O emissions for GHG reporting in a more suitable way than the estimation based on the global IPCC default approach.

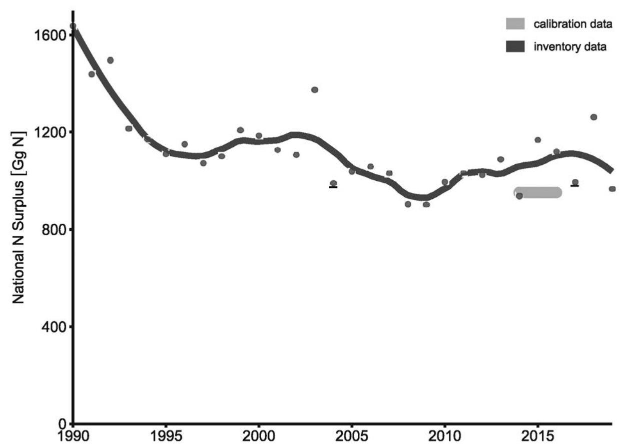

FIGURE 1 GHG inventory time series of national N surplus (Gg N) for the inventory time period and calibration data. Points depict annual inventory N surpluses. In order to highlight trends, a curve was fitted using local polynomial regression (LOESS) with a span equal to 0.3.

2 | MATERIALS AND METHODS

The aforementioned models were used and linked to model high-resolution N surplus and resulting N losses through leaching and runoff for the years 2014–2016, calculated as an average over the 3 years to reduce the impact of outliers. Estimations of N surplus excluded atmospheric N deposition. All units indicating hectare refer to hectare agricultural area, excluding all other land uses. A depiction of the workflow of the applied methodology is supplied in the supporting information (Figure 1 and Supporting Information 1).

2.1 | Data

The model input database was compiled for the years 2014–2016, primarily from official statistical information. For RAUMIS land use and livestock production, data at municipality level were taken from the Thünen-Agraratlas (Processed data. Original data from statistical offices of the federal states [district data from agricultural census 2016]; research data center of Germany and the federal states, agricultural census 2010, and und AFiD panel "Agrarstruktur" 1999, 2003, 2007, 2016 [own calculations: 1999–2016. Cluster estimator]; © GeoBasis-DE/BKG [2016]. Derived using the method of Gocht & Röder [2014]. Version 2020.). Crop yield data were obtained from the Federal Statistical Office (www.destatis.de). Data on agricultural use of compost and sewage sludge were available at NUTS-1 level (Landesamt für Statistik Niedersachsen, 2019; StBA, v.y.). Data on biogas plants and biogas production were assembled from publicly available

TABLE 1 German NUTS-1 regions and their abbreviations

Region (NUTS-1)	Abbreviation
Northrhine-Westphalia	NW
Lower Saxony North-West and Bremen	NI-W + HB
Lower Saxony South-East	NI-E
Bavaria	BY
Mecklenburg Western Pomerania	MV
Saxony-Anhalt	ST
Schleswig Holstein and Hamburg	SH + HH
Brandenburg and Berlin	BB + BE
Saxony	SN
Baden-Württemberg	BW
Thuringia	TH
Hesse	HE
Rhineland-Palatinate and Saarland	RP + SL

databases of the plant register (www.marktstammdatenregister.de) and national network operators. Substrate use data for biogas production were derived from Daniel-Gromke et al. (2017) and federal state authority data. Manure transportation data were available for some states from federal state authorities. National data on the use of mineral fertilizer were taken from the mineral fertilizer sales statistics (StBA, 2019).

For mGROWA-DENUZ, the German soil map 1:200,000 (BUEK200) (BGR, 2018) with horizon-wise data on soil type, humus content, field capacity, depth, waterlogging and groundwater influence was used. Long-term data on precipitation and the grass reference evapotranspiration were obtained from the German Meteorological Service. Land use and topography data were taken from the Federal Agency for Cartography and Geodesy. A detailed list of all data used for RAUMIS-mGROWA-DENUZ is supplied in the supporting information (Table 1 and Supporting Information 1).

For calculation of indirect N_2O emissions from leaching and runoff, N inputs as reported in the GHG inventory (Rösemann et al., 2021) were used. N removal by harvest and grazing was estimated from harvest data (StBA, FS3 R3.1.3, FS3 R3.2.1). N inputs and harvest data are a mandatory part of the annual GHG reporting for countries listed in the UNFCCC's Annex 1.

2.2 | N surplus model

N surpluses were modeled using the Regional Agricultural and Environmental Information System (RAUMIS). RAUMIS is a regional agricultural supply model based on "regional farms" at NUTS-3 level (Eurostat, 2020), developed in the 1990s as a tool for spatial agricultural policy analysis (Henrichsmeyer et al., 1996). It represents agricultural production, factor input and income on a regional level based on statistical information and a number of environmental indicators such as N balances. For the latter, an extension at municipality level is available, allowing the high-resolution estimation of N surpluses, while also being able to include a variety of heterogeneous data sources. A number of studies conducting agricultural policy analysis of agricultural N and GHG emissions in Germany have been carried out using the model system (e.g., Ackermann et al., 2016; Gömann et al., 2002; Henseler & Dechow, 2014; Kreins et al., 2007). N surpluses have been modeled in the form of net area balances for the period 2014–2016 as part of the AGRUM-DE project (Schmidt et al., 2020). The RAUMIS database also comprises regional yields, spatial information on biogas plants, and manure transportation data.

Let k represent German municipalities, A_{ck} the area of a specific crop c in a municipality k. M_k is the total amount of mineral N, and N_{jk} the total amount of organic N applied from source j (animal manure, biogas digestates, sewage sludge and compost). F_{ck} represents crop-specific N fixation rates from legumes, Y_{ck} is regional per hectare crop yields, xn_c is the respective crop's N content and G_{jk} are total gaseous emissions from organic fertilizer application. N field surpluses NS_k are thus calculated as:

$$\mathrm{NS}_k = \sum_j \left(N_{jk} - G_{jk}\right) + M_k + \sum_c F_{ck} * A_{ck} - \sum_c Y_{ck} * A_{ck} * xn_c, \tag{2}$$

with $G_{jk} = 0$ for $j \in$ (compost, sewage sludge).

Data on regional mineral fertilizer use are usually not available. Therefore, mineral fertilizer application in municipality k is modeled by means of yield-dependent and crop-dependent linear N requirement functions. The total N requirement per municipality TR_k is calculated as:

$$\mathrm{TR}_k = xs_k * \sum_c \left[\left(a_c * Y_{ck} + b_c\right) * A_{ck}\right], \tag{3}$$

where xs_k reflects local site specifics such as soil and climate conditions, affecting TR_k (Krüll, 1988; as cited in Henrichsmeyer et al., 1996), and a_c and b_c are individual parameters of the model's N requirement function for every crop (Kreins et al., 2009). These functions are derived from national fertilization recommendations and reflect regional yield levels as well as site conditions (Henrichsmeyer et al., 1996). Finally, total mineral fertilizer application at municipality level is represented by:

$$M_k = \beta * \mathrm{TR}_k - \alpha * \sum_j \left(N_{jk} - G_{jk}\right), \tag{4}$$

taking into consideration the share of total organic N being available for the crops (α) and a calibration factor (β). These factors were chosen in a way that $\sum_{k=1}^{n} M_k$ equals the amount of mineral fertilizer reported in the national mineral fertilizer sales statistics (StBA, 2019). For this study, aggregate N surpluses at NUTS-3 level were used.

2.3 | Model of nitrate leaching

The N surplus of agriculturally used soils determined with the RAUMIS model does not generally correspond with the N output from these soils. This is due to microbial conversion processes by which the surplus is reduced into gaseous N compounds that can leave the soil and enter the atmosphere. An area-differentiated simulation of these N conversion processes in the soil has been carried out using the DENUZ model (Kunkel & Wendland, 2006; Wendland, 1994).

For grassland, it is assumed that 30% of the sum of N balance surpluses from agriculture and atmospheric deposition is stored in the soil and contributes to the formation of soil organic matter (Wendland, Herrmann et al., 2020). For arable land, it is assumed that no immobilization occurs as these soils are N-saturated after decades of fertilization (Wendland et al., 2009). Accordingly, the N output from arable soils corresponds to the leachable NO_3^--N in soil (N surpluses from agriculture plus atmospheric deposition minus N immobilization) minus the denitrification losses in the root zone of the soil. For the purposes of this study, N input from atmospheric deposition was excluded to avoid double counting of indirect emissions from volatilization in the GHG inventory. The process of denitrification is simulated in the DENUZ model for both grassland and arable land based on Michaelis–Menten kinetics:

$$\frac{dN(t)}{dt} + D_{max} \times \frac{N(t)}{k + N(t)} = 0, \tag{5}$$

where $N(t)$ = N content in soil after time t (kg N [ha y]$^{-1}$); t = residence time of the leachate in soil (y); D_{max} = maximum denitrification rate (kg N [ha y]$^{-1}$); k = Michaelis constant (kg N [ha y]$^{-1}$).

The first step in modeling NO_3^- degradation in soil with the DENUZ model was to classify the denitrification conditions of soils throughout the study area. This then allowed the assignment of regional soil type-specific maximum denitrification rates (D_{max}) per year. The classification of NO_3^- degradation conditions in the soil depends on various soil properties. For example, high water storage capacities and humus contents are favorable for achieving high denitrification rates in the soil, whereas low denitrification rates can occur in soils with limited water storage capacities and reduced humus content (Köhne & Wendland, 1992; Kunkel et al., 2010; Wendland et al., 1998, 2005; Wendland, Herrmann et al., 2020; Wienhaus et al., 2008).

The D_{max} values applied in this study originated from relevant research work in the federal states of Mecklenburg-Western Pomerania (Kunkel et al., 2017), Schleswig-Holstein (Wendland et al., 2014), Saxony-Anhalt (Kuhr et al., 2014), Lower Saxony (Heidecke et al., 2016), North Rhine-Westphalia (Kuhr et al., 2013; Wendland, Bergmann et al., 2020), Rhineland-Palatinate (Wendland et al., 2021), and Thuringia (Tetzlaff et al., 2016), as well as the Weser River basin (Kuhn et al., 2016). These studies distinguished between five classes of denitrification conditions, depending on the initial substrate of the soil stratum, the humus content and the influence of groundwater and waterlogging. They found that the denitrification rates assigned to the denitrification conditions in the soil during model parameterization can differ significantly from region to region, therefore regionally differentiated D_{max} values have been allocated to the soil types indicated in the German soil map 1:200,000 (BUEK200) (Federal Institute for Geosciences and Natural Resources, 2018). Value ranges according to Wienhaus et al. (2008) were used as starting points for the regionally differentiated parameterization of D_{max} for different soil types.

The residence time of the leachate in the soil was derived from the field capacity of the soil and the leachate rate (Hennings, 2000; Müller & Raissi, 2002), in which the index i is run over all the denitrifying layers in the soil profile:

$$t = \frac{1}{Q_{SW}} \sum_i \mathrm{nFK}_i \times d_i, \tag{6}$$

where t = residence time of the leachate in soil (y); Q_{sw} = leachate rate (mm year^{-1}); nFK = effective field capacity (mm dm^{-1}); d = thickness of soil layer (dm).

Using the kinetic parameters of denitrification, the initial displaceable N surpluses in the soil and the residence times of leachate in the soil, the Michaelis–Menten differential equation can be solved numerically and the remaining N outputs from the soil can be calculated. It is then possible to combine the N emissions from the soil with the leachate rate (Q_{SW}) in order to calculate the potential NO_3^- concentration in the leachate ($C_{NO_3^-}$):

$$C_{NO_3^-} = \frac{443 \times N(t)}{Q_{SW}}, \tag{7}$$

where $C_{NO_{3-}}$ = potential NO_3^- concentration in the leachate (mg L^{-1}); $N(t)$ = N output from soil after residence NO_3^- time t in soil (kg N [ha y]$^{-1}$); Q_{sw} = leachate rate (mm year^{-1}).

The leachate rate (Q_{SW}) is an important parameter for calculating both, residence time in soil according to (6) and the NO_3^- concentration in the leachate (7). In this study, leachate rate was determined on the basis of the mGROWA model (Herrmann et al., 2015), which simulates the hydrologic processes at the earth's surface and in the root zone of soils. In particular, soil moisture dynamics including the movement of the leachate in the soil, capillary rise from groundwater to the root zone, actual evapotranspiration, and total runoff generation were calculated in daily time steps on the basis of grass reference evapotranspiration, land use-specific crop coefficients, and a topography correction function (Wendland, Bergmann et al., 2020). Leachate rates, that is, the amount of water that leaves the root zone of the soil vertically downward, are aggregated to mean long-term averages in order to exclude short-term climate-induced blurring of leachate rates and to guarantee that the modeled NO_3^- concentrations in the leachate are representative for the regional long-term hydrologic conditions (Wendland, Bergmann et al., 2020).

Against this background, the NO_3^- concentration in the leachate is calculated based on the DENUZ model. In this model, the mean long-term leachate rates from the mGROWA model are combined with the N output from the root zone of soil after residence time in soil. For the latter, agricultural N balance surpluses are considered as N input and denitrification (5) and immobilization processes in soil as N losses.

2.4 | Creating a time series of nitrate leaching for the national inventory

To enable estimation of indirect N_2O emissions from N leaching for national GHG reporting, data for the whole inventory time series are needed. Since high-quality input data for the leaching model were only available as the mean of the years 2014 to 2016, a regional transfer coefficient was calculated:

$$F_{\text{Leach,Surplus}} = \frac{N_{\text{Leach,ref}}}{N_{\text{Surplus,ref}}}, \tag{8}$$

where $N_{\text{Leach,ref}}$ is the average annual amount of N leached in 2014–2016 modeled with RAUMIS-mGROWA-DENUZ and $N_{\text{Surplus,ref}}$ is the average N surplus in the same years derived from data available in the German national inventory (Federal Environment Agency, 2021). The transfer coefficient was then multiplied with the inventory N surplus for each region and year in order to derive the time series of leached and runoff N. Since the inventory data do not currently include data on manure transports and also contain substantial uncertainties regarding spatial distributions, the transfer coefficients were calculated at NUTS-1 level. Only Lower Saxony was divided into two regions: the north-west of the state (NI-W), which has the highest livestock density in Germany, and the south-east of the state (NI-E), where cash-crop farming is more prevalent. City states were merged with neighboring federal states, that is, Hamburg with Schleswig-Holstein, Bremen with Lower Saxony (north-west), and Berlin with Brandenburg (Table 1).

For the calculation of time series, N surplus was derived from N inputs reported in the inventory (Rösemann et al., 2021), that is, synthetic fertilizers, manure application, crop residues, grazing, sewage sludge, biogas digestates, and mineralization of soil organic matter. N input from N deposition was excluded to avoid double counting of indirect emissions from volatilization, which are already estimated by the inventory and include, at least in theory, the pathway N deposition–N leaching–denitrification. N removal by harvest and grazing was estimated from harvest data (StBA, FS3 R3.1.3, FS3 R3.2.1).

As the model calculates leached N out of the root zone, the combined Tier 1 EF ($EF_5 = 0.011$ kg N_2O-N [kg N leaching/runoff]$^{-1}$) for indirect N_2O emissions from leaching and runoff in downstream water bodies can be applied. A multiplication of the leached/runoff N with the EF gave the indirect N_2O emissions. For comparison with the IPCC Tier 1 $Frac_{LEACH}$ value (IPCC, 2019), implied $Frac_{LEACH}$ values were calculated as N leached/runoff divided by the inventory's N input for the respective year and region.

2.5 | Validation of N leaching model and uncertainty estimates

Modeled N outputs from soil can be validated using measured values from soil depth profiles, suction probes, and lysimeters. However, such measurements are only available in a few cases and do not allow a plausibility check to be undertaken on a national scale (Wolters et al., 2021). Instead, modeled concentrations in leachate can be compared with measured NO_3^- values from the upper aquifer, for which more data are available.

However, monitoring sites need to meet certain preselection criteria (Wolters et al., 2021). These include the measuring points being either springs or groundwater observation wells filtered near the surface. Furthermore, the redox indicators should show an oxidized groundwater milieu so that denitrification processes in groundwater can be excluded as much as possible. In addition, the catchment area of the measuring point must be identified to calculate an average modeled NO_3^- concentration in the leachate for each area. If these criteria are met, observed NO_3^- concentrations in groundwater can be used to check the plausibility of the simulated NO_3^- concentrations in the leachate and thus indirectly the plausibility of the simulated N emissions from the soil.

Due to the different spatial and temporal reference of random point measurements in groundwater and model results for mean long-term NO_3^- concentration in leachate, but also due to the limited site-specific accuracy of the input data for modeling, an exact site-specific agreement of model values and measured values can hardly be expected. In order to assess systematically and comprehensibly if the spatial patterns and magnitudes of modeled NO_3^- concentrations in the leachate are confirmed by measured NO_3^- values from the upper aquifer, the observed and measured values were first categorized. Subsequently, the compliance of the measured and observed values to the resulting classes was assessed (Wolters et al., 2021). The class width was determined by considering the number and range of the measured values. Since there was a very large range in the measured values and the modeled values, a uniform class width of 25 mg NO_3^-/L was defined to ensure comparability. The comparison was based on seven classes (0–25, 25–50, ..., >150 mg NO_3^-/L). The agreement between modeled and observed NO_3^- levels in each class was then evaluated. The difference between the classes was used as a measure of the assessment. In this context, agreement is considered good if the observed and measured concentrations are in the same class. Acceptable agreement is when there is a deviation of one concentration class. If the deviation is two concentration classes or more, the agreement is moderate or poor.

Since the uncertainties and covariances included in many model input parameters were not available for this study, it was not possible to perform a traditional uncertainty analysis based on error propagation. Nevertheless, as modeled NO_3^- concentrations in the leachate were validated using measured values from the upper aquifer (Wolters et al., 2021), an approximate uncertainty estimate could be derived.

3 | RESULTS

The resulting 3-year average N surplus for Germany's agricultural area for the calibration data was calculated to be 951.2 Gg N year^{-1} (corresponds to 57.2 kg N ha^{-1} year^{-1}). For the same period, the inventory calculates a mean N surplus of 1074.6 Gg N year^{-1} (corresponds to 64.3 kg N ha^{-1} year^{-1}) ($N_{\text{Surplus,ref}}$). Overall, since 1990, the nationwide inventory N surplus has decreased by approximately 41% from 1637 Gg N year^{-1} to 966 Gg N a^{-1} (Figure 1). In recent years, there has been a slight increase in the N surplus due to consecutive years with very dry conditions, leading to lower crop yields and hence reduced N removal through N uptake by plants and through harvest (Klages et al., 2020). However, the development of the N surplus in Germany's NUTS-1 regions is heterogeneous (Figure 2). All regions experienced a strong

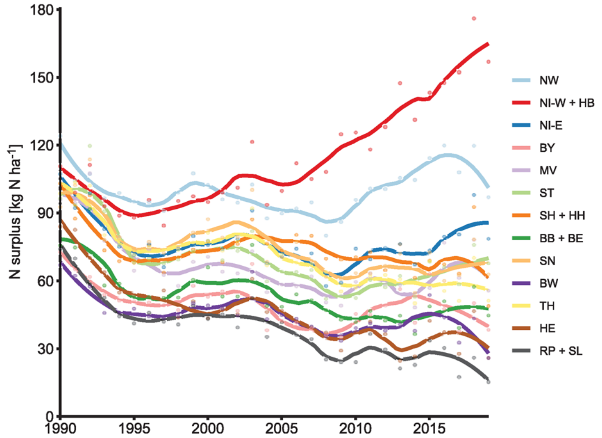

FIGURE 2 GHG inventory time series of N surplus per hectare agricultural area in the study regions. Points depict modeled annual values for each study region. In order to highlight trends, a curve was fitted using local polynomial regression (LOESS) with a span equal to 0.3.

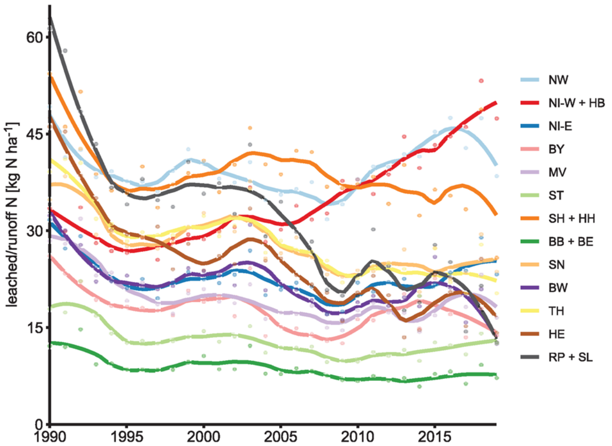

FIGURE 3 GHG inventory time series of lost N per hectare agricultural area to water bodies through leaching and runoff in the study regions. Points depict modeled annual values for each study region. In order to highlight trends, a curve was fitted and smoothed using local polynomial regression fitting (LOESS) with a span equal to 0.3.

decline until 1995, with a moderate increase in the early 2000s due to the introduction of anaerobic digestion plants for biogas production. In regions with a high and increasing livestock density (NI-W + HB), since around 2000, the N surplus has grown significantly.

In the reference period, an estimated $N_{Leach,ref}$ of 385 Gg N year^{-1} (corresponds to 23.1 kg N ha^{-1} year^{-1}) left the root zone and was lost to water bodies through leaching and runoff. The average national $F_{Leach,ref}$ (Equation 8) is 0.36. Leached N was calculated as the product of inventory N surplus and $F_{Leach,ref}$ for each year and region. Figure 3 shows the N leached per hectare since 1990. Brandenburg and Saxony-Anhalt had the lowest and most stable leaching rates because they are generally dryer regions with moderate surpluses. The manure-abundant western part of Lower Saxony and North Rhine-Westphalia,

TABLE 2 Calculated annual amounts of leached N (Gg N) from agricultural soils in German NUTS-1 regions for the GHG inventory time series

Region	1990	1991	1992	1993	1994	1995	1996	1997	1998	1999	2000	2001	2002	2003	2004
SH + HH	59.2	50.3	56.0	41.9	38.9	38.3	42.6	35.7	39.3	40.7	42.3	37.3	41.4	47.4	41.3
NI-W + HB	32.5	29.0	32.6	27.3	26.1	25.7	27.9	24.5	27.6	27.9	26.8	27.9	28.6	34.2	26.4
NI-E	55.8	48.0	51.4	43.3	39.2	37.1	39.5	34.1	38.2	40.7	38.2	37.2	39.5	45.6	34.0
NW	77.6	65.4	66.9	60.3	61.6	59.0	58.6	56.0	60.7	64.0	60.5	57.0	55.5	62.0	52.9
HE	35.7	35.0	29.8	27.5	23.7	22.9	22.5	23.8	18.6	21.4	18.2	20.0	18.6	25.5	19.1
RP + SL	48.2	45.6	38.1	34.7	29.3	27.1	30.0	27.7	27.0	32.2	28.3	29.5	25.6	34.0	22.9
BW	48.2	44.6	41.2	32.9	32.9	34.1	31.5	30.8	32.1	35.7	34.7	33.9	31.4	44.9	30.0
BY	89.1	79.5	75.1	65.5	62.4	61.9	61.0	59.4	57.0	68.3	62.2	64.7	54.5	79.1	45.1
BB + BE	17.4	15.3	18.2	12.1	12.3	11.4	11.5	11.4	11.5	13.1	14.3	11.5	11.4	16.2	10.6
MV	42.9	36.4	40.7	30.3	30.9	25.7	29.6	25.1	23.5	27.6	28.7	25.8	25.5	29.3	22.2
SN	36.6	32.2	34.4	25.1	26.9	24.9	26.4	24.7	25.7	28.1	30.1	27.5	27.5	34.4	23.3
ST	23.2	19.3	23.1	17.9	16.1	14.6	15.2	14.8	15.2	15.9	16.9	15.0	15.9	17.8	13.0
TH	34.5	31.4	31.0	25.1	24.6	22.7	23.9	23.6	23.6	24.6	25.9	23.4	24.5	29.0	21.0
Germany	600.9	532.0	538.4	443.7	425.0	405.5	420.0	391.6	400.0	440.3	427.2	410.6	400.0	499.4	361.7

Region	2005	2006	2007	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017	2018	2019
SH + HH	39.6	42.9	43.1	37.3	36.8	37.6	38.9	34.3	40.4	32.6	36.5	35.6	33.4	48.9	25.9
NI-W + HB	28.2	31.5	29.6	30.4	35.0	34.8	33.0	35.8	41.1	37.1	40.1	41.3	42.4	49.3	43.5
NI-E	35.5	37.2	36.2	28.9	29.5	36.6	34.6	37.0	37.8	33.8	36.6	39.6	39.9	48.8	38.8
NW	54.3	54.9	56.4	47.7	51.1	55.6	58.3	57.7	61.2	60.6	66.1	68.4	62.5	68.8	57.4
HE	19.8	17.9	17.0	15.8	12.5	15.7	17.7	15.3	10.4	11.2	17.9	15.7	11.8	19.8	10.9
RP + SL	27.3	23.4	22.5	16.6	15.6	15.6	23.6	19.0	13.9	14.8	21.8	19.5	11.3	16.8	10.0
BW	31.3	30.0	27.6	24.6	23.2	26.7	28.2	26.1	28.0	26.0	37.0	30.0	22.4	29.6	17.7
BY	49.4	48.0	45.0	41.5	40.4	51.0	50.7	55.1	63.4	46.7	71.3	53.4	42.2	55.7	42.7
BB + BE	10.5	11.6	11.0	10.0	9.1	8.9	9.9	9.0	9.4	7.7	10.4	10.8	8.3	12.2	9.5
MV	23.4	23.4	24.9	20.3	19.8	23.9	25.3	23.3	23.1	19.2	22.7	30.7	24.5	31.2	22.3
SN	24.2	26.4	23.8	21.2	20.9	21.8	21.6	22.8	24.6	18.6	24.7	20.4	21.2	26.5	21.3
ST	14.0	14.0	14.1	11.3	11.6	11.4	13.2	12.5	13.5	11.5	14.9	14.4	12.8	16.5	14.6
TH	22.7	21.5	21.2	20.1	17.4	17.8	19.3	19.4	18.8	15.5	21.3	17.2	15.8	21.6	15.8
Germany	380.2	382.8	372.5	325.8	323.0	357.3	374.1	367.2	385.8	335.3	421.2	397.0	348.5	445.7	330.4

TABLE 3 Annual indirect N_2O emissions (Gg N_2O) based on new implied $Frac_{LEACH}$ values in German NUTS-1 regions using the 2019 IPCC guidelines emissions factor ($EF_5 = 0.011$ kg N_2O-N [kg N leaching/runoff]$^{-1}$)

Region	1990	1991	1992	1993	1994	1995	1996	1997	1998	1999	2000	2001	2002	2003	2004
SH + HH	1.02	0.87	0.97	0.72	0.67	0.66	0.74	0.62	0.68	0.7	0.73	0.64	0.71	0.82	0.71
NI-W + HB	0.56	0.5	0.56	0.47	0.45	0.44	0.48	0.42	0.48	0.48	0.46	0.48	0.49	0.59	0.46
NI-E	0.97	0.83	0.89	0.75	0.68	0.64	0.68	0.59	0.66	0.7	0.66	0.64	0.68	0.79	0.59
NW	1.34	1.13	1.16	1.04	1.07	1.02	1.01	0.97	1.05	1.11	1.05	0.99	0.96	1.07	0.91
HE	0.62	0.6	0.52	0.47	0.41	0.4	0.39	0.41	0.32	0.37	0.31	0.35	0.32	0.44	0.33
RP + SL	0.83	0.79	0.66	0.6	0.51	0.47	0.52	0.48	0.47	0.56	0.49	0.51	0.44	0.59	0.4
BW	0.83	0.77	0.71	0.57	0.57	0.59	0.54	0.53	0.55	0.62	0.6	0.59	0.54	0.78	0.52
BY	1.54	1.37	1.3	1.13	1.08	1.07	1.05	1.03	0.98	1.18	1.08	1.12	0.94	1.37	0.78
BB + BE	0.3	0.26	0.32	0.21	0.21	0.2	0.2	0.2	0.2	0.23	0.25	0.2	0.2	0.28	0.18
MV	0.74	0.63	0.7	0.52	0.53	0.45	0.51	0.43	0.41	0.48	0.5	0.45	0.44	0.51	0.38
SN	0.63	0.56	0.59	0.43	0.46	0.43	0.46	0.43	0.44	0.49	0.52	0.47	0.47	0.59	0.4
ST	0.4	0.33	0.4	0.31	0.28	0.25	0.26	0.26	0.26	0.28	0.29	0.26	0.28	0.31	0.22
TH	0.6	0.54	0.54	0.43	0.43	0.39	0.41	0.41	0.41	0.43	0.45	0.4	0.42	0.5	0.36
Germany	10.39	9.2	9.31	7.67	7.35	7.01	7.26	6.77	6.91	7.61	7.38	7.1	6.91	8.63	6.25

Region	2005	2006	2007	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017	2018	2019
SH + HH	0.68	0.74	0.75	0.64	0.64	0.65	0.67	0.59	0.7	0.56	0.63	0.62	0.58	0.85	0.45
NI-W + HB	0.49	0.55	0.51	0.53	0.6	0.6	0.57	0.62	0.71	0.64	0.69	0.71	0.73	0.85	0.75
NI-E	0.61	0.64	0.63	0.5	0.51	0.63	0.6	0.64	0.65	0.58	0.63	0.68	0.69	0.84	0.67
NW	0.94	0.95	0.98	0.83	0.88	0.96	1.01	1	1.06	1.05	1.14	1.18	1.08	1.19	0.99
HE	0.34	0.31	0.29	0.27	0.22	0.27	0.31	0.26	0.18	0.19	0.31	0.27	0.2	0.34	0.19
RP + SL	0.47	0.4	0.39	0.29	0.27	0.27	0.41	0.33	0.24	0.26	0.38	0.34	0.2	0.29	0.17
BW	0.54	0.52	0.48	0.42	0.4	0.46	0.49	0.45	0.48	0.45	0.64	0.52	0.39	0.51	0.31
BY	0.85	0.83	0.78	0.72	0.7	0.88	0.88	0.95	1.1	0.81	1.23	0.92	0.73	0.96	0.74
BB + BE	0.18	0.2	0.19	0.17	0.16	0.15	0.17	0.16	0.16	0.13	0.18	0.19	0.14	0.21	0.16
MV	0.4	0.41	0.43	0.35	0.34	0.41	0.44	0.4	0.4	0.33	0.39	0.53	0.42	0.54	0.39
SN	0.42	0.46	0.41	0.37	0.36	0.38	0.37	0.39	0.42	0.32	0.43	0.35	0.37	0.46	0.37
ST	0.24	0.24	0.24	0.2	0.2	0.2	0.23	0.22	0.23	0.2	0.26	0.25	0.22	0.28	0.25
TH	0.39	0.37	0.37	0.35	0.3	0.31	0.33	0.34	0.33	0.27	0.37	0.3	0.27	0.37	0.27
Germany	6.57	6.62	6.44	5.63	5.58	6.18	6.47	6.35	6.67	5.8	7.28	6.86	6.02	7.7	5.71

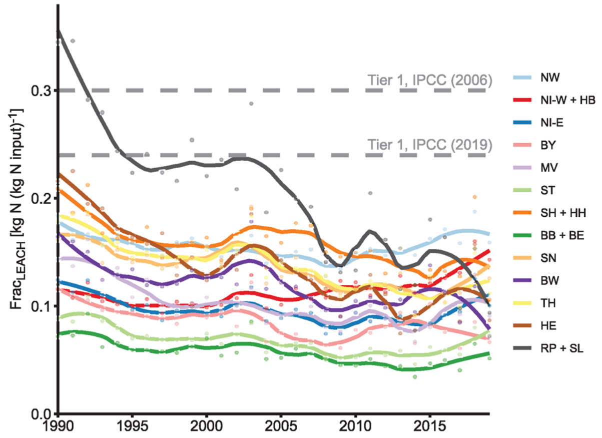

FIGURE 4 GHG inventory time series of $Frac_{LEACH}$ in the study regions compared with IPCC default values (IPCC, 2006, 2019). Points depict modeled annual values for each study region. In order to highlight trends, a curve was fitted using local polynomial regression (LOESS) with a span equal to 0.3.

both regions with the highest stocking densities in Germany, had the highest leaching rates per hectare. Most other regions showed moderate leaching rates of around 20 kg N ha^{-1}. Tables 2 and 3 shows the calculated absolute amounts of leached N leaving the root zone. Since 1990, the total amount of leached N decreased by 45% from 600.9 to 330.4 Gg N in 2019. Whereas all other regions experienced a decrease, in NI-W + HB the amount of leached N increased since 1990.

3.1 | $Frac_{leach}$

To derive a time series of implied $Frac_{LEACH}$ values, leached N was divided by the N input from the inventory. The resulting $Frac_{LEACH}$ for each year is shown in Figure 4. In 2019, $Frac_{LEACH}$ in all regions was below the IPCC default value of 0.24 kg N (kg N input)$^{-1}$ (IPCC, 2019), with a nationwide average of 0.099 kg N (kg N input)$^{-1}$ and a range between 0.051 kg N (kg N input)$^{-1}$ (BB + BE) and 0.159 kg N (kg N input)$^{-1}$ (NW) in 2019. Since 1990, most regions have shown a general downwards trend, with a slight increase recently mainly due to drought conditions during the vegetation period.

3.2 | N_2O emissions

Indirect N_2O emissions were calculated for the whole time series in accordance with the 2019 IPCC guidelines (IPCC, 2019). Based on the new estimation, emissions decreased from 10.4 Gg N_2O in 1990 to 5.7 Gg N_2O in 2019 (Figure 5, Tables 2 and 3). The largest reduction in indirect N_2O emissions from leaching and runoff occurred until 1995, with a decrease in emissions of 3.38 Gg N_2O. While lower on average, indirect N_2O emissions have experienced only a slight downwards trend since then. Due to higher N surpluses in recent years, emissions have increased slightly since 2015. In 2019, emissions were again

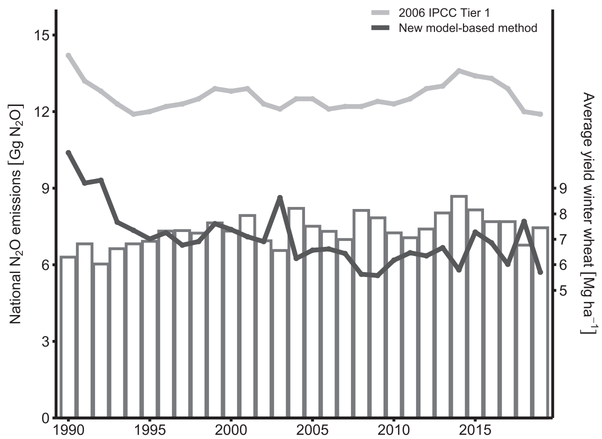

FIGURE 5 Estimated annual national indirect N_2O emissions based on the 2006 IPCC guidelines Tier 1 method and based on new implied $Frac_{LEACH}$ value in inventory time series together with national average wheat yields (StBA, FS3 R3.2.1).

below 6 Gg N_2O. Compared with the current methodology (IPCC, 2006; Tier 1) used in the German inventory (Federal Environment Agency, 2021), the new Tier 3 method leads to a nationwide reduction of indirect N_2O emission estimates of 27% in 1990 and 52.1% in 2019. Overall, indirect N_2O emissions calculated with the new method showed a greater variance, since N surplus and N leaching varied depending on the environmental conditions in the respective years, compared with the calculations with the constant IPCC default Tier 1 approach.

3.3 | Validation of nitrate leaching model and uncertainty estimates

Figure 6 shows the comparison of the class widths of modeled NO_3^- concentrations in leachate and measured NO_3^- concentrations in groundwater as a frequency distribution for 1496 preselected groundwater quality monitoring wells in the land use categories cropland (left) and grassland (right).

For the land-use category cropland, 1068 groundwater monitoring wells remained for comparison after preselection. Here, the modeled values show a good agreement at 30% of the monitoring sites, while a deviation of one class occurred at 40% of the monitoring sites. Overall, there was no tendency to systematically overestimate or underestimate the measured values. The corresponding deviations exhibit a symmetric distribution and thereby indicate that the overall system, which determines the NO_3^- concentrations in the leachate, is well represented.

For the land use category grassland 428 monitoring sites were available for comparison. At these monitoring sites, 62% show good agreement in NO_3^- concentration classes, while 29% overestimate or underestimate concentrations by one class. Although the frequency distribution shows a slightly higher number of groundwater monitoring sites where modeled NO_3^- concentrations in leachate were lower than measured NO_3^- concentrations in groundwater, the overall agreement of modeled and observed NO_3^- concentrations for the grassland land-use category can be considered very good.

For the approximate uncertainty estimate the percentage mean deviation of the modeled NO_3^- concentrations from measured concentrations in groundwater wells (−100%, +200%) was transferred to modeled $Frac_{LEACH}$ values, resulting in a 95% confidence interval of (0, 0.198) kg N (kg N input)$^{-1}$ for 2019, which is considerably narrower than that of the IPCC Tier 1 value.

4 | DISCUSSIONS

The aim of this study was to apply a model-based approach to estimate indirect N_2O emissions through N leaching and runoff from agricultural soils for Germany's national GHG inventory. A comprehensive model system was used to estimate regionally differentiated, country-specific $Frac_{LEACH}$ values to supersede the IPCC Tier 1 default value. The link of an agricultural economic model with hydrological models and the use of high-resolution spatial data allowed the representation of a wide range of different hydrological and hydrogeological conditions, as well as the drivers of the agrarian structure in Germany. Similar to the Tier 2 and Tier 3 approaches of other countries (UNFCCC, 2021), the newly estimated $Frac_{LEACH}$ was lower than the IPCC default EF, indicating an overestimation by the IPCC Tier 1 value. Germany's implied nationwide $Frac_{LEACH}$ of 0.099 kg N (kg N input)$^{-1}$ in 2019 is similar to other countries that use Tier 3 approaches. The Netherlands reports a $Frac_{LEACH}$ value of 0.13 kg N (kg N input)$^{-1}$ for 2019 based on STONE model results (Groenendijk et al., 2008; van der Zee et al., 2021; Velthof & Mosquera, 2011), Ireland uses a national average value of 0.1 kg N (kg N input)$^{-1}$ (Environmental Protection Agency, 2021) and New Zealand reports a value of 0.07 kg N (kg N input)$^{-1}$ (Ministry for the Environment, 2021).

Räbiger et al. (2020) modeled N leaching and indirect N_2O emissions for oilseed rape from five sites with different growing conditions (e.g., soil, temperature, precipitation) in the main rapeseed-growing areas in Germany. Even though oil seed rape is a crop with low N efficiency and high leaching potential (Räbiger et al., 2020), they modeled $Frac_{LEACH}$ values between 0.05 and 0.176 kg N (kg N input)$^{-1}$ depending on the site and fertilizer used. Indirect N_2O emissions were calculated to be 60–90% lower than those calculated using the IPCC default values. Fu et al. (2017) used lysimeters to measure N leaching on intensively and extensively managed montane cut grassland in southern Germany. They observed values of between 0.008 and 0.069 kg N (kg N input)$^{-1}$. Since N leaching rates from grassland are generally lower (Di & Cameron, 2002), the new estimate in the present study is in agreement with their findings.

Räbiger et al. (2020) emphasizes the need for site-specific EFs. This is confirmed by the comparatively wide range of estimated $Frac_{LEACH}$ values of the respective regions (2019: 0.051–0.159 kg N [kg N input]$^{-1}$) in the present study. As N leaching depends on multiple factors, such as soil properties of the topsoil, N denitrification potential and N input, a country-specific calculation of $Frac_{LEACH}$ based only on

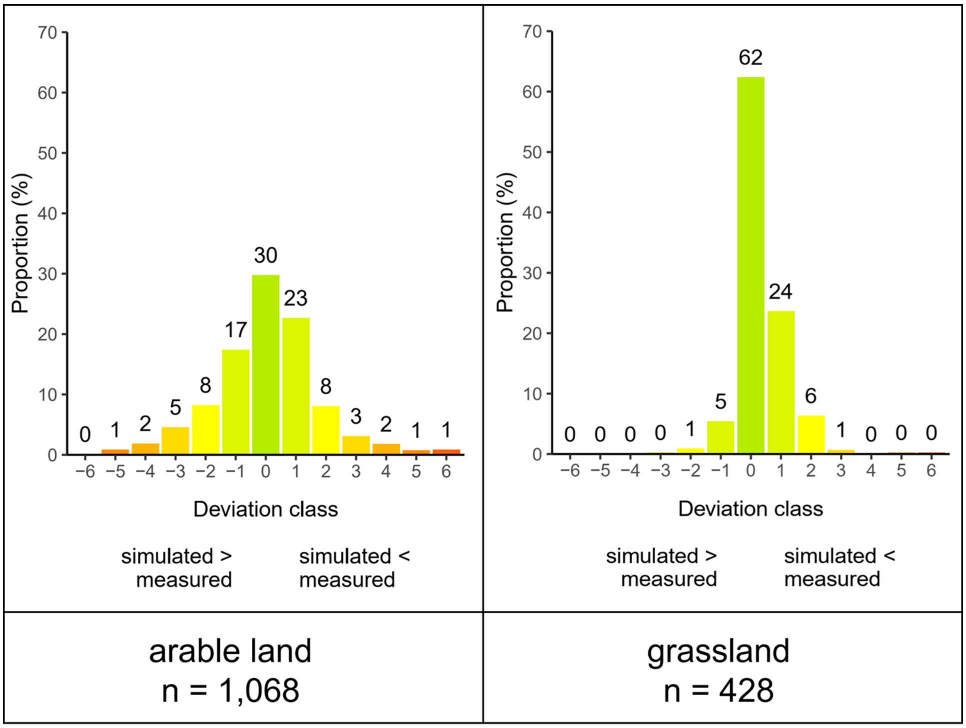

FIGURE 6 Frequency distribution of the deviation classes of simulated NO_3^- concentrations in the leachate and observed NO_3^- concentrations in the groundwater for the main land use types "arable land" (left) and "grassland" (right).

water balances, as used by some countries in their inventories as an IPCC Tier 2 approach, falls short of including all relevant controlling factors. $Frac_{LEACH}$ is highly dependent on denitrification conditions in the soil. Figure 7 shows the heterogeneity of denitrification losses in Germany. As outlined above, they depend not only on the denitrification conditions in the soil, but also on the residence time of the leachate in the soil. Thus, high denitrification rates were calculated for regions exhibiting high denitrification capacities in soil (lowland areas, soils with high organic carbon content), and regions exhibiting long residence times (loess regions), whereas low denitrification rates were calculated for the midland region, where low denitrification capacities in soil coincide with low residence times in soil. Along with differences in N surpluses in every region, this explains regionally different trends in the dynamics of $Frac_{LEACH}$. For instance, the regions of Rhineland-Palatinate and Saarland showed a strong decline in $Frac_{LEACH}$ between 1990 and 1995. In this five-year period, N surplus and N losses through leaching decreased by nearly 60%, whereas N inputs decreased by just 15%. And even though the N leaching rate in this area is the highest in Germany, $Frac_{LEACH}$ decreased greatly as a result. In contrast, denitrification capacities in the soil are generally high in north-west Germany (NW, NI-W + HB), yet high N surpluses led to the region having the highest $Frac_{LEACH}$ values in the country.

Substantial annual changes in indirect N_2O emissions could be observed because the use of N surplus rather than N inputs as the source of N leaching allowed the effects of annual changes in growing conditions to be reflected. High N inputs only result in high leaching when N uptake of the crops is low. In contrast to N input as

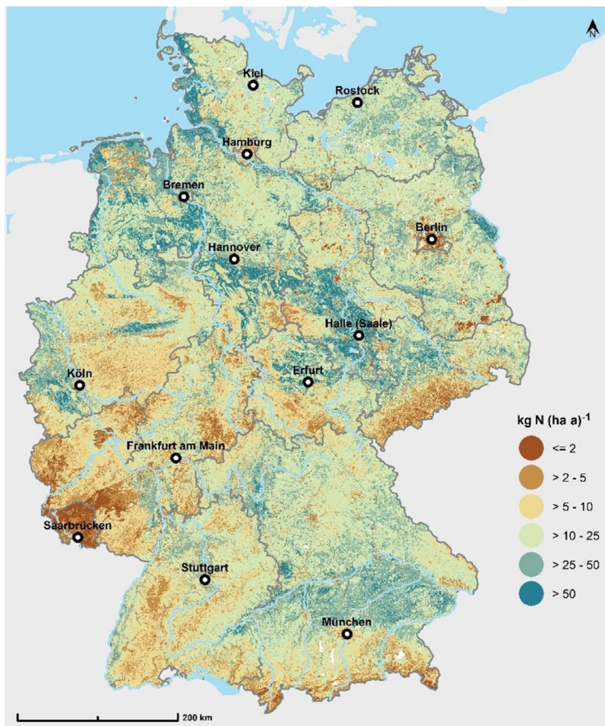

FIGURE 7 Denitrification loss in soil based on displaceable nitrogen input into soil, soil residence time, and maximum denitrification degradation according to the DENUZ model (Wendland et al., 2009).

an indicator, N surplus also considers N removal via harvest. A main cause of higher N surpluses is unfavorable growing conditions. Farmers plan crop N inputs at the beginning of the growing season, as required by the German Fertilizer Ordinance (Fertilizer Ordinance, 2020). Poor growing conditions lead to impeded crop growth and reduced N requirements. Consequently, N inputs area likely to exceed N uptake, and the increased N surpluses lead to higher N leaching risks, resulting in elevated indirect N_2O emissions. To illustrate this, national average wheat yields can be used (Figure 5). The years 2003 and 2018 were exceptionally dry and resulted in lower wheat yields. The N surplus increased N leaching and there was a rise in indirect N_2O emissions. Indirect N_2O emissions calculated based on the new $Frac_{LEACH}$ showed a highly significant, strongly negative correlation ($r = -0{,}71$, $p < 0.001$) with the national average wheat yield, whereas indirect N_2O emissions estimated based on the default $Frac_{LEACH}$ showed no significant correlation ($r = 0.19$, $p = 0.29$). Furthermore, in contrast to an input-based methodology, the N surplus-based approach was able to reflect altered management practices and technological progress regarding N-use efficiency.

In the inventory period since 1990, an overall reduction in N surplus and hence in indirect N_2O emissions can be observed. The magnitude and development of the N surpluses (Figures 1 and 2) estimated in this study agree with findings of Häußermann et al. (2020), based on a similar database as used in this study. They attribute the initial reduction of N surplus to the European Union's policy aimed at reducing N surplus and N leaching to protect water bodies from N pollution, formulated in the Nitrate Directive (The Council of the European Communities, 1991) and in its national implementation, the German Fertilizer Ordinance (Fertilizer Ordinance, 2020), which regulates N inputs and N application times. They state that increased biogas production in recent years has impeded mitigation efforts. However, the development of N surplus and thus indirect N_2O emissions is heterogeneous (Figure 2 and Table 2). Most regions showed a steady decrease in N surplus, whereas a few exhibited much higher or similar N surpluses compared with 1995 (e.g., NW, NI-E, NI-W + HB) (see Häußermann et al. [2020] for further discussion). The new, spatially differentiated method to estimate indirect N_2O emissions from N leaching allows that these developments are taken into consideration in GHG reporting.

Although the model system used in this study calculated $Frac_{LEACH}$ at a higher spatial resolution, the considerable uncertainty around input data from the 1990s necessitated aggregation of the results at NUTS-1 level for the inventory. Differences in the N surplus of the calibration data and the inventory data mainly arose as a result of different data sources being used. More accurate data from the 2016 agricultural census and additional data sources (e.g., on manure transportation) could be used in RAUMIS, whereas such detailed data are not available for the whole reporting period of the GHG inventory.

5 | CONCLUSIONS

The model system RAUMIS-mGROWA-DENUZ was designed to quantify and monitor regional water body pollution with nutrients from agricultural sources and to asses corresponding environmental policies. This study aimed to illustrate the model's capability to be also used to quantify indirect N_2O emissions for GHG reporting by deriving regionally differentiated $Frac_{LEACH}$ values. The application of the model system for GHG reporting allowed the inclusion of site-specific and spatially varying soil properties, hydrological conditions, climatic factors, and agricultural structure in the estimation of $Frac_{LEACH}$, which are not considered in the IPCC Tier 1 method. The use of N surplus rather than N input as the model driver allows the national GHG inventory to represent annual changes in cropping conditions, changes in N-use efficiency and the effects of N regulating policies and mitigation measures (The Council of the European Communities, 1991; Fertilizer Ordinance, 2020) aimed at reducing N surpluses. A combination of agricultural supply models with a water transport and a denitrification model and the use of high-resolution input data allow derivation of more accurate and less uncertain estimates of indirect N_2O emissions originating from NO_3^- leaching and runoff for national GHG inventories than the IPCC Tier 1 approach.

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SUPPORTING INFORMATION

Additional supporting information can be found online in the Supporting Information section at the end of this article.

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