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RESEARCH ARTICLE

Inventory and assessment of pH in cropland and grassland soils in Germany[#]

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Abstract

Background: Soil pH is one of the key factors affecting soil fertility. For optimal plant growth on agricultural land, suitable liming management is recommended. The basis of appropriate soil pH management in agriculture is provided by recommendations on site-specific optimum pH ranges and lime application.

Aims: This study determined the current variability of soil pH of cropland and grassland in Germany, analysed the factors associated with this variability, evaluated pH management on German agricultural land and developed a national map of current pH values in agricultural soils.

Methods: The study mainly focused on the topsoil layers of 2197 cropland sites (0–30 cm) and 812 permanent grasslands sites (0–10 cm) in the German Agricultural Soil Inventory, but reports soil pH ($CaCl_2$) down to 50 cm. Random forest models were applied to identify environmental and management factors related to soil pH and develop a map of pH values in agricultural topsoils in Germany. The current pH status of the sampled sites was classified in accordance with German lime requirement recommendations.

Results: The soil pH of both land-use types showed a bimodal distribution, with peaks at pH 6.1 and 7.3 for cropland and pH 5.0 and 7.1 for grassland. Soils with pH <5 were mainly found on sandy soils in northern Germany and acidic parent material in southern Germany. Alkaline soils predominated in central and southern Germany on loess and carbonate-rich material. The carbonate content was the major factor explaining soil pH variability, but its effect was restricted to pH values >6. Only 35.4% of the cropland sites and 23.9% of the grassland sites were within the recommended optimum pH range. The percentage of sites below the recommended pH range was greater for grassland than for cropland (52.0% and 41.0%, respectively).

Conclusions: Soil pH of German agricultural land is influenced by natural factors and pH management. The first national inventory of soil pH showed that many agricultural soils exhibited pH values lower than those recommended. More conscientious pH management could help improve soil fertility and crop yield. This should be based on the regular topsoil pH analysis conducted by most farmers every five years, together with the determination of plant-available potassium and phosphorus in soils.

KEYWORDS
agricultural soil inventory, agriculture, lime requirement, mapping, soil acidification, soil pH

1 | INTRODUCTION

One of the world's greatest challenges is to secure food production for its growing population. Therefore, it is important to manage and optimize soil fertility and yields. Besides erosion, compaction, chemical pollution and salinization, acidification is one of the main causes of soil degradation (FAO, 2015). Globally, about 30% of the ice-free land surface is occupied by acid soils with pH (H_2O) <5.5 at the soil surface (von Uexküll & Mutert, 1995). Acidification is a problem in many agroecosystems worldwide because it affects soil fertility and crop production (Guo et al., 2010; Goulding, 2016; Martins et al., 2014). The pH value is the most popular indicator of soil acidity and soil acidification. It also influences various aspects of soil fertility, such as the availability of macro and micronutrients, the occurrence of phytotoxic concentration of, for example, aluminium ions, the composition and activity of the soil microbial community influencing the decomposition kinetics of soil organic matter (SOM) and crop residues, and soil aggregation and structure (Blume et al., 2016; Rousk et al., 2010). Furthermore, soil pH can influence soil greenhouse gas exchange (Kunhikrishnan et al., 2016), change the filter and buffer functions of soils and the quality and composition of leachate, and affect different aspects of belowground and aboveground biodiversity (Komonweeraket et al., 2015; Rengel, 2003).

Soil acidification is a natural process in humid regions, mainly caused by the formation of carbonic acid (H_2CO_3) that originates from the reaction of CO_2 produced by microbial and root respiration and H_2O, atmospheric deposition of acids, and the production of organic acids in soil by roots and organic matter decomposition. In agricultural soils, the application of acidifying fertilizers and the net export of plant biomass by harvest are further reasons for decreasing pH values (Blume et al., 2016; Goulding, 2016).

Liming is the most common method for neutralizing soil acidity and keeping soil pH within a range that is favourable for crop production (Goulding et al., 1989). Suitable pH ranges depend on the crop types being grown and soil properties. As inappropriate pH management can significantly decrease crop yield, national or regional agencies provide recommendations for optimum pH levels (Defra, 2010; VDLUFA, 2000b; Teagasc Greenbook, 2016). The German classification system of the lime requirement of agricultural soils is based on soil pH measurements (in $CaCl_2$) and differentiates between land-use types (grassland soils and cropland soils) and specific soil conditions (soil texture and SOM content) (VDLUFA, 2000a). The optimum pH values decrease with decreasing clay content and increasing SOM content (Tables S1 and S2). Lower pH values of sandy soils and soils with a high SOM content should support an adequate supply of micronutrients and avoid excess SOM mineralization respectively. Higher optimum pH values in clayey soils are targeted in particular at the positive effects of high Ca saturation on soil structure and aggregation (Blume et al., 2016).

Advanced digital soil mapping approaches can offer more complete and detailed pictures of the spatial variability of soil pH and provide a general basis for large-scale modelling of all processes affected by soil pH. Fabian et al. (2014) used the pH values of 4131 topsoil samples from agricultural sites across Europe and applied kriging to produce a pH map of European agricultural soils. A more detailed map of pH in soils across Europe was recently published by Ballabio et al. (2019). They used the results of the Land Use/Land Cover Area Frame Survey (LUCAS) including more than 20,000 soil samples (0–20 cm) throughout the European Union, and produced maps for pH ($CaCl_2$) and pH (H_2O) using Gaussian process regression. No pH map of agricultural soils in Germany has previously been produced that is based on pH-controlling factors and is relevant at this scale.

Based on the first national inventory of agricultural soils in Germany (Jacobs et al., 2018; Poeplau et al., 2020), this study analysed the current pH status of grassland and cropland soils in Germany. The analysis was based on an 8 × 8 km soil-sampling grid across Germany. The objectives of this study were:

1. to determine the spatial distributions of pH in grassland and cropland soils in Germany,
2. to determine the main factors influencing the spatial distribution of pH in cropland and grassland soils on the scale of Germany,
3. to assess the current pH status of German agricultural soils with respect to the target soil fertility based on the German pH classification scheme to determine lime requirements,
4. to identify factors related to the occurrence of pH values below the optimum range and
5. to develop a national map of current pH levels in agricultural soils.

It was hypothesized that a considerable proportion of cropland and grassland soils in Germany has a topsoil pH lower than the recommended level, even when farmers apply lime to control soil pH. Based on liming recommendations, soil pH in agricultural soil should be adjusted to a specific range depending on land use (grassland or cropland), clay content and SOM content. It was also hypothesized that management factors, such as crop type within the rotation, production intensity, and natural factors such as precipitation, influence both the current soil pH status and the occurrence of pH values below the site-specific optimum range.

2 | MATERIALS AND METHODS

2.1 | Dataset

From 2011 to 2018 soil samples from 3009 sites were collected based on an 8 km × 8 km grid covering cropland (2197) and permanent grassland (812) across Germany for the German Agricultural Soil Inventory (GASI; Jacobs et al., 2018). At each site, a soil profile of 100 cm depth was excavated and characterized according to Eckelmann et al. (2006). This study focused mainly on the variability of pH in the topsoil layers (0–30 cm and 0–10 cm), but soil pH down to a depth of 50 cm was also included. All the soil samples were analysed in the same laboratory for pH ($CaCl_2$) (0.01 M $CaCl_2$ solution), texture, total nitrogen, inorganic carbon (IC) and total organic carbon (TOC).

Soil pH was determined by suspending 5 mL dry soil with 25 mL 0.01 M $CaCl_2$ solution. After 2 h, it was centrifuged for 10 min and measured by the measuring robot SKALAR SP2000 (Jacobs et al., 2018). It should be noted that soil pH as determined in 0.01 m $CaCl_2$ solution does not describe total soil acidity that includes exchangeable and nonexchangeable acids (Gavriloaiei, 2012). The pH ($CaCl_2$) is a measure of H^+ activity in soil solution that can contain small amounts of exchangeable H^+ mobilized by the addition of Ca^{2+} ions. Nevertheless, pH is the most common indicator of the acidity of agricultural soils.

Soils were supposed to contain carbonates when the topsoil pH was considerably higher than the subsoil pH and when the soil pH was >6.2. TOC was determined by combustion at 550°C and IC was analysed by subsequent combustion at 1000°C with LECO RC612 (Jacobs et al., 2018; Poeplau et al., 2020). The factor of 1.72 was used to convert TOC to soil organic matter (SOM) (Eckelmann et al., 2006). IC was multiplied by a factor of 8.34 to calculate $CaCO_3$ equivalents. An additional questionnaire, completed by farmers, provided management information for each site on liming, tillage, fertilizer practice, crop rotation, crop yield and the input of nitrogen for a period of 10–15 years before soil sampling (Jacobs et al., 2018; Jacobs et al., 2020). Exports of carbon (OC exports) were quantified using documented yields and information about by-product removal from the questionnaire of the GASI or yield statistics (Jacobs et al. 2020). Inputs of organic carbon (OC inputs) were quantified based on data about yields and organic fertilization taken from the questionnaire, while crop type specific root:shoot ratios and harvest indices (Jacobs et al. 2020) were used to quantify carbon inputs from crop residues. The soil parent material was classified according to the German soil parent material map (Federal Institute for Geosciences and Natural Resources, 2008) with small modifications. The categorization was derived from GASI parent material data and the national geological map (Federal Institute for Geosciences and Natural Resources, 2007) at each site.

2.2 | Optimum soil pH

The national recommendation scheme for the lime requirement of agricultural soils published by the Association of German Agricultural Analytical and Research Institutes (VDLUFA, 2000a) was followed to determine whether measured pH values fell within or outside the site-specific optimum pH range. This is based on the results of long-term field experiments in Germany at different cropland and grassland sites studying the impact of lime application on soil pH and yield (Kerschberger, 1996; König & Kerschberger, 1996). The recommendation scheme classifies five pH levels (Table 1). The optimum pH range depends on management (cropland or permanent grassland), soil texture (clay and silt content) and SOM content. In general, the target soil pH is higher for cropland than for permanent grassland, and it increases with increasing clay content and decreasing SOM (Tables S1 and S2). Furthermore, the recommendation scheme provides look-up tables with the recommended amount and frequency of lime application.

TABLE 1 Definition of pH levels for lime supply and requirement, according to VDLUFA (2000a)

pH level	Lime requirement
A (very low)	Very high lime requirement
B (low)	High lime requirement
C (optimal)	Regular liming to maintain the optimal level
D (high)	No liming
E (very high)	No liming; no use of fertilizers that react physiologically or chemically alkaline

2.3 | Statistical analyses and spatial distribution

To describe the relationship between measured soil pH and proxies describing climate, soil properties and management, the ensemble machine learning algorithm random forest (RF) was used (Breiman, 2001), implemented in the 'randomForest' package (Liaw and Wiener, 2002). Computations were performed with R version 3.6.1 (R Core Team, 2018). First, two models were developed to identify the main factors related to topsoil pH for cropland (0–30 cm, $RF1_{crop}$) and grassland (0–10 cm, $RF1_{grass}$) at the scale of Germany. Site-specific observations and measurements of soil properties and management (GASI data) were complemented with climate data (DWD Climate Data Center, 2013) and topographic data (Federal Agency for Cartography and Geodesy, 2018). These variables were used as independent input variables of the RF models to determine factors that explained the pH variability of croplands ($RF1_{crop}$) and grasslands ($RF1_{grass}$) (all variables are explained in Table S4). Second, the same dataset was used for the models $RF2_{crop}$ and $RF2_{grass}$ to identify factors that determine whether soil pH was within the optimum range or below the range for cropland and grassland respectively. Prior to this, redundant explanatory variables were removed using a correlation matrix. For each RF model, the number of trees was set to 900 showing the best performance, and *mtry* (the number of different variables tested at each split) corresponded to the number of potential factors. To identify the most important factors of the four models, a backward elimination algorithm was implemented using the mean square error incorporated in the RF algorithm. This algorithm removes the predictor variables that do not improve the model. Backward elimination was performed 30 times with randomly selected training datasets. The predictor variable was considered important when it was selected more than 10 times by the backward elimination method. For the ranking of the predictor variables, the variable importance quantified in the 'randomForest' package was used. It shows the increase in the mean squared error when the value of a predictor variable is randomly resampled. Partial dependence plots were used to visualize the marginal effect to show the relationships between the predictor variables and predicted soil pH obtained from the RF models (Friedman, 2001).

The Wilcox sum rank test was used to test for differences between pH distributions of different land use types (unpaired) and depth intervals (paired). The Tukey's HSD test as implemented in the '*agricolae*' package (de Mendiburu, 2019) was used for multiple comparisons (at a level of $p < 0.05$) to describe the effect of precipitation on soil pH.

Model RF3 was developed to generate an agricultural soil pH map of Germany based on pH-controlling factors that are available and relevant on a national scale. The spatial resolution of this map is 100 m. Model RF3 used spatial data covering Germany to describe soil pH distributions of grasslands and croplands across Germany. Independent variables used in RF3 included climate data (precipitation and temperature) from the DWD Climate Data Center (2013), land-use data from the Federal Agency for Cartography and Geodesy (2016) and data on soil parent material from the Federal Institute for Geosciences and Natural Resources (2013). Further predictor variables, such as texture, carbonate content, C:N ratio, TOC and soil pH, were derived from the GASI sites by calculating the mean of neighbouring GASI points within a 10 km radius. If no adjacent data point was within a 20 km radius, the measured soil properties were taken from GASI points within a 30–40 km radius. The soil pH values of the neighbouring GASI points include information on typical soil management and liming in a specific region.

To test the performance of all RF models, the data were randomly split into calibration and validation datasets (80% and 20% of the data, respectively). The accuracy of the RF models was evaluated by root mean square error (RMSE) and the coefficient of determination (R^2).

3 | RESULTS

3.1 | Distribution of soil pH in Germany

The pH ($CaCl_2$) ranged between 2.6 (raised bog, grassland) and 7.7 in the topsoil layer of agricultural land, with a mean value of 5.9 (Figure 1). For grassland, the mean soil pH increased slightly with depth from pH 5.4 (0–10 cm) to 5.6 (30–50 cm), while the mean pH of cropland was 6.1 in all soil layers. A Wilcox rank-sum test showed that soils of permanent grassland were significantly more acidic than cropland soils ($p < 0.01$) at all depth increments. Both land-use types showed a bimodal distribution of pH. Following the classification by Blume et al. (2016), the first peak of the cropland sites was within the weakly acidic range (pH 6.1), and for grassland sites was within the moderately acidic range (between pH 5.0 and 5.3 for the three depth increments). The second peak was within the weakly alkaline range for both land-use types and at all depth increments. Topsoil layers containing carbonate were more frequent at cropland sites (40%) than at grassland sites (20%). There was no significant difference between average pH in 0–30 cm and 30–50 cm, irrespective of the tillage regime (conventional ploughing or conservation tillage) in cropland soils.

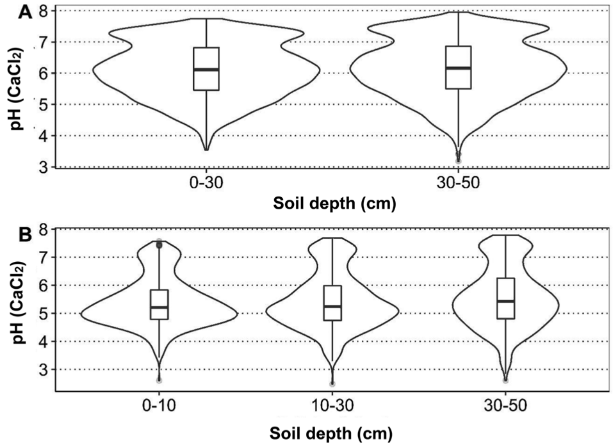

FIGURE 1 Soil pH ($CaCl_2$) at different depth increments for cropland (A; $n = 2197$) and permanent grassland (B; $n = 812$) in the German Agricultural Soil Inventory

The topsoil pH of cropland showed a distinct regional distribution. Soils with pH <5 occurred mostly in sandy soils in northern Germany, whereas high pH values (>7) dominated on loess and carbonate-rich soils in central and southern Germany (Figure 2A). For grassland sites, the regional distribution of topsoil pH was less distinct. A high frequency of sites with pH < 5 were found in northwest Germany on sandy soils and peatland, and in the Black Forest and Bavarian Forest regions (in southern Germany) on acidic parent material (Figure 2B).

3.2 | The most important predictors of spatial variability of pH

The RF approach was used to identify the most important factors determining spatial pH variability in topsoils of cropland (0–30 cm) and grassland (0–10 cm) at the scale of Germany. $RF1_{crop}$, the RF model for the cropland sites, explained 74.21% of the variance (R^2) of soil pH with a root mean square error (RMSE) of 0.44 (validation dataset: $R^2 = 73.95$, RMSE = 0.44). The RF model for the grassland sites $RF1_{grass}$ showed $R^2 = 69.98\%$ and RMSE = 0.46 (validation dataset: $R^2 = 68.55$, RMSE = 0.47). Tables 2 and 3 present the ranking of predictors by their importance.

The most important factor was the content of carbonate in cropland and grassland soils. Carbonates, mostly represented by calcium carbonate, were found at soil pH >6 (Figure 3A, B) and were detected in 43% (croplands) and 45% (grasslands) of the topsoils with a pH between >6.0 and ≤6.5, and in 85% (croplands) and 98% (grasslands) of the soils showing a pH of >6.5 and ≤7. Above soil pH 7, nearly all the topsoils (98%) contained carbonate. The importance of carbonate content on soil pH was only visible for pH values >6. Other important factors related to soil pH selected with the backward elimination were precipitation, clay content, liming, parent material and OC input for cropland, and precipitation, clay content, C:N ratio and OC export (by harvest and by grazing) for grassland. Of these factors, clay content

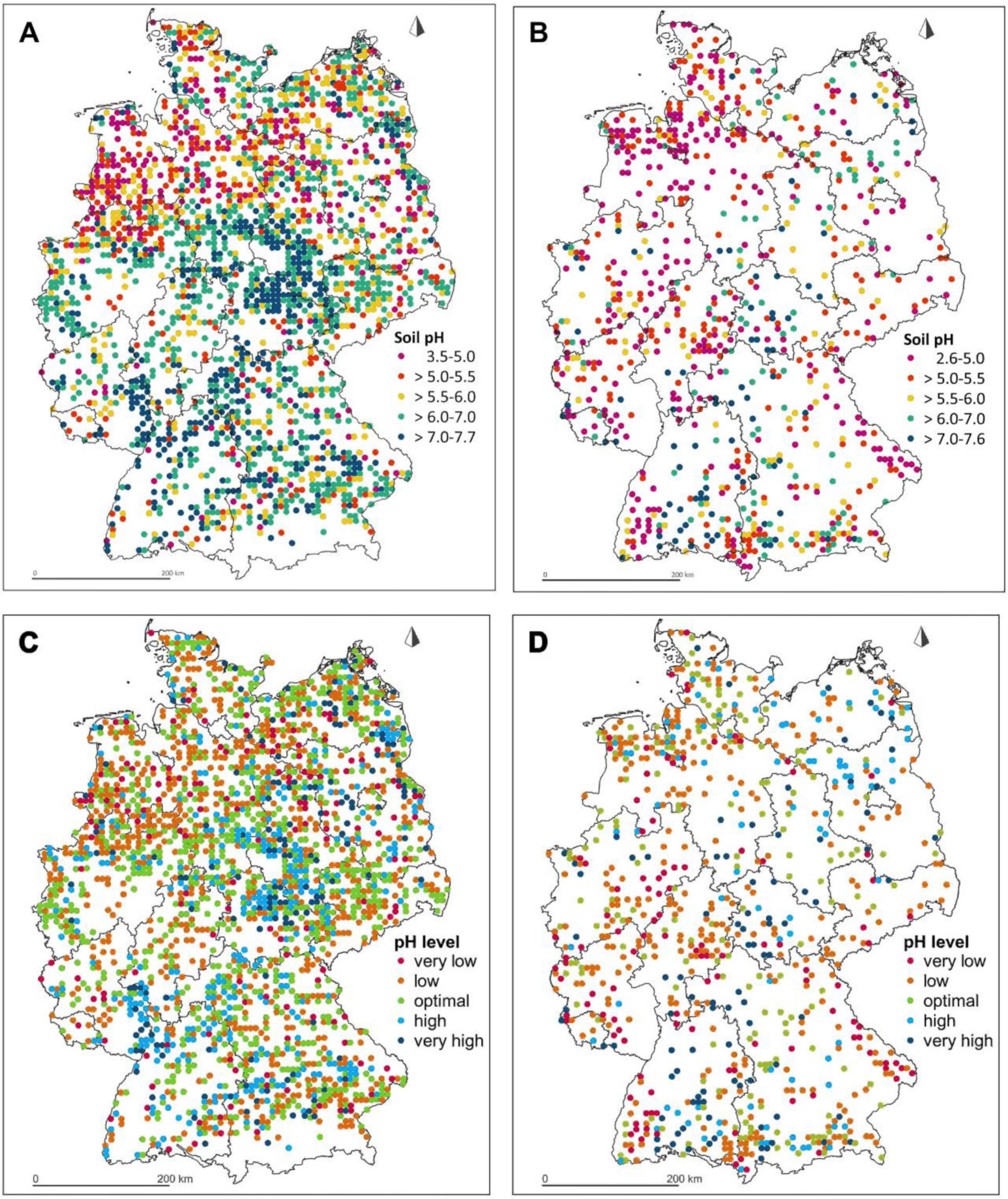

FIGURE 2 Soil pH (CaCl$_2$) in the topsoil layer of cropland (A; 0–30 cm) and permanent grassland (B; 0–10 cm) and pH levels of the topsoil layer of croplands (C; 0–30 cm) and permanent grasslands (D; 0–10 cm) according to VDLUFA (2000b) (Table 1)

(Figure 3C, D), OC input and OC export were positively correlated with soil pH in the RF models, while C:N ratio was negatively correlated.

Figure 4 shows that sites with a clay content of between 6% and 25% had a tendency of decreasing soil pH with increasing mean annual precipitation (MAP). This pH decline was significant for croplands and grasslands (with 12–18% clay content), performed with Tukey's HSD test at 5% probability. On average, MAP was higher for grasslands (mean 901 mm) than for croplands (mean 740 mm), while MAP ranged between 482 mm (southeast of the Harz Mountains) and 2610 mm (Alps).

The soil parent material was found to influence the spatial variation of soil pH. Low soil pH values were found in bogs and on acidic rocks.

TABLE 2 Variable importance for predicting soil pH (0–30 cm) of cropland generated with random forest model RF1$_{crop}$. It shows the increase of the mean squared error when the values of a predictor variable are randomly resampled. Variables selected as the most important variables by 30 backward elimination (BE) runs

Predictor variable	Variable importance	Selected frequency by BE
Carbonate content	280.08	30
Clay content	74.59	30
Lime application	49.41	30
Mean annual precipitation	37.43	30
Soil parent material	37.03	20
Organic carbon input	12.09	22

TABLE 3 Variable importance for predicting soil pH (0–10 cm) of grassland generated with random forest model RF1$_{grass}$. It shows the increase of the mean squared error when the values of a predictor variable are randomly resampled. Variables selected as most important variables by 30 backward elimination (BE) runs

Predictor variable	Variable importance	Selected frequency by BE
Carbonate content	174.56	30
Topsoil C:N ratio	24.25	30
Clay content	23.81	28
Mean annual precipitation	23.30	30
Organic carbon export	9.45	13

Soils formed on carbonate rocks had the highest median of the pH values (Figure 5).

3.3 | Soil pH management

Only 35.4% of the cropland soils and 23.9% of the grassland soils had topsoil pH values within the recommended range (Table 4). 42.8% of the sampling sites were below the optimum pH range; lime had not been applied on almost half of these sites in the 10 years leading up to sampling. Grassland had more sites with a soil pH below the recommended thresholds than cropland (52.0% and 41.0%, respectively). About 11.7% of the grassland sites and 7.0% of the cropland sites were in pH level A, indicating a very high lime requirement (Table 4). Lime was applied to 65.4% of the arable sites, but to only 22.8% of the grassland sites in the 10 years leading up to sampling. Figure 2C and D shows the spatial distribution of the five site-specific

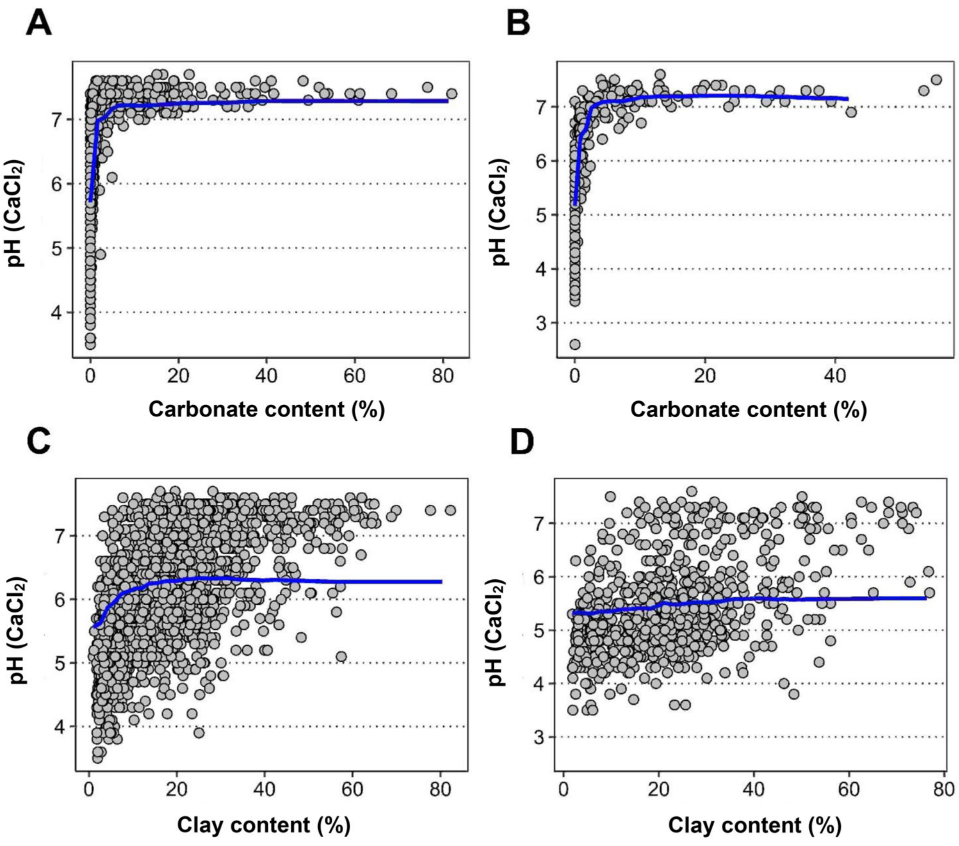

FIGURE 3 Effect of soil carbonate content (as $CaCO_3$ eq.) and soil clay content on pH ($CaCl_2$) of the topsoil layer of cropland (A and C; 0–30 cm) and permanent grassland (B and D; 0–10 cm). The blue curve visualizes the average marginal effect of carbonate content on the predicted response of soil pH derived from the random forest models RF1$_{crop}$ and RF1$_{grass}$

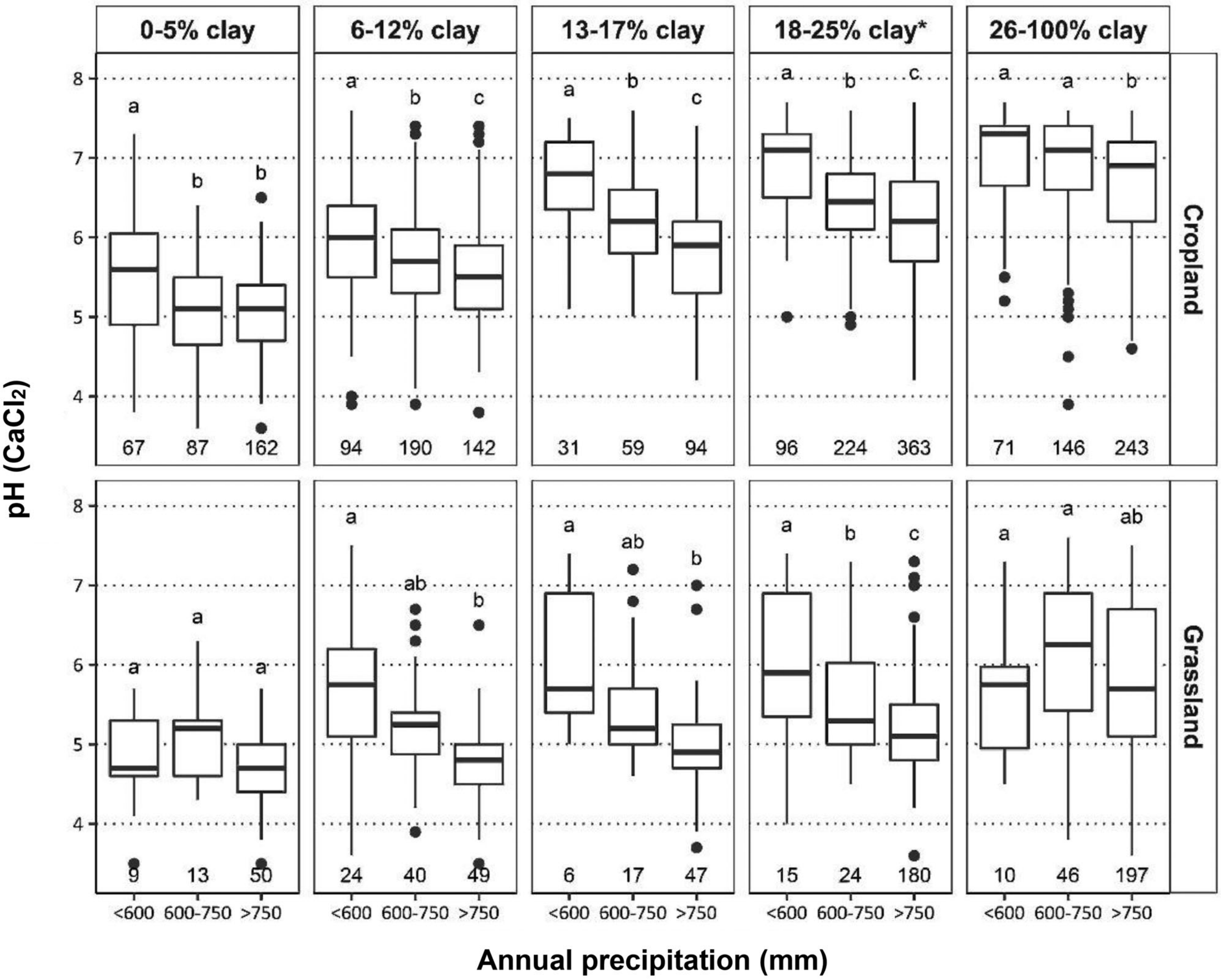

FIGURE 4 Effect of mean annual precipitation on pH ($CaCl_2$) of the topsoil layer of cropland (0–30 cm) and permanent grassland (0–10 cm) stratified by clay content. The same letters above boxplots indicate no significant difference, as determined by Tukey's HSD test ($p < 0.05$), within the texture groups. Numbers below each boxplot give the number of observations (*n*)

TABLE 4 Relative abundance of soil pH levels (see Table 1) for land use types and for sites with specific crops in the rotation (up to 18 reported years; *n* = number of observations)

		Distribution of pH levels (%)				
Land use/crop types	***n***	**Very low**	**Low**	**Optimal**	**High**	**Very high**
Cropland	2197	7.0	34.0	35.4	16.5	7.1
Grassland	812	11.7	40.3	23.9	13.7	10.4
Winter wheat	1697	4.0	31.9	38.9	18.1	7.1
Maize	1244	7.10	37.9	34.3	15.0	5.7
Winter barley	1215	4.0	35.2	39.6	15.6	5.6
Canola	1137	5.3	30.2	39.7	16.8	8.0
Winter rye	466	11.2	36.7	30.7	12.7	8.8
Summer barley	444	6.1	32.9	35.6	18.2	7.2
Sugar beet	314	0.7	22.7	43.5	26.6	6.5
Potato	244	7.8	37.3	28.3	17.6	9.0
Spring oat	198	10.6	42.9	29.8	10.1	6.7

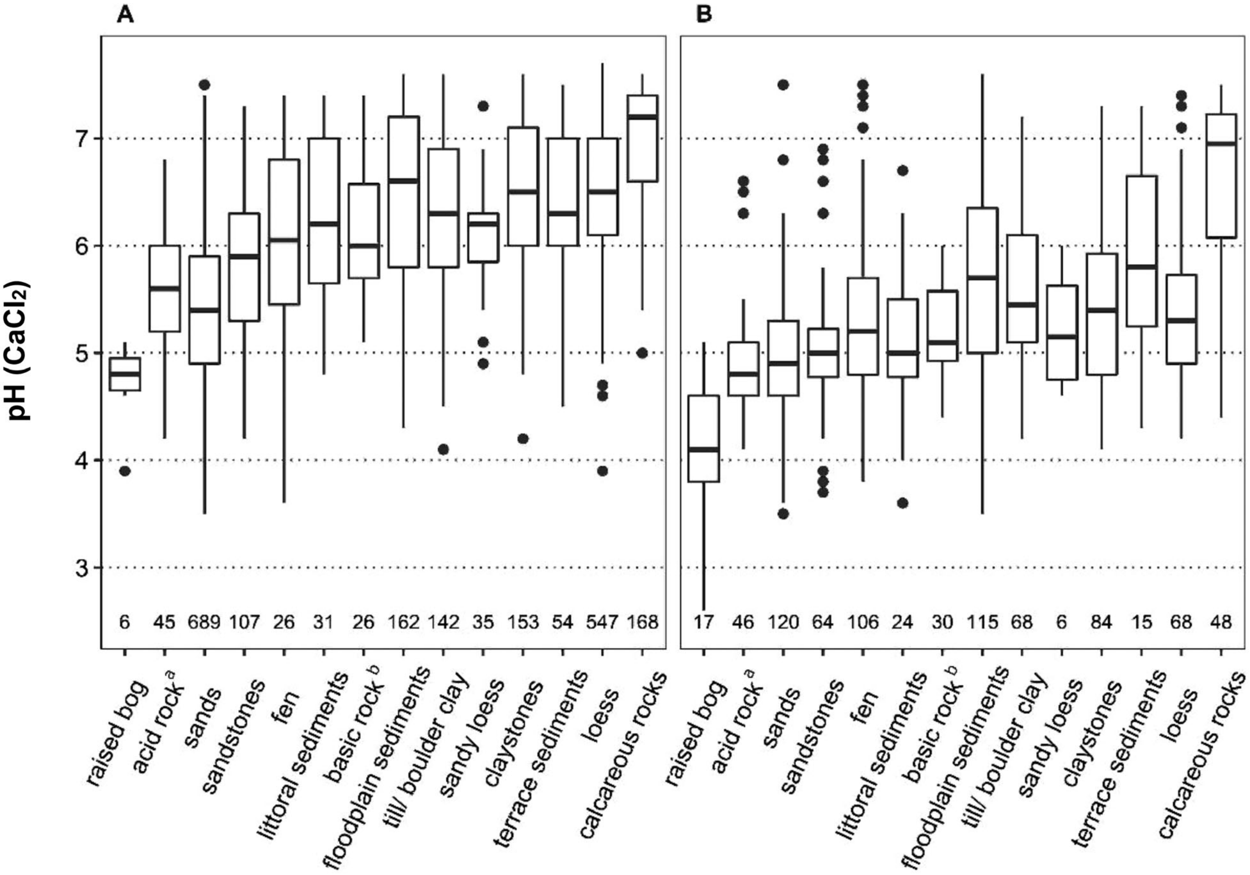

FIGURE 5 Boxplot comparison of pH ($CaCl_2$) of cropland (A; 0–30 cm) and permanent grassland (B; 0–10 cm) grouped by the parent material of the soil profile. Numbers below each boxplot give the number of observations (*n*), a: acid igneous and metamorphic rocks, b: the basic igneous and metamorphic rocks

pH levels across Germany, as defined by the German classification system of lime requirement (Table 1). Excessive pH values (pH level D and E; Table 1) were mainly associated with the occurrence of parent materials containing carbonates. Soils with pH levels A and B (pH below optimum; Table 1) were found practically everywhere in Germany, but were more abundant in regions with acidic parent material (Figure 2).

Sampling sites that included sugar beet in their crop rotation had the smallest proportion of soil pH values below the recommended optimum range (23.4%), while more than 50% of the sites with crop rotations including potatoes, winter rye, spring oats, or maize had soils with low or very low pH levels (Table 4). For grasslands, the model $RF1_{grass}$ showed a positive relationship between grass yield (OC export) and soil pH. Furthermore, the average OC export was higher on limed grassland sites (3.73 Mg C ha^{-1} y^{-1}, $\sigma = 2.54$) than on unlimed grassland sites (2.79 Mg C ha^{-1} y^{-1}, $\sigma = 2.20$).

The sampled soils of agricultural holdings managed as a primary activity showed a higher percentage within the optimum pH range at 34.1% than soils of farms managed as a sideline business (24.1%). Compared with conventional farming, the soils of sampling sites with long-term organic farming had a greater proportion of low and very low pH levels (Table S3), despite conventional and organic sites having similar distributions of clay contents and similar fractions of carbonate-containing soils (data not shown).

The models $RF2_{crop}$ and $RF2_{grass}$ were developed to identify factors related to the occurrence of pH values below the optimum range. However, the model performance was poor and therefore it was not possible to identify any of the factors tested (e.g., soil parent material, liming, TOC, texture, precipitation) as key variables explaining why specific sites had pH levels below the recommended thresholds.

3.4 | Regionalization of soil pH at the scale of Germany

The random forest algorithm for model RF3 explained 42.51% of the variance (R^2) of pH in Germany's agricultural soils with RMSE of 0.7 (calibration dataset: $R^2 = 41.82\%$, RMSE = 0.7). Figure 6 shows the soil pH map produced on the basis of model RF3. Table 5 shows the ranking of the predictor variables, with land use as most important factor followed by parent material and the average soil pH of the nearest GASI sampling points. The pH map reproduces the pH distribution of the GASI sites (Figure 2) and provides a more detailed picture of the spatial distribution of the topsoil pH (0–30 cm). Acidic soils

FIGURE 6 Map of pH ($CaCl_2$) of agricultural soils (0–30 cm) predicted with the random forest model RF3

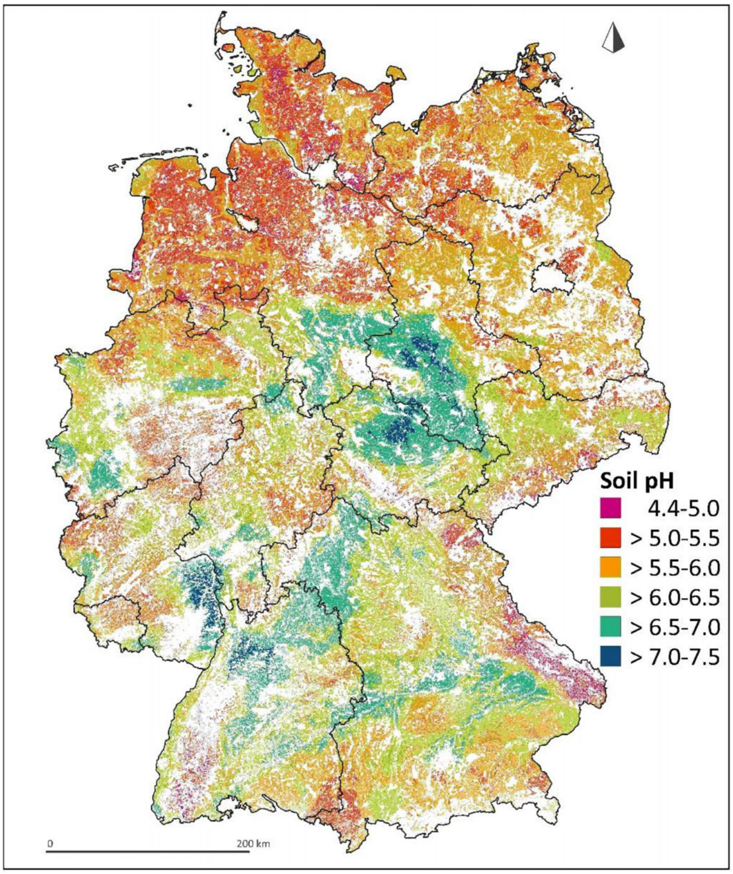

TABLE 5 Variable importance for predicting soil pH (0–30 cm) of agricultural land generated with random forest model RF3. It shows the increase of the mean squared error when the values of a predictor variable are randomly resampled

Predictor variable	Variable importance
Land use (cropland, grassland)	67.54
Soil parent material	52.23
Soil pH [a]	49.95
Precipitation	41.19
Carbonate content [a]	40.8
C:N ratio [a]	34.43
Sand content [a]	32.43
Silt content [a]	31.15
Soil organic carbon [a]	29.88
Clay content [a]	27.01
Mean air temperature	25.41

[a] Averaged values of the nearest GASI points.

(pH <5.5) predominate in northwest Germany and mountain regions in the south: Allgäu Alps, the Black Forest and the Bavarian Forest. Alkaline soils occurred predominantly in central Germany and on the Upper Rhine Plain, with slightly acidic soils in southern Germany, regions characterized by carbonate rocks and loess. Eastern Germany had mostly moderately acidic soils.

4 | DISCUSSION

4.1 | Factors influencing topsoil pH at the scale of Germany

Soil pH is a result of the acid-neutralizing capacity of soils that depends on the existence and reactivity of pH buffer systems and the input and production rates of acids of different strength (Bloom et al., 2005). Both factors are strongly influenced by agricultural management.

4.1.1 | Soil properties

The most obvious soil property determining the pH of cropland and grassland soils was carbonate content. The carbonate buffer system should stabilize soil pH (H_2O) between 6.2 and 8.6 (Eckelmann et al., 2006). It is based on the dissolution of carbonates and the reaction of H^+ with CO_3^{2-}: $CaCO_3 + H^+ \rightarrow HCO_3^- + Ca^{2+}$. The reaction is generally fast. If sufficient soluble carbonates are present, acids are consumed with little or no decrease in pH (Bloom et al., 2005; Blume et al., 2016). The results of this study showed that even small amounts of carbonates (<1%) resulted in soil pH values ≥7. The predictive power of carbonate content for soil pH is restricted to pH values >6, which is in line with the occurrence of small amounts of carbonate in many soils and the pH range of the carbonate buffer system. Small amounts of carbonate were detected in the pH range 6–7 in 60% of cropland soils and 72% of grassland soils. The bimodal distribution of the topsoil pH (Figure 1) was influenced by the carbonate buffer. Soils characterized by the presence of carbonate were mostly within the weakly alkaline range. Fabian et al. (2014) report similar findings in topsoil pH distributions at the European scale.

Topsoil clay content was another important factor influencing soil pH in croplands and grasslands. In general, GASI sites showed an increasing pH with increasing clay content. Clay content contributes to the acid-neutralizing capacity of soils by binding protons on the surface of clay minerals with permanent negative charge and by proton consumption associated with chemical weathering of silicates (Blume et al., 2016; Ulrich, 1986). In line with the present results, Fabian et al. (2014) report relatively low soil pH in the agricultural soils of Germany and Poland developed on sandy coarse-grained sediments. Moreover, liming may have contributed to the observed clay effect because the German classification scheme of lime requirement recommends increasing pH values with increasing clay content (VDLUFA, 2000b).

In very acidic soils, protons are consumed by the dissolution of aluminium hydroxides, and increasing Al^{3+} concentration can hamper root and plant growth (Blume et al., 2016). This key reaction of the aluminium buffer range becomes more important at pH (H_2O) ≤ 4.2 (Ulrich, 1986). Blake et al. (1994) report Al^{3+} concentrations in harvested hay up to eight times higher than the maximum tolerated by cattle from soils within the aluminium buffer. Almost all the mineral soils in this agricultural soil inventory had pH values above the aluminium buffer, except at six mineral soil sites. The carbonate-free mineral soils exhibit pH values where pH buffer reactions are dominated by cation exchange processes and silicate weathering. This is completely different to German forest soils. Most carbonate-free forest soils exhibit very low pH values that are typically within the aluminium buffer range (Meesenburg et al., 2019). The generally much higher pH in agricultural soils than in forest soils, which is distinct even in sites with a similar texture, is primarily the result of pH management to maintain soil fertility and yields. It indicates that the current pH level of agricultural soils is strongly determined by pH management.

4.1.2 | Climatic conditions

Negative correlations were found between the soil pH of grassland and cropland soils and MAP. Precipitation is normally slightly acidic (Goulding, 2016) and controls water movement in soil, causing the leaching of base cations (Slessarev et al., 2016). A positive correlation was found between mean annual temperature and soil pH, indicating that cold, moist conditions facilitate the low pH of agricultural soils. It has been shown that the mean annual water balance is a master variable for explaining pH distributions on a global scale (Slessarev et al., 2016). Furthermore, the pH values of agricultural soils at the European scale follow climatic gradients (Fabian et al., 2014). Replacing precipitation by the mean annual water balance for the GASI sites as a predictive factor did not improve the estimation accuracy of $RF1_{crop}$ and $RF1_{grass}$. These results showed that climatic conditions contributed to the spatial variability of the current soil pH, even at the scale of Germany. However, their effects were relatively small compared with their dominance at the global or European scale. This can be explained by a much lower variability of mean air temperature and annual precipitation, which is typical for Germany's humid temperate climate. Therefore, in the German national recommendation scheme (VDLUFA, 2000a), annual water balance is not considered a factor in determining lime requirements. One exception is the regional lime recommendation of the federal state of North Rhine-Westphalia. MAP is relatively high in this region and the state's Chamber of Agriculture generally recommends higher lime application rates than the national scheme (Landwirtschaftskammer Nordrhein-Westfalen, 2015).

4.1.3 | Land use and management

Land use and management were interacting factors influencing soil pH, with grassland soils showing generally lower pH values than cropland soils. A higher MAP at grassland sites may have contributed to this difference, but the main reason appeared to be the different target pH range and liming practice. Recommended soil pH is generally about 0.5 units lower for grassland than cropland for soils with SOM contents below 8%. The upper range of weakly acid pH values is sufficient in most grassland soils to produce high yields with high fodder value (König & Kerschberger, 1996). Thus, lime was applied more often on cropland than grassland in the 10 years leading up to soil sampling. On the European scale, Fabian et al. (2014) also observed lower topsoil pH for grasslands, and related this observation to the generally higher TOC content accompanied by higher concentrations of acidifying humic acids. Soil pH is generally adjusted by liming and the main substrate used in Germany is calcium carbonate (Destatis, 2020). In the RF1 models, lime application proved to be an important factor in the current variability of soil pH within cropland soils, while lime application had a limited impact on the variability of soil pH in grasslands. Indeed, more cropland sites than grassland sites were limed. It should be noted that the RF1 models did not capture the general dominant effect of liming on the current pH status of agricultural soils in Germany (see Section 4.1.1, much higher pH than forest soils) because they focused on factors influencing the current spatial variability of soil pH values within croplands and grasslands.

4.2 | Implications of current soil pH management

Soil pH and liming influence soil structure, the availability of primary nutrients and micronutrients, the mobility of heavy metals and aluminium and soil microbial activity. The recommended pH ranges by VDLUFA (2000a) consider all these effects and are set to find the best site-specific compromise with respect to soil fertility and crop yield. This study showed that 41% of the GASI cropland sites were below the site-specific optimum pH level recommended for arable soils (VDLUFA, 2000a). There are numerous studies on soil pH effects on crop yield (Holland et al., 2019; Kerschberger, 1996; Kerschberger & Marks, 2007; Kerschberger & Richter, 1982; Kirchmann et al., 2020).

They indicate that there is considerable potential to increase the crop yield on many fields in Germany by more regular and optimized liming strategies. pH effects on yield also depend on crop type. Kerschberger and Marks (2007) define four groups: group 1 contains high acid-sensitive crops (spring barley, canola, sugar beet), groups 2 and 3 contain intermediate acid-sensitive crops (oats, winter wheat, maize, potato, winter barley), and group 4 has low acid-sensitive crops (winter rye). Kerschberger and Preusker (2014) examined the effects of pH levels of crop yields. They report yield losses of 50–100% for spring barley (group 1) within pH level A (Table 1) on loamy sands and sands. Winter wheat (group 3) exhibited yield losses of up to 25% within the pH level A, and winter rye yields (group 4) also fell by up to 20% on a sandy soil with suboptimal pH. The GASI dataset shows that pH management followed crop requirements to a certain extent. Sites with rotations that included the crop types of group 1 were more often characterized by pH values within or above optimal ranges and less by pH ranges corresponding to pH level A (very low) compared with groups 2–4 (Table 4). For instance, fewer than 1% of sites with sugar beet in the crop rotation had pH values within level A (very low pH). This result may be due to the specific and comprehensive advice service for farmers producing sugar beets and the fact that sugar beets are produced primarily on fertile soils derived from loess deposits. The study questionnaire revealed that liming practice differed considerably. On average, cropland was limed at an interval of 5.7 ($\sigma = 3.6$) years on farms that reported liming. This is in line with official recommendations. However, 33% of all cropland sites with soil pH levels A and B had not been limed within the last 10 years. High pH values may have negative effects on crop yields due to plant nutrient deficiency. Kirchmann and Eskilsson (2010) report average yield losses of 7% by liming up to a base saturation above 70%. Above pH (H_2O) 7.2, cereal crop yield declined in a study in Sweden (Kirchmann et al., 2020). Acidifying fertilizers are recommended for calcareous soils with excessively high pH values (pH level E) (VDLUFA, 2000a). There was no detailed information on fertilizer application and it was not possible to assess whether farmers followed this rule.

The recommended optimum pH level is lower for grassland than cropland because most grass species are less sensitive to weakly acid pH values than arable crops. In general, grasslands have mostly higher SOM content than croplands. Sites with higher SOM content require a lower pH value (Tables S1 and S2). The average value of SOM content for the GASI grassland sites was 11.7% ($\sigma = 12.8$) and for the cropland sites 2.9% ($\sigma = 2.6$). Nevertheless, regular pH management is necessary on most grassland sites to support species with high fodder quality and productivity. Species richness and fodder quality are poor on acid grassland soils below pH (H_2O) 4.5 (Crawley et al., 2005; Merunková & Chytrý, 2012). In particular, productive species with a high fodder value, such as perennial ryegrass, cocksfoot, valuable herbs and legumes, prefer moderately/weakly acidic soils (König and Kerschberger, 1996; Poozesh et al., 2010). Hayes et al. (2016) report that liming increases the biomass of the acid-sensitive species lucerne by 150% and phalaris by 30%. An enhanced yield production by liming was achieved notably on grassland sites with a soil pH ($CaCl_2$) <4.5 (König & Kerschberger, 1996), comprising 10% of the grassland sites in GASI. Fifty-two per cent of the grassland sites had pH levels below the optimum (levels A and B), demonstrating that soil pH management was even less targeted for grassland than for cropland. On average, lime was applied every seven to eight years on farms that reported liming, but liming was neglected (no lime application in the last 10 years) on 77% of grassland sites with soil pH levels A and B. Compared to cropland soils, soil pH of grassland soils is more often below recommended values which might be caused by several factors; that is, the slower and more gradual changes in yield production and species richness induced by a decreasing soil pH that is too low and the fact that in mixed farms grassland is often less important for farm income than cropland. It should be noted that the German recommendation on soil pH and liming of agricultural soils focuses on soil fertility. However, soil pH affects many soil functions and biogeochemical processes that this study did not address. One example is the effect of soil pH and liming on greenhouse gas emission. Several studies suggest that increasing soil pH may substantially reduce the emission of nitrous oxide from managed soils (Hénault et al., 2019; Wang et al., 2018). However, the required lime application causes additional CO_2 emissions that have to be included in the complete greenhouse budget (Gibbons et al., 2014; Hénault et al., 2019). Yield effect is also important in order to derive yield-related emission. This example demonstrates that the new dataset on soil pH requires further evaluations.

4.3 | New map of current pH in agricultural topsoils of Germany

Many soil biochemical and physical processes are influenced by pH, while large-scale modelling of complex soil properties and processes, such as soil fertility, greenhouse gas emission and nitrate leaching, requires the spatial distribution of soil pH as an input parameter (Lugato et al., 2017; Kiese et al., 2011; Stehfest & Bouwman, 2006; Wang et al., 2018).

The soil pH map with high spatial resolution (100 m) presented in this study offers a new basis for large-scale regionalization approaches and process modelling at the scale of Germany. Major data sources used to produce this soil pH map came from GASI, which has a consistent soil sampling scheme and laboratory analysis program. At first glance, the soil pH map strongly reflects the spatial patterns of soil maps and parent material maps, indicating that a large part of pH variability can be explained by the spatial distribution of soil properties. This impression was supported by the models $RF1_{crop}$ and $RF1_{grass}$, which were developed to estimate the topsoil pH of GASI sites. For these models, about half of the determined key factors represented soil properties either directly (clay content, carbonate content, C:N ratio) or indirectly (parent material), with carbonate content being by far the most important variable for both land-use types.

Regionalization of soil pH was performed using influencing variables that are available or can be derived at a high spatial resolution across Germany. The most important soil-related variable for regionalization is parent material. The loss of the explanatory strength of carbonate content in RF3 can be explained by the derivation of this variable by averaging the carbonate contents of surrounding GASI sites, while at the same time the measured carbonate contents showed a high spatial variability, as seen in the semivariogram in Figure S1 with a range (13.5 km) just above the GASI sampling grid width. All other soil properties (texture, C:N ratio, soil pH) used in RF3 demonstrated pronounced spatial autocorrelation, with wide ranges far beyond the sampling grid width (Figure S1). While the factor of parent material used in RF1 models was specifically adjusted for GASI sites, the pH soil map is based on the soil map of Germany (Federal Institute for Geosciences and Natural Resources, 2013). Its rather low resolution of 1:1,000,000 also limits the accuracy of the soil pH map.

Land management greatly determines the soil pH of agricultural land. Farmers adjust soil pH based on the sensitivity of the crops being grown, the expected yields of liming practice and soil properties such as texture and TOC. Targeted and recommended (VDLUFA, 2000a) pH values are higher on croplands than grasslands, thus affecting the lime rates applied. Pronounced differences between cropland and grassland were also found by the RF3 model and are represented in the soil pH map. Due to the lack of regionalized liming data, the effects of farmers' pH management are underrepresented. An attempt was made to overcome this problem at least partially using the averaged pH value of surrounding GASI sites as a model predictor to minimize systematic overestimation or underestimation of pH at the regional scale and compensate for regional-specific liming characteristics. However, Figure 2 shows that sites with pH levels below or above optimal ranges according to the VDLUFA scheme are often adjacent to one another. This observed high-resolution variability in pH management was levelled out by the regionalization approach. More precise management data describing fertilization, liming and crop types would help improve the description of pH variability caused by pH management. Such data, as well as more information on spatial variability of soil pH, exist in all agricultural holdings; however, for reasons of data privacy, these data are not available.

Besides the specific pH map of German agricultural soils, two other soil pH maps have predominantly been developed for Europe that include Germany (Ballabio et al., 2019; Fabian et al., 2014). Fabian et al. (2014) used a kriging approach to produce gridded pH maps on a European scale from pH ($CaCl_2$) measurements for 2108 cropland sites (145 in Germany) and 2023 grassland sites (148 in Germany). The spatial resolution of these maps is fairly low because they depend on the spatial distribution of observed pH values only, and the number of sampling points was rather low. Ballabio et al. (2019) applied Gaussian process regression on LUCAS (Land Use Cover and Area frame Survey) data from 2009 to 2012 to produce European maps of pH ($CaCl_2$) and pH (H_2O) at a resolution of 250 m. Independent variables came from remote sensing data (MODIS, CORINNE), the European soil database and meteorological data in a monthly resolution (WorldClim). The European soil database was used to derive the spatial distribution of parent material. Similar to this study's pH map, the spatial distribution of pH strongly related to parent material, although other variables, such as derived parameters from MODIS, which were used to describe land-use types, northing (Y coordinates) and climate variables (maximum and minimum temperature and precipitation of specific months), were found to be more important. The new pH map presented in this study was based on data of higher spatial resolution than the LUCAS data (14 km × 14 km vs. 8 km × 8 km), land use was more precisely determined by information from farmers covering a time period of around ten years before sampling, and management data were indirectly included (as mean soil pH of the GASI sites) as well as site properties. Therefore, the precision of the presented pH map is slightly higher than the LUCAS-derived product and it reflects more specifically the situation in Germany. However, the absence of fine-resolution data on land use, liming practice and parent material limited the precision of both pH maps in a similar way.

Within GASI, soil pH was measured for several soil layers up to a depth of 1 m, while the present study's soil pH map represents topsoil pH. Biogeochemical models require information on the complete root zone, including subsoil pH values. Therefore, a consistent extension of the map presented here would be useful for large-scale modelling.

5 | CONCLUSIONS

Data from the first national inventory of German agricultural soils revealed that pH in many cropland and grassland soils are lower than recommended for optimizing soil fertility and crop yield. There is considerable potential on 41% of cropland sites and 52% of grassland sites to improve productivity by more regular and targeted soil pH management via liming. Also, fields with lime management should consider to apply the required amount of lime to increase the pH to the desired level. These analyses indicated that farm-scale pH management is influenced by land-use type (with agricultural areas having considerably higher pH levels than natural ecosystems such as forests), its relevance for farmers' economic income (primary activity vs. sideline business; more suboptimal pH values for grasslands than croplands) and specialization in specific crops more or less sensitive to soil pH. The regular topsoil nutrient analysis used by farmers to optimize application rates of potassium and phosphorous fertilizers provides regular and field-specific information on soil pH level. Thus, in most cases, farmers are aware of the pH levels of their soils, but this information obviously does not result in liming recommendations being implemented in full on all farms. The costs of liming and a gradual and relatively slow yield decline with decreasing soil pH probably contribute to differences in soil pH management. It is recommended that soil pH changes should be carefully observed over several years and conscientious pH management should be implemented that maintains soil fertility and considers crop-specific pH and lime requirements.

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DATA AVAILABILITY STATEMENT

The data that support the findings of this study are openly available in OpenAgrar at http://www.OpenAgrar.de. (https://doi.org/10.3220/DATA20200203151139).

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SUPPORTING INFORMATION

Additional supporting information may be found in the online version of the article at the publisher's website.

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