ASSESSMENT AND MODELING OF SOIL FUNCTIONS OR SOIL-BASED ECOSYSTEM SERVICES: THEORY AND APPLICATIONS TO PRACTICAL PROBLEMS

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ASSESSMENT AND MODELING OF SOIL FUNCTIONS OR SOIL-BASED ECOSYSTEM SERVICES: THEORY AND APPLICATIONS TO PRACTICAL PROBLEMS

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EDITORIAL
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Editorial: Assessment and Modeling of Soil Functions or Soil-Based Ecosystem Services: Theory and Applications to Practical Problems

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Keywords: ecosystem services, human, populations, soil preservation, soil degradation

Editorial on the Research Topic

Assessment and Modeling of Soil Functions or Soil-Based Ecosystem Services: Theory and Applications to Practical Problems

In the soil-related literature of the past half-century, two different perspectives have been adopted to deal with the benefits that are provided by soils (Baveye et al., 2016). The first perspective, initiated in the mid-1960s, centres on the multiple "functions" of soils, defined as the benefits that not just human populations, but also the rest of nature derive from soils. Simonson (1966) used the term of "multifunctionality" to stress the fact that these functions are numerous, and are often fulfilled simultaneously. Decision-makers quickly adopted this perspective; as early as 1972, the Council of Europe used it in some of its official documents related to the preservation of soil resources. Implementation of some of the guidelines that have resulted has been greatly facilitated by the elaboration by Blum (1988) of a detailed classification of soil functions (illustrated in **Figure 1**) and, slightly later, by the FAO of a similar, but more complete one. Both classifications have proven to be very useful communication tools to explain to lay audiences, in simple terms, what soils contribute to nature, and in particular to human populations, and therefore how vital it is to prevent their degradation. A second perspective, largely inspired by the sizeable intellectual achievement of the Millenium Ecosystem Assessment (Millennium Ecosystem Assessment, 2005), focuses on the contributions that soils make to "ecosystem services", i.e., the benefits that human populations derive from ecosystems encompassing soils.

Uncertainties and controversies resulting from the terminology in use have been associated with the concept of ecosystem services from the start (e.g., Barnaud and Antona, 2014). In the case of soils, the existence of two distinct traditions, one firmly rooted in soil science, and the other inherited from ecology, has in the last few years caused some level of confusion, because different terms are sometimes used to denote different concepts. In particular, from the soil science perspective, services, i.e., benefits that human populations derive from soils, correspond to a subset of soil functions, which by definition are not restricted to human populations. However, from the ecological perspective, the term of "function" has been traditionally associated with the physical (bio)chemical, or biological processes occurring in ecosystems that give rise to ecosystem services, and that same acception of the term has occasionally also been adopted by soil scientists (see, e.g., Keesstra et al., 2016; Pereira et al., 2018). In addition, some authors (e.g., in Issue 184 of the Philosophical Transactions of the Royal Society B, devoted in September 2021 to the topic) have also started to use the alternative expression of "nature's contribution to people" instead of ecosystem services, which adds even more to confusion, since the difference between these different terms is not obvious (Braat, 2018; Baveye et al., 2018).

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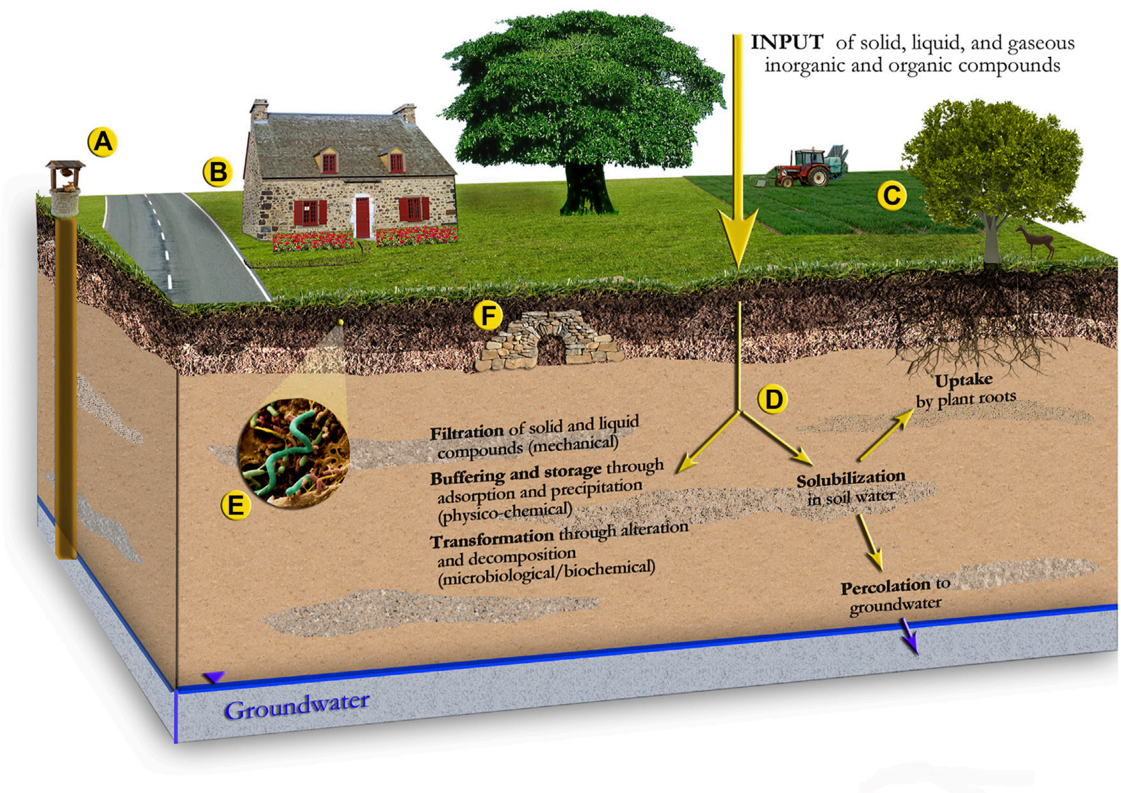

FIGURE 1 | Schematic illustration of the different functions of soils according to Blum (1988) classification. The six categories of soil functions correspond, respectively, to **(A)** the extraction of raw materials and water, **(B)** physically supporting buildings and other man-made structures, **(C)** the production of biomass, **(D)** filtration, buffering, storage, and chemical/biochemical transformations, and **(E)** the preservation of biodiversity or potentially useful genetic material, as well as of geogenic and cultural heritage **(F)**.

Regardless of the perspective that is adopted, i.e., whether we consider only the benefits of soils to human populations or we look more broadly at the benefits to nature as a whole, the hope existed 3 years ago, when we started thinking about proposing a Research Topic in the area, that soil functions/services could be used in practice in decision-making affecting the fate of soil resources. Unfortunately, in this respect, a significant hurdle at the time related to the lack of quantitative assessment of soil functions/services and of their provision under different land uses (Baveye, 2017). In the scientific literature up to that time, there were virtually no direct measurements of multiple soil functions or services at spatial and temporal scales of practical relevance. Soil functions/services tended to be estimated, rather than measured, using proxy variables or indicator parameters, leading eventually to maps of soil functions, a number of which have been produced over the last few years. An alternative assessment method relied on modelling, in which in addition to statistical correlations (e.g., pedotransfer functions), detailed process understanding could be explicitly accounted for. Modelling could in principle help us move beyond the mere quantification of functions/services at a given instant, and quantify the temporal dynamics of soil functions/services (e.g., in response to external forcing), but the approach was in dire need of verification.

To help strengthen the literature in this crucial area, the objective of the Research Topic we proposed was to serve as an outlet for articles that dealt with any aspect of the simultaneous assessment of multiple soil functions and their contributions to the provision of ecosystem services, from a conceptual standpoint, from the perspective of the development of new methodologies, or from the angle of practical applications to concrete problems and implementation for decision making about land use or land management change. Contributions on the concrete, practical side were particularly welcome, as were also papers that dealt with some of the soil functions and soil-based ecosystem services that are less frequently assessed, let alone discussed, for example the preservation of cultural artefacts, or the role of soils as stock of genetic information (e.g., in the development of antibiotics or phage therapy).

Eleven articles were eventually accepted for publication in this Research Topic. Three articles, by Vogel et al., Mikhailova et al., Gerard et al., and Lennartz and Liu, deal with different aspects of the assessment of soil functions/services. Although peripherally related to soil functions/services, the article by George et al. shows that fungal biodiversity, one of several soil biodiversity parameters that are often associated with the delivery of soil functions/services, can be measured in very different ways, potentially leading to ambiguity.

Rioux et al. address the mapping of soil functions/services, whereas Mikhailova et al. and Cope et al. also discuss the possible monetary evaluation of soil functions/services. A second group of articles focuses on modelling of soil functions/services using different approaches, including proxy parameters (Fossey et al., Van Leeuwen et al.), and three present Decision Support tools meant to facilitate the involvement of soil functions/services in practical soil management situations (Sandén et al., Debeljak et al., Van de Broek et al.).

Thanks in part to the work of the authors who contributed to this Research Topic, but also to research carried out in parallel (Chalhoub et al., 2020; Choquet et al., 2021), significant progress has been achieved recently on the measurement of soil functions/services, and on the development of various modelling frameworks to predict them in practical situations. Nevertheless, if we want the soil functions/services framework to become a useful tool for the preservation of soils in practice, it seems clear that in the next few years, the soil science community will have to devote even more attention to the methods used to assess and model soil functions, and will have to find ways to facilitate this assessment in practical applications to increase the use of relevant information for decision-making. The need is likely to become particularly acute in this area for three key reasons. The first is that climate change is forecasted to lead to pressures on soils that they have not experienced so far, e.g., in terms of regulation of the water regime under significantly more intense and less frequent rainfalls (see discussion in Baveye et al., 2020). A second reason is that at the European level the common agricultural policy and the subsidies it involves to agriculture will be increasingly tied to appropriate measures of sustainable land use. To enable this, quantitative instruments are needed to evaluate agricultural practices with respect to their impact on the ensemble of soil functions. A final reason is that heavy pressure of financial institutions and governments toward the development of carbon markets and carbon farming practices will raise tricky, and so far entirely unresolved, questions about what monetary value, if any, could be associated with specific soil functions/services.

We hope that the various articles in this Research Topic will, in some measure, foster a healthy dialogue on the assessment and modelling of soil functions/services, which will make it possible for the soil science community to address fruitfully the urgent questions that are being asked by society in this context.

AUTHOR CONTRIBUTIONS

All authors listed have made a substantial, direct, and intellectual contribution to the work and approved it for publication.

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Development of an Agricultural Primary Productivity Decision Support Model: A Case Study in France

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Agricultural soils provide society with several functions, one of which is primary productivity. This function is defined as the capacity of a soil to supply nutrients and water and to produce plant biomass for human use, providing food, feed, fiber, and fuel. For farmers, the productivity function delivers an economic basis and is a prerequisite for agricultural sustainability. Our study was designed to develop an agricultural primary productivity decision support model. To obtain a highly accurate decision support model that helps farmers and advisors to assess and manage the provision of the primary productivity soil function on their agricultural fields, we addressed the following specific objectives: (i) to construct a qualitative decision support model to assess the primary productivity soil function at the agricultural field level; (ii) to carry out verification, calibration, and sensitivity analysis of this model; and (iii) to validate the model based on empirical data. The result is a hierarchical qualitative model consisting of 25 input attributes describing soil properties, environmental conditions, cropping specifications, and management practices on each respective field. An extensive dataset from France containing data from 399 sites was used to calibrate and validate the model. The large amount of data enabled data mining to support model calibration. The accuracy of the decision support model prior to calibration supported by data mining was ∼40%. The data mining approach improved the accuracy to 77%. The proposed methodology of combining decision modeling and data mining proved to be an important step forward. This iterative approach yielded an accurate, reliable, and useful decision support model for the assessment of the primary productivity soil function at the field level. This can assist farmers and advisors in selecting the most appropriate crop management practices. Embedding this decision support model in a set of complementary models for four adjacent soil functions, as endeavored in the H2020 LANDMARK project, will help take the integrated sustainability of arable cropping systems to a new level.

Keywords: decision support model, data mining, expert knowledge, yield, soil functions, agricultural decision-making

INTRODUCTION

Soils play a unique role for agriculture and provide numerous functions to society, among them primary productivity (Schulte et al., 2014). The primary productivity function is the capacity of a soil to supply nutrients and water and to produce plant biomass for human use, providing food, feed, fiber, and fuel within natural or managed ecosystem boundaries. This function is the economic foundation for farmers and all connected sectors and is thereby directly linked to societal demands (Tóth et al., 2013; Schulte et al., 2014). The United Nations predict that, by 2050, global agricultural production must grow by 60% to feed the increasing world population (WWAP, 2015). At the same time, however, an estimated one quarter of all agricultural soils are degraded: their future potential for biomass production has decreased and will continue to decline without intervention (Conijn et al., 2013). Moreover, crops grown in short rotations or monoculture face yield declines compared to crops grown in more diverse crop rotations. This is most likely due to biotic factors, including increased plant pathogens, or abiotic factors, including agricultural management practices, both of which can reduce nutrient availability (Bennett et al., 2012; Mazzilli et al., 2016; Weiner, 2017). Soils that are not managed sustainably may lose their productivity function over the longer term (Mueller et al., 2010). More importantly, the function of agricultural soils goes beyond primary productivity to include water regulation and purification, carbon sequestration and climate regulation, provision of habitat, and soil biodiversity, as well as nutrient cycling (Mueller et al., 2010; Schulte et al., 2014; Techen and Helming, 2017). Societal demands for different soil functions pose further challenges because they involve different spatial and temporal scales (Valujeva et al., 2016), and different stakeholders have diverse demands (O'Sullivan et al., 2015). Farmers play a key role in managing agricultural soil resources, but it remains difficult to find simple tools to help them manage primary productivity, let alone simultaneously manage multiple soil functions. Therefore, sustainably managing agricultural soil resources continues to be a challenge.

Considering that primary productivity is a priority in the agricultural sector, several methods and models have been used to evaluate the productivity function of soils (e.g., Tóth et al., 2013). Mueller et al. (2010) reviewed such approaches with the aim of finding a universal strategy that could be used globally at various scales. The authors concluded that there was no common global method to assess productivity at the field level and recommended that evaluations like Muencheberg Soil Quality Rating (Mueller et al., 2007, 2012) and the Canadian Land Suitability Rating System (Bock et al., 2018) would be good basis for developing one. The target was scalability across different regions and scales in addition to integrability into existing or forthcoming evaluation frameworks (Mueller et al., 2010). Tóth et al. (2013) provided a European assessment of productivity based on available data for grasslands, croplands, and forests, showing general trends in productivity across Europe. That type of assessment, however, lacks accuracy when the need is to assess primary productivity at the field scale for farmers. Several models including DAISY (Abrahamsen and Hansen, 2000), DNDC (Gilhespy et al., 2014), EPIC (Balkovič et al., 2013), and STICS (Brisson et al., 1998) all delve deeper into the different aspects of productivity, alongside other factors such as water and nutrient dynamics. Although several detailed options are available, many evaluation tools and methods remain in the research sector and are not used in cooperation with the end-users, i.e., to advise farmers on the optimal management of their agricultural fields or to incorporate farmers' and advisors' knowledge into the evaluation tools (Rose et al., 2016). Mechanistic models—STICS (Brisson et al., 1998), CENTURY (Parton and Rasmussen, 1994), and DayCent (Parton et al., 1998)—often require many variables (Trajanov et al., 2015) that farmers rarely address. Recently, Thoumazeau et al. (2019) presented a tool consisting of a set of 12 in-field indicators to measure soil functions. That tool, however, omits measures for primary productivity and fails to take into account various management practices. Therefore, there is a demand for approaches with qualitative decision modeling in which the current or desired management practices of farmers or farm advisors can be incorporated into assessments and advice regarding production and other soil management-related targets. This would enable the main decision concept, i.e., primary productivity in the present case, to be broken down into smaller, less complex subconcept. Expert knowledge would be considered at all levels of the model (Mouron et al., 2013; Craheix et al., 2016; Bohanec et al., 2017a) and be reflected in the final outputs.

Machine learning is increasingly being used in order to utilize agricultural data to make evidence-based decisions. This includes important attributes that can be used to optimize predictions, such as on primary productivity. Machine learning has now been utilized (i) to predict single soil attributes or study what governs them (Hobley et al., 2015; Hobley and Wilson, 2016; Chang et al., 2017; Bondi et al., 2018), (ii) for continental or even global soil property predictions (Henderson et al., 2005; Hashimoto et al., 2017; Hengl et al., 2017), and (iii) to classify soils in digital soil mapping (McBratney et al., 2003; Heung et al., 2016). Trajanov et al. (2018) successfully used data mining to generate predictive models that identify the key factors governing primary productivity ($r > 0.80$). The increasing amount of earth observation data has also been applied to agricultural decision-making (Liakos et al., 2018). Such data have been used to guide water and fertilizer management for cropping systems (Vuolo et al., 2016) and, on a more regional level, to map crop rotations over time (Vuolo et al., 2018). Such data can also serve as a basis for more comprehensive qualitative decision support models that help develop simple tools to guide agricultural practices (Debeljak et al., in review[1]). Such tools can then be used together or separately by end-users including researchers, farmers, advisors, and regional agricultural governance personnel. This co-creation of a final decision support tool would support greater acceptance by farmers and advisors because it would be easier to use and more relevant to the end-users. This could be further enhanced through peer

[1]Debeljak et al. A field-scale decision support system for assessment and management of soil functions. In review in Frontiers in Environmental Science, this issue.

recommendations by farmers, who have already been testing the decision support tool. Finally, it would help develop a tool that is fit for use by advisory services (Kerselaers et al., 2015; Rose et al., 2016).

Our study was designed to develop a decision support model for agricultural primary productivity. This work was done in close cooperation with the development of decision support models for four other soil functions within the H2020 LANDMARK project (Debeljak et al., in review[1]; Delgado et al., submitted[2], Van den Broek et al., in review[3]; Van Leeuwen et al., in review[4]). To obtain a highly accurate model that helps farmers and advisors assess and manage the primary productivity of their agricultural fields, we addressed the following specific objectives: (i) to construct a qualitative decision support model to assess the primary productivity at the agricultural field level; (ii) to carry out verification, calibration, and sensitivity analysis of the model; and (iii) to validate the model with independent empirical data. The goal is to develop a generic model for primary productivity that can be applied across different environmental zones (after conducting the required standard modeling procedures to operationalize it to the respective location and scale).

MATERIALS AND METHODS

Decision Support and Data Mining Methodologies

The primary productivity decision support model was built using Multi-Criteria Decision Analyses (MCDA), in particular DEX (Decision Expert) integrative methodology (Bohanec and Rajkovic, 1990; Bohanec et al., 2013; Bohanec, 2014, 2017b) for qualitative decision modeling. The principles of this methodology follow intuitive human decision-making, where the main decision problem (concept, in our case, being primary productivity) is broken down into smaller, less complex subproblems (subconcepts, in our case, being soil, environment, crop, and management).

This breakdown is represented in the form of a hierarchy, where the main concept (primary productivity) is at the top of the hierarchy and is related to lower-level attributes on which it depends. The attributes at the lowest level of the hierarchy are the basic attributes: the soil, environment, crop, and management parameters. The intermediate attributes represent aggregations of the lower-level attributes. Their values (suitable, neutral, unsuitable) are obtained using decision rules. Decision rules (further referred to as integration rules) are a tabular representation (integration table) of a mapping from lower-level attributes to higher-level ones. The qualitative modeling approach of the DEX methodology helps formalize the input values into discrete (finite) scales. Our case unifies the scales along all basic attributes in a set of three categorical values: "Low," "Medium," and "High." Exceptions are attributes that play binary roles, represented with value scales consisting of two values: "Yes" and "No."

A standard modeling procedure was applied to obtain a reliable decision support model. It consists first of verification, sensitivity analysis, and calibration in an iterative way, followed by validation (Jorgensen and Fath, 2011). Verification is a test of the internal operational logic and behavior of the model. Domain experts (soil scientists) helped design the theoretical scenarios used to experimentally compare the model results with the expected outcomes.

The goal of the sensitivity analysis was to reduce model complexity by distinguishing between those input attributes whose values have a significant impact on model behavior, and those attributes whose values have low or no impact. After which, redundant input attributes were eliminated. This was done based on weights, which are commonly used in decision analysis to estimate the importance of attributes. The weights define the contribution of a corresponding attribute to the final evaluation of the alternative. Because the attributes had different value scales (some attributes have more values than the other), the weights had to be normalized. This adjusted all scales to the same unit interval. We used global normalized weights, which considered the structure of the entire model and the relative importance of its part. The weight of the top-most attribute in the model was 100%, whereas the weight of the basic or intermediate attributes could be 0%.

Calibration was conducted as an attempt to find the best agreement between the computed and observed data by varying the selected parameters. Calibration is usually performed on selected sets of parameters, and the model outputs are compared with the measured values of the modeled variable. The parameter set that gives the best agreement between model output and measured values is chosen. Calibration was performed by modifying the integration rules. We determined the selection of integration rules whose variation could significantly improve model performance by data mining that helps find and understand new patterns and knowledge from data based on methods from statistical modeling or machine learning. We utilized machine learning methods to supervise learning, in particular methods for learning decision trees, i.e., classification trees (Breiman et al., 1984). Classification trees (in a predictive task) predict the value of a dependent/target attribute (in our case primary productivity) from the values of independent attributes (soil, environment, crop, and management parameters). The model's structure is hierarchical. Its nodes test (compare) the values of an attribute against a splitting criterion (given as constants). The edges branching off the nodes contain the outcomes of the test. The model's terminal nodes, termed leaves, contain the predictions. To predict the class of the target attribute of a new example, it is traversed down the tree. When it reaches a leaf, the class value in this leaf determines the class value of the given example (Witten et al., 2011). We selected classification trees as a proper model because of their interpretability and comprehensibility,

[2]Delgado et al. Farming systems targeted to water regulation and purification in agricultural soils. Submitted to Frontiers in Environmental Science, this issue.

[3]Van de Broek et al. Assessing the climate regulation potential of agricultural soils using a decision support tool adapted to stakeholders' needs and possibilities. In review in Frontiers in Environmental Science, this issue.

[4]Van Leeuwen et al. Modelling of soil functions for assessing soil quality: Soil biodiversity and habitat provisioning. In review in Frontiers in Environmental Science, this issue.

as well as their stepwise approach in solving non-linear classification problems.

The decision support model for primary productivity was finally validated using a representative dataset from France containing 399 sites from Atlantic Central and Mediterranean North environmental zones across France (Metzger et al., 2005). This objective test showed how well the model output performs and fits the real data. The decision support model was validated by directly comparing the estimated values with those provided in the empirical data. The direct comparison was facilitated by discretizing the values of the dependent variable. The discretization was done similarly as for the other variables. However, the added weight of the validation step and the demand for an accurate validation process required defining accurate thresholds that reflected the statistical and expert distribution of the measured values. The thresholds of the dependent variable that expressed the primary productivity were defined in the context of a selected crop based on the differences in yields between different crops. The model validation was set up as a set of rules and defined as follows: an estimation of the primary productivity soil function was considered accurate if the estimated value or estimated most probable value (based on estimated probability distribution) was equal to the appropriate discrete value of the primary productivity of a selected site in the empirical dataset. Otherwise, the estimation was considered to be incorrect. The ratio between correct estimations and total estimations is taken as an accuracy measure for model performance.

TABLE 1 | Primary productivity attributes that underwent discretization with corresponding units and scale values.

Attribute type	Attribute name	Unit	Scale
Soil	pH ($CaCl_2$)	Unitless	High, medium, low
Soil	C:N ratio	Ratio	High, medium, low
Soil	Soil organic matter (SOM)	%	High, medium, low
Soil	Plant-available P	mg kg^{-1}	High, medium, low
Soil	Plant-available K	mg kg^{-1}	High, medium, low
Soil	Mg	mg kg^{-1}	High, medium, low
Soil	Cation exchange capacity (CEC)	cmol (IE) kg^{-1}	High, medium, low
Soil	Salinity	dS m^{-1}	High, medium, low
Soil	Bulk density (BD)	kg dm^{-3}	High, medium, low
Soil	Rooting depth	cm	High, medium, low
Soil	Clay content	%	High, medium, low
Soil	Groundwater table depth	m	High, medium, low
Environment	Annual precipitation	mm	High, medium, low
Environment	Number of days with daily average temperatures above 5°C	Days	High, medium, low
Environment	Altitude	masl	High, medium, low
Environment	Slope degree	Degree	High, medium, low
Crop	Number of crops in rotation	Absolute number	High, medium, low
Crop	Percentage of legumes in rotation	%	High, medium, low
Crop	Percentage of catch crops, cover crops, green manure (CaC/CoC/GM)	%	High, medium, low
Crop	Stocking rate	LU ha^{-1}	High, medium, low, stockless
Management	Mineral N fertilization	kg ha^{-1}	High, medium, low, without
Management	Organic N fertilization	kg ha^{-1}	High, medium, low, without
Management	Chemical pest management	Unitless	Yes, no
Management	Physical pest management	Unitless	Yes, no
Management	Biological pest management	Unitless	Yes, no
Management	Irrigation	Unitless	Yes, no
Target attribute	Yield	kg ha^{-1}	High, medium, low

Description of the Dataset

The dataset used in this study is composed of attributes underlying a soil's capacity to produce plant biomass for human use within agricultural ecosystem boundaries, i.e., primary productivity. These attributes included soil properties (S), environmental aspects (E), crop (C), and management options (M) (**Table 1**), partly based on van Leeuwen et al. (2017). Soil and management data were collected within the French Soil Monitoring Network (RMQS) that was established to provide a national framework for observing changes in soil quality across France (Arrouays et al., 2011). This dataset covered a broad spectrum of climatic, soil, and agricultural conditions at all 399 sites. It consisted of a total of 2,200 soil samples extracted from the nodes of a 16-km grid that covered the French Metropolitan Territory. We extracted data from the topsoil samples (0–30 cm) from Atlantic Central and Mediterranean North environmental zones (Metzger et al., 2005) that were sampled as described previously by Martin et al. (2009). For environmental attributes, climatic data were obtained by interpolating observational data using the SAFRAN model (Quintana-Seguí et al., 2008). The RMQS site-specific data were linked to the climatic data by finding for each RMQS site the closest node within the 12 × 12 km² climatic grid and then averaging for the 1990–2016 period. Altitude and slope information were derived from a digital elevation model (USGS, 2004). The crop attributes and management practices from the last 5 years, including the studied year at the sites where the soil was sampled, were collected by an agricultural survey with the farmers. Due to differences in management information from one site to another, the percentage of legumes and catch crops in the rotation was calculated over maximum 5 years or less, depending on the amount of available information. Three crops were used to validate the primary productivity model: winter wheat, rapeseed, and sunflower. This allowed the RMQS survey to cover 44% of sites on arable land.

Data Pre-processing

To build, calibrate, and validate the primary productivity decision support model, we pre-processed the original data. The

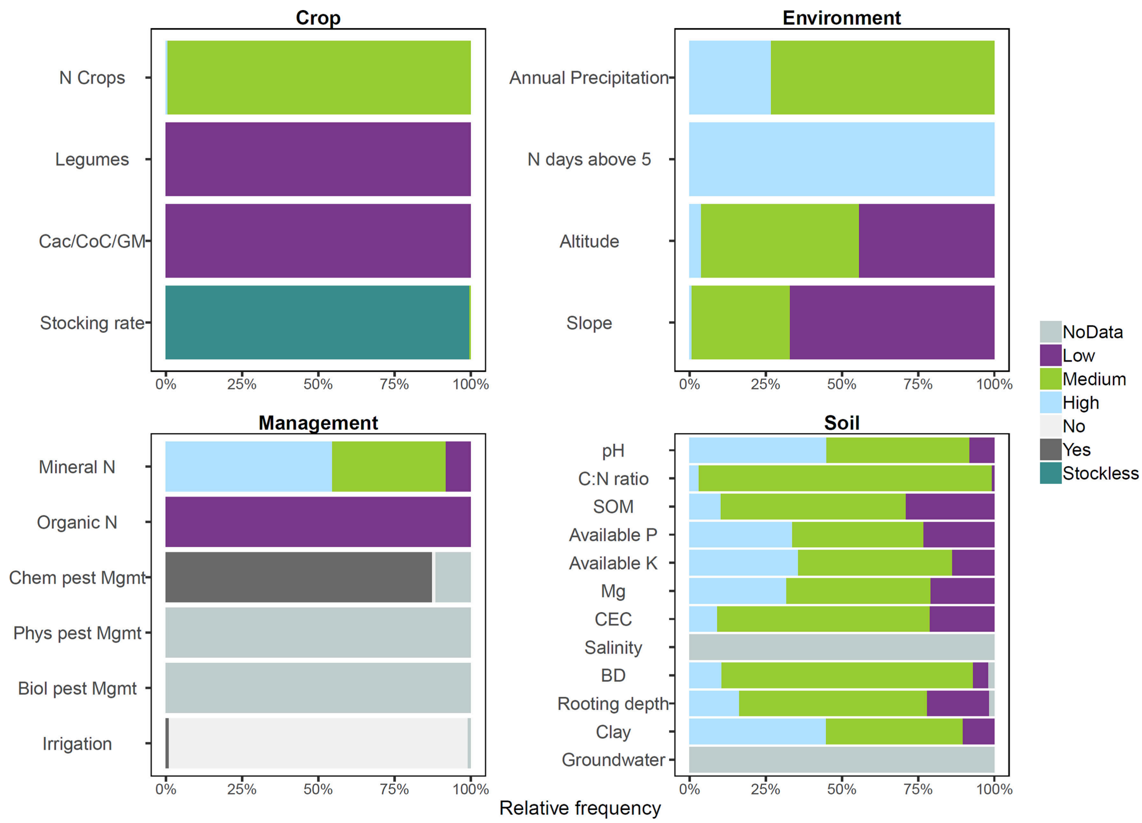

FIGURE 1 | The discretization of the dataset into values corresponding to "Low," "Medium," "High," "Yes," "No," and "Stockless".

main focus was on handling missing values and data cleansing (removing identifiers and correlated attributes).

Building and validating the DEX models requires the data to have qualitative values from a discrete scale of values (**Table 1**). All data were therefore discretized into values from a set of discrete values, using thresholds defined by domain experts (**Figure 1**). For certain attributes (e.g., soil organic matter, clay content, ground water table depth, and precipitation), different thresholds were defined for different environmental zones. The primary productivity in the soil monitoring data was expressed as a quantity (kg ha^{-1}) and was also discretized into the values corresponding to the scale of "Low," "Medium," and "High" values, meaning low, medium, and high capacity of the primary productivity soil function. In order to define the scales, the observed crop yield of the soil sampling site of the year was compared with the statistics on the agricultural yields supplied by the French Ministry of Agriculture. The quantiles (10, 25, 50, 90%) on the population of the yearly departmental statistics were calculated in order to estimate how the observed yield at the soil sampling site rated with regard to the national distribution. The quantiles yielded a score between 0 and 20 for a year yield at the site as follows: 20 points if the yield was >90%, 15 points if the yield was between the median and 90%, and so forth. For the soil sampling sites where yields were measured for many years, we averaged notes over the years available. Then, the values were discretized to an average score as follows: Low = 0–10, Medium = 10–15, and High = 15–20. Thus, the more the observed yield is situated in the superior quantiles, the more positively the function was estimated.

The next step in the data pre-processing was handling missing values during the validation process. The DEX methodology (Bohanec and Rajkovic, 1990; Bohanec et al., 2013) supports missing values and handles them considering all possible values of the attribute that has missing values. This yields a set of values and their probabilities (rather than a single value) assigned to the main attribute—the primary productivity. Hence, the missing values were not removed from the dataset but assigned with a required sign understandable for DEX.

For the data mining analyses, the same original dataset was used. The values of the attributes were not discretized, except for the values of the primary productivity attribute, which were assessed by an independent expert, and took values from the scale "Low," "Medium," and "High" as described above.

RESULTS

Structure of the Decision Support Model for Primary Productivity

The developed decision support model for primary productivity is structured in a hierarchical way to take into consideration soil (S), environment (E), crop (C), and management (M) attributes

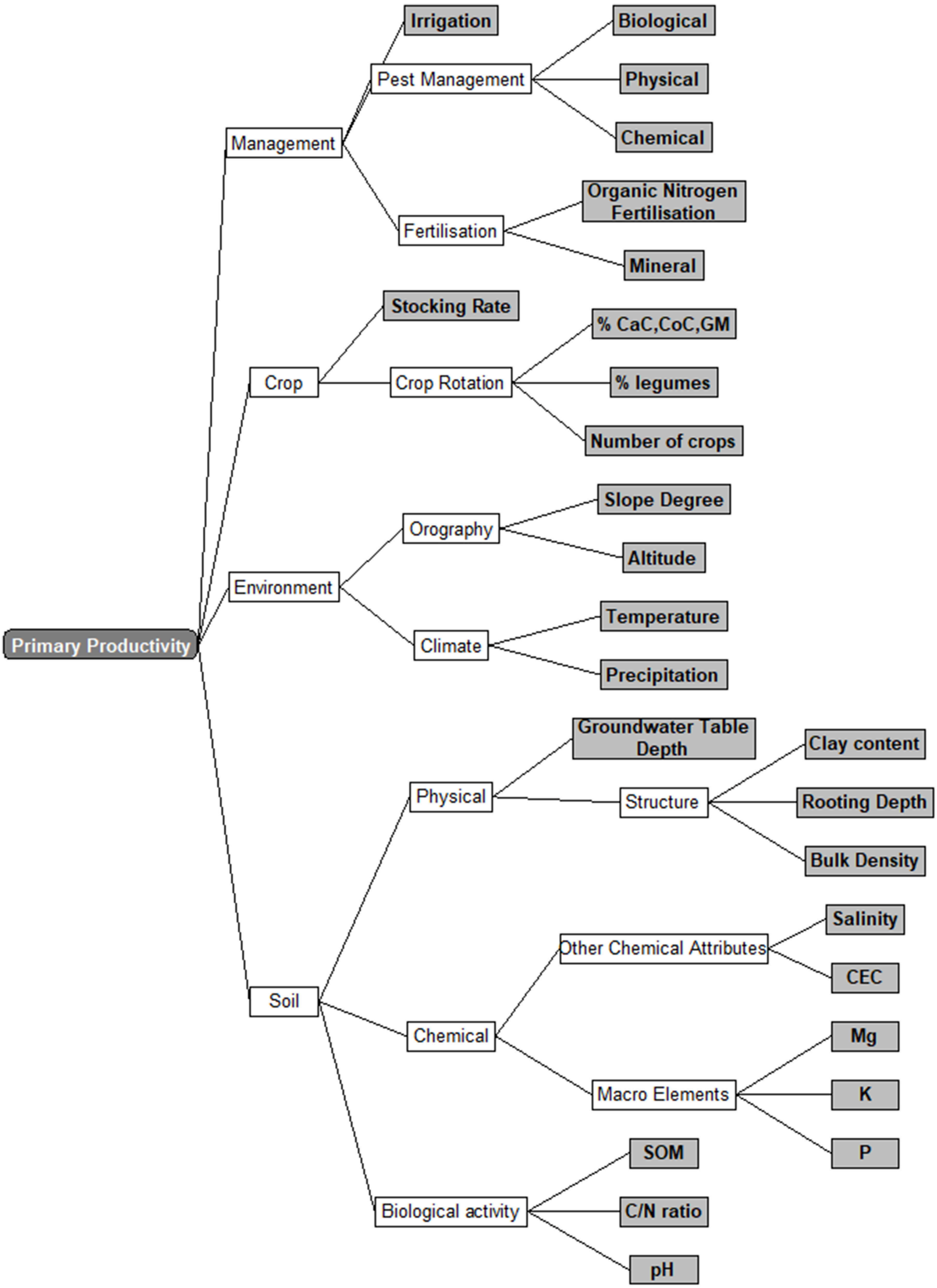

FIGURE 2 | The decision support model for primary productivity that is built up from basic attributes (gray boxes on right) via aggregated attributes (e.g., biological activity and soil) to the ultimate soil function—primary productivity.

(**Figure 2**). It comprises 4 levels and has 25 basic attributes. The top of the hierarchy represents the capacity of the primary productivity function; the intermediate levels represent attributes that integrate lower level attributes down to the basic input attributes. These S × E × C × M interactions determine whether the capacity of a soil to produce biomass is "Low," "Medium," or "High." The soil attributes consist of physical (e.g., clay content and bulk density) and chemical (e.g., macro-elements including phosphorus, potassium, and magnesium) attributes as well as attributes known to influence the biological activity of soils (soil organic matter, C/N ratio, soil pH). Environment is divided into attributes connected to orography (slope degree, altitude) and climate (temperature, precipitation). The crop consists of stocking rate as well as attributes linked to crop rotation (i.e., share of legumes, catch crops, cover crops, and green manure in the rotation, as well as the number of crops in rotation). Management attributes cover irrigation, pest management, and fertilization. Each attribute in the decision support model can have one out of three (or two) values (e.g., "High," "Medium," "Low," or "yes," "no"). Subsequently, values of a similar nature are assigned to the overarching process of each possible combination of two or three underlying attributes, until the ultimate function primary productivity (at the top) is reached.

Figure 3 shows the variability of importance of each attribute to the output (primary productivity). The first level in the hierarchy between the aggregated attributes soil, environment, crop, and management shows that these aggregated attributes each contribute 22, 30, 20, and 28%, respectively, to the overall primary productivity. This reflects similar distribution of importance (expressed as global normalized weights in **Figure 3**). This means that the inner variability of these structures contributes equally to the variability of the outcome. Nonetheless, examining the lower level of the hierarchy reveals that the water inflow ("Precipitation" and "Irrigation"), as well as orography ("Slope degree") and fertilization ("Mineral nitrogen fertilization" and "Organic nitrogen fertilization") greatly influence the variability of the primary productivity. In contrast, the least important individual attributes involve the structure of the soil properties, whereby physical properties dominate somewhat over chemical and biological ones.

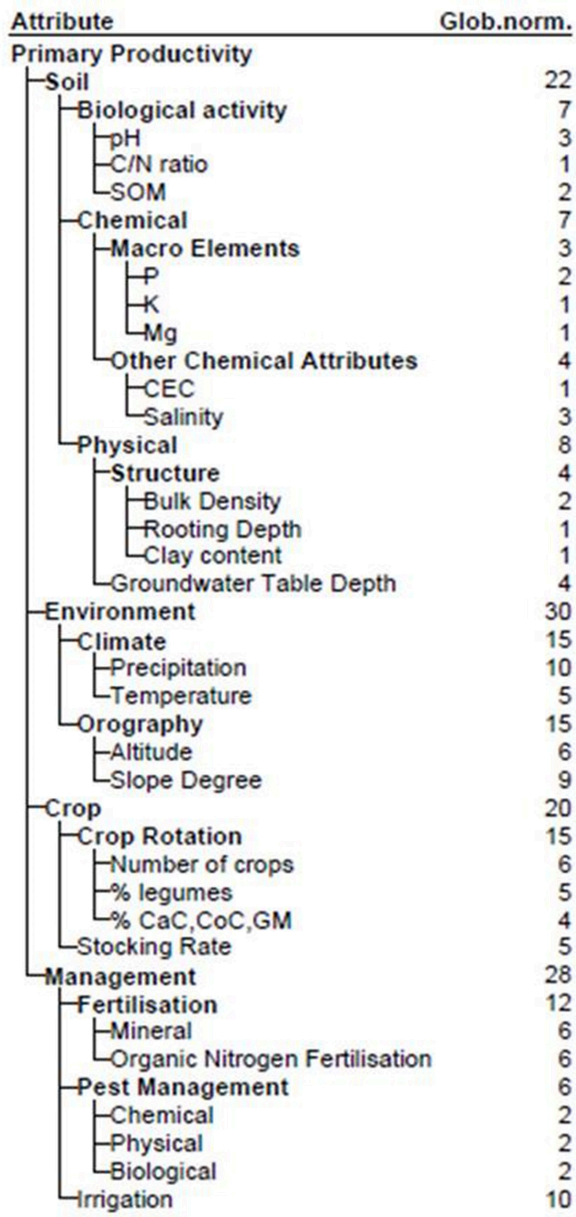

FIGURE 3 | Importance of attributes in the primary productivity model. Importance is expressed in percentage representing the contribution (ratio) of attribute's variability in outcome's variability. Hence, subconcepts (attributes at first level in the hierarchical structure) soil, environment, crop, and management contribute 22, 30, 20, and 28%, respectively, to the primary productivity value.

Operationalization of Model Structure

Once the structure of the decision model was built, we followed a standard modeling procedure to obtain a reliable decision support model ready to be used by agricultural advisors and farmers by iteratively applying verification, sensitivity analysis, and calibration. This was followed by model validation. The first model outputs showed need for further model structure modification that was done according to the knowledge and experience of the involved domain experts. Once the structure of the model was verified, sensitivity analysis was conducted. This procedure led to further structural changes and simplifications. The sensitivity analysis showed that we had to eliminate a small part describing micro-elements (not shown in the final model in **Figure 2**), because the global normalized weights of all three basic attributes (Fe, Mn, and Cu) were 0% and the global weight of their aggregated attribute (micro-elements) was only 1%. This reduced model complexity was verified, and the integration rules were modified accordingly.

The last step in the procedure was model calibration. To determine which integration rules were to be modified in order to calibrate the model to the French study area, we generated a data mining model in a form of classification tree to predict the capacity of the primary productivity soil function from the set of input attributes to the decision support model. The classification tree was generated using the French data described

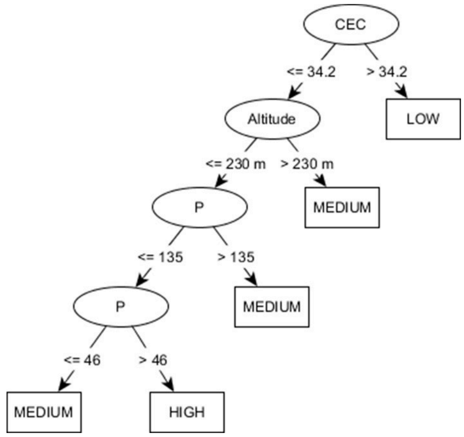

FIGURE 4 | Data mining classification tree for prediction of primary productivity in a field.

in the section Description of the Dataset and is presented in **Figure 4**. The accuracy of the data mining model was 77.7%, which was sufficiently reliable to calibrate the decision support model. The structure of this classification tree indicates that the most important initial attribute for the primary productivity at a field scale in our French dataset was the cation exchange capacity (CEC). Other important parameters were altitude and the available phosphorus (P) level in the soil. The integration tables incorporating these basic attributes were modified according to the attribute importance as they appeared in the classification tree. Accordingly, the integration rules originally defined by domain experts were modified and improved by the results of data mining modeling (see **Appendix 1** for details on changes in integration rules).

Model Validation

The last step in developing the decision support model was its validation. This was performed before and after calibrating the decision support model, which was supported by the classification model from data mining that was based on the empirical data from the same sites that were used for validation. The performance of the final decision support model, combining expert knowledge and machine learning, was expressed by its accuracy in correctly estimating the level of production compared to the local domain experts' evaluation (**Figure 5**). The local domain experts based their evaluation on the yield data they had access to. These comparisons revealed that primary productivity was more often underestimated by the domain experts compared to the outcomes of our decision support model. Since the outcome was defined by the discrete scale of "Low," "Medium," and "High," we examined model performance for each value separately, as well as its overall performance (**Table 2**). Calibration improved model performance to 83%, thus achieving overall accuracy of 77% compared to 42% before the calibration step. The primary productivity model performed best for the category of "High," followed by "Medium" and "Low" (97, 71, and 63%, respectively).

DISCUSSION

Primary Productivity Decision Support Model

Primary productivity is critical for the profitability and sustainability of agricultural systems; this makes it of pivotal importance that farmers plan for long-term maintenance of crop yields. The environment accounted for 30% of the important attributes underlying primary productivity in our decision support model (**Figure 3**). Other authors have also shown that orography (altitude and slope degree) and climate (precipitation and temperature) are among the main environmental factors that influence primary productivity (e.g., Mueller et al., 2010; Tóth et al., 2013). Primary productivity is often limited by climatic parameters such as drought, wetness, length of growing season, and irradiance (Fischer et al., 2002).

Management accounted for nearly 30% of a soil's primary productivity (**Figure 3**). The aim of management is to improve soil physical, chemical, and biological quality in order to overcome yield-limiting (e.g., soil moisture) and yield-reducing (e.g., pests) factors. In order to confirm a positive or negative effect of a management practice on primary productivity, long-term experiments can function as living laboratories (Johnston and Poulton, 2018; Sandén et al., 2018). Zavattaro et al. (2015) observed slight yield reductions following application of organic amendments, including farmyard manure and incorporation of crop residues, most likely due to N immobilization. The same authors also showed that, beyond management, the interplay between climate, soil type, and duration of management plays a role. Trajanov et al. (2018) showed that the crop grown and the compost amendment applied had major effects on primary productivity: higher yields were achieved when sufficient mineral or a combination of compost and mineral fertilization was applied compared to the application of compost amendments alone. Note, however, that independent from the chosen management practices, farm management options always have a site-specific component and should therefore ideally be tailored to as many local conditions ("supply") and requirements ("demands") as possible. Thus, practices showing benefits on one farm do not automatically result in similar benefits on a different farm. Accordingly, our decision support model often provides two or even three possible outcomes for a given location, as seen in **Figure 5B**. To decide which option should be selected, site-specific requirements need to be considered in the final decision-making process, as well as in the decision support tool to be developed (Stavi et al., 2016).

In assessing whether a field has suitable soil for primary productivity, our model further considers soil chemical and physical attributes as well as the attributes affecting biological activity. Soil properties accounted for about 20% of the total capacity to produce crops (**Figure 3**). CEC indicates the capacity of a soil to store nutrients and water—key aspects for supporting primary productivity. In our French dataset, a CEC (cobalt–hexamine method) up to 34 cmol kg^{-1} was shown to be optimal for primary productivity. This corresponds to rather high values when compared to national data (mean CEC 14 cmol kg^{-1}, 90 percentile 30 cmol kg^{-1}; Arrouays et al., 2011).

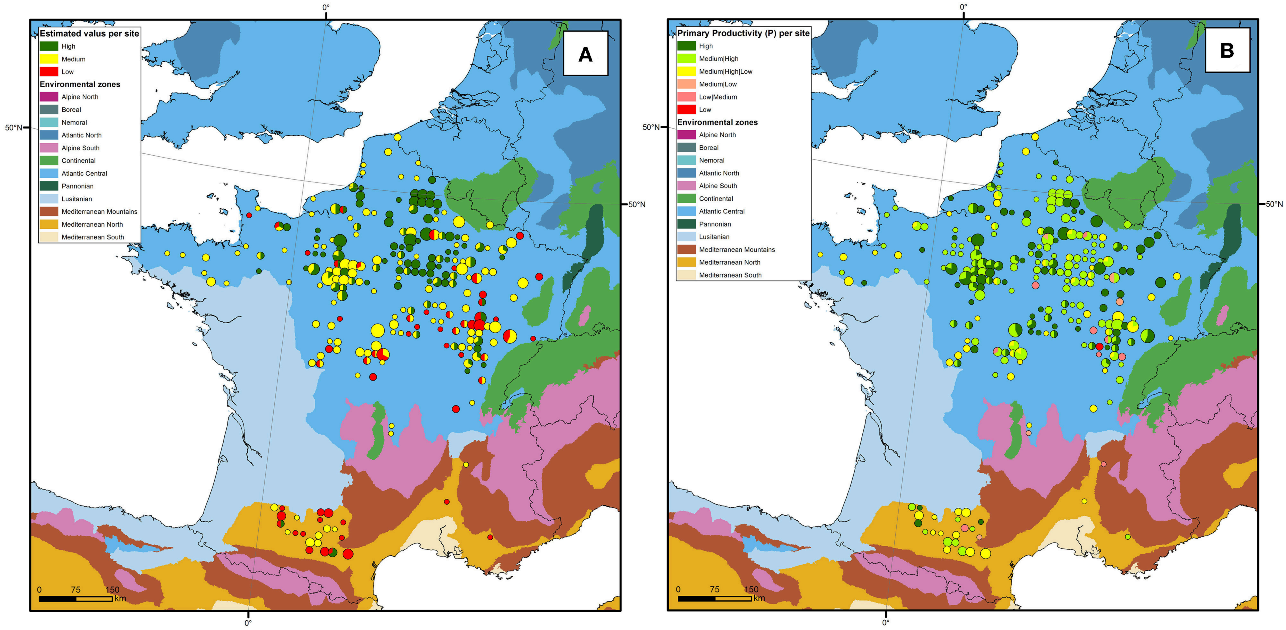

FIGURE 5 | Comparison between the estimated primary productivity as discretization of data by the domain experts (**A**, left) as low, medium, or high and the outcomes of the primary productivity decision support model (**B**, right) as low, medium, high, or combinations thereof.

TABLE 2 | Summary of the DEX primary productivity model performance before and after calibration.

	Before calibration (%)	After calibration (%)
Overall	42	77
Low	74	63
Medium	51	71
High	13	97

According to **Figure 4**, estimated primary productivity was high when plant-available phosphorus contents were between 46 and 135 mg kg^{-1}. Plant-available phosphorus contents are known to affect primary productivity (Sheil et al., 2016; Buczko et al., 2018; Trajanov et al., 2018). Furthermore, the classification tree confirms findings from Spiegel et al. (2001), who reported that very high yielding crops grown on soils with low plant available phosphorus concentrations are more likely to result in lower yields. Other factors known to limit the productivity function include shallow soils, stoniness, hardpan, anaerobic conditions, salinity, sodicity, acidity, nutrient depletion, and contamination (Mueller et al., 2010). Unfavorable soil structure can also negatively affect crop yields, for example, due to greater leaching losses (Kavdir and Smucker, 2005). Whether or not increased soil organic matter concentrations improve crop yields is still a subject of debate (e.g., Hijbeek et al., 2017), but it has been shown to greatly improve the soil biota (e.g., D'Hose et al., 2018).

The remaining 20% of our primary productivity model was affected by crop attributes (**Figure 3**). Zavattaro et al. (2015) observed that crop rotation and cover crops, in particular, had positive effects on crop yields, which is supported by our decision support model as well as by a recent study that recommended crop rotation as a promising management practice (Barão et al., 2019). Zavattaro et al. (2015) also observed that in more than 80% of the examined cases, the yield of a crop grown in a rotation practice was larger than that of a monoculture. According to their study, crop rotation worked well on sandy and loamy soils in western Europe, whereas clayey soils were less favorable for that system. Cover/catch crops had positive effects on the yields of the main crops in 60% of the cases, and it was of minor importance which cover/catch crop was grown (leguminous vs. non-leguminous) (Zavattaro et al., 2015). The positive effects of crop rotation and catch crops on primary productivity were confirmed by Sandén et al. (2018), who analyzed a total of 251 European long-term experiments. They reported an increase in yields of about 5% and 4% when crop rotation and catch crops were applied, respectively. Trajanov et al. (2018) also observed that the preceding crop had a large influence on crop yields in an Austrian long-term experiment: cereal yields were significantly lower when sugar beet or winter wheat (vs. soybean and spring wheat) preceded the crops.

Combining Expert Knowledge With Machine Learning

Expert knowledge is a central element in developing decision support models (Uusitalo et al., 2015), and modelers therefore heavily rely on such expertise and competence. Nonetheless, several issues arise when solely relying on expert knowledge (Wieland and Mirschel, 2017). The first challenge is acquiring expert knowledge, representing it in a formalized way and making it accessible for further use in decision modeling (Shaw and Woodward, 1990). Other common challenges are that such knowledge may be biased and that there may be a discrepancy between the expert's innate cognitive abilities and the complexity of the reasoning tasks required for certain scientific problems (Tversky and Kahneman, 1974). In developing our model, we worked with a wide group of experts to come up with the first ideas for the model and also incorporated experts who were very familiar with the data used to calibrate and validate the model. This approach helped minimize these challenges and tapped into varied knowledge. A further bias may arise from the data itself (**Figure 1**). In the present case, the French dataset focused on crops (e.g., winter wheat) that are usually grown in intensively managed and productive locations with suitable soil conditions, and only few are grown in less favorable conditions (**Figure 5**).

Acquisition of expert knowledge can be a hurdle: reliable experts may be unavailable or may offer opposing opinions (Shaw and Woodward, 1990). Those authors identified an even bigger challenge: the inability to verify the different opinions of the selected experts. This can partly be solved by weighing the different responses, as by Rutgers et al. (2012). Machine learning is an alternative way of obtaining domain knowledge from empirical data (Trajanov et al., 2015, 2018; Idé, 2016; Bondi et al., 2018). Machine learning algorithms for rule and tree induction are a useful framework for extracting knowledge from data and representing it in a format that can be directly used in constructing decision support models. In our case, we combined expert knowledge with data mining, which was proven successful with another dataset (Trajanov et al., 2018).

One task is to overcome these biases in expert knowledge and to satisfy the need to rely on scientific evidence and high-quality data when developing complex decision support models. This is promoted by the interplay between machine learning and decision support (Chlingaryan et al., 2018), as underlined by our decision support model. Machine learning models can provide accurate predictions (such as the capacity of the primary productivity soil function) by considering empirical data (Cherkassky and Mulier, 2007; Trajanov et al., 2018). Reliable predictions are invaluable, but in many cases, decisions must be made about the best course of action (e.g., what management practice to choose in order to increase the capacity of the primary productivity soil function). This can be achieved by feeding the predictions generated by machine learning models into a decision support model, which then evaluates alternative actions and recommends the optimal decision (Tulabandhula and Rudin, 2014). Our model aims to serve as a generic model for primary productivity that can be used across different environmental zones alongside models for four other soil functions. This requires appropriate calibration, including application of data mining.

Future Prospects: Taking the Decision Support Model From Research to Practice

An ideal decision support model will enable farmers to optimize long-term primary productivity while simultaneously accounting for management effects on other important soil functions. Improved knowledge on the effects of other soil functions on primary productivity and vice versa can help farmers make decisions on how to more holistically and sustainably manage their soils. Giving due attention to modeling scale (local, regional, national, European) is important when using decision support models: it is not trivial to upscale and/or downscale soil functions and management practices across different spatial scales (Schulte et al., 2015; Valujeva et al., 2016). Note also that not all attributes that influence primary productivity are equally relevant or have the same level of influence at every scale. While the initial development of our primary productivity model was supported by a study that focused solely on long-term experimental data in Austria (Trajanov et al., 2018), those authors suggested that a more comprehensive dataset on a larger spatial scale could more comprehensively identify the important attributes influencing primary productivity. Taking France as a case study provided us with a harmonized dataset for this purpose. Our decision support model for primary productivity will underpin the Soil Navigator decision support tool developed within the LANDMARK Horizon 2020 project. The latter is designed to integrate the simultaneous assessment of five soil functions: primary productivity, nutrient cycling, climate regulation, water regulation and purification, and biodiversity (Debeljak et al., in review[1]). The Soil Navigator is based on the concept of Functional Land Management (Schulte et al., 2014, 2015), which aims to manage soils such that the supply and demand of soil functions is balanced across a landscape. The strategy is to optimize different soil functions spatially, identifying where they have the best opportunities to thrive and where they are needed to fulfill societal demands. Engaging farmers to consider the effects of management on different soil functions requires (i) helping them to identify and understand the various influencing soil (S), environment (E), crop (C), and management (M) attributes affecting their field, and (ii) supporting them and their advisors with appropriate decision support tools. When adopting management practices, farmers will consider a range of other factors including performance, usability, relevance, cost-effectiveness, and compatibility with compliance demands (Rose et al., 2016). Furthermore, including farmers and advisors in the co-design of decision support tools has been shown to improve targeting toward user needs and ease of use as well as to provide additional benefits to end-users (Allen et al., 2017; Oliver et al., 2017). Previous research investigating farmers' knowledge on soil functions across Europe and their demands for a decision support tool showed that not all farmers want the same kind of advice (Bampa et al., 2019). That study, in agreement with Mills et al. (2018), concluded that farmer's motivations need to be taken into account to increase environmental benefits through management of agricultural landscapes. Bampa et al. (2019) observed that farmers were generally highly interested in practical solutions and in access to high-quality information in conjunction with one-on-one personal communication with soil scientists, agronomists, and advisors. Nonetheless, farmers' needs concerning mobile apps for agricultural advice and other decision support tools differed greatly between countries and even between scales (local, regional, and national) within a country (Bampa et al., 2019). These findings support a call for interactive dialogue between different stakeholders and direct involvement of farmers and advisors in the design of decision support tools. This is the most promising route to enhance and build understanding between research and practice adopters (Ingram et al., 2016).

CONCLUSIONS

Our study generated a primary productivity decision model using expert knowledge and data mining that can be used by farmers and advisors at the field level. We carried out improved standard modeling procedures to obtain a reliable decision support model by applying verification, sensitivity analysis, and calibration in an iterative manner. We then validated the primary productivity model with an extensive French empirical dataset in order to increase its usability. The proposed methodology of combining decision modeling and data mining proved to be complementary and clearly improved model performance. This approach yielded an accurate, reliable, and useful decision support model to assess the primary productivity soil function at the field level. It can also be used to improve future management practices and to maintain the primary productivity function of soils. Importantly, this model will underpin the LANDMARK H2020 project Soil Navigator, together with four other soil function models.

AUTHOR CONTRIBUTIONS

This article resulted from cooperation within the primary productivity task group in the LANDMARK H2020 project. TS, AT, HS, VK, and MD were mainly responsible for the development of the model. TS and HS as domain experts, AT with data mining, VK with model validation, and MD as the main responsible modeler throughout the study. NS and CP were responsible for the French dataset and acted as additional domain experts during the model development. CH was mainly responsible for future prospects. TS did most of the writing, with major inputs from AT, VK, NS, and MD. All authors contributed to the manuscript revision and read and approved the submitted version.

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SUPPLEMENTARY MATERIAL

The Supplementary Material for this article can be found online at: https://www.frontiersin.org/articles/10.3389/fenvs.2019.00058/full#supplementary-material

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Quantifying and Mapping Atmospheric Potassium Deposition for Soil Ecosystem Services Assessment in the United States

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National Atmospheric Deposition Program (NADP) databases are important for quantifying and mapping the contribution of atmospheric deposition to soil provisioning ecosystem services. These databases provide information about the atmospheric deposition of potassium (K^+) which is an essential element and component of many fertilizing materials. Atmospheric deposition flows (wet, dry, and total) serve as one input of K^+ to soils; however, deposition varies spatially across the United States (U.S.). This study ranked an estimated provisioning value of soil ecosystem services due to atmospheric K^+ deposition within the contiguous U.S. by state and region based on the 16-year period from 2000 to 2015. The total provisioning ecosystem value of atmospheric potassium deposition was over \$406M (i.e., 406 million U.S. dollars) (\$179M wet + \$227M dry) per year based on a 5-year moving average of \$500 per metric ton of potassium chloride (KCl) fertilizer in the U.S. The highest ranked regions for total value of K^+ deposition per year were: (1) West (\$86.5M), (2) South Central (\$80.4M), and (3) Southeast (\$80.2M). The highest ranked states for total value of K^+ deposition per year were: (1) Texas (\$44.3M), (2) California (\$18.3M), and (3) New Mexico (\$1.35M). Atmospheric potassium deposition is a source of K which is essential for human health. Given a U.S. population of 325.7 million people (2017), and a recommended daily intake of 4.7 g per person per day of K, it would require at least 1,531 metric tons/day of potassium to ensure that every person is able to meet their daily potassium requirement. In terms of monetary value, it will cost nearly \$1.5M per day based on a moving 5-year average U.S. price of \$500 per metric ton of KCl fertilizer. The results of this study provide a methodology to estimate and map the value of atmospheric potassium deposition for ecosystem services assessments, which can be helpful in conducting nutrient audits at various scales to address the United Nations (UN) Sustainable Development Goals.

Keywords: agriculture, fertilization, flow, potassium chloride, STATSGO

INTRODUCTION

The Millennium Ecosystem Assessment [Millennium Ecosystem Assessment (MEA), 2005] popularized the concept of ecosystem services as, "the benefits people obtain from ecosystems. These include provisioning services such as food, water, timber, and fiber; regulating services that affect climate, floods, disease, wastes, and water quality; cultural services that provide recreational, aesthetic, and spiritual benefits; and supporting services such as soil formation, photosynthesis, and nutrient cycling." Both direct (e.g., provisioning services) and indirect (e.g., supporting services) ecosystem services are vital components for supporting life on our planet; however, the lack of valuing these services in the form of policy is contributing to the degradation of our planet's ecological systems (Costanza et al., 1997; Gowdy, 1997; Lovett and Noel, 2008; Dominati et al., 2010; Baveye et al., 2016). These ecosystem services have been highly impacted over the last 50 years and their degradation has consequentially affected human well-being [Millennium Ecosystem Assessment (MEA), 2005]. Economics focuses more on prices than value, which is exemplified with the highly held importance on direct services (e.g., provisioning services) than indirect services (e.g., supporting services) (Heal, 2000; Lovett and Noel, 2008). Provisioning services are goods that can be extracted from the environment, while supporting services relate to soil formation and nutrient cycling [Millennium Ecosystem Assessment (MEA), 2005].

Atmospheric deposition can act as either an ecosystem service (e.g., input of essential nutrients; Mikhailova et al., 2018) or as an ecosystem disservice (e.g., input of pollution; Swain et al., 1992). Previous research has also shown derived benefits from atmospheric deposition such as the deposition of Saharan dust on increased ocean and rainforest productivity (Swap et al., 1992; Hamza, 2008; Mahowald et al., 2017). Although the atmosphere and atmospheric deposition provide numerous ecosystem services, they do not always go through the market because the atmosphere often is considered to be a "free" or "public good" which is nonrival and non-excludable (Heal, 2000; Holzman, 2012). Mikhailova et al. (2018) argued that atmospheric deposition is not always a "public good" because its contents can be deposited in the land within "private boundaries" (e.g., a farm) making "atmospheric goods" into "private goods" for which consumption is "rival" and "excludable" (Heal, 2000). Very often, ecosystem services are difficult to monetize, because "nature is the most complex system" (Holzman, 2012). One commonly used valuation technique is based on estimating "replacement cost" (Holzman, 2012). This method, in which one evaluates the cost of replacing an ecosystem service with a perfect human-derived substitute, is used as a measure of the economic value of ecosystem services.

Groshans et al. (2018a,b) stressed the importance of translating science-based "biophysical accounts" into boundary-based "administrative accounts" and used this accounting framework to estimate the replacement cost of soil inorganic carbon (SIC) by soil order, state, region, land resource region (LRR) using the State Soil Geographic (STATSGO) soil database. Mikhailova et al. (2018) used this accounting framework and identified the input of atmospherically deposited Ca^{2+} ions to the continental United States (U.S.) as a provisioning ecosystem service because it is a component of "raw" agricultural liming material ($CaCO_3$). Mikhailova et al. (2018) ranked an estimated provisioning value of soil ecosystem services due to atmospheric Ca^{2+} deposition within the contiguous U.S. by state and region. According to their calculations, the total provisioning ecosystem value of atmospheric Ca^{2+} deposition was \$65M (i.e., 65 million U.S. dollars) based on an average 2014 price of \$10.42 per U.S. ton of agricultural limestone ($CaCO_3$) or nearly \$355M based on an average 2014 price of \$33.00 per U.S. ton gypsum ($CaSO_4{\bullet}2H_2O$) (Mikhailova et al., 2018). In another study related to atmospheric deposition, Groshans et al. (2018c) ranked the provisioning ecosystem services value of atmospheric Mg^{2+} deposition in the United States by soil order, state, and region. The total value of provisioning ecosystem services contributed from atmospheric Mg^{2+} deposition was \$47M (e.g., 47 million U.S. dollars) based on a national average price (2014) of \$12.90 per U.S. ton of agricultural dolomite ($CaMg(CO_3)_2$).

Potassium plays an important role in the ecosystem services and Sustainable Development Goals (SDGs) in order to sustain global human societies (Keestra et al., 2016). First of all, potassium belongs to soil chemical properties, and it plays an important role in soils, plants, human and animal nutrition (Hasanuzzaman et al., 2018; Islam et al., 2018). The significance of potassium in agriculture (especially as a soil macronutrient) is well documented (Manning, 2010) and the following examples are specifically linked to the selected SDGs (Keestra et al., 2016) (numbers 2, 3, and 15 correspond to the specific SDGs):

2. End hunger, achieve food security and improve nutrition and promote sustainable agriculture;

Potassium is an important nutrient, and Sheldrick et al. (2002) reported that the depletion of K is particularly severe which results in an annual global deficit of 20 kg K ha^{-1}. In terms of monetary cost, this annual global deficit is valued at just over \$19 ha^{-1} based on a moving 5-year average price of U.S. \$500 per metric ton of potassium chloride (KCl) (Yager, 2016). According to Sheldrick et al. (2002), soil and surface balances for potassium can vary by different regions in the world. Sardans and Peñuelas (2015) reported global potassium contents in various soils with Aridisols, Mollisols, and Vertisols having the highest potassium contents, and Inceptisols, Andisols, and Spodosols having the lowest potassium contents.

3. Ensure healthy lives and promote well-being for all at all ages;

Potassium is extremely important for human health and various biological functions such as being a co-factor for many enzymes, required for insulin secretion, creatine phosphorylation, carbohydrate metabolism, and protein synthesis (Ringer and Bartlett, 2007). Given a global population of 7.7 billion people (2018), and a recommended daily intake of 4.7 g per person per day of potassium (U.S. Department of Health Human Services U.S. Department of Agriculture, 2015-2020), it would require at least 36,190 metric tons/day of potassium to ensure that every person is able to meet their daily potassium requirement. In terms of monetary value, this potassium requirement would cost \$34.5M each day based on

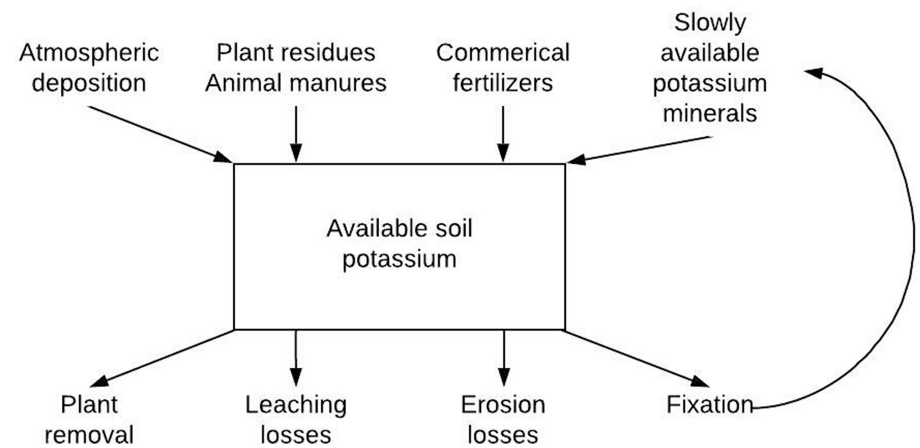

FIGURE 1 | The role of atmospheric potassium deposition in the gains and losses of available soil potassium under average field conditions (adapted from Brady and Weil, 2002).

a moving 5-year average price of U.S. $500 per metric ton of potassium chloride (KCl) (Yager, 2016). Given a U.S. population of 325.7 million people (2017), and a recommended daily intake of 4.7 g per person per day of K, it would require at least 1,531 metric tons/day of potassium to ensure that every person is able to meet their daily potassium requirement. In terms of monetary value, it will cost nearly $1.5M per day based on a moving 5-year average U.S. price of $500 per metric ton of KCl fertilizer (Yager, 2016).

15. Protect, restore and promote sustainable use of terrestrial ecosystems, sustainably manage forests, combat desertification and halt and reverse land degradation and biodiversity loss.

Potassium is important for activation of 80 different enzymes responsible for various plant and animal processes (e.g., energy metabolism, starch synthesis, nitrate reducation, photosynthesis, sugar degradation etc.), and helping plants to adapt to environmental stress (e.g., drought, winter, diseases, et al.) (Brady and Weil, 2002). Potassium is a key soil nutrient for agricultural crops and a deficit in soil potassium can reduce plant yields and increase plant susceptibility to disease (Rawat et al., 2016). Plant ecosystems, including forests and grasslands growth can be limited by available potassium (Sardans and Peñuelas, 2015). Potassium is also involved in physiological water use mechanisms in plants and can help mitigate plant drought stress (Sardans and Peñuelas, 2015).

Unlike other soil nutrients, potassium is present in the soil solution only as K^+ (**Figure 1**; Brady and Weil, 2002). Retention of K^+ is dependent on cation exchange capacity (CEC) which is largely affected by the predominant clay minerals (e.g., illite, vermiculite, etc.) (Manning, 2010). Soil K^+ retention is different for the 12 soil orders, with the lowest retention associated with highly leached and weathered soils (e.g., Ultisols, Oxisols). For soils with potassium deficiencies, the two most common soil fertilizers used for supplementing potassium are muriate of potash (MOP; more commonly referred to as potassium chloride or KCl) and sulfate of potash (SOP); more commonly referred to as potassium sulfate or K_2SO_4) (Havlin et al., 1999). United States consumption of KCl was 6,411,121 short U.S. tons in 2014 (USDA/ER, 2019), which would have cost almost 3 billion dollars assuming a 5-year moving average of $500 per metric ton of potassium chloride (KCl) in the U.S. (Yager, 2016).

Although significant research has been done on potassium in soils and atmosphere, the contribution of atmospheric deposition of potassium to soils often is not accounted for in ecosystem services valuations (Manning, 2010) (**Figure 1**). For example, quantifying the gains and losses of available potassium in soil due to fixation dynamics, potassium release from soil minerals, erosional and leaching losses, etc., limit our ability to quantify the stocks and flows of potassium associated with ecosystem services (Bilias and Barbayiannis, 2019). The objective of this study was to assess and rank the contribution of atmospheric potassium (K^+) deposition flows to soil provisioning ecosystem services within the contiguous U.S. by state and region. A monetary valuation of atmospheric wet, dry, and total K^+ deposition was calculated based on a moving 5-year average price of U.S. $500 per metric ton of potassium chloride (KCl) (Yager, 2016). This method, in which we evaluate the cost of replacing an ecosystem service with a human-derived substitute (potassium chloride, KCl), is called the replacement cost approach, and it is commonly used as a measure of the economic value of ecosystem services.

MATERIALS AND METHODS

The Accounting Framework

Atmospheric potassium deposition (flow) from atmospheric capital into soil capital represents the amount of potassium defined in a spatial and temporal context, which is in this study is the quantity of potassium deposition (kg) per area (ha) per unit time (year) (**Figure 2**). **Table 1** provides a conceptual overview of the accounting framework for valuation of various atmospheric potassium deposition flows: wet, dry, and total.

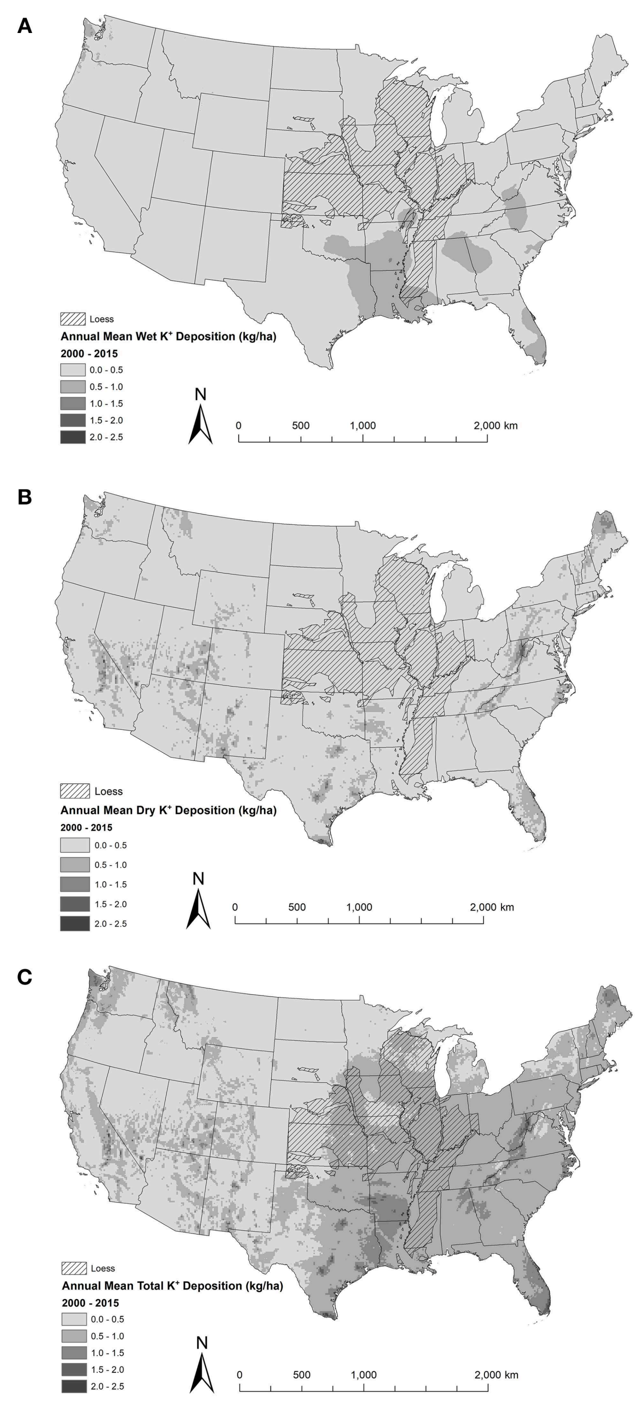

FIGURE 2 | Area-normalized annual mean K^+ deposition (kg/ha) for the years 2000–2015 in the contiguous United States: **(A)** wet, **(B)** dry, and **(C)** total.

The Monetary Valuation of the Atmospheric K^+ Deposition Flows

The overall monetary valuation procedure used to calculate atmospheric deposition of K^+ was adapted from the approach reported by Mikhailova et al. (2018) for calcium and by Groshans et al. (2018c) for magnesium deposition from the atmosphere. Briefly, annual atmospheric K^+ deposition (kg ha^{-1}) gradient maps were downloaded from the National Atmospheric Deposition Program (NADP) website (National Atmospheric Deposition Program (NRSP-3), 2018) in Grid format (**Table 1**). The maps' estimates of annual atmospheric K^+ deposition were calculated using samples from field sites operated by the NADP and National Trends Network (NTN). Samples were collected from field sites weekly. Details on sample collection, laboratory methods, quality control, and mapping methods can be found in several open-source publications using the NADP website (National Atmospheric Deposition Program (NRSP-3), 2018). An inverse distance weighting algorithm was used to spatially interpolate precipitation-weighted annual mean K^+ concentration (mg/L) measured at field sites to a continuous raster map layer with an approximate 2 km resolution. The resulting concentration map was then multiplied by annual precipitation maps developed using the PRISM precipitation model (Daly et al., 2008). The annual mean atmospheric K^+ deposition (kg ha^{-1}) over the study period was computed for each map cell using the Cell Statistics function in ArcGIS® 10.4 (ESRI, 2016) and then converted to U.S. dollars per area (i.e., hectare) and U.S. dollars in Microsoft Excel using the following equations:

$$\$/ha = \left(K^{+} deposition,\ kg/ha\right) \times \frac{74.55\ g\ KCl}{39.10\ g\ K^{+}} \times \frac{1\ metric\ ton}{1000\ kg} \times \frac{\$\ price}{metric\ ton\ KCl} \quad (1)$$

$$\$ = \left(price\ per\ area\ from\ eqn.\ 1\right) \times \left(area\ in\ ha\right) \quad (2)$$

Note that the price values calculated in U.S. dollars and dollars per ha represent the money that would be required simply to purchase potassium chloride (KCl) without consideration of other important costs, such as the equipment, fuel, and labor that would be required to incorporate the potassium fertilizers into the soil, nor any external costs associated with extracting and processing of potassium chloride etc. (Groshans et al., 2018b). There is an implicit assumption that potassium deposition onto the soils is not lost because of erosion, runoff, etc. Also potassium sources found in deposition cannot be distinguished between redistribution and recycling. Potassium found in dust and rainfall likely comes from terrestrial sources that can quickly be re-deposited or be transported for large distances across the U.S. (Mikhailova et al., 2018). Dust deposition can be influenced by the loess extent. Therefore, loess distribution was incorporated into the maps based on previously mapped loess distribution using 0.1 × 0.1° gridded map layers derived from USGS (2016) maps (Lineback et al., 1983; Miller et al., 1988; Holbrook et al., 1990; Gray et al., 1991; Hallberg et al., 1991; Denne et al., 1993; Whitfield et al., 1993; Swinehart et al., 1994), and complied by Kohfeld and Harrison (2001).

RESULTS

Atmospheric K^+ deposition provides a substantial monetary value to the U.S. in the form of goods (e.g., K^+, etc.) and services

TABLE 1 | Conceptual overview of the annual atmospheric K^+ deposition accounting framework used in this study (adapted from Groshans et al., 2018b).

Biophysical accounts (science-based)	Administrative accounts (boundary-based)	Monetary accounts	Benefits	Total value
Soil extent	Administrative extent:	Ecosystem good(s) and service(s):	Sector:	Types of value:
		Separate constituent flow 1: Annual mean atmospheric wet K^+ deposition **Separate constituent flow 2:** Annual mean atmospheric dry K^+ deposition **Composite flow (sum of flows: wet + dry):** Annual mean atmospheric total K^+ deposition		
Not determined	– Country – State – Region	Goods: – K^+ Services: – Provisioning (e.g., food) – Commodity	Agriculture: – Fertilizer equivalent – Essential nutrient	Direct market valuation using replacement cost method based on market-based value of commodities: – Price of potassium-containing fertilizers (e.g., potassium chloride, KCl)

(e.g., provisioning, etc.) for agricultural benefit (e.g., fertilizing, etc.) and therefore can be evaluated using commodity prices for potassium chloride (KCl) (**Table 2**). The total provisioning ecosystem value of atmospheric potassium deposition was \$406M (i.e., 406 million U.S. dollars) (\$179M wet + \$227M dry) per year based on a 5-year moving average of \$500 per metric ton of potassium chloride (KCl) in the U.S. The value of average annual K^+ deposition varies across the country at the state and region scales based on data from time period of 2000–2015.

The highest ranked states for total value of wet K^+ deposition per year were: (1) Texas (\$18.2M), (2) Arkansas (\$7.83M), and (3) Louisiana (\$7.42M) (**Table 2**, **Figure 3A**). Area-normalized total mean annual values of wet K^+ deposition varied by state from a low of \$0.06 ha^{-1} (Nevada) up to 0.63 ha^{-1} (Louisiana) (**Table 2**, **Figure 3A**). The highest ranked regions for total value of wet K^+ deposition were: (1) Southeast (\$43.7M), (2) South Central (\$40.1M), and (3) Midwest (\$30.6M) (**Table 2**, **Figure 4A**). Area-normalized total mean annual values of wet K^+ deposition varied by region from a low of \$0.11 ha^{-1} (West) up to 0.41 ha^{-1} (Southeast) (**Table 2**, **Figure 4A**).

The highest ranked states for total value of dry K^+ deposition were: (1) Texas (\$26.1M), (2) California (\$14.0M), and (3) New Mexico (\$10.5M) (**Table 3**, **Figure 3B**). Area-normalized total mean annual values of dry K^+ deposition varied by state from a low of \$0.14 ha^{-1} (South Dakota) up to 0.54 ha^{-1} (West Virginia) (**Table 3**, **Figure 3B**). The highest ranked regions for total value of dry K^+ deposition were: (1) West (\$63.2M), (2) South Central (\$40.3M), and (3) Southeast (\$36.5M) (**Table 3**, **Figure 4B**). Area-normalized total mean annual values of dry K^+ deposition varied by region from a low of \$0.20 ha^{-1} (Northern Plains) up to 0.41 ha^{-1} (East) (**Table 3**, **Figure 4B**).

The highest ranked states for total value of total K^+ deposition were: (1) Texas (\$44.3M), (2) California (\$18.3M), and (3) New Mexico (\$13.5M) (**Table 4**, **Figure 3C**). Area-normalized total mean annual values of total K^+ deposition varied by state from a low of \$0.29 ha^{-1} (North Dakota) up to 0.95 ha^{-1} (Arkansas) (**Table 4**, **Figure 3C**). The highest ranked regions for total value of total K^+ deposition were: (1) West (\$86.5M), (2) South Central (\$80.4M), and (3) Southeast (\$80.2M) (**Table 4**, **Figure 4C**). Area-normalized total mean annual values of total K^+ deposition varied by region from a low of \$0.36 ha^{-1} (Northern Plains) up to 0.75 ha^{-1} (Southeast) (**Table 4**, **Figure 4C**).

DISCUSSION

Losses of potassium from the soil, particularly from highly leached and weathered soils, is a major problem causing soil degradation and threatening sustainable agriculture and development. Although several studies have attempted to conduct potassium audits at various scales, these audits lack monetary evaluation and rarely include the atmospheric K^+ contribution (Sheldrick et al., 2002). An important distinction related to the potential impact of potassium deposition is if agricultural productivity increases with potassium additions which depends on the soil type and existing potassium stocks. Areas where deposition may have more significant impact are indicated by states where a higher percentage of soil samples require potassium additions to avoid profit loss (**Figure 5**). Deposition of potassium from the atmospheric to land surfaces can be a source of K^+ to soils as well, for example, potassium in the rain across the U.S. tends to have relatively small and uniform concentrations (0.1–0.2 mg/l) over the whole country (Junge and Werby, 1958). Potassium from marine sources accounts for about 10% of K^+ in the U.S. continental rain (Berner and Berner, 1996). Non-marine sources of K^+ vary from area to area and include: dissolution of soil dust, potassium-containing fertilizers, pollen and seeds, biogenic and anthropogenic aerosols, and burning (e.g., forest, grasslands, etc.) (Berner and Berner, 1996). It is interesting to note that some states which have relatively high deposition rates of K^+ (**Figure 2**) also have high crop needs for K^+ fertilization (**Figure 5**); these states tend to be in the Southeast U.S. with Ultisols being the dominant soil order. Ultisols are highly weathered and leached soils, with low ability to retain nutrients in the soil matrix that are enriched in kaolinitic clays. Das et al. (2019) also reported a high need for K^+ fertilization in cultivated kaolinitic red soils in eastern India.

The fact that atmospheric K^+ deposition is not accounted for in the market can result in externalities leading to the inefficient use of soil resources, human-derived fertilizers, and

TABLE 2 | Total value (rankings) and area-averaged value (rankings) of annual atmospheric wet K^+ deposition for each state (region) for the 16-year period 2000–2015 based on a moving 5-year average price of U.S. $500 per metric ton of potassium chloride (KCl) (Yager, 2016).

State (Region)	Area (ha)		Mean wet K^+ deposition (kg ha^{-1})		Mean value ($ ha^{-1}) based on average price of KCl		Total value ($) based on average price of KCl	
Connecticut	1.28E+06	(46)	0.36	(16)	0.34	(16)	4.41E+05	(46)
Delaware	5.24E+05	(47)	0.37	(13)	0.35	(13)	1.85E+05	(47)
Massachusetts	2.08E+06	(44)	0.29	(23)	0.28	(23)	5.75E+05	(43)
Maryland	2.48E+06	(42)	0.32	(19)	0.31	(19)	7.57E+05	(41)
Maine	8.26E+06	(38)	0.21	(34)	0.20	(34)	1.65E+06	(39)
New Hampshire	2.38E+06	(43)	0.22	(30)	0.21	(30)	5.00E+05	(45)
New Jersey	1.93E+06	(45)	0.39	(9)	0.37	(9)	7.17E+05	(42)
New York	1.25E+07	(29)	0.23	(28)	0.22	(28)	2.75E+06	(31)
Pennsylvania	1.17E+07	(32)	0.30	(21)	0.29	(21)	3.36E+06	(21)
Rhode Island	2.61E+05	(48)	0.28	(24)	0.27	(24)	6.96E+04	(48)
Vermont	2.49E+06	(41)	0.22	(31)	0.21	(31)	5.21E+05	(44)
West Virginia	6.28E+06	(40)	0.38	(10)	0.36	(10)	2.28E+06	(37)
(East)	**5.22E+07**	**(6)**	**0.28**	**(3)**	**0.26**	**(3)**	**1.38E+07**	**(6)**
Iowa	1.46E+07	(22)	0.32	(20)	0.31	(20)	4.44E+06	(13)
Illinois	1.46E+07	(23)	0.28	(25)	0.27	(25)	3.89E+06	(18)
Indiana	9.43E+06	(37)	0.30	(22)	0.29	(22)	2.70E+06	(32)
Michigan	1.50E+07	(21)	0.18	(36)	0.17	(36)	2.57E+06	(34)
Minnesota	2.18E+07	(11)	0.22	(32)	0.21	(32)	4.58E+06	(12)
Missouri	1.81E+07	(17)	0.37	(14)	0.35	(14)	6.38E+06	(7)
Ohio	1.07E+07	(34)	0.28	(26)	0.27	(26)	2.85E+06	(30)
Wisconsin	1.45E+07	(24)	0.23	(29)	0.22	(29)	3.18E+06	(27)
(Midwest)	**1.19E+08**	**(3)**	**0.28**	**(4)**	**0.26**	**(4)**	**3.06E+07**	**(3)**
Arkansas	1.37E+07	(26)	0.60	(2)	0.57	(2)	7.83E+06	(2)
Louisiana	1.18E+07	(31)	0.66	(1)	0.63	(1)	7.42E+06	(3)
Oklahoma	1.81E+07	(18)	0.38	(11)	0.36	(11)	6.57E+06	(5)
Texas	6.83E+07	(1)	0.28	(27)	0.27	(27)	1.82E+07	(1)
(South Central)	**1.12E+08**	**(4)**	**0.38**	**(2)**	**0.36**	**(2)**	**4.01E+07**	**(2)**
Alabama	1.34E+07	(27)	0.47	(5)	0.45	(5)	5.99E+06	(8)
Florida	1.43E+07	(25)	0.48	(4)	0.46	(4)	6.54E+06	(6)
Georgia	1.52E+07	(20)	0.41	(8)	0.39	(8)	5.93E+06	(9)
Kentucky	1.04E+07	(35)	0.33	(17)	0.31	(17)	3.29E+06	(24)
Mississippi	1.23E+07	(30)	0.49	(3)	0.47	(3)	5.76E+06	(10)
North Carolina	1.26E+07	(28)	0.45	(6)	0.43	(6)	5.41E+06	(11)
South Carolina	7.96E+06	(39)	0.42	(7)	0.40	(7)	3.19E+06	(26)
Tennessee	1.09E+07	(33)	0.38	(12)	0.36	(12)	3.95E+06	(17)
Virginia	1.03E+07	(36)	0.37	(15)	0.35	(15)	3.62E+06	(20)
(Southeast)	**1.07E+08**	**(5)**	**0.43**	**(1)**	**0.41**	**(1)**	**4.37E+07**	**(1)**
Colorado	2.70E+07	(7)	0.15	(38)	0.14	(38)	3.86E+06	(19)
Kansas	2.13E+07	(13)	0.33	(18)	0.31	(18)	6.70E+06	(4)
Montana	3.81E+07	(3)	0.12	(42)	0.11	(42)	4.36E+06	(14)
North Dakota	2.00E+07	(14)	0.14	(40)	0.13	(40)	2.67E+06	(33)
Nebraska	2.00E+07	(15)	0.22	(33)	0.21	(33)	4.20E+06	(16)
South Dakota	2.00E+07	(16)	0.17	(37)	0.16	(37)	3.24E+06	(25)
Wyoming	2.53E+07	(8)	0.10	(44)	0.10	(44)	2.42E+06	(36)
(Northern Plains)	**1.72E+08**	**(2)**	**0.17**	**(5)**	**0.16**	**(5)**	**2.74E+07**	**(4)**
Arizona	2.94E+07	(5)	0.09	(47)	0.09	(47)	2.53E+06	(35)
California	4.08E+07	(2)	0.11	(43)	0.10	(43)	4.27E+06	(15)
Idaho	2.16E+07	(12)	0.15	(39)	0.14	(39)	3.09E+06	(28)
New Mexico	3.15E+07	(4)	0.10	(45)	0.10	(45)	3.01E+06	(29)
Nevada	2.87E+07	(6)	0.06	(48)	0.06	(48)	1.64E+06	(40)
Oregon	2.51E+07	(9)	0.14	(41)	0.13	(41)	3.35E+06	(22)
Utah	2.20E+07	(10)	0.10	(46)	0.10	(46)	2.10E+06	(38)
Washington	1.74E+07	(19)	0.20	(35)	0.19	(35)	3.31E+06	(23)
(West)	**2.16E+08**	**(1)**	**0.11**	**(6)**	**0.11**	**(6)**	**2.33E+07**	**(5)**
Totals or averages	**7.78E+08**		**0.24**		**0.23**		**1.79E+08**	

Bold type indicates regions consisting of the states listed immediately above.

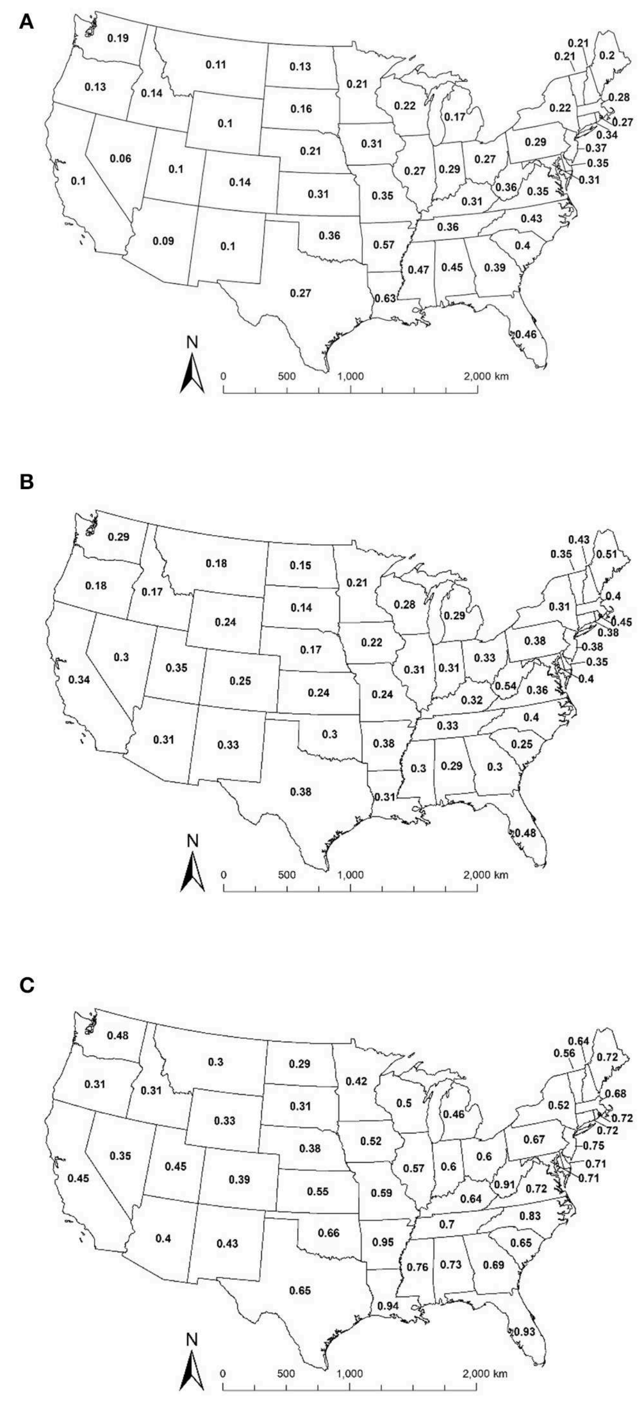

FIGURE 3 | Area-normalized value of annual K^+ deposition ($/ha) for different states in the contiguous United States based on a moving 5-year average price of U.S. $500 per metric ton of potassium chloride (KCl) (Yager, 2016): **(A)** wet, **(B)** dry, and **(C)** total.

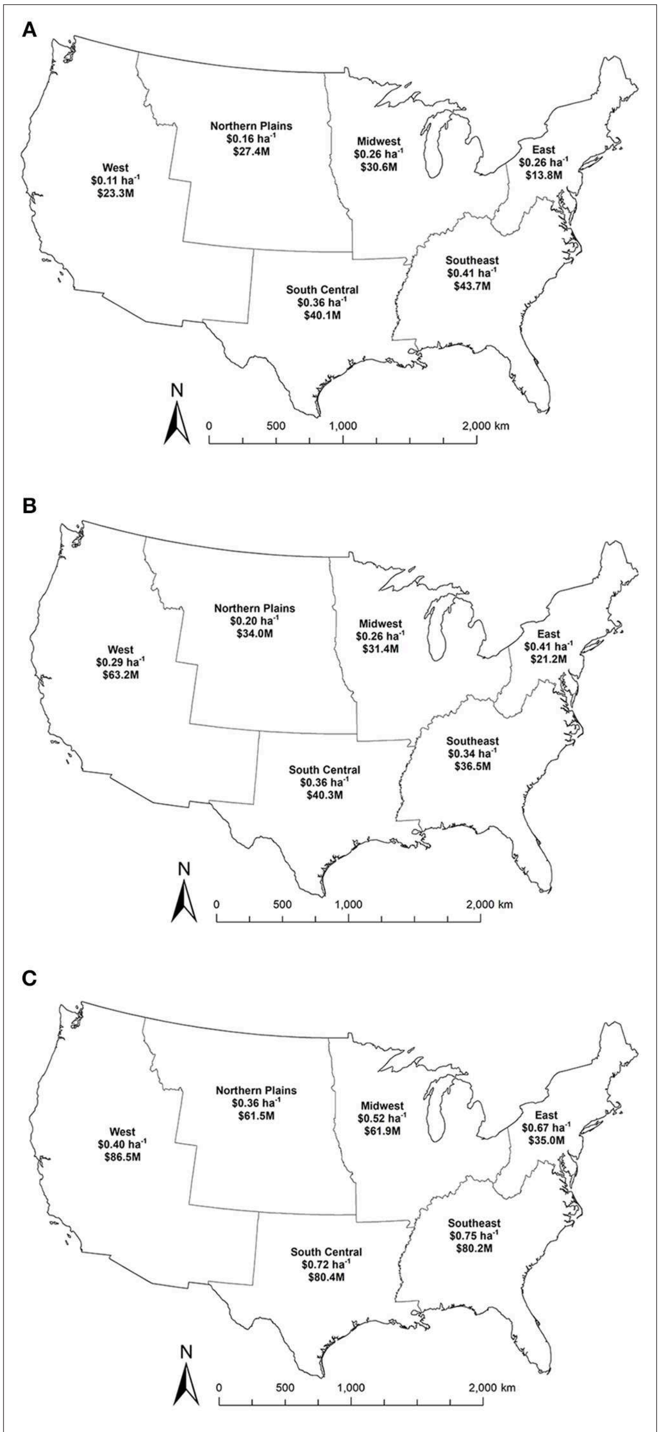

FIGURE 4 | Area-normalized value of annual K^+ deposition ($/ha, top number), and value of total storage ($, bottom number) and for different regions in the contiguous United States based on a moving 5-year average price of U.S. $500 per metric ton of potassium chloride (KCl) (Yager, 2016): **(A)** wet, **(B)** dry, and **(C)** total.

decision-making about agricultural production (Groshans et al., 2018a,b). This study quantified and mapped contribution of atmospheric K deposition to soil provisioning ecosystem, services in the contiguous United States based on fertilizer replacement costs. The replacement cost method is best used in cases such as this, where it is employed to establish the economic value of a single, rather than multiple, ecosystem services (Sundberg, 2004).

TABLE 3 | Total value (rankings) and area-averaged value (rankings) of annual atmospheric dry K^+ deposition for each state (region) for the 16-year period 2000–2015 based on a moving 5-year average price of U.S. $500 per metric ton of potassium chloride (KCl) (Yager, 2016).

State (Region)	Area (ha)		Mean dry K^+ deposition (kg ha^{-1})		Mean value ($ ha^{-1}) based on average price of KCl		Total value ($) based on average price of KCl	
Connecticut	1.28E+06	(46)	0.40	(9)	0.38	(9)	4.90E+05	(46)
Delaware	5.24E+05	(47)	0.37	(15)	0.35	(15)	1.85E+05	(47)
Massachusetts	2.08E+06	(44)	0.42	(6)	0.40	(6)	8.33E+05	(44)
Maryland	2.48E+06	(42)	0.42	(7)	0.40	(7)	9.94E+05	(42)
Maine	8.26E+06	(38)	0.54	(2)	0.51	(2)	4.25E+06	(23)
New Hampshire	2.38E+06	(43)	0.45	(5)	0.43	(5)	1.02E+06	(41)
New Jersey	1.93E+06	(45)	0.40	(10)	0.38	(10)	7.35E+05	(45)
New York	1.25E+07	(29)	0.32	(26)	0.31	(26)	3.82E+06	(26)
Pennsylvania	1.17E+07	(32)	0.40	(11)	0.38	(11)	4.48E+06	(19)
Rhode Island	2.61E+05	(48)	0.47	(4)	0.45	(4)	1.17E+05	(48)
Vermont	2.49E+06	(41)	0.37	(16)	0.35	(16)	8.77E+05	(43)
West Virginia	6.28E+06	(40)	0.57	(1)	0.54	(1)	3.41E+06	(34)
(East)	**5.22E+07**	**(6)**	**0.43**	**(1)**	**0.41**	**(1)**	**2.12E+07**	**(6)**
Iowa	1.46E+07	(22)	0.23	(41)	0.22	(41)	3.19E+06	(36)
Illinois	1.46E+07	(23)	0.32	(27)	0.31	(27)	4.45E+06	(20)
Indiana	9.43E+06	(37)	0.33	(23)	0.31	(23)	2.97E+06	(38)
Michigan	1.50E+07	(21)	0.30	(32)	0.29	(32)	4.29E+06	(22)
Minnesota	2.18E+07	(11)	0.22	(42)	0.21	(42)	4.58E+06	(16)
Missouri	1.81E+07	(17)	0.25	(38)	0.24	(38)	4.31E+06	(21)
Ohio	1.07E+07	(34)	0.35	(19)	0.33	(19)	3.56E+06	(32)
Wisconsin	1.45E+07	(24)	0.29	(35)	0.28	(35)	4.01E+06	(24)
(Midwest)	**1.19E+08**	**(3)**	**0.28**	**(5)**	**0.26**	**(5)**	**3.14E+07**	**(5)**
Arkansas	1.37E+07	(26)	0.40	(12)	0.38	(12)	5.22E+06	(12)
Louisiana	1.18E+07	(31)	0.33	(24)	0.31	(24)	3.71E+06	(28)
Oklahoma	1.81E+07	(18)	0.31	(28)	0.30	(28)	5.36E+06	(11)
Texas	6.83E+07	(1)	0.40	(13)	0.38	(13)	2.61E+07	(1)
(South Central)	**1.12E+08**	**(4)**	**0.38**	**(2)**	**0.36**	**(2)**	**4.03E+07**	**(2)**
Alabama	1.34E+07	(27)	0.30	(33)	0.29	(33)	3.83E+06	(25)
Florida	1.43E+07	(25)	0.50	(3)	0.48	(3)	6.82E+06	(8)
Georgia	1.52E+07	(20)	0.31	(29)	0.30	(29)	4.48E+06	(18)
Kentucky	1.04E+07	(35)	0.34	(22)	0.32	(22)	3.38E+06	(35)
Mississippi	1.23E+07	(30)	0.31	(30)	0.30	(30)	3.64E+06	(30)
North Carolina	1.26E+07	(28)	0.42	(8)	0.40	(8)	5.05E+06	(14)
South Carolina	7.96E+06	(39)	0.26	(36)	0.25	(36)	1.97E+06	(40)
Tennessee	1.09E+07	(33)	0.35	(20)	0.33	(20)	3.64E+06	(31)
Virginia	1.03E+07	(36)	0.38	(14)	0.36	(14)	3.72E+06	(27)
(Southeast)	**1.07E+08**	**(5)**	**0.36**	**(3)**	**0.34**	**(3)**	**3.65E+07**	**(3)**
Colorado	2.70E+07	(7)	0.26	(37)	0.25	(37)	6.68E+06	(9)
Kansas	2.13E+07	(13)	0.25	(39)	0.24	(39)	5.08E+06	(13)
Montana	3.81E+07	(3)	0.19	(43)	0.18	(43)	6.90E+06	(7)
North Dakota	2.00E+07	(14)	0.16	(47)	0.15	(47)	3.05E+06	(37)
Nebraska	2.00E+07	(15)	0.18	(45)	0.17	(45)	3.44E+06	(33)
South Dakota	2.00E+07	(16)	0.15	(48)	0.14	(48)	2.86E+06	(39)
Wyoming	2.53E+07	(8)	0.25	(40)	0.24	(40)	6.04E+06	(10)
(Northern Plains)	**1.72E+08**	**(2)**	**0.21**	**(6)**	**0.20**	**(6)**	**3.40E+07**	**(4)**
Arizona	2.94E+07	(5)	0.33	(25)	0.31	(25)	9.26E+06	(4)
California	4.08E+07	(2)	0.36	(18)	0.34	(18)	1.40E+07	(2)
Idaho	2.16E+07	(12)	0.18	(46)	0.17	(46)	3.70E+06	(29)
New Mexico	3.15E+07	(4)	0.35	(21)	0.33	(21)	1.05E+07	(3)
Nevada	2.87E+07	(6)	0.31	(31)	0.30	(31)	8.47E+06	(5)
Oregon	2.51E+07	(9)	0.19	(44)	0.18	(44)	4.55E+06	(17)
Utah	2.20E+07	(10)	0.37	(17)	0.35	(17)	7.75E+06	(6)
Washington	1.74E+07	(19)	0.30	(34)	0.29	(34)	4.96E+06	(15)
(West)	**2.16E+08**	**(1)**	**0.31**	**(4)**	**0.29**	**(4)**	**6.32E+07**	**(1)**
Totals or averages	**7.78E+08**		**0.31**		**0.29**		**2.27E+08**	

Bold type indicates regions consisting of the states listed immediately above.

TABLE 4 | Total value (rankings) and area-averaged value (rankings) of annual atmospheric total K^+ deposition for each state (region) for the 16-year period 2000–2015 based on a moving 5-year average price of U.S. $500 per metric ton of potassium chloride (KCl) (Yager, 2016).

State (Region)	Area (ha)		Mean total K^+ deposition (kg ha^{-1})		Mean value ($ ha^{-1}) based on average price of KCl		Total value ($) based on average price of KCl	
Connecticut	1.28E+06	(46)	0.76	(9)	0.72	(9)	9.31E+05	(46)
Delaware	5.24E+05	(47)	0.74	(13)	0.71	(13)	3.70E+05	(47)
Massachusetts	2.08E+06	(44)	0.71	(17)	0.68	(17)	1.41E+06	(44)
Maryland	2.48E+06	(42)	0.74	(14)	0.71	(14)	1.75E+06	(41)
Maine	8.26E+06	(38)	0.75	(10)	0.72	(10)	5.91E+06	(36)
New Hampshire	2.38E+06	(43)	0.67	(22)	0.64	(22)	1.52E+06	(42)
New Jersey	1.93E+06	(45)	0.79	(7)	0.75	(7)	1.45E+06	(43)
New York	1.25E+07	(29)	0.55	(30)	0.52	(30)	6.57E+06	(33)
Pennsylvania	1.17E+07	(32)	0.70	(18)	0.67	(18)	7.84E+06	(24)
Rhode Island	2.61E+05	(48)	0.75	(11)	0.72	(11)	1.86E+05	(48)
Vermont	2.49E+06	(41)	0.59	(28)	0.56	(28)	1.40E+06	(45)
West Virginia	6.28E+06	(40)	0.95	(4)	0.91	(4)	5.69E+06	(38)
(East)	**5.22E+07**	**(6)**	**0.70**	**(3)**	**0.67**	**(3)**	**3.50E+07**	**(6)**
Iowa	1.46E+07	(22)	0.55	(31)	0.52	(31)	7.63E+06	(26)
Illinois	1.46E+07	(23)	0.60	(27)	0.57	(27)	8.34E+06	(21)
Indiana	9.43E+06	(37)	0.63	(24)	0.60	(24)	5.66E+06	(39)
Michigan	1.50E+07	(21)	0.48	(34)	0.46	(34)	6.86E+06	(30)
Minnesota	2.18E+07	(11)	0.44	(38)	0.42	(38)	9.16E+06	(19)
Missouri	1.81E+07	(17)	0.62	(26)	0.59	(26)	1.07E+07	(11)
Ohio	1.07E+07	(34)	0.63	(25)	0.60	(25)	6.41E+06	(34)
Wisconsin	1.45E+07	(24)	0.52	(32)	0.50	(32)	7.20E+06	(29)
(Midwest)	**1.19E+08**	**(3)**	**0.55**	**(4)**	**0.52**	**(4)**	**6.19E+07**	**(4)**
Arkansas	1.37E+07	(26)	1.00	(1)	0.95	(1)	1.31E+07	(5)
Louisiana	1.18E+07	(31)	0.99	(2)	0.94	(2)	1.11E+07	(10)
Oklahoma	1.81E+07	(18)	0.69	(19)	0.66	(19)	1.19E+07	(6)
Texas	6.83E+07	(1)	0.68	(20)	0.65	(20)	4.43E+07	(1)
(South Central)	**1.12E+08**	**(4)**	**0.75**	**(2)**	**0.72**	**(2)**	**8.04E+07**	**(2)**
Alabama	1.34E+07	(27)	0.77	(8)	0.73	(8)	9.82E+06	(17)
Florida	1.43E+07	(25)	0.98	(3)	0.93	(3)	1.34E+07	(4)
Georgia	1.52E+07	(20)	0.72	(16)	0.69	(16)	1.04E+07	(14)
Kentucky	1.04E+07	(35)	0.67	(23)	0.64	(23)	6.67E+06	(32)
Mississippi	1.23E+07	(30)	0.80	(6)	0.76	(6)	9.40E+06	(18)
North Carolina	1.26E+07	(28)	0.87	(5)	0.83	(5)	1.05E+07	(13)
South Carolina	7.96E+06	(39)	0.68	(21)	0.65	(21)	5.16E+06	(40)
Tennessee	1.09E+07	(33)	0.73	(15)	0.70	(15)	7.59E+06	(27)
Virginia	1.03E+07	(36)	0.75	(12)	0.72	(12)	7.34E+06	(28)
(Southeast)	**1.07E+08**	**(5)**	**0.78**	**(1)**	**0.75**	**(1)**	**8.02E+07**	**(3)**
Colorado	2.70E+07	(7)	0.41	(40)	0.39	(40)	1.05E+07	(12)
Kansas	2.13E+07	(13)	0.58	(29)	0.55	(29)	1.18E+07	(8)
Montana	3.81E+07	(3)	0.31	(47)	0.30	(47)	1.13E+07	(9)
North Dakota	2.00E+07	(14)	0.30	(48)	0.29	(48)	5.72E+06	(37)
Nebraska	2.00E+07	(15)	0.40	(41)	0.38	(41)	7.64E+06	(25)
South Dakota	2.00E+07	(16)	0.32	(46)	0.31	(46)	6.10E+06	(35)
Wyoming	2.53E+07	(8)	0.35	(43)	0.33	(43)	8.45E+06	(20)
(Northern Plains)	**1.72E+08**	**(2)**	**0.38**	**(6)**	**0.36**	**(6)**	**6.15E+07**	**(5)**
Arizona	2.94E+07	(5)	0.42	(39)	0.40	(39)	1.18E+07	(7)
California	4.08E+07	(2)	0.47	(35)	0.45	(35)	1.83E+07	(2)
Idaho	2.16E+07	(12)	0.33	(45)	0.31	(45)	6.79E+06	(31)
New Mexico	3.15E+07	(4)	0.45	(37)	0.43	(37)	1.35E+07	(3)
Nevada	2.87E+07	(6)	0.37	(42)	0.35	(42)	1.01E+07	(15)
Oregon	2.51E+07	(9)	0.33	(44)	0.31	(44)	7.91E+06	(23)
Utah	2.20E+07	(10)	0.47	(36)	0.45	(36)	9.85E+06	(16)
Washington	1.74E+07	(19)	0.50	(33)	0.48	(33)	8.27E+06	(22)
(West)	**2.16E+08**	**(1)**	**0.42**	**(5)**	**0.40**	**(5)**	**8.65E+07**	**(1)**
Totals or averages	**7.78E+08**		**0.55**		**0.52**		**4.06E+08**	

Bold type indicates regions consisting of the states listed immediately above.

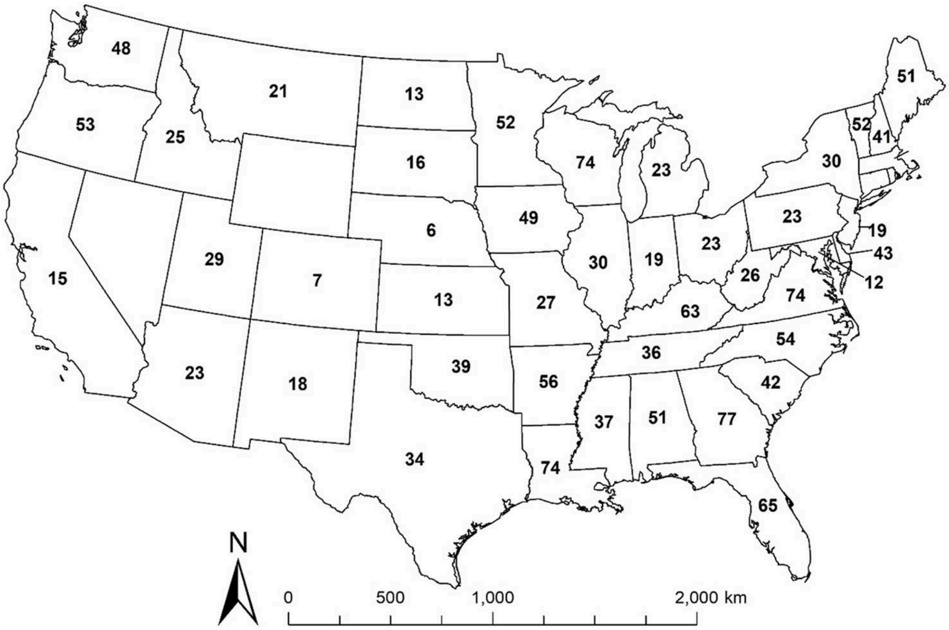

FIGURE 5 | Percent of soil samples, which need yearly K additions to prevent loss of profit for the majority of agricultural crops in 2005 for different states in the contiguous United States (modified from Fixen et al., 2007).

According to Heal (2000), there are pros and cons associated with the replacement cost approach. One of the advantages is that "it can work even if there is no marketed service for which the natural service contributed" (Heal, 2000). In other words, it allows one to estimate the monetary values of ecosystem services in an indirect way, even when ecological data are absent in the market. On the other hand, "replacements rarely replace all the services, so they capture only a part of the value" (Heal, 2000). Therefore, under some conditions, the replacement cost method may overestimate or underestimate the value of an ecosystem service (Pearce et al., 1996). It has also been argued that replacement cost "is not a proper estimate of the value unless the cost is incurred, however, if the supply were to start running out, then the market price would rise toward the replacement cost, which would become more relevant as an indicator of value" (Heal, 2000). Finally, the replacement cost method is based on the idealized assumption that the replacements used are perfect substitutes for ecosystem services and environmental goods. Such perfect substitutes, however, rarely exist (Edwards-Jones et al., 2000). Atmospheric K^+ deposition is an important source of potassium because it is currently considered to be a "free public good," which does not cost anything to produce, purchase, and distribute compared to commercial potassium fertilizers. It is not evenly distributed within the landscape and can fluctuate depending on the dynamic nature of the atmospheric deposition.

Failure to account for the value of atmospheric K^+ deposition in the market can result in externalities that lead to the inefficient use of soil resources and poor decision-making about agricultural production (Groshans et al., 2018a). There are two potential methods for assessing the economic value of environmental resources. The first of these, the preference-based method, measures value in terms of individuals' willingness to pay (WTP) for environmental resources or their willingness to accept (WTA) compensation if they were deprived of those resources. The higher the WTP or WTA, the more the resource is worth. The second method for assessing the value of ecosystem resources is the cost-based method. This typically employs the "replacement cost" method, which measures the value of ecosystem goods and services by determining how much it would cost to replace them if they were damaged.

Both methods have their own strengths and weaknesses. When market information about the ecosystem service in question is adequate, the preference-based system can be quite useful, since WTP or WTA can be measured directly, as individuals can easily express their WTP or WTA based on the available market information. Although such direct measurement of WTP and WTA is the most straightforward and accurate approach, it's not frequently used in the evaluation of environmental resources, as the market information is usually inadequate in such cases.

When market information is inadequate, however, WTP or WTA can still be indirectly measured by examining the demands for related goods in the market. The Hedonic Pricing Method (HPM) is the most popular used method for indirectly measuring WTP and WTA. This method works by comparing the market prices of two goods that differ only in their ecosystem characteristics and services (De Groot et al., 2002). A classic example of this method is a study conducted by Wilson and

Carpenter (1999) to determine the value of freshwater ecosystem services in the US. In their study, two properties were identified that were identical with the exception of the water quality for wetlands, rivers, streams, and lakes. The value of the water quality was determined by the difference in value between these two properties. While the HPM can be quite useful, the biggest challenge is to find two identical sites that differ only with respect to the particular ecosystem characteristic being studied. This is especially difficult when ecosystem services overlap and interact with each other, making it nearly impossible to isolate a single characteristic for study. Given these considerations, the preference-based method—whether direct or indirect—is not the appropriate approach for this study. This is because the market information regarding the atmospheric deposition of K^+ is lacking, thereby ruling out the possibility of direct measurement, while indirect measurement is also ruled out by the fact that it would be nearly impossible to find the sort of nearly identical sites, differing only in their atmospheric K^+ deposition, that would be necessary to conduct such a measurement. Thus, the cost-based approach is a more appropriate alternative for this study.

The replacement cost method is well-suited to cases such as this, where it will be employed to establish the economic value of a single ecosystem service, rather than several at once (Sundberg, 2004). According to Heal (2000), there are other pros and cons associated with the replacement cost approach. One of the advantages is that "it can work even if there is no marketed service for which the natural service contributed" (Heal, 2000). In other words, it allows one to estimate the monetary values of ecosystem services in an indirect way, even when ecological data are absent in the market, as is the case for the present study. On the other hand, "replacements rarely replace all the services, so they capture only a part of the value" (Heal, 2000). Thus, under some conditions, the replacement cost method may over- or underestimate the value of an ecosystem service (Pearce et al., 1996). It has also been argued that replacement cost "is not a proper estimate of the value unless the cost is incurred, however, if the supply were to start running out, then the market price would rise toward the replacement cost, which would become more relevant as an indicator of value" (Heal, 2000). Finally, the replacement cost method is based on the idealized assumption that the replacements used are perfect substitutes for ecosystem services and environmental goods. Such perfect substitutes, however, rarely exist (Edwards-Jones et al., 2000). Despite these drawbacks, however, the replacement cost method is still the most appropriate approach for the present study, as it at least makes possible the assessment of the economic value of atmospheric K^+ deposition, even if those evaluations are somewhat idealized.

CONCLUSIONS

Atmospheric deposition contains remarkable quantities of potassium (K^+), which can be considered a fertilizing material, but it has not been included in economic valuations of ecosystem services. These flows represent potential quantifiable ecosystem services provided by the atmosphere and deposited on land which provides important information across the contiguous United States for potassium audits on a more site-specific basis. Local audits could use the deposition information combined with soil and crop information to determine its realized value. NADP contains data on wet, dry, and total K^+ deposition within the contiguous U.S. The amount of this atmospheric K^+ fertilizing material varies by science-based biophysical accounts (e.g., soil order, parent material, climate etc.), and boundary-based administrative accounts (e.g., country, state, region etc.). This spatial distribution information could be linked to existing or future policy with regards to sustainable soil nutrient management. The fact that atmospheric K^+ deposition has positive value but zero market price results in the negative externality and the inefficient use of land. Estimating the replacement cost of atmospheric K^+ deposition is the crucial step to correcting the market failure. The results of this study provide market-based replacement costs of atmospheric K^+ deposition within the administrative boundaries. Future research on atmospheric K^+ deposition and ecosystems services should combine spatial and temporal variation in atmospheric replacement costs or other methods of valuation. Another important future research consideration is understanding supply and demand for atmospheric K^+ deposition in terms of ecosystem services to meet the SDGs.

AUTHOR CONTRIBUTIONS

EM: conceptualization. EM and MS: methodology. GP and MC: visualization. EM, GP, CP, MS, and LZ: writing—review and editing.

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Hydraulic Functions of Peat Soils and Ecosystem Service

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Keywords: hydraulic functions, ecosystem service, peat soils, available water capacity, preferential flow

Peatlands cover ~3% of the Earth's land area, but store ~30% of the global soil carbon (C), 10% of the global soil nitrogen (N), and 10% of global fresh water (Joosten and Clarke, 2002; Limpens et al., 2008). Drainage of peatlands induce aerobic conditions, which leads to carbon mineralization, peat degradation and concomitant emissions of carbon dioxide (CO_2) to the atmosphere. It is estimated that 15% of global peatlands have been drained and are currently being used for agriculture and forestry (Joosten and Clarke, 2002). The drained fraction can be as high as 95% (e.g., Northern Germany). Drainage leads to subsidence of peat deposits by 0.5–4 m (Wösten et al., 1997; Pronger et al., 2014), and oxidation of peat organic matter from 100 to 20 wt% (Rezanezhad et al., 2016; Liu and Lennartz, 2019), causing a loss in their water storage and water filter function. Little is known about the function of peat soils with respect to water quantity and quality (Baveye et al., 2016; Rabot et al., 2018; Vogel et al., 2018). We combine key properties such as available water capacity and hydraulic conductivity to classify peat soils with respect to their function in the water cycle. We, also, identify soil physical parameters in order to estimate the filter and buffer potential of peat soils. We established a rating scheme that takes soil degradation into account and classifies the water related ecosystem services provided by peat soils. The classification scheme shall be further developed and may serve as a decision support tool for peatland restoration projects.

SOIL STRUCTURE AND HYDRAULIC FUNCTIONS OF PEAT

Pristine peat is formed of decayed plants and characterized by a low density and high organic matter content (e.g., >90 wt%; **Figure 1**). The most extraordinary feature of pristine peat is its high porosity, which easily exceeds 90 vol% with a dominance of macropores (>50 μm; **Figure 2A**). These macropores facilitate water movement and solute transport (Quinton et al., 2009; Rezanezhad et al., 2016). Therefore, greater saturated hydraulic conductivity values (K_s) are observed in pristine peat than in degraded peat (**Figure 2B**). Drainage of peatland accelerates carbon mineralization, resulting in a higher bulk density and a lower porosity. Here, we propose bulk density as a proxy for peat degradation (Liu and Lennartz, 2019). The relationship between physical properties and peat degradation has been studied (Boelter, 1969; Schindler et al., 2003). Macropores in low to moderately degraded peat soils (e.g., bulk density <0.2 g cm^{-3}) are formed by the undecomposed parent plant material, which functions as a channel/pipe system (**Figure 1**). With increasing bulk density from 0.2 to 1.0 g cm^{-3}, macroporosity remains constant because of the formation of secondary macropores (e.g., root channels; **Figure 1**; Liu and Lennartz, 2015).

A strong negative linear relationship was observed between total porosity and bulk density ($R^2 = 0.82$, $p < 0.001$; **Figure 2A**). In contrast, a power-law relationship was detected between macroporosity (>50 μm) and bulk density (**Figure 2A**). With an increase in bulk density, from 0.01 to 0.2 g cm^{-3}, K_s decreased dramatically (**Figure 2B**), because macroporosity is markedly reduced with peatland degradation. A negative linear relationship was observed between $\log_{10}K_s$ and bulk density. With increasing bulk density, from 0.20 to 1.0 g cm^{-3}, K_s almost remains constant with a large variance (Liu and Lennartz, 2019).

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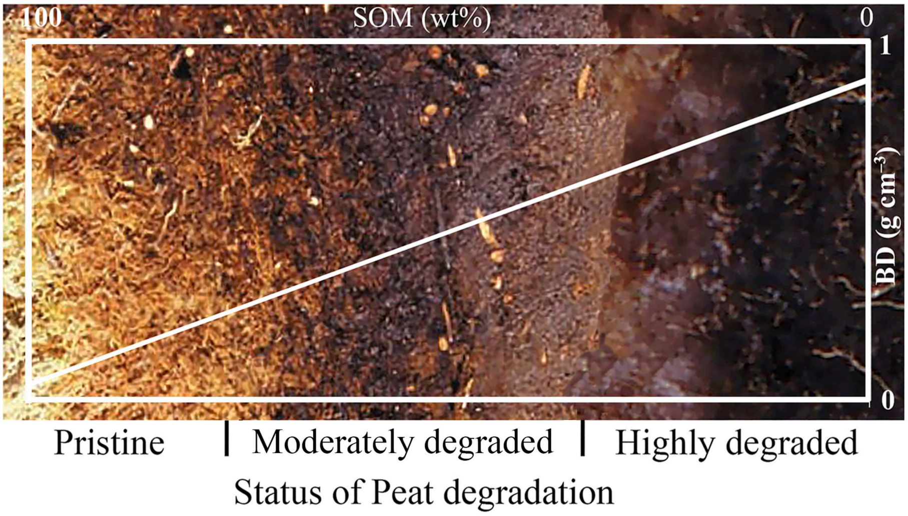

FIGURE 1 | Morphological structure of peat soils at various degradation stages (pristine, moderately degraded, and highly degraded). SOM, soil organic matter; BD, bulk density.

CLASSIFICATION OF PEAT SOIL HYDRAULIC FUNCTION

We categorized degraded peat soils according to their function in the water cycle. We created five classes of peat soils from pristine (P) to extremely degraded (E). This classification scheme is not based on an expert system (e.g., von Post degradation scheme; Von Post, 1922) but on independently measured bulk density, which assures easy applicability and—more importantly—comparability with different studies.

We suggest a combination of saturated hydraulic conductivity (K_s) with available water capacity as core parameters of soil-water-interactions to characterize a given site in a hydrological sense (**Table 1**). The available water capacity (AWC) is defined as the volumetric soil water content between matrix potentials at −60 and −15 000 hPa (Schwärzel et al., 2002). It has to be noted that the AWC for peat soils (0.1–0.7 cm^3 cm^{-3}) has a broader range than that for mineral soils (0.1 to 0.3 cm^3 cm^{-3}; Merdum, 2010). Pristine peat has a low AWC (0.05 to 0.3 cm^3 cm^{-3}). However, *water storage*, defined as the total water content in length units ($W = \theta^*z$, with θ = volumetric soil water content and z = considered soil depth) at the actual ground water table, is nonetheless high because the ground water table in pristine peat is always near the surface. In this situation, macroporosity is included as a part of storage capacity. Soil subsidence and the associated loss of water storage is not reflected in the AWC. We employed the AWC because it is the most commonly and readily available parameter in soil science, even though it does not correctly depict water storage. Also, the definition of *water storage capacity* depends on various assumptions (e.g., soil volume change by shrinkage and subsidence; Price, 2003), which adds uncertainty to any classification scheme.

Interpretation of the classification scheme must consider current and future management of peatland sites. For instance, if a site is to be rewetted as a restoration measure, minimum requirements of water conductance need to be fulfilled. Difficulty may arise when managing the groundwater table in highly degraded peat soils because of the low hydraulic conductivity.

In cases where water is supplied through storm surges and flooding, as in coastal wetlands, highly degraded peat horizons at the soil surface may hinder water infiltration, causing the formation of shallow lakes. This would mean a system-shift from a (degraded) peatland to a lake ecosystem with severe consequences to bio-geochemical cycling and the biota (Jurasinski et al., 2018). In this context, the derived scheme (**Table 1**) may help create an appropriate management strategy.

Table 1 indicates that the AWC of pristine and minor degraded peat soils spans a wide range of values (Liu and Lennartz, 2019). High K_s values are only found for pristine and minor degraded peat soils. The high variance in AWC values for pristine and minor degraded peat reflects the presence of a significant fraction of macropores, which easily exceeds 50% of the total porosity. Small changes in pore structure and/or the method of AWC determination may lead to higher or lower values of AWC. Even highly degraded peat soils might have AWC values exceeding 0.5 cm^3 cm^{-3}, which makes them an important component in overall landscape water storage. If the degradation is severe and the bulk densities are >0.4 g cm^{-3}, AWC decreases, resulting in a loss of ecosystem service.

Soil function is categorized into three classes (**Table 1**). Green indicates that the peatland provides maximum ecosystem services in terms of water holding capacity and conductance. Such circumstances are found in pristine, minor degraded and moderately degraded peat soils only. Peat soils having K_s values below 1 or even below 0.01 cm h^{-1} are limited in the service they can provide because they function as a hydraulic barrier, which hampers restoration efforts. Gabriel et al. (2018) created an evaluation scheme that classifies the hydraulic properties of

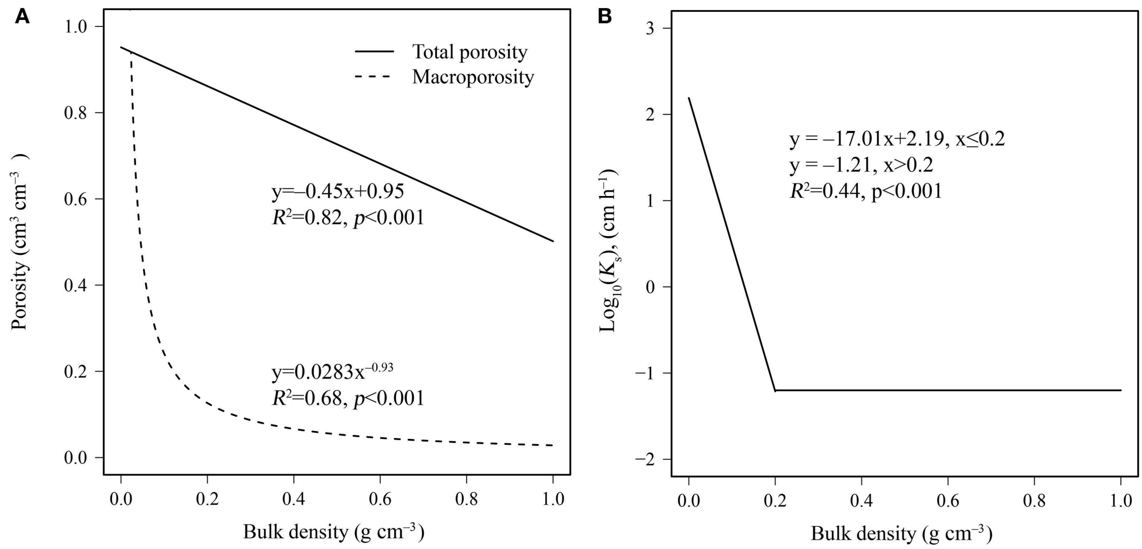

FIGURE 2 | Pore structure (total porosity and macroporosity; **A**) and saturated hydraulic conductivity (K_S; **B**) of peat soils along a bulk density gradient. Data source from Liu and Lennartz (2019).

TABLE 1 | Hydrological classification of degraded peat soils based on saturated hydraulic conductivity (K_S) and available water capacity (AWC, cm^3 cm^{-3}).

K_S \ AWC	0–0.1	0.1–0.3	0.3–0.5	>0.5
>100 cm h^{-1}	P	P	Mi	Mi
1–100 cm h^{-1}		Mi	Mi, M	M
0.01–1 cm h^{-1}		M, E	M, H, E	M, H
<0.01 cm h^{-1}			H	H

Value combinations marked in green, yellow, and red provide a high, moderate, and low ecosystem service, respectively. Data source from Liu and Lennartz (2019). P, pristine peat, BD ≤ 0.05 g cm^{-3}; Mi, minor degradation, 0.05 < BD ≤ 0.10 g cm^{-3}; M, moderate degradation, 0.10 < BD ≤ 0.20 g cm^{-3}; high degradation, 0.20 < BD ≤ 0.40 g cm^{-3}; E, extreme degradation, BD > 0.4 g cm^{-3}.

various peat soils. The classification scheme provided in this study differs from the aforementioned in the way hydraulic properties are combined and the way peat degradation is explicitly addressed.

SOLUTE TRANSPORT AND THE RISK FOR PREFERENTIAL FLOW

The filter and buffer functions of soil are of prime importance in the estimation of ecosystem services. Peatlands play a crucial role in this because they are frequently located in ecosystem transition zones connecting mineral soils with aquatic ecosystems. For instance, in lowland catchment areas, fen peat is often formed along rivers (riparian fen). Surface and groundwater movement between land and water could pass through a fen. In agricultural settings, where mineral soils are intensively used, and fertilizers and pesticides are massively applied, the filter and buffer function of a riparian fen is the sole element protecting water quality. However, depending on the history of the peat (e.g., agricultural usage) and current water management, riparian fens may also act as a source, especially for nutrients such as phosphorus (Zak and Gelbrecht, 2007). Coastal wetlands are another example of transition ecosystems that contain peat soils. Coastal peatlands are found, for instance, along the southern Baltic Sea coast where they form unique habitats (Kreuzburg et al., 2018). Rising sea levels and a sinking coast may increase the frequency of flooding of coastal areas. In cases where dunes and dykes are removed for restoration purposes, coastal peatlands might get frequently flooded with seawater. In such situations, the role of peat soil is two-fold. Seawater might carry pollutants such as micro-plastics, which get filtered out in the peatland. Additionally, peat soils are a source of nutrients and complex organic molecules, which might reach coastal waters either with the retreating seawater or with submarine groundwater fluxes originating from the wetland. In either case, sink or source, physical peat properties will determine the extent of exchange and solute transport.

In peat soils, filter and buffer functions will depend on state variables such as hydraulic head and properties, which determine how homogeneously the soil matrix is penetrated by any given compound. It is well-known that solute transport, including preferential transport, in soils is non-equilibrated (Flury et al., 1994; Jarvis, 2007; Vogel et al., 2010). In such cases, a solute bypasses the soil matrix and retention mechanisms are non-operational. Early arrival of high concentrations of hazardous substances in ground and surface waters is a clear indication of non-equilibrium transport (Heathwaite and Dils, 2000; Jørgensen et al., 2002).

Several studies have suggested that a variety of parameters will help quantify non-equilibrium in solute transport (Lennartz et al., 1997; Kamra and Lennartz, 2005; Koestel et al., 2011). Here we suggest the mobility index (MI) as a parameter to

TABLE 2 | Classification scheme for the "filter and buffer function" of peat soils as based on the macro-porosity and mobility index (MI).

Macroporosity \ MI	>1.2	0.8–1.2	0.3–0.8	<0.3
>25 vol%	Mi			
10–25 vol%	M	M	M	
5–10 vol%	M	M, H	M,H	
<5 vol%			E	E

Value combinations marked in green, yellow, and red are considered to provide a high, moderate, and low buffer function, respectively. The mobility index may serve as an indicator for preferential flow and the risk of fast solute transport (Liu et al., 2017); the lower the value the higher the risk of fast solute transport. MI will depend on the tracer; an ionic tracer, such as bromide, might behave differently in organic rich soils than, for instance, tritium. Data source from Liu et al. (2017). P, pristine peat, BD ≤ 0.05 g cm^{-3}; Mi, minor degradation, 0.05 < BD ≤ 0.10 g cm^{-3}; M, moderate degradation, 0.10 < BD ≤ 0.20 g cm^{-3}; high degradation, 0.20 < BD ≤ 0.40 g cm^{-3}; E, extreme degradation, BD > 0.4 g cm^{-3}.

characterize the extent of preferential flow in soils. The MI is the ratio of measured pore water velocity (v_{measure}) to fitted pore water velocity (v_{fit}) as obtained from a model (Lennartz et al., 1997; Liu et al., 2017). It should be noted that the solute transport database for peat soils is very limited. Only recently a few studies provided solute transport data, which classified peat soils with respect to solute transport (e.g., Liu et al., 2017). Our results have to be considered in the light of data scarcity.

The macro-pores of undegraded peat soil are part of the primary pore space formed by plant residues and form a highly connected space. The macro-porosity of peat soil differs from those of mineral soils because macro-pores in mineral soils belong to the secondary pore space originating from biological activity (worm burrows, plant roots) and formation of soil peds (aggregation). In mineral soil, the macro-pores are often less connected to the rest of the pore space than in pristine peat soil. In landscapes with pristine peat soil and water tables that are close to the soil surface, macro-porosity is also an indicator of connectivity. It can be expected that macro-porous peat soil (macroporosity >50 vol%) is well-connected to adjacent ecosystems (e.g., mineral soils), because a high saturated hydraulic conductivity ensures (horizontal) water exchange between ecosystem compartments.

We combined macro-porosity with the mobility index, as derived from leaching studies employing conservative tracers [**Table 2**; data source from Liu et al. (2017)]. This combination is used to assess the potential filter and buffer functions provided by a soil (e.g., ecosystem services). For peat soils, conservative tracers such as bromide, are retarded resulting in MI values > 1 (Boudreau et al., 2009; Liu et al., 2017). No solute transport data is available for pristine peat, which could be related to experimental difficulties in handling pristine peat samples with a porosity above 90 vol%.

In accordance with the scheme for water storage and conductance (**Table 1**) we developed a system that ranks a peat soil's ability to filter and buffer dissolved compounds. From **Table 2**, it is evident that extremely degraded peat soils possess a high risk of preferential transport. The risk that these extremely degraded soils are penetrated by compounds from the (permeable) adjacent mineral soils is, however, low because they are not well-connected. A risk for preferential flow might be relevant if a site is to be rewetted. Peat soil may become a source of various compounds. Ground and surface water may become contaminated because mobilized substances are transported along preferential pathways (e.g., DOC, phosphorus etc.). Our classification may help in determining remediation measures; however, the scheme is in the discussion phase and the database needs to be expanded. The suggested approach creates new pathways for creating classification schemes for peat soils.

AUTHOR CONTRIBUTIONS

HL and BL conceived the study. HL collected data and performed statistical analyses. BL prepared the manuscript.

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How Land Cover Spatial Resolution Affects Mapping of Urban Ecosystem Service Flows

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In urban areas, estimating the effect of land cover (LC) data spatial resolution on ecosystem services (ES) mapping remains a challenge. In particular, mapping spatial flows of ES, from greenspaces to beneficiaries, may be more sensitive to LC data resolution than mapping potential supply or demand separately. Our objectives were to compare the sensitivity of global- and local-flow ES maps to LC data resolution, and to assess the effect of LC data resolution within different types of urban land uses. A case study was conducted in the city of Laval, Canada. Carbon storage (a global-flow ES), urban cooling and pollination (two local-flow ES) were mapped using LC data aggregated from 1 to 15 m. Results were analyzed for districts (comprising various types of urban land uses), and for 480 × 480 m residential and commercial zones. Greenspace cover was generally underestimated at coarser spatial resolutions; as a result, so were ES potential supply and flow. For urban cooling and pollination, the effect of LC data spatial resolution on ES flow also depended on changes in the spatial configuration of ES potential supply relative to ES demand. The magnitude of the effect differed among land use types. However, the effect was also highly variable between similar landscapes, suggesting that it is very sensitive to LC structure. To adequately map the ES provided by the small greenspaces scattered throughout the urban matrix, using land cover data with a spatial resolution of 5 m or finer is recommended, especially for local-flow ES.

Keywords: ecosystem services modeling, spatial scale, uncertainty, urban greenspace, supply, demand, land use, landscape metrics

INTRODUCTION

Urban greenspaces provide several ecosystem services (ES), such as recreation, runoff mitigation and air cooling or purification, that contribute to citizens' security, health and quality of life (Bolund and Hunhammar, 1999; Tratalos et al., 2007; Bowler et al., 2010; Gomez-Baggethun and Barton, 2013; Irvine et al., 2013; Mexia et al., 2018). In this regard, a recent review on the economic value of urban greenspaces concluded that the flow of benefits largely surpass the management costs of these infrastructures (Tempesta, 2015). For example, the value of air pollution removal by urban trees in the United States has been estimated at $3.8 billion annually (Nowak et al., 2006), with $9.2 million for the city of Chicago alone (McPherson et al., 1997). In California, urban trees reduce peak energy load by 10%, resulting in annual savings of $779 million (McPherson and Simpson, 2003). Considering that two-thirds of the world's population is expected to live in cities by 2050 (United Nations, 2015), the role of urban greenspaces is unequivocal, especially since economic studies have demonstrated their efficiency.

There is a growing interest worldwide in integrating ES to guide urban planning with the aim of increasing the well-being (quality of life) of city dwellers (Gomez-Baggethun et al., 2013). To this end, ES mapping represents a useful tool (Pulighe et al., 2016). Yet, ES mapping is still an evolving field and the diversity of methods and data in use can produce divergent estimates of the amount and location of a given ES in the landscape (Crossman et al., 2013; Schulp et al., 2014; Bagstad et al., 2018). Accordingly, there is often a high level of uncertainty about the accuracy of the maps produced, which is seldom assessed (Hou et al., 2013; Boerema et al., 2017; Ochoa and Urbina-Cardona, 2017). One of the challenges is to develop a better understanding of these sources of uncertainty (Hamel and Bryant, 2017), in order to adapt the choice of methods and data to the objective of mapping (Schroter et al., 2015).

Land cover (LC) maps describing the biophysical characteristics of the land surface are one of the most common data sources used in ES mapping (Martínez-Harms and Balvanera, 2012). The spatial resolution of the data is an important feature of LC maps that has been shown to influence ES mapping, but the magnitude of the effect was found to vary depending on the ES and the landscape under study (Konarska et al., 2002; Schulp and Alkemade, 2011; Grêt-Regamey et al., 2014; Grafius et al., 2016; Bagstad et al., 2018; Zhao and Sander, 2018). For example, when mapping urban ES using 5 and 25 m resolution LC data, Grafius et al. (2016) estimated 1.3 times more carbon storage but 2.8 times less potential sediment erosion at the finer resolution. In another study, ES value for the conterminous United States was three times higher when calculated using 30 m LC data compared to 1 km data, but the magnitude of the difference varied between states (Konarska et al., 2002). Estimating the effect of LC data resolution on a given ES in a given landscape thus remains a challenge.

Part of the difficulty lies in estimating the effect of spatial resolution on the LC map itself. While the general effect of decreasing the spatial resolution of a LC map is an increase in the area of dominant classes at the expanse of rarer classes and a loss of information on fine-scale spatial heterogeneity (Turner et al., 1989; Wu, 2004), the precise changes depend on the actual structure of the landscape represented. For example, the effect of decreasing spatial resolution on the proportion of a LC class on a map depends on the proportion of this class in the landscape, the size of its patches and its level of clumpiness (Moody and Woodcock, 1995). Another part of the challenge is to relate changes in the LC map to the spatial processes involved in mapping the ES. In particular, spatially explicit ES models were found to be highly sensitive to LC data resolution in spatially heterogeneous environments (Schulp and Alkemade, 2011; Grafius et al., 2016; Bagstad et al., 2018).

For urban areas that are characterized by fine-scale spatial heterogeneity (Small, 2003; Cadenasso et al., 2007), the differences between very fine and coarser resolution urban LC maps may have a significant effect on urban ES mapping. This effect will also likely vary within the urban area as a function of land use (LU), which refers to the function to which a land parcel is dedicated. For example, the effect may be more pronounced in fine-grained, highly heterogeneous residential areas than in coarse-grained, more homogeneous commercial ones (Herold et al., 2002; Zhao and Sander, 2018). Advanced technology allows the production of urban LC maps with a very fine (i.e., $\leq$1 m) resolution (e.g., Zhou and Troy, 2008). Yet, such fine resolution LC maps are not readily available for all locations (Gong et al., 2019), and the resources needed to produce them may not be affordable for every ES mapping project, especially in low-income countries and outside academic institutions. When available, detailed maps often need to be aggregated to coarser resolution, due, amongst several reasons, to computational limitations or constraints on integrating them with other datasets (Raj et al., 2013). A better understanding of the effect of LC data spatial resolution on fine-scale urban ES mapping is thus needed to weigh the cost of investing in fine resolution LC maps against their benefits.

The high demand for ES in urban areas (Gomez-Baggethun and Barton, 2013) makes it important to understand the effect of LC data resolution on mapping not only ES supply, but also spatial flows of ES, i.e., the actual delivery of ES from greenspaces to beneficiaries (Villamagna et al., 2013; Haase et al., 2014). Spatial flows of ES result from the spatial relationship between the supply of ES and the demand for this ES, and can take different forms (Serna-Chavez et al., 2014). While some ES like wild fruit picking must be performed (used) *in situ* (spatial congruence of ES supply and demand), most ES are used at some distance from greenspaces. There is thus a spatial discrepancy between ES supply and beneficiaries. In particular, global-flow ES, like carbon storage, are totally independent of beneficiaries' location relative to the area of service production, while local-flow ES, like urban cooling, depend on the proximity between beneficiaries and greenspaces (Cimon-Morin et al., 2014; Cimon-Morin and Poulin, 2018). The effect of LC data spatial resolution on those two scales of spatial flows of ES may thus be different. Land use planning based solely on ES supply may not be adequate for ensuring that ES benefits are provided where beneficiaries need them and where these benefits can sustain their well-being (Cimon-Morin and Poulin, 2018). Yet, as most cities worldwide will continue to grow (Seto et al., 2011), mapping ES flow will be increasingly important for urban planners and decision makers in the years to come. This will require a comprehensive understanding of the relation between ES supply and demand (i.e., ES fluxes) and how spatial resolution of LC maps can modulate this relationship.

The aim of this study is therefore to provide empirical results that shed light on the effect of LC data spatial resolution on the three components of fine-scale urban ES mapping, which are supply, demand and flow. To this end, we documented the magnitude of the differences in LC structure and ES quantity between maps produced using LC data aggregated from 1 to 15 m, for a typical North American city. Three ES representing different scales of spatial flows were compared: carbon storage,

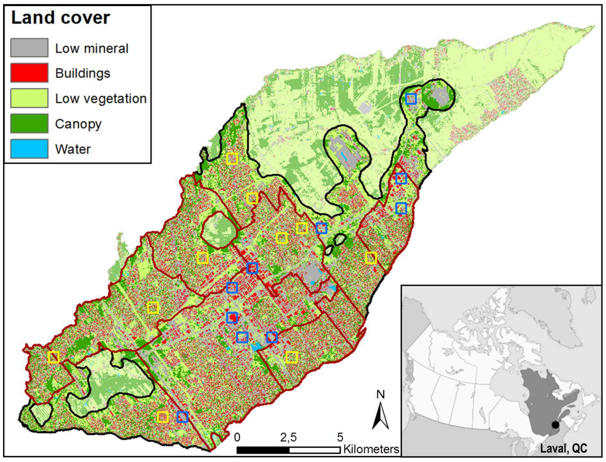

FIGURE 1 | Location and land cover map of the study area. The land cover map also shows the delineation of the urban area in black, urban districts in dark red, residential zones in yellow, and commercial zones in blue. Land cover data source: Communauté Métropolitaine de Montréal (2017).

a global-flow ES, as well as urban cooling and pollination, two local-flow ES. Results were analyzed for two levels of landscapes: large urban districts, and 480 × 480 m residential and commercial zones. Analysis at the district level aimed to assess the global effect of spatial resolution in the urban area, as districts were assumed to capture the overall heterogeneity of the urban landscape. Analysis at the level of residential and commercial zones aimed to assess the local effect of spatial resolution, as each LU type was assumed to exhibit a specific LC structure (Herold et al., 2002; Van de Voorde et al., 2011) and thus a specific scaling behavior. These two levels of analysis were used to better assess the variability of the effect of LC data resolution within the urban area.

DATA AND METHODS

Study Area

We conducted our study in Laval, a city located in southern Québec, Canada (**Figure 1**) with a land area of 247 km^2 and a population of 422,993 inhabitants in 2016 (Statistics Canada, 2016). Laval is part of Greater Montreal, Canada's second most populous metropolitan area. Originally an agricultural territory, the city has experienced accelerated urban sprawl since the 1950s (Nazarnia et al., 2016). Its form of development, typical of North American suburbs, is characterized by spatial segregation of uses, with extensive low-density residential and commercial areas intersected by a road network designed for automobile travel (Dupras et al., 2016; Nazarnia et al., 2016; Ville de Laval, 2017b). Yet, agricultural lands still occupy about a third of Laval's territory, mainly in the east.

Land Cover Data

We used an existing 1 m spatial resolution raster land cover (LC) map of Laval's entire territory (Communauté Métropolitaine de Montréal, 2017). This map was created using color-infrared orthophotos taken in August 2015. Four LC classes were distinguished based on the normalized difference vegetation index (NDVI) and height: low mineral (NDVI < 0.3; height < 3 m), buildings (NDVI < 0.3; height > 3 m), low vegetation (NDVI > 0.3; height < 3 m) and tree canopy (hereafter referred to as "canopy") (NDVI > 0.3; height > 3 m). A fifth class corresponding to water was added from ancillary data; however, as it covered only a small proportion of the study area (<1%), we treated it as a background class for the remainder of the study. Visual analysis of the original LC map revealed some systematic classification errors related to agricultural fields, water bodies and buildings that were corrected in a data preparation step (see **Supplementary Material** for more information on these corrections, as well as other methodological details).

The corrected 1 m LC map (**Figure 1**) was then aggregated to spatial resolutions of 3, 5, 10, and 15 m following a majority rule. To do so, the raster map was first converted to vector format, keeping the edges of the polygons the same as the raster's cell edge. This vector map was then converted back to rasters of coarser resolution using the "maximum combined area" cell assignment type in ArcMap (ESRI, 2015), so that the dominant LC class (the class covering the most extensive area) within a cell was assigned to this cell. In case of a tie between two LC classes, the cell was randomly assigned to one of the two.

Selection of Landscapes

Urban Districts

Since the focus of this study was on the urban landscape, urban areas of the territory had to be distinguished from the rural portions, which represented one third. Yet, there is no standard or universal definition of what constitutes an urban area (McIntyre et al., 2000; Raciti et al., 2012; Short Gianotti et al., 2016), as urbanization represents a multidimensional phenomenon (Hahs and McDonnell, 2006). A pragmatic solution to this issue is to develop and use a clearly-described working definition, adapted to the objective of the study (McIntyre et al., 2000).

Considering that surface imperviousness is a characteristic feature of urban areas (Hahs and McDonnell, 2006), the following LC based method was used to delineate and select urban districts in a quantitative and reproducible way, adapted from Raciti et al. (2012). It involved reclassifying the LC map into "impervious surfaces" (low mineral and buildings) and "greenspaces" (low vegetation and canopy). This reclassified map was used to calculate the impervious surface area in a 500 m radius moving window around each cell. A 15% imperviousness threshold was used to distinguish between urban (≥15%) and non-urban (<15%) cells. After testing many combinations of radius sizes and imperviousness percentages, the combination 500 m radius/15% imperviousness was chosen because it represented the best balance between cohesion in the urban area and distinction between urban and agricultural land uses. In addition, a radius of 500 m or less is often used in urban ecology to study the effects of the surrounding matrix on urban ecosystems (e.g., Coutts et al., 2007; Petralli et al., 2014; Schütz and Schulze, 2015; Melliger et al., 2018).

The 14 districts of Laval (Ville de Laval, 2017a) were then clipped to the urban area. The result of this operation corresponded to the "urban districts" as defined in this study. Urban districts too small or irregular in shape as a result of the clipping operation were excluded from the analysis. In the end, eight urban districts were selected for the analysis (**Figure 1**). These urban districts varied in size from about 3 to 40 km², and were all composed of a heterogeneous mix of different LU types.

Residential and Commercial Zones

In addition to these large heterogeneous urban districts, zones homogeneous in terms of land use (LU) were selected using an existing LU map (Communauté Métropolitaine de Montréal, 2016) that was reclassified into three broad LU types: residential, commercial (including commercial, industrial and office workplaces) and "other" (including every other LU, for example, parks, agricultural lands, the highway network and vacant lots). From a grid composed of 480 × 480 m polygons positioned over the urban area, two sets comprising the 25 polygons with the highest proportion of residential or commercial area were selected. For both residential and commercial sets of 25 polygons, 10 non-contiguous polygons were randomly chosen, which represent the 10 zones of analysis for each LU type (**Figure 1**).

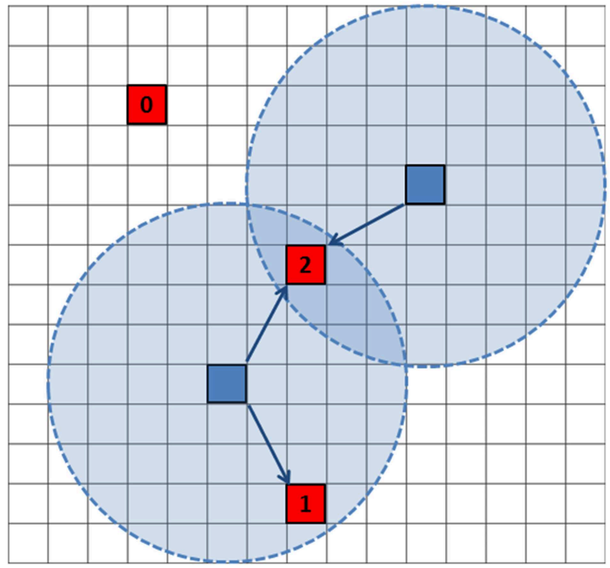

FIGURE 2 | Illustration of the ecosystem services mapping method used. The figure depicts provisioning area as blue cells, benefiting area as red cells, flow area as transparent blue circles and ecosystem service flow as blue arrows. Ecosystem service flow is mapped as supplied to benefiting cells, and is quantified as the amount of supply received by a benefiting cell (numbers shown).

Ecosystem Services Mapping

Conceptual Framework

Based on the conceptual framework proposed by Villamagna et al. (2013), our ecosystem services (ES) mapping method identified three components: potential supply, demand, and flow. ES potential supply refers to the "ecosystem's capacity to deliver services based on biophysical properties"; ES demand refers to "the amount of a service required or desired by society"; and ES flow refers to "the actual use of the service." From a spatial perspective, an ES flow can be viewed as the spatial connection between the area of service production (provisioning area) and the area of service use by beneficiaries (benefiting area). For each provisioning area, the area within which the ES can potentially be used is defined as the flow area (Serna-Chavez et al., 2014). The presence of beneficiaries (expressing a demand) in the flow area gives rise to the actual ES flow.

Figure 2 illustrates how we applied these concepts in our mapping method. A distinctive feature of the method is that provisioning and benefiting areas were allocated to individual raster cells, while the flow area corresponded to a circular radius in and around each provisioning cell. A potential supply value was first attributed to every provisioning cell. This potential supply was then redistributed to every cell in the flow area around the provisioning cell. Doing so for every provisioning cell on the map determined the total potential supply received by each cell. A binary demand value of 1 (for model simplicity) was then attributed to each benefiting cell on the map, and a null value was assigned to other cells. Finally, the demand map was multiplied by the potential supply map to produce the flow map (Watson et al., 2019). In other words, the ES flows were quantified as the amount of supply received by each benefiting cell.

ES Selection and Mapping

The effect of LC data resolution was compared for two scales of spatial flows of ES: global-flow ES, which is independent of beneficiaries' location relative to provisioning areas, and local-flow ES, which depends on the proximity between provisioning and benefiting areas. Three ES were selected: (1) carbon storage, a global-flow ES; (2) urban cooling and (3) pollination, which are two local-flow ES. These three ES were mapped using simple models, and the five LC maps at different resolutions were used as input data. More complex models were not necessary to map ES for the purpose of our study, but would be needed to make concrete management decisions (Eigenbrod et al., 2010).

Carbon storage

The carbon storage model corresponded to global climate regulation by carbon storage in live biomass (Weissert et al., 2014). Based on data from the literature, a carbon storage value of 7.69 kgC/m² was attributed to canopy (Nowak et al., 2013), 0.22 kgC/m² to low vegetation (Jo and Mcpherson, 1995) and zero to impervious surfaces. As a global-flow ES, the flow area of carbon storage is the entire planet: carbon storage at any location contributes to global climate regulation. Therefore, all the carbon stored in the study area benefits people, and potential supply equals flow.

Urban cooling

The cooling model corresponded to the cooling effect of vegetation on the surrounding air temperature (Bowler et al., 2010). A relative cooling effect value of 10 units/m² was attributed to canopy, 5 units/m² to low vegetation and zero to impervious surfaces. These relative values reflect the fact that trees have a higher cooling effect on air temperature than grass (e.g., Huang et al., 2008). The cooling effect of vegetation can be perceived as far as several hundred meters from large greenspaces (e.g., Sugawara et al., 2016). As we attributed a value to small individual raster cells, we choose a conservative cooling distance of 60 m to determine the flow area around each provisioning cell. Cooling potential supply received by each cell on the map was thus computed as the mean cooling effect value of the cells in a circle 60 m in radius around that focal cell. Regarding cooling demand, a binary value of 1 unit/m² was attributed to buildings, and zero to all the other classes. The cooling demand map was then multiplied by the cooling potential supply map to produce the cooling flow map, representing the quantity of cooling received by each building cell.

Pollination

The pollination model corresponded to urban garden pollination by wild bees (Lowenstein et al., 2015). Pollination potential supply was mapped using the InVEST pollination model (Sharp et al., 2016). This model first calculates an index of the relative abundance of bees nesting in each cell on the map, based on the nesting suitability of the cell and the floral resources in the flight range around this cell, giving more weight to nearby cells. From this output, an index of the relative abundance of bees foraging in each cell on the map (potential supply received by each cell) is computed, again based on the flight range of the species. We modeled a single type of bee species, representative of small ground-nesting bees with a short flight range, which was set to 60 m. Regarding the other model parameters, a relative nesting suitability value of 1 was attributed to canopy and 0.5 to low vegetation, and a relative floral resources value of 0.25 was assigned to canopy and 1 to low vegetation. Impervious surfaces received null values. These values were estimated based on previous use of the InVEST model in urban areas (Grafius et al., 2016; Davis et al., 2017). Pollination demand was attributed to residential vegetable gardens. Since no map of gardens was available for the study area, we randomly attributed a 5 × 5 m garden to 5% of low-density residential lots in the city [based on results from Taylor and Lovell (2012)], for a total of ∼4,600 gardens. During the process of random attribution, all gardens were constrained to be allocated in the greenspace LC of residential lots only, in order to avoid gardens being allocated to unlikely places like buildings or roads. A binary demand value of 1 unit/m² was attributed to gardens and zero to the rest of the study area. The pollination demand map was then multiplied by the pollination potential supply map to produce the pollination flow map, representing the relative abundance of bees pollinating each garden cell. It is important to note that the spatial resolution of the pollination demand map was kept constant at 1 m for each model run, as all gardens would have disappeared from the map over 5 m resolution.

Data Analysis

Analyses of landcover (LC) and ecosystem services (ES) maps were performed for each landscape (urban districts as well as residential and commercial zones) at each resolution. LC structure was quantified with three class-level landscape metrics, using FRAGSTATS 4.2 (McGarigal et al., 2012): proportion of landscape, mean patch size and clumpiness index. Patches were delineated using the 8 cells neighbor rule. As it is based on cell adjacency, calculating the clumpiness index is sensitive to cell size: for identical LC maps (in term of structure), the clumpiness index value decreases as cell size increases, because the ratio of interior to border cells decreases (McGarigal, 2015). To isolate the real changes in LC structure from this calculation bias, each of the coarser resolution LC maps was resampled (cell-center method) to a spatial resolution of 1 m before computing the clumpiness index. This resampling clipped larger cells into several smaller cells, but had no effect on LC structure *per se*. For the ES maps, the mean ES component quantity/m^2 of the landscape (ES quantity) was computed for carbon storage, and for cooling and pollination potential supply, demand and flow. Results obtained at 1 m resolution were considered to be the reference against which results from the coarser resolution maps were compared. The effect of data resolution on LC and ES metrics was calculated as the percentage of variation in the value of the metric at a coarser resolution compared to 1 m resolution, following Equation (1):

$$\text{Metric variation} = (V_{ir} - V_{io})/V_{io} * 100 \quad (1)$$

where V_{ir} = value of metric i at resolution r, and V_{io} = value of metric i at the original resolution of 1 m. In addition to the three landscape metrics described above, the total percentage of cells that changed LC class with aggregation (cell-by-cell analysis) was calculated in ArcMap. For residential and commercial zones, the spatial location of these LC changes from one class to another was also analyzed visually.

RESULTS

Representation of Land Cover Structure at 1 m Spatial Resolution

Land cover (LC) structure at 1 m spatial resolution was different for residential zones, commercial zones and urban districts (**Figure 3**). Residential zones were more similar to one another than commercial zones, as shown by the lower variability in LC structure. On average, the low mineral class was dominant for both land use (LU) types, but this was particularly true in commercial zones, which exhibited a higher proportion of low mineral and building cover and a lower proportion of low vegetation and canopy cover than residential zones. Overall, the grain of the landscape was coarser in commercial than in residential zones, as low mineral and buildings classes were larger and more clumped. Regarding urban districts, even if they were composed of a mix of different LU types, variability in overall LC structure between individual districts was low. Class proportion was similar to residential zones, while configuration attributes were intermediate to residential and commercial zones.

Effect of Map Aggregation on Representation of Land Cover Structure

On maps of residential and commercial zones as well as urban districts, the proportion of impervious surfaces (low mineral and buildings) generally increased, while the proportion of

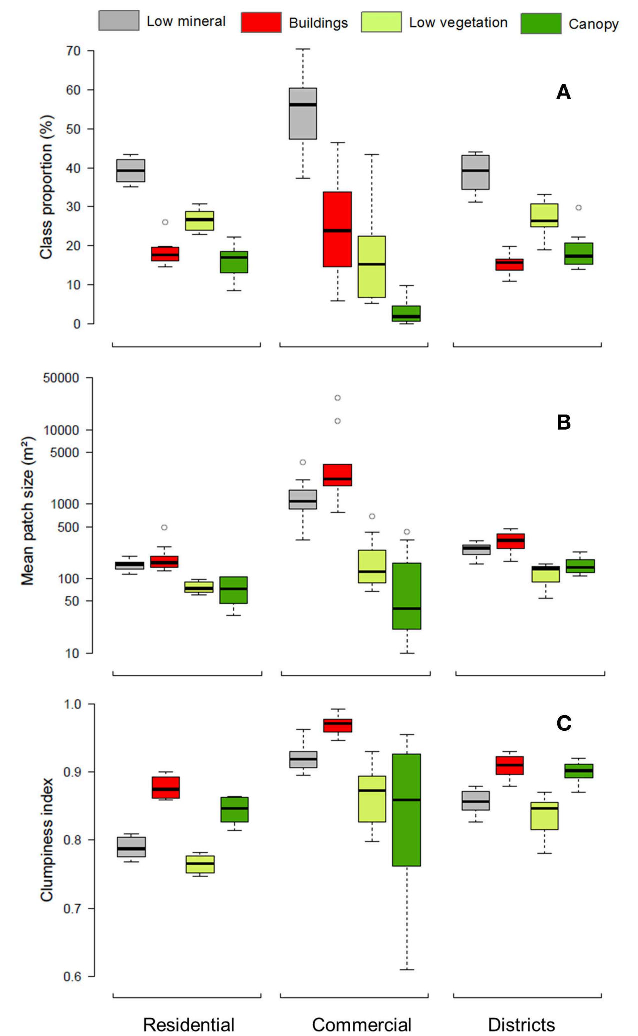

FIGURE 3 | Land cover structure at 1 m spatial resolution. Each boxplot shows the distribution of a landscape metric value (y-axis) for residential (n = 10) and commercial zones (n = 10) as well as urban districts (n = 8) (x-axis). Each subfigure corresponds to a landscape metric: **(A)** class proportion; **(B)** mean patch size; **(C)** clumpiness index. Note that for mean patch size, the y-axis is on a logarithmic scale.

greenspaces (low vegetation and canopy) generally decreased with spatial aggregation (**Figure 4**). These effects were generally accentuated with increasingly coarse spatial resolution, but the magnitude varied between the three types of landscapes. On average, the proportion of impervious surfaces in residential zones increased by about 10%, while the proportion of greenspaces decreased by about −15% throughout the entire gradient of spatial resolution. In comparison, in commercial zones, the increase in proportion of impervious surfaces was less pronounced (+6% for low mineral and about zero for buildings), while the decrease in proportion of greenspaces was more pronounced (−27% for low vegetation and −46% for canopy). At the district level, the increase in proportion of impervious surfaces was intermediate to that of residential and commercial zones (+8% for low mineral and +4% for buildings), while the decrease in proportion of greenspaces was less pronounced than that of residential and commercial zones (−13% for low vegetation and −4% for canopy). In addition to these average values, the magnitude of the effect varied substantially within each type of landscape. For example, the variation in canopy proportion in commercial zones ranged from a +9% increase to a −100% decrease at 15 m, depending on which commercial zone was analyzed.

Regarding LC configuration, mean patch size and clumpiness index increased for each LC class and each landscape with map aggregation (**Figure 4**). Increase in mean patch size was generally more pronounced for low mineral, followed by low vegetation, canopy and then buildings (Y axes vary in scale). Regarding clumpiness, all LC classes tended to converge up to a high level of clumpiness at 15 m. Total percentage of changes was higher in residential (41% on average at 15 m) than commercial zones (14%), and intermediate in urban districts (29%) (**Table 1**). Visual analysis showed that changes occurred along the edge of large patches (stair-step effect), while small patches disappeared to the benefit of the dominant class surrounding them (**Supplementary Figures A2.3, A2.6**). The very large increase in mean patch size at 15 m in many landscapes could be related to the loss of almost all the very small LC patches with aggregation. In residential zones, low mineral gains occurred mainly at the expense of low vegetation, and mostly around roads. Small buildings and canopy patches disappeared from the map, while larger buildings and canopy patches coalesced into more clumped patches. In commercial zones, changes at the interface between low mineral and building patches resulted in gains and losses that mostly offset each other, while small low vegetation and canopy patches disappeared massively, mainly to the benefit of low mineral patches.

Quantity of Ecosystem Services Estimated at 1 m Spatial Resolution

Carbon storage (0.25 kgC/m^2), cooling (1.19 units/m^2) and pollination (0.05 units/m^2) potential supply at 1 m resolution were on average lower in commercial than in residential zones and urban districts (**Figure 5**). Cooling flow (0.11 units/m^2) was also lower in commercial zones, while null pollination flow was associated with the absence of gardens in these areas, and thus of demand. Comparing residential zones and urban districts, carbon storage (1.28 vs. 1.50 kgC/m^2), cooling (2.91 vs. 3.24 units/m^2) and pollination (0.09 vs. 0.11 units/m^2) potential supply were on average similar, but pollination (1.52*10^{-3} vs. 0.72*10^{-3} units/m^2) demand as well as cooling (0.5 vs. 0.35 units/m^2) and pollination (0.15*10–3 vs. 0.08*10^{-3} units/m^2) flow were on average higher in residential zones.

Effect of Land Cover Resolution on Quantity of Ecosystem Services Estimated

For the three ecosystem services (ES) and each group of landscapes, ES potential supply and flow generally decreased with increasingly coarse LC data resolution (**Figure 6**). Carbon storage decreased in most landscapes (except the few where canopy cover increased with spatial aggregation; not shown). The effect of LC resolution on carbon storage was more

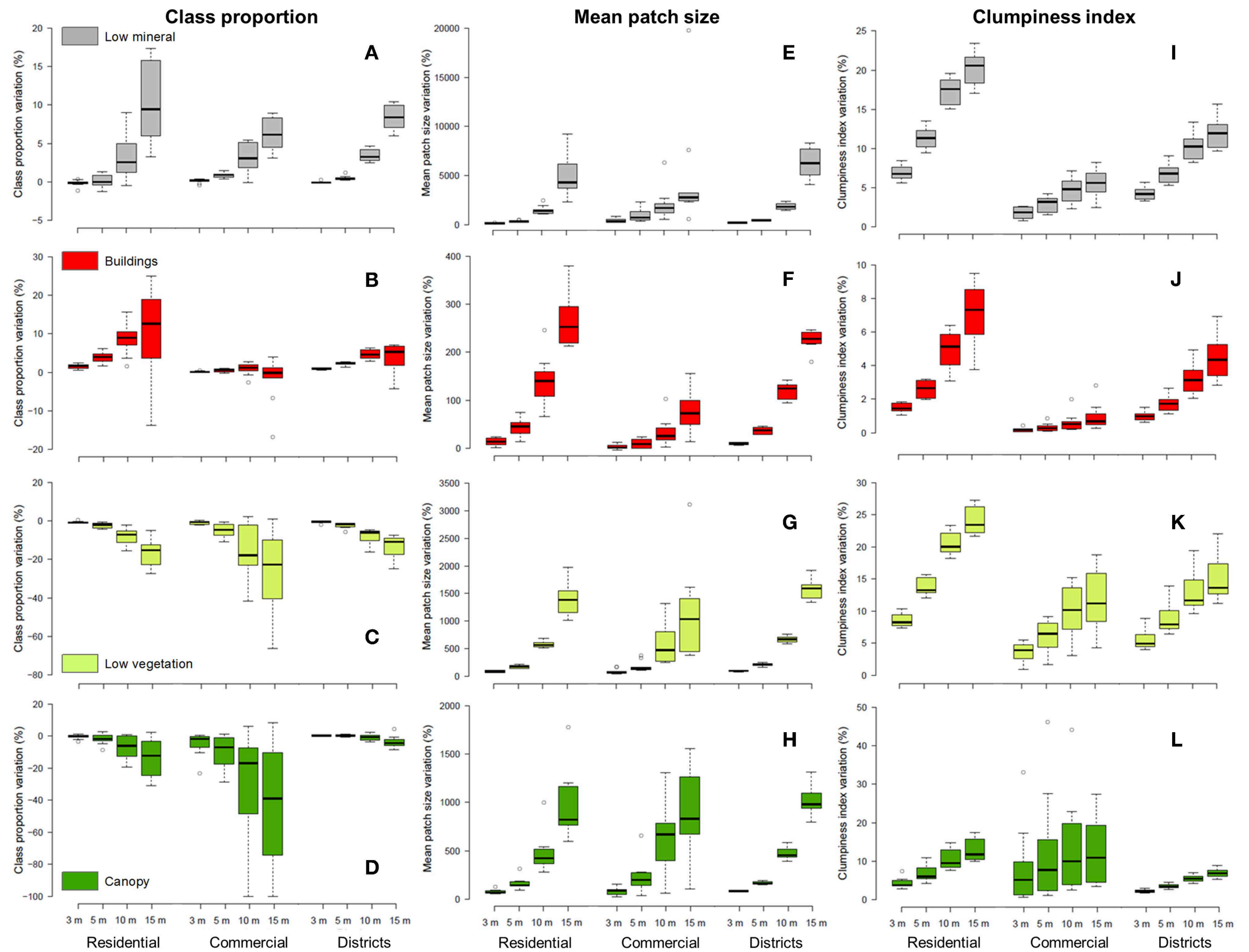

FIGURE 4 | Variation of land cover structure at spatial resolutions of 3, 5, 10, and 15 m compared to land cover structure at a spatial resolution of 1 m. Each boxplot shows the distribution of a landscape metric variation (y-axis), each boxplot quartet shows variation at 3, 5, 10, and 15 m, and the three boxplot quartets in each subfigure correspond to residential zones ($n = 10$), commercial zones ($n = 10$) and urban districts ($n = 8$) (x-axis). Each column of subfigures corresponds to a landscape metric, while each row corresponds to a land cover class: **(A)** class proportion variation for low mineral; **(B)** class proportion variation for buildings; **(C)** class proportion variation for low vegetation; **(D)** class proportion variation for canopy; **(E)** mean patch size variation for low mineral; **(F)** mean patch size variation for buildings; **(G)** mean patch size variation for low vegetation; **(H)** mean patch size variation for canopy; **(I)** clumpiness index variation for low mineral; **(J)** clumpiness index variation for buildings; **(K)** clumpiness index variation for low vegetation; **(L)** clumpiness index variation for canopy. Note that the scale of y-axes differs between subfigures.

TABLE 1 | Total percentage of cells that have changed LC class at spatial resolutions of 3, 5, 10, and 15 m compared to LC class at a spatial resolution of 1 m.

	3 m	5 m	10 m	15 m
Residential	13.4 (0.8)	20.8 (1.2)	33.4 (1.9)	41.5 (2.3)
Commercial	4.2 (1.3)	6.7 (2.1)	11.2 (3.5)	14.3 (4.5)
Districts	9.0 (1.1)	14.0 (1.6)	22.7 (2.6)	28.7 (3.3)

Mean (SD) for residential and commercial zones as well as urban districts.

variable and on average more pronounced in commercial (−38% at 15 m) than in residential zones (−13%) and urban districts (−4%).

Following a pattern similar to that of carbon storage, the quantity of cooling flow decreased in most landscapes, with the effect of LC resolution again being more variable and on average more pronounced in commercial zones (−41% at 15 m) than in urban districts (−12%) and residential zones (−9%) (**Figure 6**). Variability in the effect of LC resolution on cooling flow was very low for districts, but intermediate for residential zones, where cooling flow increased in some zones. This increase likely resulted from an increase in cooling demand that largely compensated for the decrease in potential supply in these zones. However, variation in the quantity of cooling flow was not simply the sum of variation in the quantity of potential supply and demand, but also depended on changes in their spatial configuration. Indeed, cooling flow generally decreased more than would be expected

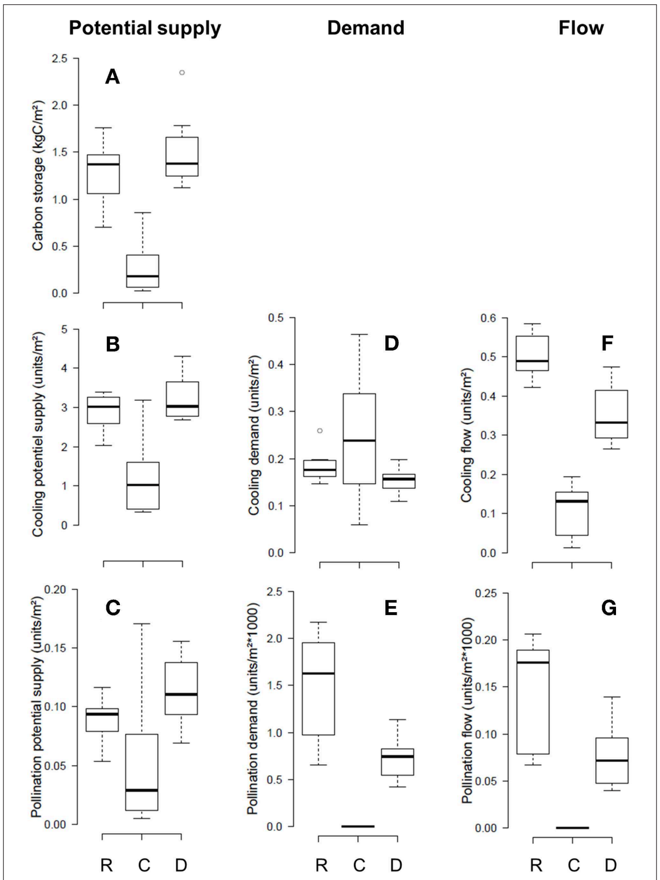

FIGURE 5 | Ecosystem services quantity at 1 m spatial resolution. Each boxplot shows the distribution of ecosystem services quantity (y-axis) for residential (R; $n = 10$) and commercial zones (W; $n = 10$) as well as urban districts (D; $n = 8$) (x-axis). Each subfigure corresponds to an ecosystem service component: **(A)** carbon storage potential supply; **(B)** cooling potential supply; **(C)** pollination potential supply; **(D)** cooling demand; **(E)** pollination demand; **(F)** cooling flow; **(G)** pollination flow. Note that the scale of y-axes differs between subfigures.

based on the variation in potential supply and demand, indicating that the decrease in potential supply was more pronounced near buildings than, on average, in the entire landscape (**Figure 7**). In other words, this indicates that the decrease in greenspace cover was more pronounced in a 60 m radius around buildings than in the landscape as a whole.

Pollination flow decreased in every residential zone and urban district (**Figure 6**). This decrease was slightly more variable and more pronounced in residential zones than in urban districts (−22 vs. −19% at 15 m). While demand did not vary in either of these types of landscapes, the decrease in pollination flow was not equal to that in pollination potential supply, again indicating that the variation in potential supply was not uniform across the landscape. In residential zones, decrease in flow was generally less pronounced than that in potential supply, indicating that the latter was less pronounced around gardens than elsewhere (**Figure 7**). Conversely, in districts, decrease in flow was generally more pronounced than that in potential supply, indicating that the latter was more pronounced around gardens than elsewhere.

DISCUSSION

Effect of Spatial Resolution on Maps of Urban Land Cover and Ecosystem Services

Our results suggest that using land cover (LC) data with a spatial resolution coarser than 1 m can be expected to lead to underestimating greenspace cover and ecosystem services (ES) potential supply in urban areas. However, a decrease in ES potential supply with LC aggregation did not necessarily result in a proportional reduction in ES flow. For example, in some residential zones, a higher demand for urban cooling counterbalanced a lower potential supply at a coarser resolution, leading to a higher cooling flow. In addition, variation in ES flow also depended on changes in the spatial configuration of ES potential supply relative to demand. Decrease in cooling and pollination flow depended on changes in greenspace cover specifically around buildings and gardens, which were usually different from changes calculated for entire landscapes. These differences between potential supply, demand, and flow variation demonstrate the importance of considering the specific location of LC changes when assessing the effect of LC resolution on mapping spatial flows of ES from provisioning to benefiting areas.

All other factors being equal, the effect of LC resolution should thus be easier to estimate for global-flow ES that depend only on changes in potential supply, than for local-flow ES that also depend on the specific location of changes in potential supply relative to demand. These two scales of spatial flow represent extremes on a continuum from local to global scale, and the sensitivity of regional-flow ES (i.e., flood control or water provisioning) will probably be intermediate. For example, the specific location (e.g., meter-accurate) of changes in LC may not be significant for modeling water provision in a watershed, but it could be necessary to distinguish between changes that occur upstream and downstream from water intake. Changes in LC configuration would also need to be assessed to estimate the effect of LC resolution on mapping of potential supply using a spatially explicit model. For instance, potential supply often depends on the location of a provisioning area in the landscape (e.g., riparian vs. non-riparian) or on its position relative to other LC classes (e.g., connecting areas) (Andersson et al., 2015; Verhagen et al., 2016).

The trend toward a decrease in low vegetation and canopy cover to the benefit of low mineral and building cover observed with aggregation in this study is coherent with findings in the literature (e.g., Qian et al., 2015a,b; Zhou et al., 2018). As cell size increases, classes with a higher initial proportion and clumpiness tend to increase in proportion, at the expanse of rarer and more dispersed classes (Turner et al., 1989). Likewise, the increase in clumpiness and mean patch size observed with aggregation for every class and landscape was expected, as it is the consequence of small patches coalescing into larger ones (Moody and Woodcock, 1995). These changes in LC configuration probably increased the average distance between buildings and greenspace cells, the former falling outside of the flow area, which could explains the accentuated decrease in cooling flow. Such loss of information on fine-scale spatial heterogeneity may thus be particularly crucial for local-flow

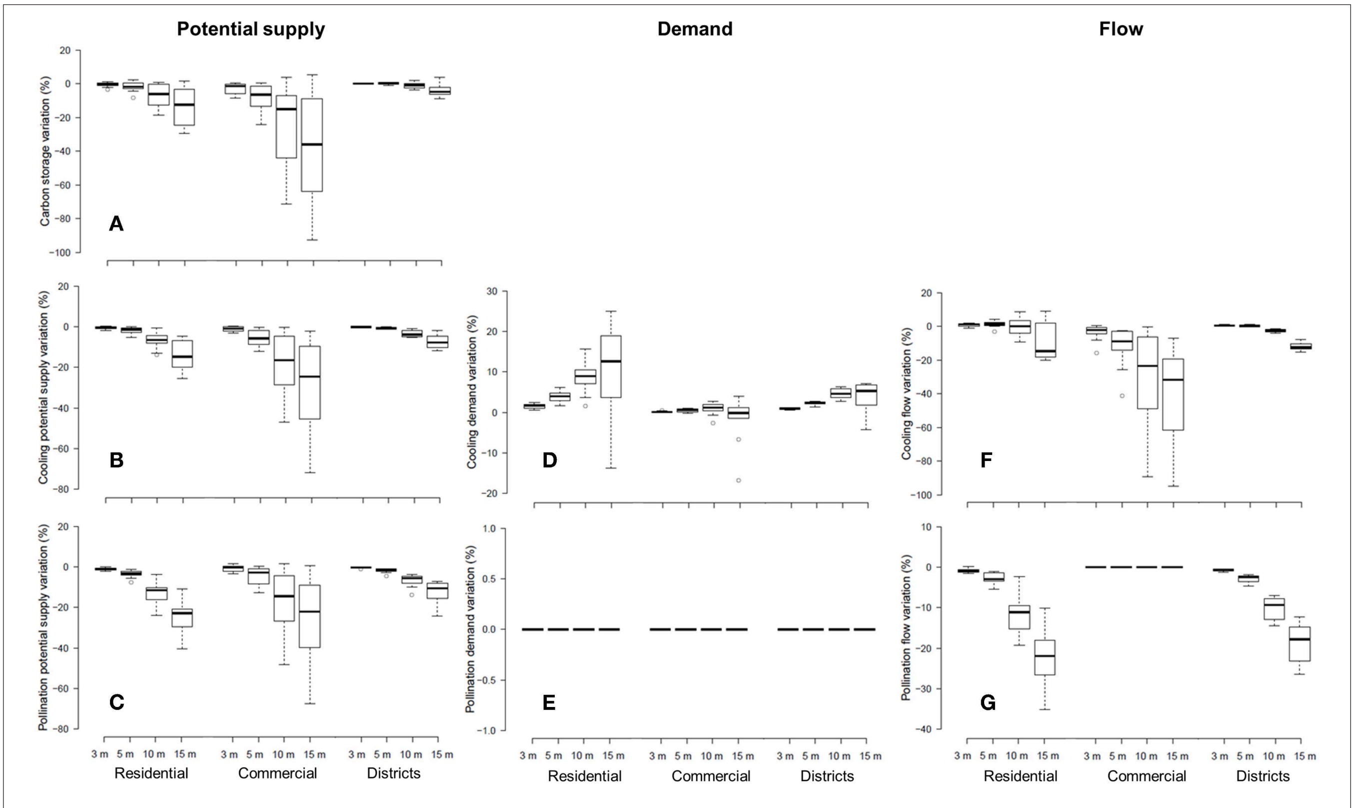

FIGURE 6 | Variation of ecosystem services quantity at spatial resolutions of 3, 5, 10, and 15 m compared to ecosystem services quantity at a spatial resolution of 1 m. Each boxplot shows the distribution of ecosystem services quantity variation (y-axis), each boxplot quartet shows variation at 3, 5, 10, and 15 m, and the three boxplot quartets in each subfigure correspond to residential zones ($n = 10$), commercial zones ($n = 10$), and urban districts ($n = 8$) (x-axis). Each subfigure corresponds to an ecosystem service component: **(A)** carbon storage potential supply variation; **(B)** cooling potential supply variation; **(C)** pollination potential supply variation; **(D)** cooling demand variation; **(E)** pollination demand variation; **(F)** cooling flow variation; **(G)** pollination flow variation. Pollination demand variation is null because the spatial resolution of the pollination demand map was kept constant at 1 m for each model run. Pollination flow variation in commercial zones is null because there was no pollination demand and thus no pollination flow in these zones. Note that the scale of y-axes differs between subfigures.

ES that depend on the proximity between provisioning and benefiting areas.

The underestimation of greenspace cover with increasingly coarse spatial resolution must, however, be viewed as a tendency rather than a definitive pattern, as the effect of LC aggregation varied between types of landscapes. In particular, the decrease in greenspace cover and ES potential supply was less pronounced in urban districts than in residential and commercial zones. This indicates that variation in greenspace cover was positive (or less negative) in the "other" land use (LU) types composing the districts, which can be related to the presence of large greenspaces like parks. More generally, the differences between districts and residential and commercial zones underscore the importance of considering intra-urban variability in LC structure when estimating the effect of LC resolution on mapping of urban ES. Analysis at the level of local zones homogeneous in terms of LU allowed us to control some of this variability and highlight meaningful differences between residential and commercial LU types. For example, decrease in greenspace cover was on average more pronounced in commercial than in residential zones, because the initial proportion of greenspaces was lower and there were fewer gains possible for low vegetation and canopy patches against the large impervious surfaces patches surrounding them. A better understanding of these local characteristics can support a more accurate estimate of the effect of LC aggregation within the urban area. For example, knowing that low vegetation losses with aggregation in residential areas mostly occur in front yards can be useful when mapping an ES for which location relative to the road network is important, like surface runoff attenuation (Alberti et al., 2007).

The variable effect of LC aggregation found for urban districts and residential and commercial zones was also evident within each type of landscape. For residential and commercial zones, one factor that partially explains this variability is that LU is only an imperfect approximation of LC structure (Vanderhaegen and Canters, 2017). This was particularly apparent for commercial zones, where the initial LC structure at 1 m was highly variable. However, even for residential zones where the initial LC structure was similar between zones, large differences in LC response were observed, indicating that even a small change in initial LC structure could influence the effect of aggregation. This sensitivity can be expected to be particularly high when cell size is near the grain of the landscape (Woodcock and Strahler, 1987), as was the case in fine-grained residential

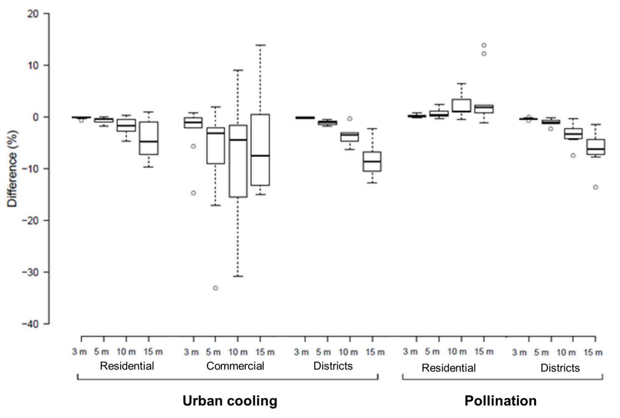

FIGURE 7 | Difference between (1) variation of ecosystem services flow at spatial resolutions of 3, 5, 10, and 15 m compared to ecosystem services flow at a spatial resolution of 1 m, and (2) the sum of variation of ecosystem service potential supply and demand at spatial resolutions of 3, 5, 10, and 15 m compared to ecosystem service potential supply and demand at a spatial resolution of 1 m. Each boxplot shows the distribution of the difference (y-axis), each boxplot quartet shows variation at 3, 5, 10, and 15 m, and the five boxplot quartets correspond to residential zones ($n = 10$), commercial zones ($n = 10$), and urban districts ($n = 8$) for cooling and pollination (x-axis). Note that two outlier data points are excluded from the figure to optimize presentation.

zones, where a high number of changes was observed on a cell-by-cell basis. A way to reduce the variability found for residential and commercial zones would be to refine the definition of LU types by, for example, distinguishing several residential densities (e.g., low, medium, and high density). However, some levels of variability will always persist because any LU classification system remains an abstraction of an urban continuum (Vanderhaegen and Canters, 2017). Consequently, rather than using LU as a proxy, it may be possible to characterize the LC structure of a landscape unit directly with a set of landscape metrics, and then assess the relationship between this structure and the effect of spatial resolution using statistical analysis. This approach has proved effective for correcting errors in class area estimates at coarser resolution in forested landscapes (Moody and Woodcock, 1995). However, the statistical model developed for a given landscape may not apply in another landscape, as many LC attributes are interactive (Moody and Woodcock, 1996; Francis and Klopatek, 2000). A combination of the empirical LU based approach tested in this study, establishing the general landscape structure, with the statistical approach mentioned above, specifying landscape attributes with a subset of significant metrics, would merit further investigation.

The generally lower variability observed for urban districts compared to residential and commercial zones was surprising, since the former were composed of a heterogeneous mix of different LU types and were not selected for their similarity. The larger expanse of urban districts, compared to the smaller sized residential and commercial zones, probably buffered the results by moderating the influence of "extreme" local effects. As well, our focus only on the urban part of each district, rather than its entirety, may have fostered LC similarity between districts and contributed to convergence of results. Using a quantitative method based on surface imperviousness to delineate the urban area may thus provide a way to control the variability in LC structure and help estimate the effect of spatial resolution on LC representation and ES mapping. However, the low variability observed for urban districts may also be specific to our study area. It would be interesting to compare these results with those of other cities, using the same definition of urban area, to assess their robustness. In particular, the effect of LC resolution in cities exhibiting alternative forms of development (e.g., level of density), history (e.g., former LU), and natural setting (e.g., climate) should be assessed. Our results should be representative of low-density suburban areas, as the city of Laval is a typical example of such suburbs (Dupras et al., 2016; Nazarnia et al., 2016), but caution should be taken when applying our quantitative results to more compact cities, such as those in Europe or Asia (Welch, 1982). For instance, European cities have been shown to develop differently than North American ones, mainly due to stronger planning legislation and availability of public transportation (Nazarnia et al., 2016).

Before considering whether the empirical results presented in this study are applicable elsewhere, it is also essential to be aware of the methodological factors that influence the effect of LC aggregation. First, the LC classification system used defines the initial LC map structure and therefore its response to aggregation (Ju et al., 2005). For example, disaggregating the "low mineral" class into asphalt, concrete and other types of material would result in less dominant classes that would probably not increase with aggregation as much as "low mineral" did. Second, our results cannot be readily extrapolated beyond the range of spatial resolution considered (1–15 m), as landscape structure is scale dependent (Wu, 2004). Third, we documented the effect of LC aggregation following a majority rule, which is only one method among many others (e.g., Raj et al., 2013). We chose the majority method because it is commonly used in ecology and remote sensing (Wu, 2004) and for its similarity to producing LC maps directly from aerial or satellite images of variable resolutions (Benson and MacKenzie, 1995). However, the outcomes of aggregating an existing LC map and producing several LC maps from images of different resolutions are not identical (Turner et al., 2000; Schulp and Alkemade, 2011). In addition, between two distinct LC products representing a given landscape, there will always be differences other than those caused by spatial resolution, stemming, for example, from temporal differences or classification errors. These additional differences should also be considered when assessing the effect of LC data input on ES mapping.

Implications for Mapping Urban Ecosystem Services

The continuous growth of urban areas and human populations poses a great challenge for ensuring human well-being in cities (Haase et al., 2014). Urbanization processes, either sprawl or densification, generally result in the reduction of land areas covered by vegetation within the urban matrix. Planning for urban greenspaces may be a solution that would contribute to the development of sustainable cities, since these spaces promote physical activity, psychological well-being, and the general public health of urban dwellers through the delivery of essential ES benefits (Bolund and Hunhammar, 1999; Tzoulas et al., 2007; Niemalä et al., 2010; Irvine et al., 2013). However, to make informed management choices, planners and decision makers need to rely on data that are consistent with the level of accuracy required. Our results showed that aggregating LC data from 1 to 15 m can result in substantially underestimating greenspace cover and, as a direct consequence, ES quantity. Considering the difficulty of making accurate estimates, and subsequently correcting for this effect, our study reaffirms the importance of choosing data of appropriate resolution for mapping urban ES (see also Grafius et al., 2016). Although the aim of this study was not to identify a single optimal spatial resolution for mapping urban ES, our results suggest the use of LC data with a spatial resolution of 5 m or higher. Such high resolution LC data is needed to detect the small greenspaces scattered throughout the urban matrix, which can represent a significant proportion of total urban vegetation cover (Qian et al., 2015a,b; Zhou et al., 2018) and thus of ES potential supply.

Using high resolution LC data is recommended to accurately map the ES produced by greenspaces, particularly for local-flow ES like urban cooling, which must be supplied near the beneficiaries, inside the urban matrix. Indeed, those small greenspaces scattered throughout the urban matrix will often be located closer to ES demand and thus provide the actual ES flows. An accurate representation of the spatial configuration of ES potential supply relative to ES demand is also essential to adequately map these local flows of ES. Failing to capture the fine-scale spatial relation between ES provisioning and benefiting areas could lead to erroneous greenspace management decisions, such as displacing management interventions (e.g., conservation, restoration, creation, etc.) toward locations that are suboptimal in terms of ES benefits delivery. For instance, when the ES being evaluated is supplied only by large greenspaces (e.g., recreation in urban parks), the consequences of using coarser LC maps may not be significant but finer resolution maps may be necessary for making decisions on specific management options, such as where trees should be planted along city streets in order to obtain maximal benefits (e.g., McPherson et al., 2011). Benefits for a tree planting program in the city of Los Angeles have been estimated \$1.33 billion on average over the next 35 years (McPherson et al., 2011), indicating that management decisions on where to locate trees may indeed have significant economic consequences. Estimating where the most important ES flows would be following plantation, and avoiding location errors, could increase the effectiveness of such management decisions.

Our results also provide a number of meaningful insights into the quantification of ES that should be considered in most analyses and applications. First of all, in addition to the total quantity of ES in an area, it could be important to consider the effect of LC resolution on other aspects of ES maps, like the location of ES hotspots, bundles or mismatches (Bennett et al., 2009; Geijzendorffer et al., 2015; Schroter and Remme, 2016). For example, Cimon-Morin and Poulin (2018) used ES supply, demand and flows to assemble a conservation network for protecting ES delivered by urban wetlands. It would therefore be interesting to assess whether changing LC resolution modifies site priority status and network costs (efficiency), or if site ranking remains similar despite the overall change in ES supply, demand and flow. Our results could also help reconcile urban management challenges with environmental justice issues. Indeed, many studies on urban greenspace have revealed that the distribution of such infrastructures often predominantly benefits specific groups, such as more affluent, predominantly white communities in American cities (Wolch et al., 2014). A better quantification of ES flows, and thus, of accessibility to ES benefits for a diversity of groups and communities, may foster effective strategies to lower such inequalities by directly targeting areas that reap few greenspace benefits. It should also be helpful for determining the greenspace surface area required to avoid counteractive effects of greening strategies, such as increased housing costs and property values, gentrification and displacement of the residents who were the intended beneficiaries (Dooling, 2009; Wolch et al., 2014).

DATA AVAILABILITY

The datasets generated for this study are available on request to the corresponding author.

AUTHOR CONTRIBUTIONS

J-FR organized the database, performed the analyses, and wrote the first draft of the manuscript. All authors contributed to the conception and design of the study, manuscript revision, read, and approved the submitted version.

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SUPPLEMENTARY MATERIAL

The Supplementary Material for this article can be found online at: https://www.frontiersin.org/articles/10.3389/fenvs.2019.00093/full#supplementary-material

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A Field-Scale Decision Support System for Assessment and Management of Soil Functions

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Agricultural decision support systems (DSSs) are mostly focused on increasing the supply of individual soil functions such as, e.g., primary productivity or nutrient cycling, while neglecting other important soil functions, such as, e.g., water purification and regulation, climate regulation and carbon sequestration, soil biodiversity, and habitat provision. Making right management decisions for long-term sustainability is therefore challenging, and farmers and farm advisors would greatly benefit from an evidence-based DSS targeted for assessing and improving the supply of several soil functions simultaneously. To address this need, we designed the Soil Navigator DSS by applying a qualitative approach to multi-criteria decision modeling using Decision Expert (DEX) integrative methodology. Multi-criteria decision models for the five main soil functions were developed, calibrated, and validated using knowledge of involved domain experts and knowledge extracted from existing datasets by data mining. Subsequently, the five DEX models were integrated into a DSS to assess the soil functions simultaneously and to provide management advices for improving the performance of prioritized soil functions. To enable communication between the users and the DSS, we developed a user-friendly computer-based graphical user interface, which enables users to provide the required data regarding their field to the DSS and to get textual and graphical results about the performance of each of the five soil functions in a qualitative way. The final output from the DSS is a list of soil mitigation measures that the end-users could easily apply in the field in order to achieve the desired soil function performance. The Soil Navigator DSS has a great potential to complement the Farm Sustainability Tools for Nutrients included in the Common Agricultural Policy 2021–2027 proposal adopted by the European Commission. The Soil Navigator has also a potential to be spatially upgraded to assist decisions on which soil functions to prioritize in a specific region or member state. Furthermore, the Soil Navigator DSS could be used as an educational tool for farmers, farm advisors, and students, and its potential should be further exploited for the benefit of farmers and the society as a whole.

Keywords: soil functions, field scale, decision support system, multi-criteria decision models, method DEX, soil management

INTRODUCTION

Soil functions are fundamental for the provision of many ecosystem services, as soils contribute to the generation of goods and services beneficial to human society and the environment (Blum, 2005; Schulte et al., 2014; Adhikari and Hartemink, 2016; Baveye et al., 2016). The five main soil functions in agriculture and forestry are primary productivity, water purification and regulation, climate regulation and carbon sequestration, soil biodiversity and habitat provision, and provision and cycling of nutrients (Haygarth and Ritz, 2009; Creamer and Holden, 2010; Bouma et al., 2012; Rutgers et al., 2012; Schulte et al., 2014). If one or more soil functions are impeded, threats to soil functions may arise (e.g., soil sealing, compaction, erosion, loss of biodiversity, loss of organic matter, salinization, contamination, and desertification) (Blum et al., 2004; Creamer and Holden, 2010; Creamer et al., 2010; Stolte et al., 2016) and the rational use and protection of soil would fail (European Commission, 2006; Stankovics et al., 2018).

All soils can perform these functions simultaneously, but the extent and the relative composition of this functionality depend on soil characteristics (physical, chemical, and biological), environmental variables (regimes for temperature, humidity, hydrology, slope), land use (cropland, grassland, forestry), and soil management practices (e.g., drainage and irrigation, tillage, nutrient and pest management, crop choice, and rotation) that reflect the specific demands for soil functions (Schulte et al., 2015; Vogel et al., 2019).

Until now, research and corresponding soil-related policies have mostly focused on increasing the provision of individual soil functions. This has resulted in inconsistent and sometimes even conflicting recommendations (ten Berge et al., 2017). Making correct management decisions for soils is therefore challenging and farmers have to make these decisions on their farm/land daily. Therefore, farmers and farm advisors would greatly benefit from evidence-based decision support systems (DSSs) to support their decision making process. DSS are web-based or app-based software systems and are designed to guide the end-users through different stages of decision making in order to reach a final decision (Dicks et al., 2014). DSS targeted for optimizing the supply of soil functions could be used to provide farmers and farm advisors with information about the potential effects of external physiochemical, biological, and management factors. In addition, DSS could inform stakeholders about whether particular targets for selected soil functions have been reached, and if not, how management could enable them to reach those targets.

The usefulness of DSS has been confirmed in different agricultural domains like pest management, nutrient management planning, farm economy, livestock, and crop management (Jones et al., 2017a,b). The national farm advisory services in several European member states are offering access to DSS as an integrated part of supporting their clients. Examples of such DSS are MarkOnline in Denmark (Bligaard, 2014), Mesp@rcelles in France (APCA, 2019), NMP Online in Ireland (Teagasc, 2016), AgrarCommander in Austria (AGES, 2019), and Web Module Düngung in Germany (LWK Niedersachsen, 2019). Furthermore, in the new 2021–2027 Common Agricultural Policy (CAP) proposal (European Commission, 2018) adopted by the European Commission, member states are suggested to implement nutrient management plans, supported by the use of Farm Sustainability Tools for Nutrients (FaST). This is specifically part of the new framework of standards for good agricultural and environmental condition of land (GAECs). A recent review of app-based DSS in agriculture concludes that there is a demand for and value in systems able to address individual farm management issues for achieving the sustainability goals (Eichler Inwood and Dale, 2019). However, nearly all DSS on the market can be characterized as "single solution" DSS that provide limited data to improve only a specific aspect of farm management practices and lack an integration of sustainability aspects (Eichler Inwood and Dale, 2019). Evaluating several soil functions in the same DSS would overcome this lack of integration. Furthermore, although agricultural DSS are becoming increasingly advanced, the uptake and use of DSS by farmers and farm advisors is still very low compared to the number available and accessible DSS (Rose et al., 2016; Bampa et al., 2019). Several studies show that one of the main reasons for this is the lack of end-user involvement in the design and development of the DSS since the beginning of the process (Rose et al., 2016; Lindblom et al., 2017; Rodela et al., 2017). Rose et al. (2016) argue that a successful uptake of DSS requires end-users to be actively involved in the development of the DSS. In addition, these tools should be designed in such a way that they are easy to use, fit the existing workflow of users, and are trustworthy.

The main goal of the European-founded project LANDMARK (Land Management: Assessment, Research, Knowledge base) is to develop a scientific framework for the quantification and management of the five aforementioned soil functions. Furthermore, it aims to provide guidelines for the optimization of these soil functions at the local, regional, and European scale. In order to quantify the soil functions at the local level, a web-based DSS, the Soil Navigator, was developed. It provides an integrated assessment of the five soil functions, which allows an assessment of trade-offs between soil functions for a specific agricultural management practice. In addition, the DSS proposes a suite of management practices that foster an optimal balance among soil functions, recognizing the different function priorities and requirements across different European pedo-climatic zones (Metzger et al., 2005).

The main aim of this paper is to explain the methodological framework for the development of the Soil Navigator DSS. First, we describe the general principles for DSS development and the methodological and theoretical background of the DSS architecture. Then, we present the methodology used for the development of decision support models and their integration into a final DSS, including the active involvement of end-users in the development of the Soil Navigator.

MATERIALS AND METHODS

Decision Problem

The initial step in the process of decision modeling and developing DSS is to define the decision problem. For farmers and farm advisers, most existing decision models deal with primary productivity, which helps the farmer to achieve crop or livestock production targets and economic revenue. However, in the majority of cases, there are no strong drivers and limited legislation to enhance the multi-functionality of soils (Bünemann et al., 2018). Nevertheless, farmers and farm advisors often try to enhance the multi-functionality of their soils, and are more likely to do so where they have observed reduction in crop yields, due to soil degradation, or due to climate change effects (Olesen et al., 2011). However, information on whether the applied agricultural management practices provide support to the multi-functional performance of their soils or how management needs to be modified in order to achieve better performance are not trivial to find or have access to. Hence, decisions on what agricultural management practices will need to be adopted to achieve better performances of all soil functions remains a complex decision problem.

In our study, the decision problem was defined in two steps:

i) Assessing the performance of the five soil functions under specific management practices, environmental/climatic conditions, and soil characteristics;
ii) Choosing appropriate management practices that will improve the performance of the soil functions under given environmental/climatic conditions and soil characteristics.

Decision Support System

To address this complex decision problem, an integration of existing data and knowledge into a DSS using information technologies is required. We designed our DSS as an interactive computer-based system intended to help farmers and advisors to utilize data, knowledge, and models to make decisions about the management measures that would improve the performance of the soil function (Power, 2019). Furthermore, as recommended by Rose et al. (2016), we involved end-users throughout the development process by consulting farmers and farm advisors in Denmark, Austria, France, Germany, and Ireland. This was done systematically by (i) conducting stakeholder workshops before initiating the development of the DSS, (ii) establishing and consulting National Reference Groups (NRGs) for the Soil Navigator in the development phase, and (iii) organizing workshops with farmers and farm advisors to guide the further development of the DSS prototype.

The developed DSS belongs to the group of cooperative and dynamic DSS (Hättenschwiler, 1999), which allows the decision maker to modify the decision suggestions provided by the system. The process is then repeated until a satisfying solution is generated for the user. Given the nature of the DSS and the complexity of the decision problem, we structured the DSS in accordance with Turban et al. (2004), who suggest that the DSS should include data and knowledge bases, models, and a user interface. The structure thus comprises the following seven parts: knowledge base, database, data transformation, decision models, output, user interface, and user (**Figure 1**).

The DSS methodological elements are linked through the following types of information and data flows:

(1) User communication channel: The communication channel through which the user inputs the required data about the field of interest and the constraints about the available soil management measures. This information channel provides also the outputs from the DSS to the end-users. The textual and graphical form of the input and output information are provided in a user-friendly form.
(2) Steering information channel: The information entered by the end-user through the interface are sent to the decision support models, where the modeling constraints and operations are set, and the data required for the performance of the demanding modeling tasks are selected.
(3) Data flow: Flow of data that are transformed according to the requirements of the individual decision models.
(4) Raw data flow: Information for the required data are sent to the data and knowledge bases and available data are sent back to the data transformation part for their further formatting in order to be used in the decision support models.
(5) Flow of modeling results: Outputs from the individual decision support models are sent for further meta-analysis and translation into a set of applicable soil management measures.
(6) Output information flow: Information about the proposed management measures are sent back to the user interface and are communicated to the end-users.

Knowledge Base

DSS rely heavily on expert knowledge as their central element (Uusitalo et al., 2015). However, relying on expert knowledge poses several challenges. The first is the acquisition of expert knowledge and its representation in a formalized way for the purposes of decision modeling (Shaw and Woodward, 1990). Another challenge is that the expert knowledge may differ between experts (Tversky and Kahneman, 1974). In addition, finding a sufficient number of experts, which are knowledgeable on the subject matter is often difficult (Shaw and Woodward,

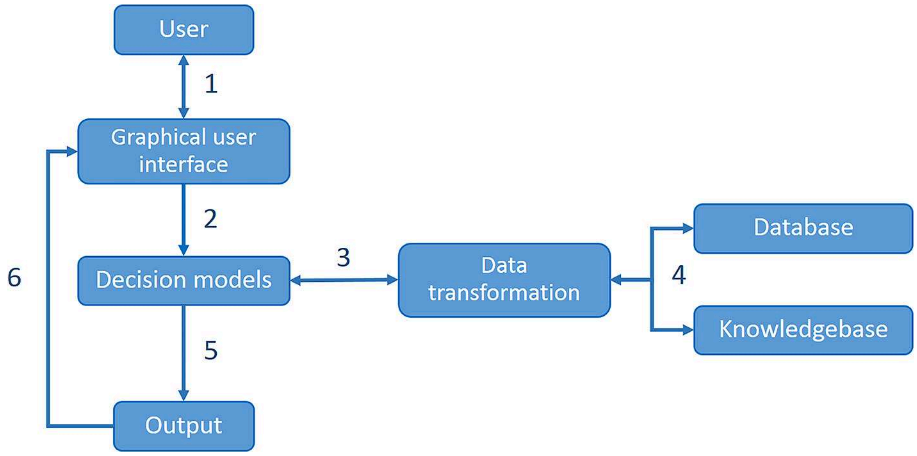

FIGURE 1 | Methodological structure of the DSS for the assessment and management of five soil functions.

1990). There is also an issue of elicitation of the different opinions of the selected experts.

In our study, groups of scientists from the LANDMARK consortium and stakeholders from the NRGs were involved in participatory modeling approach (Bohanec and Zupan, 2004; Jakku and Thorburn, 2010), where they participated in the development, calibration, and validation of the different soil function decision models. Besides working with experts, we also obtained domain knowledge from empirical data using machine learning and data mining (Trajanov et al., 2015, 2018; Bondi et al., 2018). Machine learning algorithms represent a useful tool to extract knowledge from data and representing it in a format that can be easily used for constructing decision models (Trajanov et al., 2018).

Database

Input data for the DSS came from the end-users that provided specific attributes about their field and the applied management practices. Another part of the data was collected from existing databases (soil, meteorological databases) to which the system is internally connected. Specifically, we used soil, environment, and management data from the LANDMARK project (Micheli et al., 2017; Saby et al., 2018). During the development of the individual decision models, data were used for their verification, calibration, and validation. Later, data were used as an input into the DSS.

Data Transformation

During data transformation, input data are transformed to a format suitable for feeding all models. Transformations performed within this segment included (i) data discretization, (ii) derivation of synthesized input attributes, and (iii) attribute harmonization.

Data discretization is applied to numerical values and discretizes them into nominal (qualitative) values. This step is important, as inputs in the decision models are qualitative values from a predefined scale of values. The discretization process uses thresholds defined in accordance with different ecosystems and climatic zones. The former specify the thresholds regarding the purpose of land use (cropland or grassland). The latter capture the spatial distribution of the thresholds according to six predefined climatic zones (Metzger et al., 2005): Central Atlantic, North Atlantic, Continental, South Alpine, Pannonian, and North Mediterranean region.

The derivation of synthesized input attributes is a process of integration of one or more input attributes through an aggregation function that can be defined as a simple mathematical expression or a set of mathematical expressions and can result in a qualitative or quantitative value. The aggregation is performed using predefined mathematical expression (e.g., functions) for each synthesized attribute.

Attribute harmonization matches the name of each empirical (measured) attribute to the name of the corresponding models' input attribute. This process is required to avoid mismatch in the names and meaning of attributes among different models.

Methodology for Construction of Decision Models

The decision models perform the central tasks of the decision-making process and are at the core of the DSS. In general, they are used for prediction of the outcome of the decision choice that we might make (Mallach, 1994). The decision models help the decision makers to rank a set of decision alternatives and choose the best one according to their preferences. In the Soil Navigator, the ranking of a set of decision alternatives is based on a list of selected criteria, which are relevant for the soil functions. Since we were dealing with a multi-criteria decision problem, we used multi-criteria decision models (MCDM) for the analysis of our decision problem (Kangas et al., 2015). Our approach is based on the application of analytical hierarchical processes (Saaty, 1990) for building decision models. Following this approach, a complex decision problem is decomposed into less complex sub-problems represented by attributes structured into a hierarchy, where hierarchical levels are linked by integrative functions.

The simultaneous assessment of the five soil functions could be addressed by qualitative MCDM (Mendoza and Martins, 2006;

A

Attribute	Scale
Climate regulation	Low; Medium; High
├**Carbon sequestration**	Low; Medium; High
│ ├Carbon inputs	Low; Medium; High
│ ├Potential carbon loss	High; Medium; Low
│ └Organic carbon content	Low; Medium; High
├**N2O emissions**	High; Medium; Low
│ ├Direct N2O emissions	High; Medium; Low
│ └Indirect N2O emissions	High; Medium; Low
└**CH4 emissions**	High; Medium; Low
├Artificial drainage	No; Yes
└Soil type	Organic; Mineral

B

Direct N2O emissions	Indirect N2O emissions	N2O emissions
High	High	**High**
High	Medium	**High**
High	Low	**High**
Medium	High	**Medium**
Medium	Medium	**Medium**
Medium	Low	**Medium**
Low	High	**Medium**
Low	Medium	**Low**
Low	Low	**Low**

FIGURE 2 | Top part of the DEX model for the climate regulation and carbon sequestration soil function. **(A)** Hierarchical structure and scale values of attributes. **(B)** Integration rules for integration of direct and indirect N_2O emissions into N_2O emissions.

Greco et al., 2016). To build qualitative MCDM, we used the DEX (Decision Expert) integrative methodology (Bohanec and Rajkovič, 1990; Bohanec et al., 2013; Bohanec, 2017), which combines the approach of hierarchical MCDM with rule-based expert systems and fuzzy sets. DEX enables the acquisition and the representation of decision knowledge, as well as evaluation and analysis of decision alternatives. DEX is based on attributes with a finite set of nominal values. The integrative functions (integration rules) in DEX are represented with if–then rules, which are given in a tabular form (**Figure 2B**). These rules are a tabular representation of a mapping from lower-level to higher-level attributes. The DEX methodology enables the construction of transparent and comprehensive models, and it provides mechanisms for presenting aggregation rules in a user-friendly way, i.e., in the form of decision trees.

Beside the mere evaluation of alternatives, the DEX methodology provides what-if analysis of alternatives (e.g., effects of changing one or more initial attribute values on model outputs). In addition, DEX is able to handle missing or non-exact data using probabilistic or fuzzy distribution of attributes' values. The evaluation of alternatives was used for the assessment of the performance of all five soil functions, while the what-if analyses were used for the selection of soil management measures that would improve the performance of soil functions if needed. The decision models were built with the software modeling tool DEXi (Bohanec, 2017, 2019).

Output

The output of the developed DSS consists of (i) an assessment of the performance of each soil function and (ii) suggestions of how to improve the performance of the preferred soil function(s). Both outputs utilize the same DEX decision models developed for each soil function. However, they differ in their purpose, format, and the approach of utilization of the DEX tree structures.

The assessment of the performance of the soil functions considers the outputs of the DEX decision models. Each decision model is fed with data prepared in the data transformation step, after which the input basic attributes are aggregated to the upper level of the model structure. Such aggregation to higher level continues until the top node is reached. The aggregated value in the top node is the overall assessment of the performance of a particular soil function. The same approach is applied across all soil functions; thus, the format of the DSS output is a set of qualitative values describing the performance of the five soil functions.

The set of suggestions for improving the performance of the preferred soil function(s) is an output obtained by generative design approach (Lohan et al., 2016) over the DEX decision models. This approach traverses the DEX tree structure from the top to the bottom, i.e., from the top node (output attribute) to the basic (input) attributes. The idea of the generative design approach is to find a suitable combination of input values for a given output of the model. In this case, the input to the DEX decision models represents the current situation of a particular agricultural field represented through a set of qualitative input values. The generative design approach allows identifying attributes that need to be changed in order to achieve the desired performance of a soil function. The generative design can be constrained by users' preferences and only a subset of inputs undergo the generative approach. The same approach is applied for each soil function, which leads to a set of suggestions for improving their performance.

However, each soil function model generates a different set of suggestions of management practices, which leads to a long list of suggestions and they might be sometimes contradicting (some management practices might improve certain soil functions, but decrease other). Thus, an optimal set of management practices is chosen through a combinatorial process, where contradicting management practices are eliminated and only the acceptable sets of suggestions are further propagated to the user interface.

Graphical User Interface

The graphical user interface (GUI) enables the communication between the user and the DSS. The UI of our DSS is divided into two parts. In the first part, the users insert the required data (management, soil, and environmental properties) related to their field or modify the default data obtained from existing databases that the system is connected to.

In the second part, the GUI communicates the results of the DSS to the end-user. The results are represented textually and graphically and show an estimation of the performance/potential of each of the five soil functions in a qualitative way, using three values: low, medium, and high. The GUI also enables the end-users to choose the level of improvement for a certain soil function, as well as to set weights (preferences) to certain soil functions. The system then searches through all possible combinations of management practices that could be taken in order to improve the preferred soil functions and provide the end-user with several suggestions, if they exist.

Users

The target users of the Soil Navigator are farmers and farm advisors. To define the preferred type of communication between our DSS and the users, 32 workshops with 473 stakeholders (farmers, farm advisors, and regional, national, and European stakeholders) were conducted as part of the LANDMARK project (Bampa et al., 2019). The results from these workshops show good to very good understanding among potential end-users of the meaning and need for soil quality and the participants demonstrated their inherent understanding of soil functioning. In addition, in many cases, they showed a reasonable understanding of the four soil functions other than primary production, but found it difficult to assess how multiple soil functions interact and respond to management measures under local conditions. These consultations demonstrated a knowledge gap regarding the existence of soil data and the possible use of such data in decision support tools for assessment and management of soil functions. This knowledge gap exists despite the fact that the importance of having data, providing advice and simple tools to support decisions on soil and land management, was well-recognized. The results of Bampa et al. (2019) showed a strong interest by famers for independent and scientifically supported advice to be provided at field level.

Following these initial stakeholder workshops, NRGs for the Soil Navigator were established with farmer and farm advisors in Denmark, Austria, France, Germany, and Ireland in order to involve them in the development of the Soil Navigator. The NRGs were consulted using an online survey and a follow-up interview to ensure that the Soil Navigator DSS was designed in such a way that it (i) is easy to use; (ii) provides trustworthy, relevant, and valuable information; and (iii) uses terms that are recognized and meaningful for both farmers and farm advisors. In the survey, the NRG members were asked about (i) the most meaningful terms for describing the five soil functions, (ii) the availability of data required for running the DSS, (iii) their preferences for the functionality and design of the DSS, and (iv) what would make the DSS trustworthy, relevant, and valuable for them. After the first DSS prototype was developed, we subsequently organized hands-on evaluation workshops with farmers and farm advisors in Denmark, Austria, France, Germany, and Ireland to get feedback and expertise for the further development of the DSS. This participatory approach taken toward continuously involving end-users along the development process has proved successful in creating a sense of ownership and trust toward the tool finalization.

Construction of the Decision Models

In our study, DEX decision models were developed for all five soil functions using the following five standard steps of building ecological models: construction of the models, verification, sensitivity analysis and calibration in an iterative way, and validation (Jørgensen and Fath, 2011).

The construction of the DEX models started by breaking down the concept of each soil function into smaller and less complex parts using the software DEXi (Bohanec, 2019). The structure of the model is given as a hierarchy of attributes (**Figure 2A**). It consists of basic attributes (input data), aggregated attributes (internal nodes), which provide the assessment of the alternatives at various hierarchical levels, and the root attribute (top attribute), which gives the overall assessment of the alternatives and presents the final output of the model. The same initial or aggregated attribute can participate in several integration rules and such attributes are named linked attributes.

The involved experts assigned a finite set of qualitative (nominal) values (e.g., low, medium, high; suitable, not suitable; wet, dry) to each attribute in the model. Their value scales were ordered preferentially from "bad to good" or were left unordered in cases when the attributes' values could not be ordered (**Figure 2A**). The integration from basic attributes (e.g., soil pH, salinity or tillage) to the soil function (the attribute at the top of the hierarchy) was defined by integration rules given in a form of decision tables that were formulated by the involved experts (**Figure 2B**).

An example of the structure of a DEX model is presented in **Figure 2A**, where the first three hierarchical levels of the climate regulation and carbon sequestration soil function are shown. Each attribute has an ordered scale of values, which are integrated in a decision table as presented in **Figure 2B**. The rows in the table represent integration rules, which map the values of lower-level attributes into an integrated (higher-level) attribute. A detailed description of the DEX model for the climate regulation and carbon sequestration soil function is explained in Van de Broek et al. (unpublished)[1].

When the models were constructed, a model verification was performed in order to test their internal operational logic and behavior. The verification was performed by domain experts and end-users (farm advisors and farmers) who designed several theoretical case study scenarios, covering a wide spectrum of possible evaluation alternatives (e.g., variability of soil samples). The outputs from the models were compared to the results of a ranking made by experts and end-users of the soil function performance. If the experimental results were not as expected, the integration rules were re-examined. If this did not make a significant change, the model structure was modified as well.

When the verification of all soil function decision models was completed, a sensitivity analyses was carried out. This was used to find input attributes whose values had a negligible impact on the model behavior. These attributes were removed from the models to reduce the model complexity. The sensitivity analysis of the DEX models was based on the contribution of a corresponding attribute to the final evaluation result. Because the attributes had different value scales (some attributes have

[1]Van de Broek, M., Henriksen, C. B., Ghaley, B. B., Lugato, E., Kuzmanovski, V., Trajanov, A., et al. (unpublished). Assessing the climate regulation potential of agricultural soils using a decision support tool adapted to stakeholders' needs and possibilities. *Front. Environ. Sci.*

more values than others), the weights had to be normalized to the same unit interval. In our study, we used global normalized weights, which take into account the structure of the entire model and the relative importance of every part (Bohanec, 2019). In cases when the weights of the basic attributes were negligible (<1%), the attributes were removed from the model structure and the integration rules in the corresponding integration table were modified accordingly. After that, the verification process was repeated.

To adjust the sensitivity of the decision models to specific pedo-climatic conditions, calibration of the models was performed. Since we developed qualitative multi-attribute models where tables with integration rules are used (**Figure 2B**), the sensitivity analysis was performed by the variation of the integration rules. When data were available, we applied data mining to obtain additional knowledge about the integration rules in order to improve the model sensitivity and performance (Sandén et al., 2019).

To check how well the model outputs fit real-world data, a validation of the decision models was performed. First, an estimation of the real performance of the soil function on a certain field was calculated from empirical data or was estimated by experts and end-users. Subsequently, the model's output was compared to the estimated level of the soil function performance. Finally, the ratio between the number of correctly predicted soil function performance levels and the total number of estimations was calculated. Different validation criteria were formulated for each soil function due to the differences in the availability and quality of empirical data (Rutgers et al., 2019; Sandén et al., 2019; Delgado et al., unpublished[2]; Van de Broek et al., unpublished[1]). The data used for validation were not used for model calibration.

SOIL NAVIGATOR

Conceptual Structure of the DSS Soil Navigator

The conceptual structure of the DSS Soil Navigator (**Figure 3**) consists of two parts. In the first part, the assessment of the soil functions was carried out, while the second part searches for appropriate soil management practices to improve the performance of the soil functions in accordance with the expectations and goals of the user.

The assessment of the performance of all five soil functions is based on the inputs to the DSS, which comprises data describing the properties of the assessed field. There are three categories of input data. The first category describes environmental conditions (climatic and orographic data), the second category describes soil properties of the assessed field (e.g., water pathways, physical, chemical, and biological soil properties), and the last category provides data about the current soil and agronomic management activities (crop management, fertilization, water management, pest management, harvest) for that field. Once the input data are pre-processed, they are sent to the soil function decision models, which provide an assessment of the performances of the five soil functions.

If the performance of the assessed soil functions is not in accordance with the expected levels, the DSS proposes appropriate changes in management practices that will increase the performance of these soil functions. This is performed in the second part of the system. The mechanism of iterative what-if analysis searches through all theoretical combinations of the values of input attributes to find combinations that provide the accepted performance level of the soil functions. The number of suitable combinations of mitigation measures could theoretically be very large. Therefore, the selection is based on the collection of mitigation options that are actually criteria representing the end-users' management preferences or constraints. The final output from the DSS is a list of mitigation measures that end-user could apply on the field in order to achieve the desired performances of the soil functions.

Soil Function Decision Models

In this section, we provide a brief overview of the individual soil function decision models. Since the decision models of soil functions should address both cropland and grassland soils, some of the decision models have been split into two separate decision models, one for cropland and one for grassland. By doing so, the sensitivity of the outputs for changes in the input data has been increased. The detailed descriptions of each model are provided in separate papers in this issue (Rutgers et al., 2019; Sandén et al., 2019; Delgado et al., unpublished[2]; Van de Broek et al., unpublished[1]). The model for nutrient cycling was developed earlier and published by Schröder et al. (2016).

The primary productivity decision model consists of sub-models describing the environmental conditions (E), inherent soil conditions (S) (physical: structure, groundwater table depth; chemical: micro- and macro-elements; biological: pH, C/N ratio, soil organic matter), soil management (M), and crop properties (C). Primary productivity, as the top attribute, integrates the sub-models, which leads to an assessment of the capacity of a soil to produce biomass. A detailed description of the primary productivity model is given in Sandén et al. (2019).

The structure of the nutrient cycling decision model consists of three sub-models, integrated into the top attribute, describing the ability of a soil to provide and cycle nutrients. The first sub-model comprises nutrient fertilizer replacement value, which describes the extent to which nutrients, particularly those in left or applied organic residues, are as available to plants as manufactured mineral fertilizers. The second part of the model describes the extent to which plant-available nutrients are effectively taken up by crops and the last part addresses the harvest index describing the extent to which the nutrients taken up by crops are eventually leaving the field in the form of successful harvests (Schröder et al., 2018).

The climate regulation and carbon sequestration decision model integrates carbon sequestration, N_2O emissions and CH_4 emissions. The carbon sequestration sub-model is determined by the magnitude of carbon inputs, carbon losses, and the soil organic carbon concentration. The N_2O emissions sub-model makes a distinction between direct N_2O emissions occurring on

[2]Delgado, A., O'Sullivan, L., Debeljak, M., Creamer, R. E., Henriksen, C. B., Wall, D. P. (unpublished). Farming systems targeted to water regulation and purification in agricultural soils. *Front. Environ. Sci.*

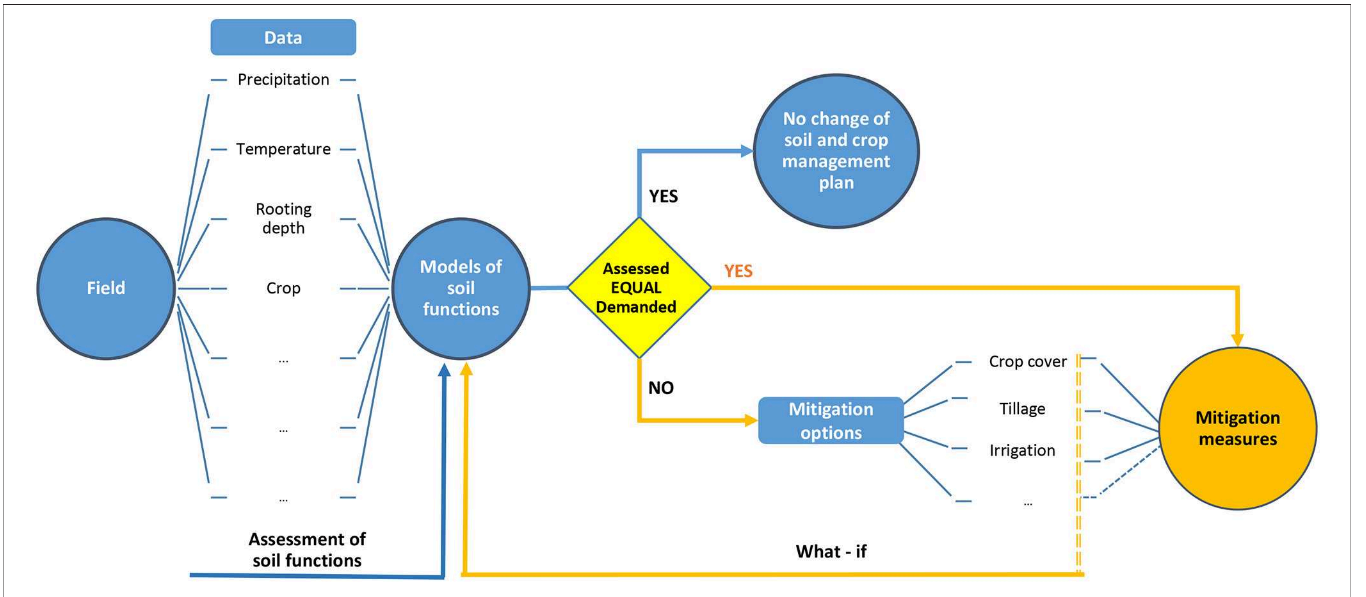

FIGURE 3 | Conceptual representation of the Soil Navigator.

agricultural fields, and indirect N_2O emissions, after reactive N species have been transported through the landscape. The part of the model addressing CH_4 emissions are determined by the extent to which artificial drainage is applied on organic soils. Detailed information about the model are given in Van de Broek et al. (unpublished)[1].

The water regulation and purification soil function decision model integrates three sub-models describing the prevailing soil water pathways: water storage, water runoff, and water percolation. Water storage is determined by the attributes used for assessing the water holding capacity and soil moisture deficit. Water runoff is determined by the attributes used for assessing the water-, sediment-, and nutrient-related runoff. The water percolation sub-model is determined by the attributes used for assessing the resulting drainage of excess of water above that potentially stored in the soil and the resulting nutrient leaching and losses (Wall et al., 2018).

The soil biodiversity and habitat provisioning decision model integrates four sub-models describing soil nutrients (status, trends, turnover, and nutrients availability), soil biology (available information on diversity, biomass, and activity of soil organisms), soil structure [structure and density, ranging from mesoscale (coarse fractions, soil particles, organic matter, air, and water-filled space) to macroscale (soil layers, terrain, slope)], and soil hydrology (soil humidity and the soil water flow pathways) (Rutgers et al., 2019).

The structural properties of the DEX decision models of all five soil functions are given in **Table 1**. All decision models have similar hierarchical structure (number of hierarchical levels), as well as the number of basic attributes. From the number of integration rules, it is evident that the water regulation and purification and the biodiversity and habitat models are more complex than the others, because of the total number of attributes and their scales of values. However, the decision models for all five soil functions use the same subset of basic attributes, so the total number of distinctive input attributes for all decisions models is 75.

Graphical User Interface

The GUI enables the interactions between the user and the DSS through a series of steps: (i) data entry, (ii) specification of soil function preferences, and (iii) selection of the changes of factors or states in an agricultural field. The development and testing of the GUI was based on end-user preferences indicated in the surveys and follow-up interviews with the members of NRGs for the Soil Navigator.

The data entry form (**Figure 4**) allows the user to provide all available data for a particular agricultural field. The required set of input data includes data about the agroecosystem, environment, soil, and management (rightmost column, **Figure 4**). The middle panel shows the input forms for the required attributes within each of the data categories, while the field "Scenario" (at the top of the page) allows the user to specify a name for the particular scenario under consideration. The DSS has an option of importing data from the external corresponding databases.

The user is required first to specify his preferred soil function (**Figure 5**) that is based on the outputs from the assessment of the soil functions (given on the right side of the screen) and includes an input form for specifying a preference for improvement the performance of one or more soil functions (bottom panel). The preferences can be specified through the given sliders that have a value corresponding to the initially assessed level of performance.

The final step/output that is presented through the Soil Navigator GUI is the proposed set of suggestions for the improvement of the performance of a soil function

TABLE 1 | Structural properties of the DEX models of all five soil functions.

Soil function models	Total number of attributes	Number of aggregated attributes	Number of input attributes	Number of hierarchical levels	Number of integration rules
Primary productivity	42	16	25	4	294
Nutrient cycling	51	27	24	5	302
Climate regulation	540	21	19	5	301
Water regulation and purification	116	77	39	6	800
Biodiversity and habitat	55	24	31	5	612

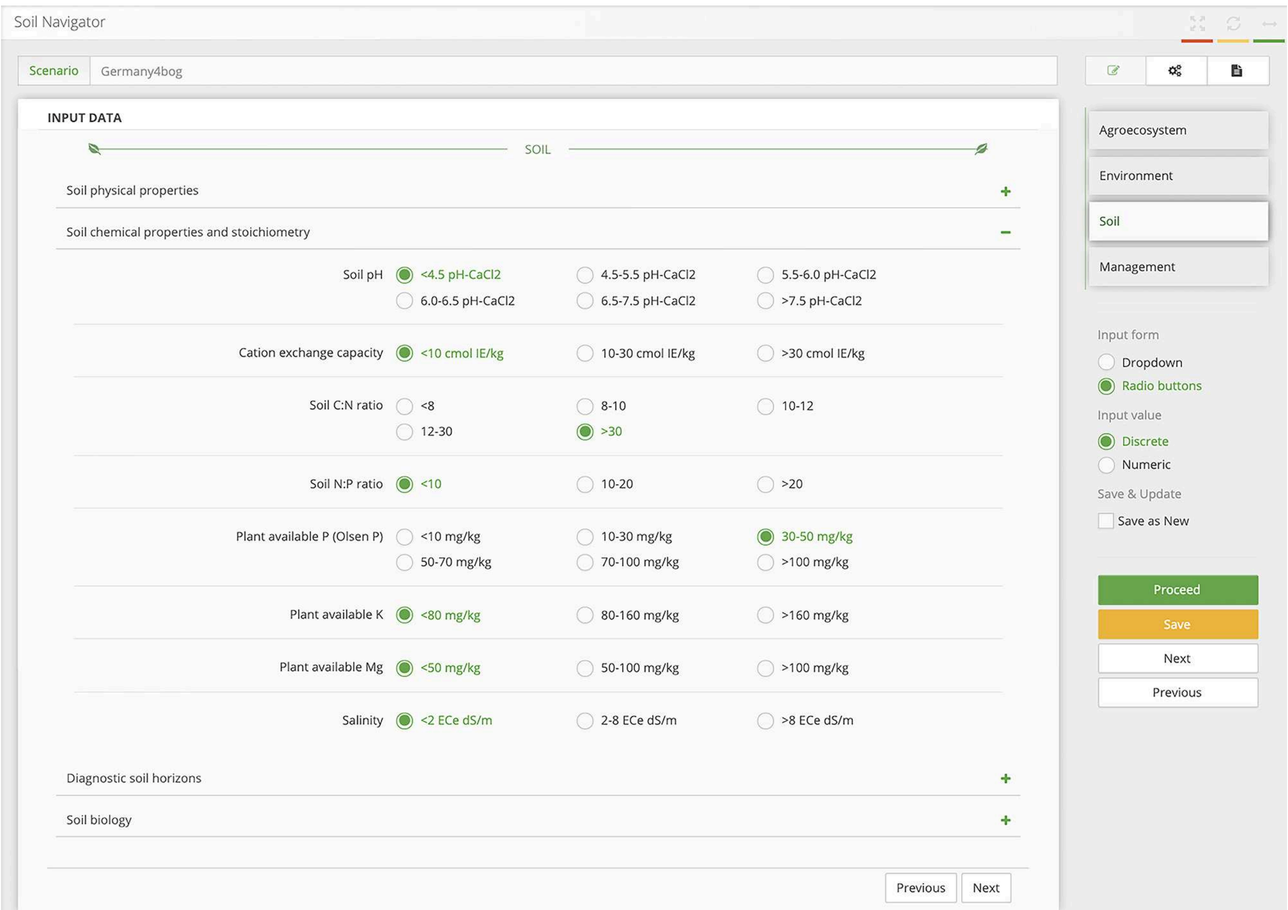

FIGURE 4 | Data entry form for a particular agricultural field.

(**Figure 6**). In this step, the user can also request to find other suggestions if the ones that are offered do not satisfy the user's expectations and possibilities. All input data for an assessed field and the suggestions for the improvement of its soil functions can be saved and later used for the purpose of validation of the results, as well as its re-evaluation in the future.

In **Figures 4–6**, we present the Soil Navigator GUI using a scenario that involves an agricultural field located in Germany, within the Central Atlantic climatic zone. The purpose of the land use is crop production within a mixed farm type (crop and livestock production). **Figure 4** shows some of the input data for the soil from the selected field.

In the second step (**Figure 5**), the system provides an initial assessment of the performance of all five soil functions. The soil functions primary productivity and water regulation and purification are assessed as most efficient (high performance capacity), climate regulation and carbon sequestration as medium-scaled performance, and cycling of nutrients along with soil biodiversity and habitat provision as lowest level of performance (low performance). Consequently, the overall improvement can be achieved by improving the performance of

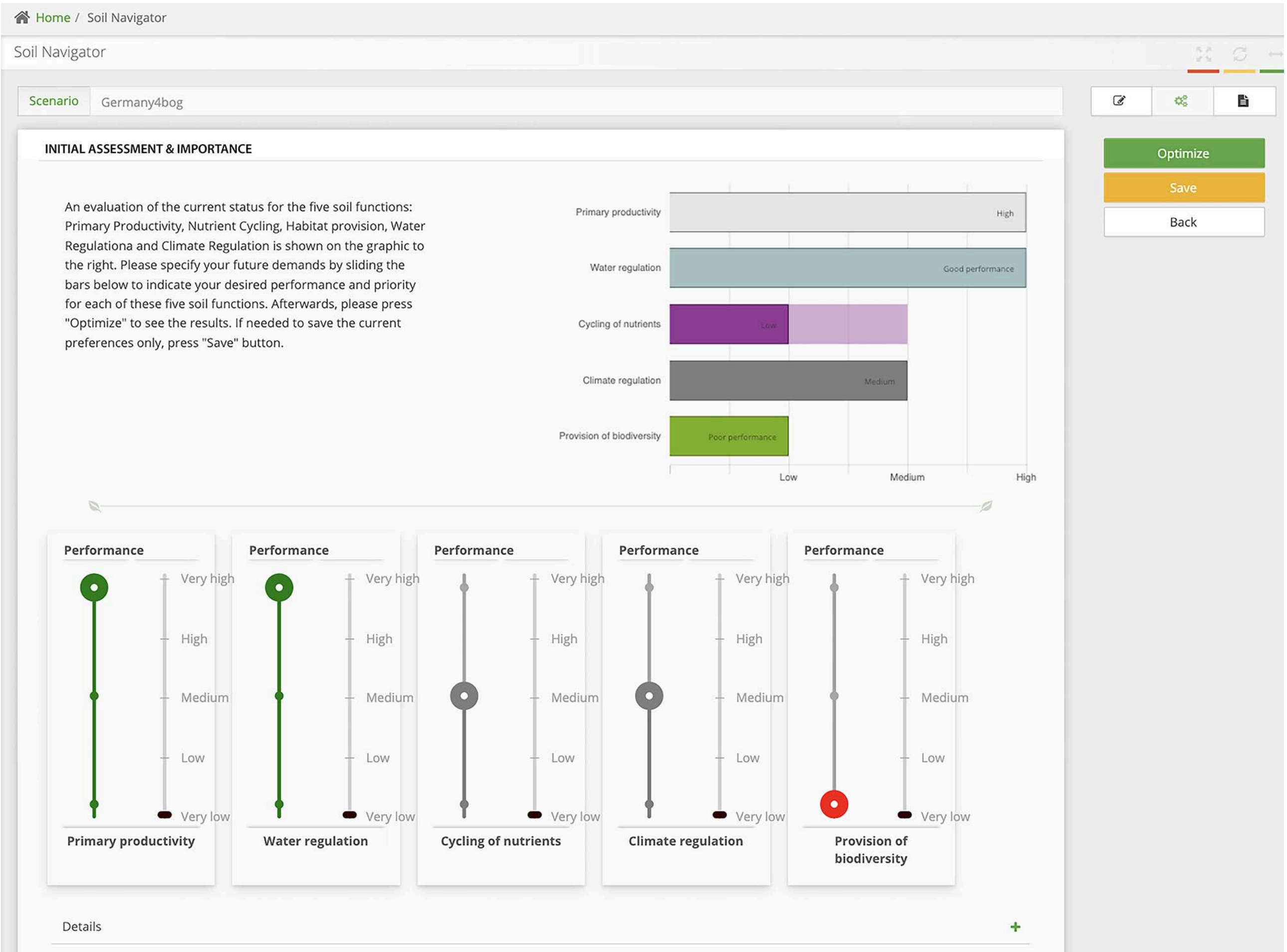

FIGURE 5 | Outputs from the assessment of the soil functions and specification of their preferences.

the last three functions. In the given example (**Figure 5**), the user selected the function Nutrient Cycling as the only function of interest and target/level for improvement of the capacity of this soil function to medium performance level (visually given on the bar chart with violet color with reduced opacity).

In the final step, the system performs a search of all possible combinations of values of the input attributes in order to identify a smaller number of combinations that would improve the capacity of the soil to deliver the nutrient cycling function. When a suitable combination is found, the bar chart in the top right corner shows more colors (**Figure 6**). The inner rectangles with bold colors represent the initial assessment. The outer rectangles show the user's preferences, stated in the previous step, the borders of which are bolded only to those that are successfully improved. In our case, the system found a solution, which would improve the performance of the function cycling of nutrients, without compromising the other functions. The solution shows that the share of legumes needs to be increased drastically in order to achieve the desired performance of the soil functions in this particular field.

DISCUSSION

Jones et al. (2017a,b) highlighted the lack of integrated DSS for farm system management. They envisioned a DSS platform that connects various models, databases, analyses, and information synthesis tools in an easy-to-use interface to enable analyses and outputs to answer questions relating to the management of particular farming "systems" biophysical resources and/or socio-economic situations. Jones et al. (2017a,b) concluded that such DSS are required, but still not developed. The Soil Navigator DSS encompasses the above-listed components, performs similar tasks, and communicates with the end-users through user-friendly graphical interface designed according to Rose et al. (2016). Furthermore, the Soil Navigator meets the documented needs for a DSS that will assist farmers and advisors to achieve sustainability of the agricultural landscape (Eichler Inwood and Dale, 2019), by enabling field-specific assessment and the enhancement of five soil functions simultaneously while integrating sustainability concerns from multiple dimensions or themes. In addition, the Soil Navigator DSS has the potential

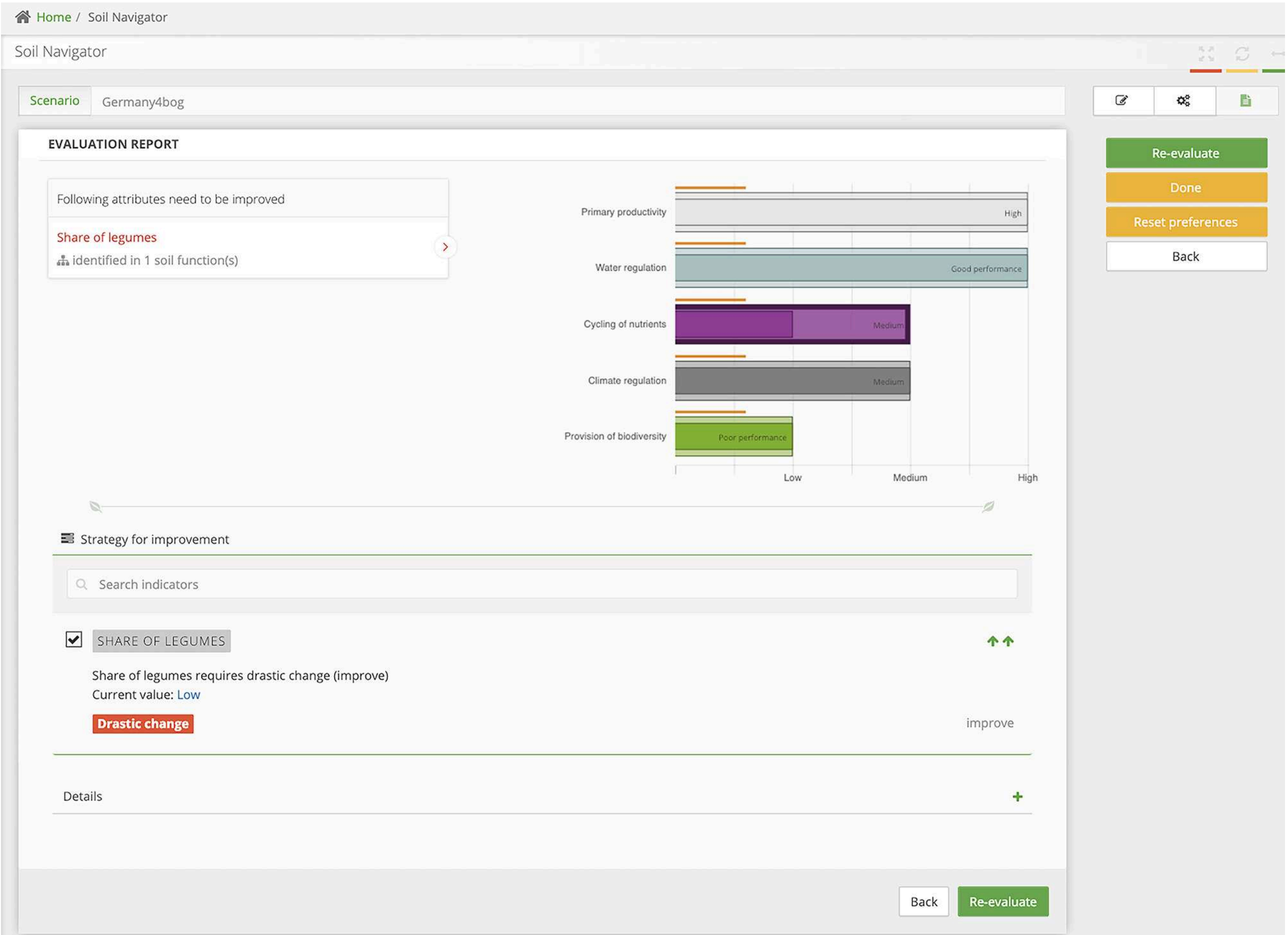

FIGURE 6 | Proposed suggestions for improvement of the performance of soil functions.

to complement the FaST tools required by the proposal on the 2021–2027 CAP (European Commission, 2018). As part of the GAESs framework, farmers will be required by Member States to use FaST tools in order to establish nutrient management plans and support the agronomic and the environmental performance on their farms. The tool should provide on-farm decision support featuring minimum nutrient management functionalities. However, the capacity of a soil to provide and recycle nutrients is determined not only by nutrient management practices but also by environmental or climatic/weather conditions and farm- or soil-related management practices. This implies that for the same level of functioning, if attainable at all, soils will require different managements under different pedo-climatic conditions.

Another consequence of the interplay of factors is that some environments are better suited to perform certain functions and deliver specific services than others, regardless of management efforts. Decisions favoring nutrient cycling may compromise one or more other functions, as for example increased cycling of phosphorus (P) nutrient may have negative consequences for the quality of water (water purification function) even if losses from the soil are relatively small. This complicates the decision making process even further. Consequently, there is no such thing as a one size (or soil) fits all soil strategy, which is in line with the findings of Sandén et al. (2018). Decisions must therefore be based on careful considerations accounting for local demands, their soils' potential to deliver functions and even ecosystem services, as well as synergies and trade-offs between soil functions and the weightings of alternative options for achieving these services.

It is in this space that the Soil Navigator DSS could support the objectives of the CAP post-2020. Based on the European Commission commitment to make FaST interoperable and modular, it should be possible to couple the Soil Navigator DSS with FaST. Whereas, FaST is focusing on nutrients, the Soil Navigator DSS could make it possible for the farmer to perform a combined assessment and optimization of nutrient cycling, primary productivity, biodiversity and habitat provisioning, water regulation and purification, and climate regulation and carbon sequestration. In addition, farmers will be able to assess the potential change in GHG emission as a consequence of the management they apply, and to make them aware of trade-offs between, e.g., C sequestration and N_2O emissions. Obvious trade-offs occur, e.g., between application of fertilizer and manure, leading to increased carbon sequestration on one side and potentially leading to increased N_2O emissions on the other side, if not managed correctly (Tubiello et al., 2015; Zhou et al., 2017; Lugato et al., 2018). Thus, the Soil Navigator could facilitate activities that will reduce the impact of agricultural sector on climate change and provide support actions to achieve the European Union commitments under the Paris Agreement (United Nations/Framework Convention on Climate Change, 2015).

Besides the potential to integrate the Soil Navigator in the CAP post-2020, there is also potential to use the DEX models at larger spatial scales (e.g., regional or European) in order to improve the provision of soil functions in a spatially explicit context. Such an application of the developed DEX models could be used to indicate which soil functions should be prioritized by a specific region or member state. However, in order to produce reliable results, the different DEX models would have to be adjusted to match the specific scale. This can be handled easily, since the embedded DEX models can be improved upon request (e.g., for a higher tier assessment, other systems, such as forestry). By applying a set of harmonized models, it is possible to use the available data and knowledge as efficient as possible.

The Soil Navigator DSS also has the potential to function as an educational tool for farmers, farm advisors, and students. The Soil Navigator DSS presents an opportunity to gain knowledge about different soil functions and how they are affected by management strategies under certain soil and environmental conditions. The tool could potentially guide discussions between the farmers and farm advisors and demonstrate that primary productivity is closely linked with other soil functions. The stakeholders would be able to visualize the effect of the implementation of a specific management practice not only toward primary productivity but also toward the performance of other soil functions. Such demonstrations may incentivize farmers to obtain the data needed to run more specific Soil Navigator scenarios for particular farms or soil conditions in order to obtain more reliable results (e.g., soil pH, organic matter content, or soil texture). The Soil Navigator DSS could also be linked to regional soil maps and thereby educate the farmers about new sources of information. Finally, it can be used as a tool to assess the influence of the global climatic changes on the soil functions, which will enable experts to perform risk assessment and risk management and to propose practical and effective climate adaptation measures for farmers and other stakeholders.

As outlined in this paper, the integrated field-scale assessment and optimization of soil functions delivered by the Soil Navigator DSS have many different potential applications that should be further exploited for the benefit of farmers and the society as a whole.

DATA AVAILABILITY

The datasets for this manuscript are not publicly available because they contain personal data about applied soil management practices. Requests to access the datasets should be directed to RC, rachel.creamer@wur.nl.

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AUTHOR CONTRIBUTIONS

JS, TS, HS, DW, MV, and MR contributed to the development of the soil function decision models. MD, AT, VK, and CH developed the decision support system, while FB and RC contributed to reading and structuring of the paper. MD and AT wrote most of the paper with major inputs from VK, CH, JS, FB, TS, HS, MV, MR, and RC.

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Modeling of Soil Functions for Assessing Soil Quality: Soil Biodiversity and Habitat Provisioning

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Soil biodiversity and habitat provisioning is one of the soil functions that agricultural land provides to society. This paper describes assessment of the soil biodiversity function (SB function) as a proof of concept to be used in a decision support tool for agricultural land management. The SB function is defined as "the multitude of soil organisms and processes, interacting in an ecosystem, providing society with a rich biodiversity source and contributing to a habitat for aboveground organisms." So far, no single measure provides the full overview of the soil biodiversity and how a soil supports a habitat for a biodiverse ecosystem. We have assembled a set of attributes for a proxy-indicator system, based on four "integrated attributes": (1) soil nutrient status, (2) soil biological status, (3) soil structure, and (4) soil hydrological status. These attributes provide information to be used in a model for assessing the capacity of a soil to supply the SB function. A multi-criteria decision model was developed which comprises of 34 attributes providing information to quantify the four integrated attributes and subsequently assess the SB function for grassland and for cropland separately. The model predictions (in terms of low—moderate—high soil biodiversity status) were compared with expert judgements for a collection of 137 grassland soils in the Netherlands and 52 French soils, 29 grasslands, and 23 croplands. For both datasets, the results show that the proposed model predictions were statistically significantly correlated with the expert judgements. A sensitivity analysis indicated that the soil nutrient status, defined by attributes such as pH and organic carbon content, was the most important integrated attribute in the assessment of the SB function. Further progress in the assessment of the SB function is needed. This can be achieved by better information regarding land use and farm management. In this way we may make a valuable step in our attempts to optimize the multiple soil functions in agricultural landscapes, and hence the multifaceted role of soils to deliver a bundle of ecosystem services for farmers and citizens, and support land management and policy toward a more sustainable society.

Keywords: ecosystem service, soil function, soil biodiversity, land management, qualitative modeling, Europe, habitat provisioning

INTRODUCTION

Soil is an extremely valuable resource for life on our planet. Soils contribute essentially to agricultural productivity, the environmental cycling of energy, carbon and nutrients, water regulation, climate regulation, disease suppressiveness, natural attenuation and purification, and the provision of biodiverse communities below–and aboveground. Ongoing human activities form severe threats to our soils, in terms of land use change, soil contamination, soil degradation, desertification, and soil sealing leading to the loss of the soils functionality for ecosystems and mankind (JRC, 2010a; FAO ITPS, 2015; Orgiazzi et al., 2016).

In the last decades, starting with a monodimensional view on soil health (e.g., Doran and Zeiss, 2000), soil quality has been increasingly approached by expressing it in terms of the capacity of the soil to deliver multiple ecosystem services (e.g., Lavelle et al., 2006; Dominati et al., 2010; Mulder et al., 2011; Robinson et al., 2013; Schulte et al., 2014; Baveye et al., 2016; Keesstra et al., 2016; Vogel et al., 2018). The reason to do so lies in our ambition to use, protect and manage our soils in such a way that the soil sustainably delivers the ecosystem services we request. This approach implies that in order to make our soil management effective and successful, we should have measurable indicators of the soil's contribution to independently deliver a suite of ecosystem services, in this study we use the term soil functions. For some soil functions relatively easy indicators can be used, for example agricultural yield for the agricultural productivity service. For other soil functions it becomes more difficult. For example, soil as environmental buffer for nutrients should be based on the multidimensional complex of nutrient pools and fluxes present in soil at several spatial and temporal scales, and the interplay among them.

A soil function that poses also a challenge for defining measurable and understandably indicators of the provision of ecosystem services by the soil is the so-called habitat function, i.e., the provision of habitats for species rich communities, below as well as aboveground. Belowground, soils harbor an incredible amount of organisms with a vast diversity exceeding that in all other environmental compartments (Orgiazzi et al., 2016). The soil biota are seen as key players in many soil functions, such as nutrient cycling and carbon sequestration, but are thought to be also important for the soil as habitat for aboveground biological diverse communities (Lavelle et al., 2006; Mulder et al., 2011).

In the H2020 project LANDMARK (Land Management: Assessment, Research, Knowledge base), "Soil biodiversity and habitat provision" (SB) is one of the five soil functions that is considered as part of sustainable land management (Schulte et al., 2014). One of the aims of the LANDMARK project is to come up with science based sustainable soil management schemes, with the development of five indicators for the various soil functions. In this issue, these indicators are presented in a set of articles.[1] The fifth soil function indicator was published earlier (Schröder et al., 2016). Up until now no formula or index to quantify soil biodiversity that is universally accepted and applicable (Bastida et al., 2006; Bünemann et al., 2018) and no comprehensive decision-support model for the assessment of SB is available (Havlicek, 2012). This is due to the lack of a clear and accepted definition of the SB function, to the low standardization in soil biological methods, and to the difficulties in addressing spatial scale (Bastida et al., 2006). Hence we lack affordable, yet robust and reliable, proxy-indicator systems for the SB function that capture the different dimensions of the SB function, such as presence, abundance and activity of the soil organisms, soil ecosystem process rates, and the provision of habitats for aboveground species rich communities (Maes et al., 2016; Yu et al., 2017). Many contributions in the field of soil ecology have only focused on separate species of functional groups of organisms, for instance earthworms (Lavelle et al., 2006), micro-arthropods (Parisi et al., 2005; Menta et al., 2011, 2018), nematodes (Yeates et al., 1997), microorganisms (Winding et al., 2005; Bloem et al., 2006; Romaniuk et al., 2011). On the other side of the scientific spectrum, there have been built complex models for soil functioning and biodiversity which need a vast amount of essential soil attribute information, making these models less appropriate for routine analysis (De Ruiter et al., 1993; Mulder et al., 2011). An exception is the approach by Lima et al. (2013) who showed practical options to reduce the number of indicators while retaining enough discriminatory power to assess soil quality. This analysis did however only include a small part of soil biodiversity (microbes, earthworms) neglecting the presence and abundance of e.g., nematodes and micro-arthropods, which makes it, in our view, less appropriate for the assessment of the SB function. In addition, important aspects of soil management were not assessed in the analysis.

The present paper describes a novel approach to assess the SB function and its first application on two soil datasets covering information on soil biodiversity, soil ecosystem functioning, and soil management. These datasets comprise of 137 grassland soils in the Netherlands and 52 soils in France (Brittany), of which 29 grasslands and 23 croplands.

[1]This issue of Frontiers in Environmental Science will contain all or a selection of the following papers on soil function models from the H2020 LANDMARK project: Debeljak et al. (2019), Sandén et al. (2019), Delgado et al. (submitted), Van de Broek et al. (submitted).

BOX 1 | The multitude of soil organisms and processes, interacting in an ecosystem, making up a significant part of the soil's natural capital and providing society with a wide range of ecosystem services.

Dissecting the definition:

1. Multitude of soil organisms: this comprises communities, populations, species, genes, molecules and enzymes. It is focusing specifically on the living parts of the soil.
2. Processes: this comprises ecological processes.
3. Interacting in an ecosystem: together with 1 and 2 this comprises dynamics, food webs, trophic interactions, non-trophic interactions, and soil habitat characteristics.
4. Natural capital: this links the soil function to the stocks of soil biodiversity and to contributions to the habitat for above ground organisms (Maes et al., 2013).
5. Providing society with soil-related ecosystem services: this configures the soil function for usage in National Ecosystem Assessments (Maes et al., 2013), and contributes to solving the Sustainable Development Goals (Dominati et al., 2010; Mulder et al., 2011; Robinson et al., 2013; Baveye et al., 2016; Keesstra et al., 2016).

Basic in the proposed approach is our working definition of SB as "the multitude of soil organisms and processes, interacting in an ecosystem, providing society with a rich biodiversity source and contributing to a habitat for above ground organisms" (**Box 1**).

The approach toward the SB function will be specifically focused on the community of soil organisms, including trophic and non-trophic interactions of soil organisms, together with habitat modifying properties such as nutrient availability, and physical and chemical soil conditions. In this way the definition of the SB function also captures aboveground biodiversity, e.g., in terms of diversity in plant communities (e.g., De Deyn and Van Der Putten, 2005), or bird populations (e.g., Roodbergen et al., 2008).

The search for an indicator for the SB function has recently gained momentum given the goals of the Convention on Biological Diversity (CBD) and the Sustainable Development Goals (SDGs) (Keesstra et al., 2016). In addition, the recently held UN-CBD meeting (COP 14) has requested the FAO to perform a world-wide assessment of soil biodiversity by 2020.

Our methodology will approach the SB function by gathering information on soil biodiversity in a multi-attribute manner. In our approach we assembled attributes for an indicator system of the SB function using a hierarchical structure of four integrated attributes: (1) soil nutrient status, (2) soil biological status, (3) soil structure, and (4) soil hydrological status, following Van Leeuwen et al. (2017). The total amount of soil information provided by these four integrated attributes was used to assess the SB function together with the assessment of four other soil functions using partly the same input data in order to support farmers and farm advisors at local scale and policymakers at regional scales.

The proposed approach is meant to be seen as a first attempt and as a proof of concept. Upon further development additional attributes may foster an improved soil function assessment. As a first attempt we have restricted our concept to focus on belowground biodiversity and soil ecosystem processes, excluding information on aboveground biodiversity. As proof of concept we will compare the outcome of the proposed methodology with an alternative assessment of the soil SB function based on expert judgement for 137 grasslands in the Netherlands (Mulder et al., 2005b; Rutgers et al., 2009; Schouten et al., 2014) as well as for 52 sites in Brittany France (Cluzeau et al., 2012; Ponge et al., 2013; Villenave et al., 2013).

MATERIALS AND METHODS

Structure of the Decision Model (DEX Model)

We developed a decision model according to the DEX (decision expert) model structure (Bohanec et al., 2007) to quantify the capacity of a soil to supply the function soil biodiversity and habitat provision (SB function). The model quantifies the capacity of a soil to support the supply SB function at three levels, i.e., low, moderate or high. The structure of the model has the form of a Multi-Criteria Decision Analysis, including quantifiable or measurable "attributes" of the soil combined with expert judgement (Debeljak et al., this issue). Within the DEX model we developed two sub-models, one for grassland and one for cropland, as they function very differently with respect to the management attributes. Approaching grasslands and croplands in the same way would reduce the versatility and sensitivity of the model for the SB function and limit the provisioning of useful advice to farmers and other stakeholders.

In total, 32 (grassland model) or 31 (cropland model) attributes (**Table 1**, **Figure 1**), were combined in a hierarchical DEX model to make a first-tier assessment of the SB function. Data availability may sometimes be limited (especially for the biological attributes) leading to an incomplete set of attributes to make an assessment. For this reason, we implemented a no data category for these attributes, to ensure that the model is able to provide a performance estimate despite incomplete input data, responsibly addressing the amount of information that is available in the remaining quantified attributes. Obviously, the model output improves considerably, the more input data are available.

An attribute is defined as a piece of quantifiable information of the ecosystem, including the information from the environment, climate, hydrology, geographic characteristics, land and soil management and which can be used to quantify and to assess the SB function. Only attributes that can be linked in a statistical or mechanistic way to the SB function were used in these models. The models distinguish attributes in three categories, i.e., soil properties (S), environmental factors (E), and management practices (M). These attributes together fill the S × E × M matrix (Turbé et al., 2010; Schulte et al., 2014; Vogel et al., 2018). This three-dimensional matrix addresses the interrelationships between the various attributes. Soil properties (S) include static attributes such as soil texture, and dynamic attributes, such as soil biological attributes (e.g., soil organism abundance, richness) and soil organic matter content. S attributes can have a different effect

TABLE 1 | Description of attributes used in the decision model of soil biodiversity and habitat provisioning and their respective units used.

Type	Attribute	Unit	Description
E	Annual precipitation	mm	Average yearly precipitation
E	Average annual temperature	°C	Average yearly temperature
S	Soil pH	–	Soil pH, measured as pH ($CaCl_2$ soil: water 1:2.5)
S	Soil organic matter	%	Soil organic matter content in the topsoil
S	Thickness of organic layer	cm	Thickness of organic layer (A horizon)
S	Soil C:N ratio	–	Soil C:N ratio (Total C/Total N)
S	Soil N:P ratio	–	Soil N:P ratio (Total N/Total P)
S	Bacterial biomass	mg C/kg dry soil	Bacterial biomass
S	Fungal biomass	mg C/kg dry soil	Fungal biomass
S	Earthworm richness	# species per 100 individuals	Earthworm specie richness
S	Earthworm abundance	# m^{-2}	Earthworm abundance
S	Nematode richness	# genera per 150 individuals	Nematode genus richness
S	Nematode abundance	# 100 g^{-1} fresh soil	Nematode abundance
S	Microarthropod richness	# families per 100 individuals	Microarthropod family richness
S	Microarthropod abundance	# m^{-2}	Microarthropod abundance
S	Enchytraeid richness	# species per 70 individuals	Enchytraeid species richness
S	Enchytraeid abundance	# m^{-2}	Enchytraeid abundance
S	Soil texture	–	3 classes: WRB classification system
S	Soil bulk density	kg dm^{-3}	Soil bulk density
S	Groundwater table depth	m	Depth of groundwater table
M	Liming	Yes/no	Application of liming
M	Mineral N fertilization	kg N ha^{-1} y^{-1}	Amount of plant-available N applied per ha per year
M	Manure type	–	Type of manure applied (slurry, manure, compost, etc.)
M	Legume presence	%	Percentage of legumes in grassland
M	Chemical pest management	Yes/no	Application of chemical pesticides
M	Mechanical pest management	Yes/no	Application of mechanical weeding
M	Grassland type	–	Type of grassland
M	Grassland diversity	#	Number of grass/herb species sown
M	Grassland in rotation	Yes/no	Inclusion of grassland in rotation
M	Number of crops in rotation	#	Number of crop types during last 5 years
M	Type of crops in rotation	–	Cash crops, grass or grains, legumes, crop mixtures, and intercropping
M	Catch crops	#3 years	Frequency of catch crops in rotation during last 5 years
M	Tillage	–	No tillage, non-inversion or intermittent tillage, or conventional tillage
M	Stocking density	LSU ha^{-1}	Livestock density in Livestock units
M	Months in field	# month	Time spent in the field by livestock
M	Irrigation	Yes/no	Presence of sprinklers, drippers or ditches for providing water
M	Artificial drainage	Yes/no	Presence of tile drains, ditches, furrows, or pipes

on the SB function depending on the value of environmental (E), for example climatic zone, and management (M) attributes, for example application of manure or tillage. Similarly, particular management practices can be highly valued in one climatic zone, but may have little influence in other climatic zones. These differences in the model between climatic zones are not visible in the model structure, but threshold values have been created (based on available literature and expert knowledge) for each climatic zone separately, marking model responses as low, moderate or high per attribute (**Table 2**). Hence, the absolute value for any one attribute, may fall into category "high" in one climatic zone but "moderate" or even "low" in another climatic zone (for example, a soil pH($CaCl_2$) of 5 is considered "moderate" in the Atlantic zone, but "low" in the Mediterranean zone) (JRC, 2010b).

Following decision rules according to the method described by Bohanec et al. (2007) and Debeljak et al. (this issue) the basic attributes appear as the leaves of a decision tree and these are aggregated at multiple steps into small branches and then larger branches. The largest branches of the decision tree are referred to as "integrated attributes" (**Figure 1**). Four integrated attributes exist in the DEX model: (1) soil nutrient status: representing the pools and fluxes and availability of nutrients for plants and soil organisms (including C, N, P, K, and micronutrients); (2) soil biodiversity status: representing diversity, abundance, and activity of soil organisms and related management practices; (3) soil structure: representing information on soil structure, ranging from mesoscale (coarse fractions, soil texture classes, organic matter, air and water-filled space, density, and compaction) to macroscale (soil layers, terrain, slope); and (4) soil hydrological

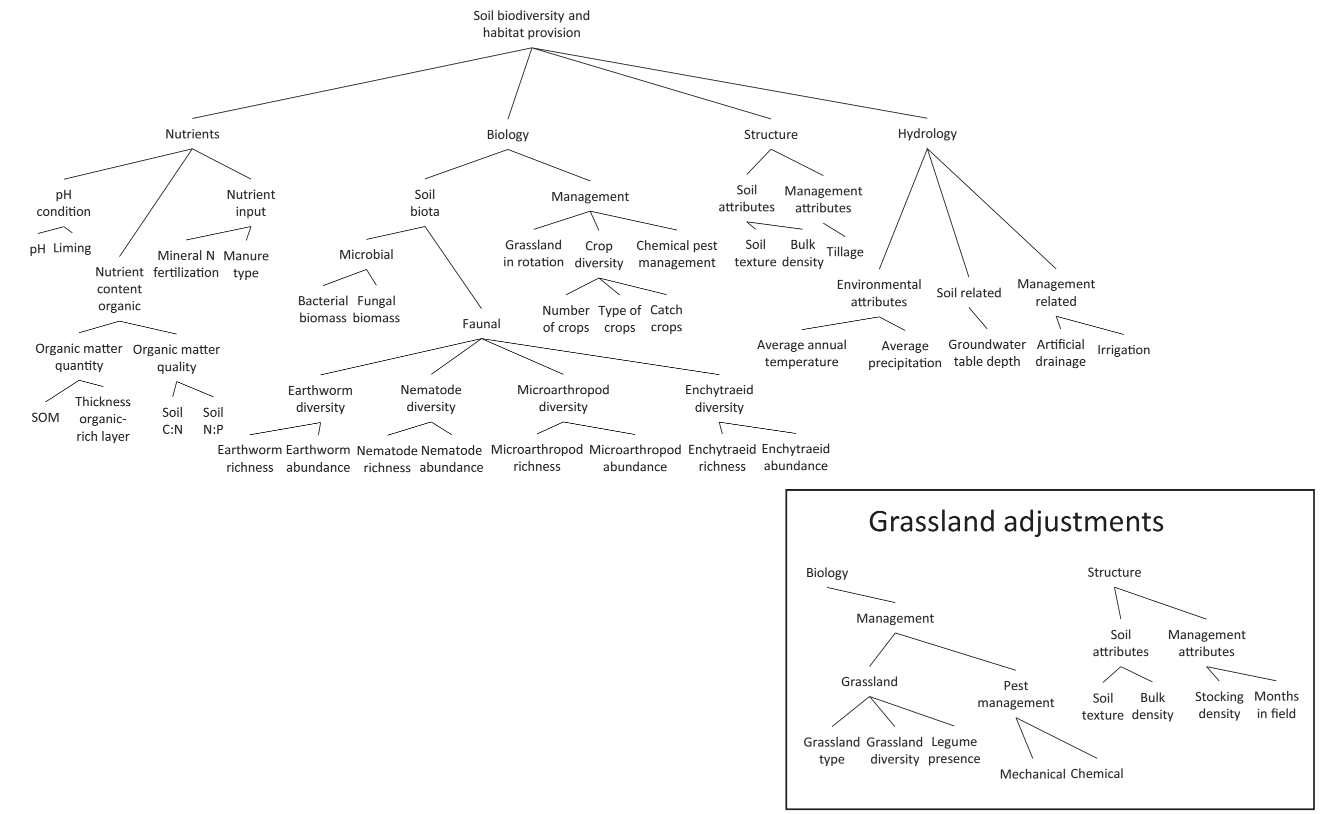

FIGURE 1 | Cropland model structure, showing the build-up of the soil function from basic attributes, via one or more aggregation steps, into four "integrated attributes" and finally to the holistic assessment of the SB function. Some of the management attributes in the integrated attributes biology and structure were changed to adjust the model to grassland cases (inset).

status: representing all processes and elements that contain information on the hydrological status of the soil, such as humidity, the flows of water, and drainage status. The combination of these four integrated attributes together provide the information for the assessment of the SB function in terms of "low," "moderate," and "high."

The decision rules of the model were defined by soil ecology experts (i.e., the authors of this paper, with the exception of Guenola Pérès who was an independent expert for the French sites). The threshold and categorical values of attributes to be used in the decisions rules can be found in **Table S1** (Supplementary section). At each stage of branching of the model, integration rules apply, for example, a "high" earthworm abundance and "low" earthworm richness lead to "moderate" earthworm diversity (Rutgers et al., 2016). Another example is that in acidic soils liming leads to a higher soil biodiversity, in particular for earthworms (McCallum et al., 2016). In this process of integrating attributes, some attributes were considered as more important than others, and thereby having a larger effect in the decision rules. The weights (importance) of attributes are presented in **Table 2**. There are two types of weights. Local weights represent the importance of an attribute for the following (or next) aggregated attribute, for example earthworm abundance and richness each count for 50% of earthworm diversity, at the next level of attributes, which by itself counts for 25% of the next level attribute "faunal." Global weights represent the importance of the attribute in the overall model, for example earthworm abundance then only determines 1% of the overall model output.

Two sub-models were developed, one for croplands (**Figure 1**) and one for grasslands (**Figure 1**-inset), which differed in incorporation of specific management practices, e.g., tillage and crop rotation characteristics in the cropland model, grazing and grass management characteristics in the grassland model. Also the threshold values of some attributes classifying data in low, moderate, or high classes are different between models. For example, in grassland most values of biological attributes (abundances, richness) are higher than in cropland due to the often lower agricultural land use intensity (Eggleton et al., 2005; Plassart et al., 2008; Rutgers et al., 2009; Cluzeau et al., 2012; Tsiafouli et al., 2015), and threshold values were set accordingly (higher in grasslands).

Netherlands Soil Monitoring Network Expert Assessment

As comparison for the DEX model we used a soil biodiversity/quality assessment obtained by expert judgements.

TABLE 2 | Weights of attributes in grassland and cropland models.

Attribute	Grassland		Cropland	
Soil biodiversity and habitat	**Local**	**Global**	**Local**	**Global**
Nutrients	39	39	38	38
pH condition	30	12	31	12
Liming	50	6	50	6
Soil pH	50	6	50	6
Nutrient content	35	14	38	15
Organic matter quantity	50	7	50	7
Soil organic matter	50	3	50	4
Thickness organic-rich layer	50	3	50	4
Organic quality	50	7	50	7
Soil C:N ratio	50	3	57	4
Soil N:P ratio	50	3	43	3
Nutrient inputs	35	14	31	12
Mineral N fertilization	50	7	50	6
Manure type	50	7	50	6
Biology	33	33	29	29
Soil biota	35	11	44	13
Faunal	50	6	50	6
Earthworm diversity	25	1	25	2
Earthworm richness	50	1	50	1
Earthworm abundance	50	1	50	1
Nematode diversity	25	1	25	2
Nematode richness	50	1	50	1
Nematode abundance	50	1	50	1
Microarthropod diversity	25	1	25	2
Microarthropod richness	50	1	50	1
Microarthropod abundance	50	1	50	1
Enchytraeid diversity	25	1	25	2
Enchytraeid richness	50	1	50	1
Enchytraeid abundance	50	1	50	1
Microbial	50	6	50	6
Bacterial biomass	50	3	50	3
Fungal biomass	50	3	50	3
Management*	65	21	NA	NA
Grassland	57	12	NA	NA
Grassland type	32	4	NA	NA
Grassland diversity	36	4	NA	NA
Legume presence	32	4	NA	NA
Pest management	43	9	NA	NA
Chemical pest management	67	6	NA	NA
Mechanical pest management	33	3	NA	NA
Management*	NA	NA	56	16
Grassland in rotation	NA	NA	34	5
Crop diversity	NA	NA	32	5
Number of crops in rotation	NA	NA	27	1
Type of crops in rotation	NA	NA	38	2
Catch crops	NA	NA	35	2
Chemical pest management	NA	NA	34	5
Structure	14	14	20	20
Soil attributes	50	7	50	10
Soil texture	50	4	50	5
Soil bulk density	50	4	50	5
Management attributes*	50	7	NA	NA
Stocking rate	50	4	NA	NA
Number of months in fields	50	4	NA	NA
Management attributes*	NA	NA	50	10
Tillage	NA	NA	100	10
Hydrology	14	14	13	13
Environmental attributes	33	5	33	4
Average annual temperature	17	1	17	1
Annual precipitation	83	4	83	4
Soil related	33	5	33	4
Groundwater table depth	100	5	100	4
Management related	33	5	33	4
Irrigation	50	2	50	2
Artificial drainage	50	2	50	2

*The weights are the result of the integration rules, and not determined beforehand. The Management sections marked with a *represent parts of the model trees that differ between the grassland and cropland models.*

The outcome of the DEX model for the 137 Dutch sites were compared with the expert ranking of the data from the Netherlands Soil Monitoring Network [NSMN; (Mulder et al., 2005a; Rutgers et al., 2009)]. In the NSMN biological and chemical soil attributes and land management attributes were analyzed in a routine procedure, each year with a sampling period in the spring (March–June) at approximately 40 sites. The monitoring and sampling design is described in Rutgers et al. (2009). In total, data from 137 grasslands (for dairy farming) on sand were selected from the first monitoring cycle from 1999 to 2003. This set was selected because some additional data on land management were also available. Four types of grasslands of dairy farms were present in the dataset: organic, conventional, intensive, and extensive dairy farms with an additional livestock system (pigs and/or poultry).

Eight professionals involved in the NSMN with track records in soil quality assessment were asked to use their expertise in soil and land management attributes and independently rank this set of 137 sites according to their estimation of the performance of the SB function. The judgements were based on biological information, including presence, abundance, activity and diversity of enchytraeids, earthworms, nematodes, micro-arthropods, bacteria, and soil management, including percentage of grassland and livestock density. For more details regarding the methods for analyzing the underlying data in the NSMN see Rutgers et al. (2009).

The following rules were applied for the ranking (between brackets the weight factor of the information contributing to the attribute score) (Schouten et al., 2014):

- Enchytraeid community: number of genera (2), abundance (4), percentage of *Friderica* species (1), Functional group diversity [1/ sum (0.0001+N^2)] (2)
- Earthworm community: abundance (4), number of taxa (2) percentage of litter decomposers (2) percentage of anecic earthworms (2), functional group diversity (1)
- Nematode community: abundance (1), Shannon diversity (3), Maturity index 2–5 (3), plant parasitic index (2), 1-NCR (nematode channel ratio) (2), percentage of CP1 nematodes (2), abundance of carnivore plus omnivore nematodes (1)
- Micro-arthropod community: total abundance (1), abundance of a-sexual long living micro-arthropods (1), abundance of phoretic species (1), abundance of nematode predators (1), abundance of general predators (1), abundance of parasite micro-arthropods (1), abundance of fungivore browsers (1)
- Bacterial processes: bacterial biomass (1), potential N mineralization rate (2)
- Bacterial metabolic diversity: hillslope of the community level physiological profile (CLPP) (1)
- Management attributes: percentage of grassland (1), 1/(livestock density) (1)

First, the 137 sites were ranked for each sub attribute. Subsequently the ranking score was multiplied by a weighting factor (also based on expert judgement) leading to a total score for all attributes and their weighting factors. Although the NSMN methodology includes valuation on the basis of management, information regarding management was sometimes missing, hence this was in this case not taken into account for the final ranking. The final ranking was used as an expert driven dataset with information on soil quality for the evaluation of the DEX model.

French (Brittany) Soil Biodiversity Monitoring Network Expert Assessment

A second dataset used for the comparison with output from the DEX model was obtained from the Soil Biodiversity Monitoring Network (RMQS-BioDiv) which is part of the French Soil Monitoring Network (RMQS). The RMQS was established to provide a national framework for observing changes in soil quality across France (Arrouays et al., 2002) and consisted of 2,200 sites located at the nodes of a 16-km grid that covered the French Metropolitan Territory. The RMQS-BioDiv is part of the RMQS but limited to the region of Brittany (West of France) and consisted of a total of 109 sites (https://ecobiosoil.univ-rennes1.fr/page/programme-rmqs-biodiv). Biological attributes were collected in 2006 or 2007 during the spring season, with sampling design and sampling protocol as described in (Cluzeau et al., 2012). Chemical and physical attributes correspond to the topsoil samples (0–30 cm) from Atlantic Central (Metzger et al., 2005) that were sampled as described previously in Martin et al. (2009). For environmental attributes, climatic data were obtained by interpolating observational data using the SAFRAN model (Quintana-Segui et al., 2008). The RMQS-BioDiv data were linked to the climatic data by finding for each RMQS site the closest node within the 12×12 km² climatic grid and then averaged for the 1990–2016 period. Altitude and slope information were derived from a digital elevation model (USGS, 2004). The crop attributes and management practices from the last 5 years, including the year in which the biodiversity was studied, were collected by an agricultural survey with the farmers. Due to differences in management information from one site to another, the percentage of legumes and catch crops in the rotation were calculated on maximum 5 years or less (if less information was available). In total, from the 109 sites, 52 sites (29 grasslands, 23 croplands) were selected where both biological attributes and other attributes were available.

The expert judgement of RMQS-BioDiv was carried out independently by one of the co-authors (GP) in order to evaluate this set of 52 sites. The evaluation was done following a separate expert judgement using an a priori approach. The judgments were based on (i) biological information including presence, abundance, and richness of earthworms, nematodes, bacteria, (ii) management attributes including fertilization (mineral vs. organic, solid vs. liquid), grazing and mowing intensity, percentage of grassland, tillage, type of crops, (iii) soil properties including pH, organic matter content, bulk density and organic layer thickness. The thresholds used were independent from those used for the NSMN sites.

The following rules were applied for the evaluation (between brackets the weight of factor of the information contributing to the attributes score, based on expert judgement):

- Earthworm community: abundance (4), number of taxa (2)
- Nematodes community: abundance (1), Shannon diversity (3)
- Bacterial processes: bacterial biomass (1)
- Management attributes: fertilization (3), grazing and mowing intensity (1), percentage of grassland (3), tillage (3), type of crop (1)
- Soil properties: pH (1), organic matter content (1), bulk density (1) and organic layer thickness (1).

The sites were ranked based on the sum of weighted attributes, and the cut-off between high, moderate and low evaluations was based on quantiles, i.e., the highest 13 sites (1st quantile), were ranked as "high," the lowest 13 sites (4th quantile) were ranked as "low," and the 26 sites in between as "moderate."

Statistical Comparison

The analyses of the two test datasets both produced values of the performance of the SB function in terms of "low," "moderate" and "high." For the Netherlands dataset we made two comparisons between the output of the two approaches, one for the full set of 137 farms, and one for a subset of 50 farms (top and bottom 25 farms from the ranked list). The two stage process was adopted because we expected a large variation in the assessments which resulted in moderate and low performance (see discussion section). For the French data-set we made one comparison of the two approaches using all 52 soils and by distinguishing the SB is the three categories "low," "moderate" and "high." For all comparisons, we calculated three measures of similarity in output. First, we calculated the Pearson correlation coefficients between the two outputs (DEX model and expert weighted ranking) (scoring low as "1," moderate as "2" and high as "3"). Second, we quantified a similarity index in output by assigning values to the fit, i.e., a score of "+1" when both outputs had the same performance, a score of "0" when the two outputs gave different, but not contrasting performance, i.e., "low" vs. "moderate," or "moderate" vs. "high," and a score of "−1" when the two outputs predict contrasting performance, i.e., "low" vs. "high." When both outputs produced completely random results, the overall value is slightly positive (0.11). Third, we counted the number of perfect fits, i.e., the percentage of "+1" scores. With random models this percentage would be 33.3%.

In addition, we performed a sensitivity analysis of the DEX model for missing data and for the contribution of each category of attributes. For each of the sensitivity runs we calculated all three values of similarity between the results of the DEX model in comparison to the expert weighted rankings.

RESULTS

A multi-attribute DEX model was built for quantifying the SB function with two sub-models for grassland and cropland management systems. To complement the assemblage of DEX models for three other soil functions (described elsewhere in this issue). Together with the nutrient cycling and regulation function of soils (Schröder et al., 2016) this set of five soil functions embraces the major contributions of soils to deliver a coherent set of most important ecosystem services to society.

Model Performance

The comparison between the DEX model and the ranking based on expert judgement was made for both the 137 grassland soils from the Netherlands (Schouten et al. (2014) and for the 52 soils from Brittany France. For the Dutch soils, two comparisons were made, one using all 137 sites, using the categories "low," "moderate," and "high" (**Figure 2**), and one using the 25 "low" ranked and 25 "high" ranked sites. For the French soil only a comparison using all 52 sites was made, and using the same categories as the Dutch sites, i.e., "low," "moderate," and "high" (**Figure 3**).

For the 137 sites from The Netherlands we found a statistically significant positive Pearson correlation coefficient between the model and the expert weighted ranking ($r = 0.35$, $p < 0.01$), with 43% correctly evaluated (**Table 3B**). Restricting the analyses to the 25 "low" and 25 "high" sites, we found a higher statistically significant positive Pearson correlation coefficient between the model and the expert weighted ranking ($r = 0.53$, $p < 0.001$), with 54% correctly evaluated (**Table 3A**).

The similarity index value of goodness of fit was made by assigning the value of −1 to sites with a contrasting prediction, the value of 0 to sites that had different predictions, i.e., "low" vs. "moderate" or "moderate" vs. "high, and +1 when both approaches gave the same prediction. Hence, with a random generated model the goodness of fit parameter should be (around) 0 (zero), while if the DEX model predictions and expert weighted rankings always result in the same prediction, the similarity index has a value of 1. Using the 25 "low" ranked and 25 "high" ranked sites we found a similarity index of 0.38 and using the 137 sites a similarity index of 0.37.

For the set of 52 grassland soils from Brittany France we found a significant positive Pearson correlation coefficient between the outcome of the DEX model and the expert weighted rankings ($r = 0.57$, $p < 0.001$), with 58% correctly evaluated (**Table 3C**).

It should be noted that when we had used random models the percentages predicted correctly would have been 33.3% using all sites divided over the three categories, and 50% using the 50 Dutch sites divided over two categories. This means that we have an improved prediction of 4 and 10% for the two analyses of the Dutch sites and an improved prediction of 25% for the French soils.

Sensitivity Analysis

To assess the sensitivity of the model to data inputs we excluded data for each of the four integrated attributes one by one, where the decrease in correlation coefficient gives an indication how much the data is needed for model accuracy. We performed this sensitivity analysis for the Dutch dataset of 25 "low" and 25 "high" sites, for the Dutch sites including all 137 sites, and for the French sites including all 52 sites.

For the 25 "low" and 25 "high" sites the results are given in **Table 3A**, for the 137 sites in **Table 3B**, and for the 52 French sites in **Table 3C**. The clearest conclusion from all analyses is that information on nutrients is critical. This includes dominant attributes such as pH, SOM content, C-N ratio. Also, the high global weight of this integrated attribute explains the relative dominance of information on the nutrient status on the SB function. From the comparison with the French data also the presence of data on soil organisms came out as important. Furthermore, all analyses showed that parameters in the integrated attribute hydrology that were excluded and didn't have any effect were average temperature and average annual precipitation. Excluding data for these parameters leads to default values that are quite similar and did not change the model performance.

Data for irrigation and drainage were not available for the full model in the Netherlands, but information for these attributes was included for many of the French soils. An important remark here: when data for some attributes is not provided, the model assumes default values, which often represent the moderate category. Hence, if the dataset used for validation contains many farms in the category moderate, removing input values leads to a better fit (the more input values are missing, the higher the change that the model output will be moderate). Therefore, we consider the sensitivity analysis presented in **Table 3A** as the better assessment, as no moderate farms were included here.

DISCUSSION

The results show that the proposed DEX model for the SB function was meaningful, i.e., the outputs were positively and statistically significant correlated with the rankings based on independent expert judgements on the status of the SB function at 137 grasslands in the Netherlands (sandy soils, Atlantic climate) and 52 sites in France, 29 grasslands and 23 croplands. Yet, in a substantial number of cases the two approaches

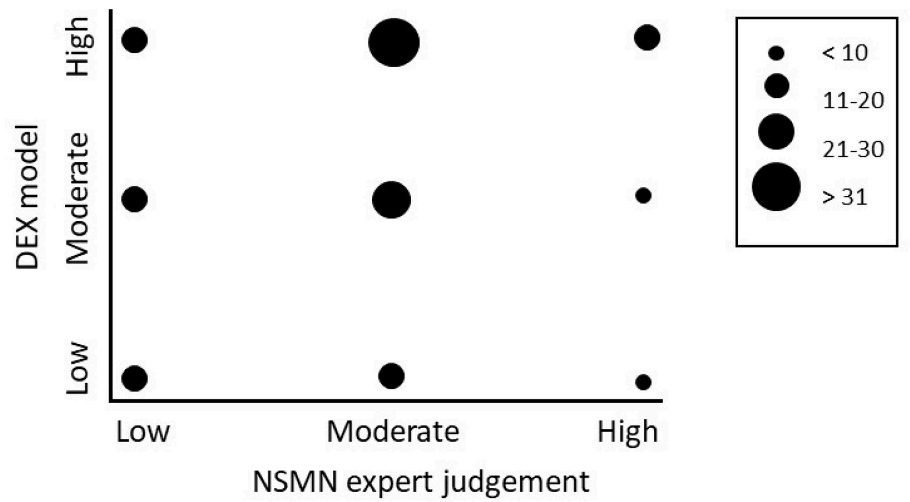

FIGURE 2 | Comparison of the output of the DEX model with the expert judgements on 137 sites in the NSMN in the Netherlands. In the ranking of the sites, the top 25 was classified as "high performance," the bottom 25 sites were scored as "low performance" and all in between as "moderate." Bubbles represent the number of sites scoring a particular combination.

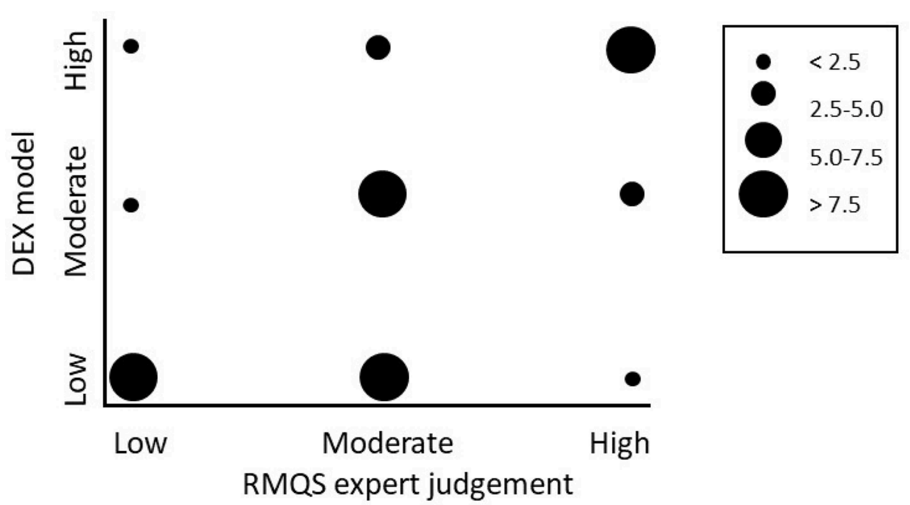

FIGURE 3 | Comparison of the output of the Decision support model with the expert judgements on the 52 soils from sites in the RMQS in Brittany France. In the ranking of the sites, 13 sites were classified as "high" performance, 13 sites were scored as "low" performance and all in between (26 sites) as "moderate." Bubbles represent the number of sites scoring a particular combination.

predicted different performance. When we look at the similarity indices we found values of 0.38 (50 Dutch sites), 0.37 (137 Dutch sites) and 0.54 (52 French sites), all clearly above 0 (zero).

For the Dutch soils, the percentage of correct predictions were relatively low. Using all 137 soil this percentage was 43%, which is 10% higher than the random null model (which would have been 33% correctly predicted by chance), and using the 50 sites it was 58%, again only 8% higher than a random null model (which would have been 50% correctly predicted by chance). The percentage of correct prediction was much higher using the 52 French sites, i.e., 58% which is 25% higher than with a random null model. Overall, we therefore conclude that both the DEX model and the expert weighted ranking seem in line when it comes to the assessment of the SB function.

The differences between the performance of the model with respect to the Dutch and French datasets may arise from three circumstances:

First, looking at the data available for the French sites we might assume that the significantly higher correct prediction is at least partly due to the available information regarding land use and soil management. In the Netherlands, this information had limited availability and was not used for the expert weighted ranking of the sites. Consequently, the ranking in the Netherlands was only based on information from soil biological

TABLE 3A | Outcome of the sensitivity analysis using the 25 "low" and 25 "high" sites.

Model ($n = 50$)	Correlation coefficient	*P*-value	Similarity	Perfect fit
Full model	0.525	<0.001	0.38	0.54
Nutrients excluded	0.378	0.007	0.26	0.4
Biology excluded	0.464	<0.001	0.22	0.44
Structure excluded	0.493	0.003	0.4	0.58
Hydrology excluded	0.525	<0.001	0.38	0.54

TABLE 3B | Outcome of the sensitivity analysis using the 137 Dutch sites.

Model ($n = 137$)	Correlation coefficient	*P*-value	Similarity	Perfect fit
Full model	0.347	<0.001	0.37	0.43
Nutrients excluded	0.248	<0.001	0.43	0.48
Biology excluded	0.281	<0.001	0.29	0.37
Structure excluded	0.310	<0.001	0.33	0.39
Hydrology excluded	0.347	<0.001	0.37	0.43

TABLE 3C | Outcome of the sensitivity analysis using the 52 French sites.

Model ($n = 52$)	Correlation coefficient	*P*-value	Similarity	Perfect fit
Full model	0.565	<0.001	0.54	0.58
Nutrients excluded	0.597	<0.022	0.54	0.56
Biology excluded	0.372	0.002	0.38	0.44
Structure excluded	0.548	<0.001	0.54	0.58
Hydrology excluded	0.565	<0.001	0.54	0.58

attributes, which were collected over a larger time span of time (6 years) and from a somewhat larger geographically area which adds to the variation in the observations.

Differences in the methodological approaches can also explain the differences. Differences in sampling protocols can be a reason for differences in performance. For instance, in the Netherlands the samples in the NSMN were mixed at the farm level (Rutgers et al., 2009), while in France the samples in the RMQS were mixed according to small plots with a fixed orientation (Cluzeau et al., 2012).

Interestingly, it seems that soils which were assessed as having a "high" biodiversity were more often predicted right (i.e., as similar in both approaches), than soils with "low" or "moderate" performances. Probably disturbed soils with respect to the SB function are more different from each other than soils with a healthy soil life. One aspect might be the variability in types and levels of disturbances, resulting in differences in disturbed soils, which are more difficult to predict correctly.

The most important category of attribute in the assessment of the SB function was found to be the nutrient status of the soil. This was found for especially the Dutch soils. This clearly shows the interrelationship between the SB function and the nutrient cycling function (Schröder et al., 2016), and the importance of soil pH for soil biodiversity (Griffiths et al., 2016). Although the goodness of fit clearly dropped when leaving out information on soil organisms from the French data, it is interesting to note that the predictions of the DEX model, without information on soil biological attributes, were still significantly positively correlated with the expert judgements based on soil biological information.

The DEX model for the SB function was developed for a European-wide application to assess five soil functions in agricultural soils. However, the present results with the SB function suggest some caution, as there were several major restrictions in this study. First, the comparison was restricted to one climatic zone (Atlantic). Unfortunately, no better independent datasets were available that could have been used as a tool for validation for the other climatic zones. Although the present comparisons were not ideal for testing of the DEX model, we think it is based on the currently best available data and can therefore be seen as a first step of testing the performance of the model. As such it can be a starting point of our future aim to build a comprehensive model for Europe, fully including cropland, all different soil types and climatic zones. Although for some countries detailed data for a large number of attributes is available (for example from the Netherlands, Ireland, and France, dominant in the Atlantic climatic zone), testing the model properly throughout Europe requires data from all (climatic zone $\times$ soil type $\times$ land use) categories. Recently, the introduction of the General Data Protection Regulation of the EU has however added another complicating factor in gathering and storing management information from farms, limiting the available data sources to be used in European wide biodiversity assessments.

Second, the approach distinguished only three broad output categories (i.e., in "low," "moderate," and "high" categories), starting from quantitative data. This has two consequences; on the one hand, the categorization makes the data input less critical, as only classes of values are needed as an input, which is easier to provide, and the output is an estimate of the soils' capacity to support the SB function. On the other hand, the categorization requires a lot of expert knowledge and reference data for setting the threshold values for each attribute within each climatic zone. For example, the soil pH is on average higher in the Mediterranean area than in the Atlantic area, while soil organic matter content shows the opposite pattern (JRC, 2010a).

Furthermore, with only three output categories, the DEX model is insensitive to small changes in the values of the input data for the attributes. Only if a sufficient number of thresholds is passed, a switch to another performance can be expected. Debeljak et al. (this issue) discussed advantages and disadvantages of this. For instance semi-quantitative modeling makes the model easier to run with a simple interface for farmers and farm advisors, the "Soil Navigator." With the Soil Navigator and the outputs of the DEX models, it is possible to set preferences for soil functions, and explore management options to reach these targets. Finally it is possible to build continuous quantitative models based on the DEX trees for the five soil functions, in order to improve sensitivity.

Third, all the data collected in the datasets used were collected for other reasons than validation of the DEX model (both were part of soil monitoring programs) and therefore present incomplete data inputs which were not optimally designed to test a holistic assessment of the soil biodiversity function, with a broad set of attributes such as compiled in the DEX model. In general, soil data are collected without a solid basis in analyzing soil biological attributes, and very often with no or poor information on soil management attributes, in particular for the Dutch sites. The Dutch soil monitoring system was designed to capture the biological soil attributes, with few attributes for nutrient condition, structure, and hydrologic condition.

The performance of the DEX model might be significantly improved when more data are available about land use and farm management, as can be seen from the results obtained for the French sites. The more data that exists at field, farm or local level and that can be fed into the model, the better the accuracy of the output will be. For example, when more detailed data on soil texture or organic matter quality is available, this can be easily implemented and will most likely improve the model output through reducing uncertainty. Ultimately, the data provided by the farmer, on for example management practices or plant available nutrients at the plot scale, will also lead to better predictions.

The conceptual structure of the DEX model for the SB function is based on the notion that we have to deal with a multidimensional concept for which no unified proxy-indicator system exists, and that we have very few standardized and reliable data for producing quantitative predictions for the SB function. Consequently, any source of information which could be plausibly linked to quantification of the SB function was appreciated, even if the data is of chemical (such as pH, nutrients, water) or physical (such as temperature, slope, soil structure) origin. The idea to use all information there is to quantify soil functions, was also applied in other contributions (Rutgers et al., 2012; Van Wijnen et al., 2012; Wagg et al., 2014). The structure of the decision tree of the DEX model represents an improvement to the former studies, as four integrated attributes were agreed and combined: nutrient status, soil biology status, structure and hydrological status. In this way information from different origins can be transparently processed in a quantification system for the SB function, and new environmental data can also be implemented easier, and reduce uncertainty in the assessment.

Progress in monitoring and improving the SB function of soils will most strongly depend on the farmers' and stakeholders' acceptance of the importance of this function. Even though primary productivity, high yields and short term profitability is bound to be the main focus for contemporary agriculture, there is acknowledgment in the farming community that our intensive way of farming is not sustainable when environmental and public health trade-offs are not taken into account. In order to combat the loss of fertile soil and to counteract these trade-offs, many farmer initiatives are adopted in all EU member states, such as the 'Initiative Agriculture de conservation in France (https://agriculture-de-conservation.com) and Veldleeuwerik in the Netherlands (www.veldleeuwerik.nl). Based on the LANDMARK stakeholder workshops (Sturel et al., 2018) it is evident that the SB function has a positive connotation for most farmers and is even associated with the concept of life itself, i.e., in Germany and Austria the soil function is recognized as "Soil life" in France as "Living soil" and in Ireland as "Active and healthy soil." Furthermore, the same stakeholders associate soil biodiversity often to sustaining aboveground biodiversity, thereby adopting the concept of a system approach with living soils as an integral part of healthy ecosystems. For instance, earthworms are the staple feed for some field birds, like the black-tailed godwit in the Netherlands. High metal (Pb, Cu) concentrations in peatland had negative effects on the earthworm community (lower average body weight, and total biomass) with effects accumulating in the bird population (Klok et al., 2006; Roodbergen et al., 2008). Future developments in the assessment of the SB function should addressing this aspect of habitat provision in a broad sense, as in its present form the assessment has no specific linkage to any aboveground biodiversity target (protection of a species, a nature target type, etc.).

In conclusion, the present DEX model predictions of the SB function are converging to the current and combined expert judgements of the SB function. In this way, quantification of the SB function, together with the quantification of the other four soil functions (Schröder et al., 2016; Sandén et al., 2019; and described elsewhere in this issue) is better placed in our attempts to optimize the multiple soil functions in agricultural landscapes, and hence the multifaceted role of soils to deliver a bundle of ecosystem services for farmers and citizens, and supporting land management and policy toward a more sustainable society.

DATA AVAILABILITY

Requests to access the raw data supporting the conclusions of this manuscript should be directed to the corresponding author.

AUTHOR CONTRIBUTIONS

JvL: model development, validation, and writing. RC: conceptual framework, writing. CP, DC and GP: acquisition and analysis of French data. MD, AT, VK and GV: model development. FG, CM, and IT-G: conceptual framework. CH: development of decision support system. NS: database management. MR: conceptual framework, acquisition and analysis of Dutch data, writing.

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SUPPLEMENTARY MATERIAL

The Supplementary Material for this article can be found online at: https://www.frontiersin.org/articles/10.3389/fenvs.2019.00113/full#supplementary-material

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Assessing the Climate Regulation Potential of Agricultural Soils Using a Decision Support Tool Adapted to Stakeholders' Needs and Possibilities

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Soils perform many functions that are vital to societies, among which their capability to regulate global climate has received much attention over the past decades. An assessment of the extent to which soils perform a specific function is not only important to appropriately value their current capacity, but also to make well-informed decisions about how and where to change soil management to align the delivered soil functions with societal demands. To obtain an overview of the capacity of soils to perform different functions, accurate and easy-to-use models are necessary. A problem with most currently-available models is that data requirements often exceed data availability, while generally a high level of expert knowledge is necessary to apply these models. Therefore, we developed a qualitative model to assess how agricultural soils function with respect to climate regulation. The model is driven by inputs about agricultural management practices, soil properties and environmental conditions. To reduce data requirements on stakeholders, the 17 input variables are classified into either (1) three classes: low, medium and high or (2) the presence or absence of a management practice. These inputs are combined using a decision tree with internal integration rules to obtain an estimate of the magnitude of N_2O emissions and carbon sequestration. These two variables are subsequently combined into an estimate of the capacity of a soil to perform the climate regulation function. The model was tested using data from long-term field experiments across Europe. This showed that the model is generally able to adequately assess this soil function across a range of environments under different management practices. In a next step, this model will be combined with models to assess other soil functions (soil biodiversity, primary productivity, nutrient cycling and water regulation and purification). This will allow the assessment of trade-offs between these soil functions for agricultural land across Europe.

Keywords: soil functions, climate regulation, carbon sequestration, N_2O emissions, agroecosystems, qualitative decision modeling

INTRODUCTION

Soils in agroecosystems play an important role regulating the global climate as they have contributed substantially to the increase in atmospheric greenhouse gases such as carbon dioxide (CO_2) and nitrous oxide (N_2O) during the past centuries (Ciais et al., 2013; Le Quéré et al., 2018). The conversion of soil organic carbon (SOC) to CO_2 in agroecosystems mainly occurs as a consequence of the conversion of native vegetation to arable land. This process results in an average loss of topsoil organic carbon (OC) of ca. 32 ± 20 % in temperate regions (Poeplau et al., 2011). N_2O is mainly emitted as a consequence of microbial transformations of fertilizer containing reactive nitrogen (N) that is applied on agricultural land. N_2O emissions occur both directly after application on the field or indirectly, after reactive N has been transferred to other ecosystems, as nitrate (NO_3^-) losses or ammonia (NH_3) emissions (Galloway et al., 2003; Zhou et al., 2017). These emissions are not trivial, as greenhouse gas emissions from agroecosystems have constituted ca. 11.2 % of total emissions (mainly as N_2O and CH_4), while the share resulting from land use changes associated with food production was ca. 10.0 % in 2010 (mainly as CO_2) (Tubiello et al., 2015).

The regulation of the global climate is thus an important ecosystem function that soils perform through carbon storage and a reduction of greenhouse gas emissions, referred to as the climate regulation soil function. This soil function is defined here as the capacity of a soil to reduce the negative impact of increased greenhouse gas emissions on climate, among which its capacity to store carbon (C) and to minimize N_2O emissions. In line with the recognition of the importance of the climate regulating function of soils (Schulte et al., 2014), the *4 per mille Initiative: Soils for Food Security and Climate* has been proposed (https://www.4p1000.org/). This initiative aims to increase the amount of OC in soils around the world, not only to reduce atmospheric CO_2 concentrations, but also to improve food production and mitigate soil degradation. The *4 per mille* initiative has received many criticisms (Minasny et al., 2018), mainly related to the magnitude of achievable gains in SOC over the coming decades and social and economic constraints, despite the many benefits associated with increasing SOC stocks (Paustian et al., 2016; Chabbi et al., 2017; Soussana et al., 2017).

Although uncertainties about the achievable magnitude of future soil C sequestration exist, many long-term experiments (LTEs) have shown that the consistent application of certain management practices does increase the OC content of agricultural soils (Paustian et al., 1997; Ogle et al., 2005; Minasny et al., 2017; Chenu et al., 2018). An increase in SOC stocks is achievable through management practices that increase C inputs to the soil, such as the addition of organic fertilizers (Haynes and Naidu, 1998; Sandén et al., 2018), the incorporation of crop residues in the soil after harvest (Lehtinen et al., 2014) or the cultivation of cover crops (Poeplau and Don, 2015). In contrast, practices that aim to reduce SOC losses, such as no-till, generally lead to a mere redistribution of OC along the soil profile while not significantly increasing total SOC stocks (Luo et al., 2010; Powlson et al., 2014). The application of no-till combined with an increase in C inputs to the soils has, however, been shown to be an effective strategy to increase the SOC content (Luo et al., 2010; Virto et al., 2012). When discussing changes in SOC stocks through changes in management practices, two important considerations have to be taken into account (Minasny et al., 2017; Chenu et al., 2018). First, the efficiency with which SOC stocks are increased is negatively correlated to the initial SOC stock. Second, the rate of the increase in SOC stocks is highest in the first years after the initiation of improved management practices and decreases substantially in the following years or decades. Both effects are a consequence of the maximum amount of OC that can be stored in mineral soils, as a function of the applied management (Six et al., 2002; Stewart et al., 2007; Castellano et al., 2015).

Although increasing the OC content of soils can lead to a net removal of CO_2 from the atmosphere, trade-offs with N_2O emissions should be taken into account, as these can reduce or completely offset the climate mitigation effect of certain management practices (Gao et al., 2018). For example, while the application of farmyard manure (FYM) can significantly increase topsoil OC stocks (Bai et al., 2018; Sandén et al., 2018, 2019b), an accompanying increase in N_2O emissions can offset this benefit (Zhou et al., 2017). Similar observations have been made for crop rotations including cover crops, which can increase topsoil OC stocks significantly (Poeplau and Don, 2015), while N_2O emissions can increase substantially when their biomass is decomposed (Basche et al., 2014). The same pattern has been observed in a modeling study at the European scale by Lugato et al. (2018), who found that the climate mitigation obtained by increasing SOC stocks can be canceled out by increased N_2O emissions due to changing management practices in the long term. Also the practice of crop residue incorporation has been shown to increase losses of reactive N in the form of N_2O and NH_3, despite its positive effect on the SOC content of upland soils (Xia et al., 2018). In contrast, also positive interactions are possible. For example, the potential of cover crops to uptake nitrate (NO_3^-) can substantially decrease indirect N_2O emissions and therefore increase their climate mitigation potential (Tonitto et al., 2006; Basche et al., 2014). These trade-offs thus show that the climate regulation potential of soils in agroecosystems depends on both C sequestration and losses of reactive N species, such as N_2O, NH_3, and NO_3^-.

A thorough evaluation of the climate regulation function of soils in agroecosystems therefore requires a holistic assessment of the effect of different management practices on this soil function (Vogel et al., 2018). In addition, interactions between different management practices, the effect of local environmental conditions and trade-offs between C sequestration and losses of reactive N need to be taken into account. As a consequence, evaluating the climate regulation function of soils is not straightforward, with models generally being used to achieve this goal. Ideally, these models should assess different aspects of this soil function for a given combination of environmental conditions and management practices based on knowledge of the relevant processes. In addition, these models should be simple enough to be applicable by non-expert users, while providing reliable simulations based on the limited amount of data that is generally at hand.

A problem associated with existing models is that data requirements often exceed available data, which limits their application to a regional or national scale. For example, the 1D-ICZ (one-dimensional Integrated Critical Zone) model quantifies four different soil functions (biomass production, C and nutrient sequestration, water filtration and biodiversity) using process-based simulations at the soil profile scale (Giannakis et al., 2017), with a focus on the simulation of temporal changes in soil structure and aggregate dynamics. Although these types of models greatly improve our ability to use process understanding to quantify different soil functions, the simulation of these processes requires a large amount of data, while the range of management practices on which this model has been tested is currently still limited (Kotronakis et al., 2017). Other existing tools that have been developed to quantify different soil functions have been calibrated for North America [Fieldprint calculator (https://calculator.fieldtomarket.org), Comet-Farm (http://cometfarm.nrel.colostate.edu/) and HOLOS (Little et al., 2008)] or the global scale (Coolfarm (https://coolfarmtool.org/), which may limit their applicability to European agroecosystems.

To overcome these problems, we developed a relatively simple, qualitative model to assess the climate regulation potential of agricultural soils that can be coupled to similarly structured models assessing other soil functions. This qualitative model aims to inform different stakeholders, such as farmers or farm advisors, about the directional effects of combinations of different agricultural practices on the climate regulation capacity of mineral, non-peatland, agricultural soils. The aim of this tool is not to provide a detailed quantitative assessment of different fluxes of greenhouse gases from agricultural soils, as other tools are available to achieve this [e.g., DayCent; (Parton et al., 1998) or DNDC; (Li et al., 1992)]. Rather, this tool provides the user with qualitative information regarding the capacity of an agricultural soil to perform the climate regulation function. In addition, the aim of this tool is to increase awareness among model users about the multifunctionality of agricultural soils, and the existence of important trade-offs between the performance of these soil functions as a consequence of the applied management. The model has been developed in the framework of the Horizon 2020 Landmark project, which aims to quantify the current and potential supply of different soil functions from farm scale application to the scale of Europe. These are (i) primary productivity, (ii) water regulation and purification, (iii) soil biodiversity and habitat provision, (iv) nutrient cycling and provision and (v) climate regulation. To achieve this goal, decision support tools for every soil function have been developed. These tools have been brought together to assess the trade-offs between different soil functions for a given set of management practices across Europe (Debeljak et al., 2019). The main aims of this paper are (1) to present the model developed to assess the climate regulation function of agricultural soils and (2) to test this model based on available data from long-term field experiments across Europe.

MATERIALS AND METHODS

Model Description

The model has been developed based on the rationale that it should make a reliable assessment of the climate regulation function of agricultural soils based on data that is readily available. It is built using multi-criteria decision analyses, in particular the DEX (Decision Expert) integrative methodology for qualitative decision modeling (Bohanec and Rajkovič, 1990; Bohanec et al., 2013; Bohanec, 2017). Using this methodology, the main decision problem (assessing the climate regulation soil function) is broken down into smaller, less complex sub-problems in a hierarchical way. The main concept (the climate regulation soil function) is at the top of the hierarchy and is related to lower-level attributes on which it depends. These attributes represent the characteristics of the system, which are environmental variables, soil properties and management practices. The attributes on the lowest level of the hierarchy are the basic attributes. The intermediate attributes are obtained using integration rules, which also determine how the attributes are combined into the final climate regulation function.

The developed model has two distinct parts that separately simulate (i) C sequestration and (ii) N_2O emissions, both direct (from soils) and indirect (originated from NH_3 volatilization/deposition or NO_3^- leaching) (**Figure 1**), as presented in more detail in the following sections. Although the term ‘C sequestration’ is generally used to describe changes in the SOC stock that result from a net transfer of C from the atmosphere to the soil (Powlson et al., 2011; Chenu et al., 2018), this term is used here in the broad sense of the capacity of a soil to store C. The assessments are made for the upper 0.3 m of agricultural soils. If one aims to evaluate the current climate regulation function of a soil, input data should represent the average environmental conditions and management practices for the past 5 years. This time span was chosen to account for previous management practices, while avoiding problems with providing the average management for a longer period of time, which might be characterized by multiple changes in management practices. If the aim is to evaluate the effect of potential future management practices, input data should represent the current conditions with the desired change in management practices adjusted accordingly, with predictions being made for the medium term (<10 years). It is noted that the model does not account for potential legacy effects from a previous land use. Consequently, the model only provides information about the effect of the applied management practices on the climate regulation soil function. In the model, all attributes are classified into the categorical variables “low,” “medium,” and “high,” or “yes” and “no.” Thresholds to classify quantitative variables into these categories were agreed upon by the members of the Landmark project, as shown in **Table 1**. The model result, i.e., how well a soil performs the climate regulation function, is similarly expressed as “low,” “medium,” or “high.” The latter categories are not explicitly coupled to a quantitative value, due to the lack of a quantitative definition of this soil function. The model has been developed to be applicable to agroecosystems throughout Europe, regardless of crop type.

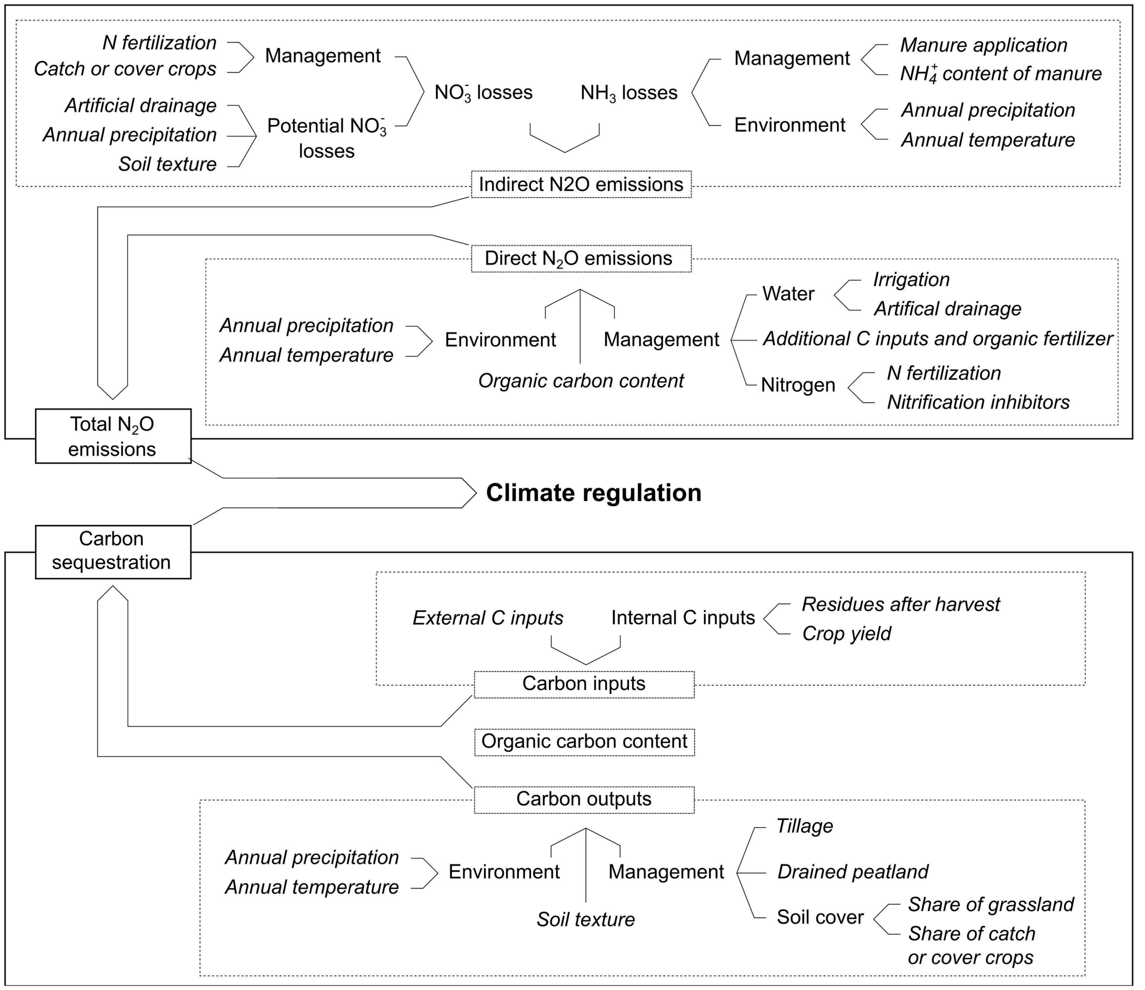

FIGURE 1 | Structure of the model assessing the climate regulation soil function. Input attributes (shown in italic) are classified into "low," "medium," and "high," or "yes" and "no," as shown in **Table 1**. Internal integration rules determine how input attributes are combined into the final climate regulation function, which is similarly classified into "low," "medium," and "high".

More information about how different management practices are translated into model input variables is provided in **Table 1**.

Nitrous Oxide Emissions

The model simulates direct and indirect N_2O emissions separately. Direct emissions are considered as emissions occurring *in-situ* in the field, as a result of the nitrification and denitrification of mineral N derived from applied fertilizer or mineralized organic N. The two sources of reactive N in the model are (i) mineral N fertilizer and (ii) additional C inputs and organic fertilizers (e.g., farmyard manure, slurry and plow-in crop residues). Together with attributes influencing the moisture content of the soil (irrigation and artificial drainage), the magnitude of N inputs determines how management practices influence direct N_2O emissions. The integration rules that determine how the rate of N inputs affects total N_2O emissions are chosen so that the N_2O emissions increase with increasing rates of N application. This is in line with empirical observations, showing that once the amount of applied N exceeds the crop demand, N_2O emissions increase exponentially with every additional unit of applied N (Bouwman et al., 2002; Hoben et al., 2011; Shcherbak et al., 2014). The calculated magnitude of N_2O emissions is further constrained by climatic conditions [N_2O emissions are enhanced by high values of average annual temperature and precipitation, with a higher weight assigned to precipitation (Groffman and Tiedje, 1991; Barnard et al., 2006; Butterbach-Bahl et al., 2013)] and the SOC concentration (high OC concentrations increase N_2O production by providing a substrate for denitrifying bacteria).

Indirect N_2O emissions are the result of the management applied on the field, but occur at downstream locations due to cascading effects (Syakila and Kroeze, 2011; Butterbach-Bahl et al., 2013). The two simulated sources of indirect N_2O emissions occur after leaching of nitrate (NO_3^-) to groundwater, or after NH_3 emissions that are deposited back on the soil surface (Sommer and Hutchings, 2001; Galloway et al., 2003).

TABLE 1 | Thresholds used to categorize input variables into "low," "medium," and "high," or "yes" or "no". Input variable should reflect the average management practices for the past 5 years, while temperature and precipitation inputs should be based on climatic data (30-year average).

		Categories	
Environmental variables			
Temperature (°C)	Low: <6	Medium: 6–10	High: >10
Precipitation (mm yr^{-1})	Low: <400	Medium: 400–900	High: >900
Soil texture	Clayey	Silty	Sandy
Management variables			
Manure application		Yes/No	
NH_4^+ content of manure	Low: Cattle slurry and solid manure; cattle and pig litter; liquid cattle manure		High: Pig and poultry slurry and solid manure; poultry litter
N fertilizer (kg N ha^{-1} yr^{-1})	Low: <50	Medium: 50–100	High: >100
Nitrification inhibitors		Yes/No	
External C inputs for C sequestration	None	Slurry, sewage sludge, digestates	Farmyard manure, compost
Additional C inputs for N_2O emissions	None	Farmyard manure	Slurry, sewage sludge, residues from the main crop, catch crops and cover crops
Organic carbon content (%)	<1	1–3	>3
Tillage	No-till	Non-inversion tillage	Inversion tillage
Residues after harvest left on the field[a] (% of yield)	<10	10–30	>30
Artificial drainage		Yes/No	
Irrigation		Yes/No	
Share of catch or cover crops (years in last 5 years)[b]	<1	1–3	>3
Share of grassland (years present in last 5 years)[b]	<1	1–2	>2
Crop yield (t ha^{-1} yr^{-1})	<4	4–8	>8
Drained peatland		Yes/No	

[a] *Only the aboveground biomass of crop residues should be accounted for.*
[b] *If catch crops, cover crops or grasses are present in the crop rotation, the biomass produced by these crops should be added to the estimation of total crop yield.*

NO_3^- losses are enhanced by the application of N fertilizer and reduced by the presence of catch or cover crops (Hansen and Djurhuus, 1997; Di and Cameron, 2002; Kirchmann et al., 2002). The potential for NO_3^- losses to actually occur is further determined by the presence or absence of artificial drainage, the rate of precipitation and soil texture (Di and Cameron, 2002). The calculation of NH_3 losses is driven by whether or not manure is applied and its NH_4^+ content (Sommer and Hutchings, 2001), while being enhanced by high average annual temperature and precipitation. Attributes that are known to influence N_2O emissions but are not present in the model include the effect of soil pH and different types of (i) compost, (ii) cover crops, (iii) tillage and (iv) irrigation, as discussed in section Discussion.

Carbon Sequestration

The model evaluates the extent to which a soil sequesters C based on (i) C inputs, (ii) C losses, and (iii) the OC concentration of the soil. This soil function is assessed based on the following integration rules: (i) a soil that loses C (outputs > inputs) receives a low value, while (ii) a soil with an increasing C content (inputs > outputs) receives a high value. When (iii) the C stock is in equilibrium (inputs = outputs), the assigned value equals the value of the C concentration. The rationale behind this last rule is that a soil with a high OC content performs the climate regulation soil function better than a soil with a low OC content. It is noted that the model is not designed to make predictions of the OC concentration of the soil. Instead, it evaluates the capacity of a soil to perform the climate regulation soil function while using the SOC concentration as a model input. In addition, the model has not been designed to account for legacy effects on the current SOC concentration, e.g., caused by a recent previous land use. Therefore, the model assumes that the soil has been under cultivation for a timespan of multiple decades. In the model, inputs of C are divided into external and internal inputs (**Table 1**). The former can consist of e.g., farmyard manure or slurry, while the latter consist of the amount of crop residues (as a percentage of the total yield) that is left on the field after harvest and the mean annual crop yield. C outputs are evaluated based on a combination of soil texture, environmental conditions (mean annual precipitation and temperature) and management practices. These include tillage intensity, the share of grasslands and cover crops in the crop rotation and whether or not the soil is a drained peatland. To correctly represent the effect of cover crops or grass in the model, in addition to indicating the number of years a cover crop or grass was present in the past 5 years, an estimate of its biomass has to be added to the mean annual net primary productivity. Attributes that are known to affect C sequestration but are not present in the model include the effect of N fertilizer application, biochar application and soil pH, as discussed in section Discussion.

The Climate Regulation Soil Function

The final climate regulation soil function is determined based on the combination of the magnitude of N_2O emissions and C sequestration. The integration rules that define the magnitude of the climate regulation soil function are shown in **Table 2**. These are a logical combination of the simulated values for N_2O emissions and C sequestration, while a higher weight is given to N_2O emissions because N_2O is a much more potent greenhouse gas than CO_2 and often dominates the GHG balance of agroecosystems. For example, a medium value for C sequestration and a high value for N_2O emissions lead to a low overall climate regulation value.

Sensitivity Analysis

A sensitivity analysis was performed to assess the extent to which the results of the model are influenced by changes in management practices. This was done separately for the simulated magnitude of N_2O emissions and C sequestration, as the combinations of both attributes are straightforward to interpret (**Table 2**). The assessment of how the magnitude of C sequestration is affected by changes in management practices was done relative to a reference management. This reference management was chosen not to favor C sequestration, resulting in low C inputs, high C outputs and therefore low C sequestration (**Figure 3**). The model sensitivity was assessed by gradually changing different management practices which are expected to increase C sequestration. The sensitivity of the N_2O component of the model was assessed using a similar procedure. Here, the reference management was chosen to favor N_2O emissions. Gradually, one, two or three management practices were changed to reduce N_2O emissions. In addition, the effect of average temperature and precipitation on C sequestration and N_2O emissions was assessed for soils with different textures.

TABLE 2 | Integration rules used to classify the climate regulation soil function as "low," "medium," or "high" based on the determined magnitude of N_2O emissions and carbon sequestration.

Carbon sequestration	N_2O emissions	Climate regulation
Low	High	Low
Low	Medium	Low
Low	Low	Medium
Medium	High	Low
Medium	Medium	Medium
Medium	Low	High
High	High	Medium
High	Medium	High
High	Low	High

Model Testing Using Long-Term Field Experiments

An assessment of the accuracy of the model was made by simulating agricultural soils in long-term experiments (LTEs) and comparing the model outcomes to reported changes in N_2O emissions or C sequestration. LTEs were chosen because they facilitate the assessment of a range of different management practices on the component parts of the climate regulation function on a decadal timescale. The geographical location of the LTEs was limited to Europe, in line with the intended geographical extent of model application. For this purpose, the database constructed by Sandén et al. (2018) was used. This database contains publications on 251 European LTEs in which the effect of alternative management practices on soil quality were assessed. From these, 78 LTEs reported on changes in SOC stocks and 40 reported on changes in N_2O emission or NO_3^- leaching. A large portion of these LTEs studied the effect of tillage ($n = 18$ for N_2O, $n = 33$ for C stocks). As the effect of tillage on these soil properties has been summarized in multiple meta-studies, it was chosen not to run all these studies separately by the model, but instead, model performance was assessed based on these meta-analyses (Luo et al., 2010; Powlson et al., 2014; Meurer et al., 2018). After excluding studies on the effect of tillage and studies using parameters that are not simulated by the model, the number of studies that was retained to test the model was 6 for N_2O emissions, 2 for NO_3^- leaching and 12 for changes in SOC stocks. This includes one additional study on NO_3^- leaching (Hansen and Djurhuus, 1997) and one on C sequestration (Spiegel et al., 2018) that were added to the dataset.

The aim of this exercise was to test if the model is able to correctly predict the climate regulation function of (i) a soil with a constant management through time and (ii) a soil which experiences a change in management practices. For the first purpose, the climate regulation function of the control treatments of the LTEs were predicted and compared to reported values. As it was assumed that the OC concentration of the control treatments was constant through time (C inputs equal C outputs), the simulation of the control treatments was used to test if this equilibrium was predicted correctly by the model. Therefore, the classified value of C sequestration by the control treatments was equal to the SOC concentration of these treatments (see section carbon sequestration). For the second purpose, the treatment studied in the LTEs was simulated and compared to the reported change in the soil function. To this end, the results of the LTEs had to be classified into low, medium and high. This was done based on the results reported in the articles presenting the outcomes of the LTEs. The outcomes of the LTEs that were used to validate the C sequestration part of the model were classified based on differences in the SOC concentration between the controls and treatments, as reported in **Table 3**. The outcomes of the LTEs used to validate the N_2O part of the model were classified based on the reported differences in N_2O emissions and NO_3^- leaching between controls and treatments, as reported in **Table S1**. For N_2O, the intensity of emissions for the control situation and the change in management practices was classified (i.e., into low, medium or high) based on the data provided.

The classification of the magnitude of N_2O emissions for the treatment was based on the relative change in N_2O emissions. For example, if the control management (without N fertilizer application) led to low N_2O emissions, a low value was assigned. If the treatment (which included N fertilizer application) resulted in a substantial increase in N_2O emissions, a value higher than low was assigned. Thus, if the model predicted N_2O emissions for the treatment to be medium or high, this was assumed to be a correct model outcome. Also for C sequestration, the classification of the outcomes of the LTEs was based on the data provided in the articles. This information was used to derive the direction of change in SOC concentration as a consequence of the change in management practices, according to the rules outlined in section carbon sequestration. It is noted that term "control treatment" is used to refer to the treatments in the LTEs to which changes in management practices are compared, while the term "reference management" is used to refer to the management practices to which the outcomes of the sensitivity analyses are compared.

RESULTS

Sensitivity Analysis

Carbon Sequestration

The environmental variables (precipitation and temperature) and the soil texture have a substantial effect on the predicted magnitude of C sequestration (**Figure 2**). On average, higher C sequestration is predicted for clayey soils, while this decreases for soils with a coarser texture. Furthermore, the predicted C sequestration is highest for environments with a low temperature and precipitation and decreases when temperature and precipitation increase simultaneously.

The results of the sensitivity analysis of the C sequestration part of the model are shown in **Figure 3**. Increasing the amount of C inputs to the soil (through crop residue incorporation or the addition of external C inputs, not through an increase in yield) from low to medium does not improve the predicted value for C sequestration. When high values for these C inputs are chosen, the predicted value for C sequestration increases from low to medium. When crop residue incorporation and the addition of external C inputs are both at high levels, similar outcomes are obtained. Consequently, for the considered combination of environmental conditions and management practices, only increasing the amount of C inputs while C losses remain high increases the magnitude of C sequestration from low to medium, but not to high. Similarly, the adoption of minimum tillage or no-till does not lead to an increased prediction of C sequestration. As a consequence, only reducing C outputs, while C inputs remain low, does not lead to high predictions of C sequestration. When a management practice that increases C inputs and one that decreases C outputs are jointly applied, medium or high values for C sequestration are predicted. Improving multiple management practices together thus consistently leads to a high predicted value for C sequestration.

N_2O Emissions

The effect of precipitation and soil texture on predicted indirect N_2O losses via NO_3^- and NH_3 losses is shown in **Figure 4**. For the particular combination of management practices chosen (see **Figure 4**), low values of precipitation do always lead to medium predicted values for NO_3^- losses, while medium and high precipitation rates lead to higher losses. On a clayey soil, only high values of precipitation lead to high NO_3^- losses, while coarser soils result in high NO_3^- losses for medium and high precipitation values. This is in line with studies showing that higher NO_3^- losses occur in sandy vs. clayey soils (Gaines and Gaines, 1994; Vinten et al., 1994). Predictions of low NH_3 losses are only obtained at low rates of precipitation, while high losses are consistently predicted for medium and high rates of precipitation. In contrast, temperature and precipitation do not have a marked effect on direct N_2O emissions (data not shown). This is a consequence of the fact that a higher weight is given to the rate of N fertilizer application in the internal decision rules of the model.

The results of the sensitivity analysis of the N_2O emissions part of the model are shown in **Figure 5**. High values for direct and total N_2O emissions are consistently predicted when high rates of N fertilizer are applied. The model predicts decreased N_2O emission when N fertilization is improved (i.e., lower application rates of N fertilizer). Predictions of low total N_2O emissions are not obtained as a consequence of high predicted indirect N_2O emissions in the reference management. Predictions of low direct N_2O emissions are obtained consistently when low rates of N fertilizer are applied.

When management practices that influence indirect N_2O emissions are improved (e.g., no manure application, reduced NH_4^+ content of manure or planting catch crops instead of a fallow period), reduced indirect emissions are only predicted when no manure is applied, or when two or more of these management practices are applied together. However, this does not lead to a decrease in total N_2O emissions in each of these cases, since the reference management leads to high direct N_2O emissions. Optimizing one management practice that reduces direct N_2O emissions and one management practice that reduces indirect emissions only leads to lower predictions of total N_2O emissions when the amount of applied N fertilizer is reduced. Similarly, improving four or six management practices only leads to lower predictions of total N_2O emissions when the amount of N fertilizer applied is reduced.

Model Testing Using Long-Term Field Experiments

For C sequestration, 11 of the 14 control treatments were predicted correctly by the model (**Table 3**, see **Table S1** for additional information), indicating that the model is able to correctly predict the C sequestration function of agricultural soils when no change in OC concentration occurs over time. The model thus correctly simulates that C outputs were equal to C inputs in the control treatments of the LTEs. For treatments that included a change in management practice, 7 out of 14 experiments were predicted correctly by the model. The

TABLE 3 | Model performance using reported data from European long-term field experiments.

References	OC (%)	Texture	T (°C)	P (mm yr^{-1})	Management practice	Expert classification	Model prediction	Correct?
Carbon sequestration								
Blair et al., 2006	1.03	Silt	9.1	693	Control	Low	Low	Y
	2.73				FYM addition	> Low	Low	N
Bolinder et al., 2010	2.3	Silt	3.4	567	Control	Medium	Medium	Y
	2.8				Forage crops and manure	High	High	Y
Jäger et al. (2011) – Spröda	0.71	Sand	8.3	540	Mineral N	Low	Low	Y
	0.83				+ manure	Low	Low	Y
Jäger et al. (2011) – Methau	0.99	Silt	8	600	Mineral N	Low	Low	Y
	1.53				+ manure	> Low	Low	N
Kismányoky and Tóth, 2013	1.07	Silt	10.8	683	Control	Medium	Medium	Y
	1.24				+ manure	High	Medium	N
Triberti et al., 2008	0.54	Silt	13	700	Control	Low	Low	Y
	0.82				+ manure	> Low	Low	N
van Eekeren et al., 2008	1.22	Silt	9.5	726	Control	Low	Low	Y
	1.97				Ley-arable crop rotation	> Low	Medium	Y
Moeskops et al., 2012	1.05	Silt	9.5	726	Control	Low	Medium	N
	1.38				+ FYM	> Low	High	Y
Bertora et al., 2009	1.00	Silt	11.8	740	Control	Medium	Low	N
	1.35				+ FYM	> Medium	Low	N
Monaco et al., 2008	1.04	Sand	11.8	792	Control	Low	Low	Y
	1.41				+ manure/mineral N	> Low	Low	N
Perucci et al., 1997	0.81	Silt	12.6	873	Residue removal	Low	Low	Y
	0.94				Residue incorporation	Low	Low	Y
Šimon et al., 2013	1.17	Sand	7.5	750	Control	Medium	Low	N
	1.49				+ FYM	High	Medium	N
Spiegel et al. (2018) – Marchfeld	1.99	Silt	9.1	540	Control	Low	Low	Y
	2.16				+ crop residues	Medium	Medium	Y
Spiegel et al. (2018) – Alpenvorland	0.84	Silt	8.5	836	Control	Low	Low	Y
	0.87				+ crop residues	Low	Low	Y
Direct N_2O emissions								
Abalos et al., 2013	0.82	Sand	13.2	430	Control	Low	Low	Y
					+ residues	Low	Low	Y
					+ residues & mineral N	High	High	Y
Abdalla et al., 2012	1.6	Sand	9.3	823	Control	Low	Low	Y
					+ N fertilizer	> Low	High	Y
Jeuffroy et al., 2013	1.8	Silt	8	400	Control	Low	Low	Y
					+ N fertilizer	> Low	Medium	Y
Sanz-Cobena et al., 2012	0.8	Sand	13.2	430	Urea addition	High	High	Y
					Urea + nitrification inhibitors	< High	Medium	Y
Sanchez-Martín et al., 2010	0.82	Sand	13.2	430	Control	Low	Low	Y
					+ N fertilizer	> Low	High	Y
Baggs et al., 2006	1.5	Sand	8.4	668	Control	Low	Low	Y
					+ N fertilizer	> Low	High	Y
					+ N fertilizer & residues	> Low	High	Y
Nitrate leaching								
Hansen and Djurhuus (1997) – Jyndevad	1.5	Sand	9	1616	Plowing	High	High	Y
					+ catch crop	< High	High	N
Hansen and Djurhuus (1997) – Ødum	1.5	Silt	7.3	1260	Plowing	High	High	Y
					+ catch crop	Medium	Medium	Y
Constantin et al. (2010) – Thibie	1.5	Silt	10.8	605	No catch crops	High	High	Y
					Catch crops	< High	Low	Y

T, the mean annual temperature; P, the mean annual precipitation; FYM, farmyard manure; N, fertilizer refers to mineral N fertilizer. The classification of the results for the carbon sequestration part of the model were based on changes in the OC concentration, as reported in the table. More information about the classification of the reported results for N_2O emission and nitrate leaching can be found in ***Table S1***.

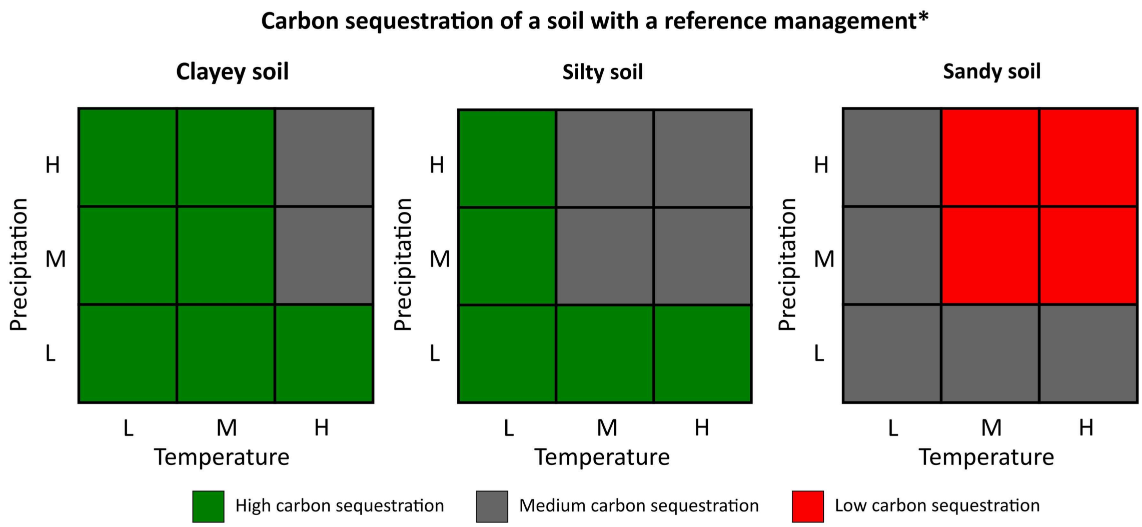

FIGURE 2 | Example of the effect of temperature and precipitation on the predicted C sequestration function of soils with different textures. *Reference management: a mineral soil with medium values for yield, OC content, share of cover crops, external C inputs and residues after harvest; low share of grassland and non-inversion tillage.

management practice that was varied most often was the addition of external C inputs (e.g., manure). The outcomes of the LTEs differed, with some experiments reporting no substantial increase in SOC stocks (Jäger et al., 2011; Kismányoky and Tóth, 2013), while others did report an increase (e.g., Blair et al., 2006; Monaco et al., 2008). In most cases, however, the model did not predict an increase in C sequestration following the addition of manure, in line with the results of the sensitivity analysis. This is a result of the prediction of high C losses for the majority of these experiments, because of the combination of inversion tillage and the absence of cover crops applied in most of these LTEs. As a result, modeled C losses were higher than C inputs in most cases, resulting in low predictions of C sequestration. It should be noted that since most LTEs only report changes in C concentration without reporting changes in bulk density, this may overestimate the amount of sequestered C.

The three LTEs that assessed the effect of crop residue incorporation reported relatively small absolute increases in OC concentrations (0.03–0.17% OC) after multiple decades (Perucci et al., 1997; Spiegel et al., 2018). This was correctly predicted by the model, with no modeled increase in C sequestration for two experiments (with a SOC concentration below 1%) and an increase for one experiment (with ca. 2% SOC). For all these experiments, the incorporation of crop residues led to a high predicted value for C inputs, which was balanced by high predicted OC losses, as a consequence of the application of a combination of inversion tillage and the absence of cover crops in these LTEs. Since modeled C inputs and outputs had an equal magnitude (high), the modeled increase in C sequestration in the experiment with higher SOC (ca. 2 %) in Spiegel et al. (2018) from low to medium was a consequence of the medium OC concentration of this soil.

The only experiment that resulted in high modeled values for C sequestration included both manure application and the presence of forage crops in the rotation (Bolinder et al., 2010), thereby increasing C inputs while reducing C outputs. This was in line with the results from the sensitivity analysis, which showed that the predicted magnitude of C sequestration generally increases when C inputs are increased and C losses are reduced.

The model was successful in predicting the magnitude of direct N_2O emissions for all control (no N fertilizer application) (6/6) and management treatments (8/8) of the LTEs. In most of the LTEs, the control treatment resulted in low N_2O emissions, while most of the treatments included the application of high rates of mineral N fertilizer, leading to higher N_2O emissions. This was predicted well by the model. As shown in the sensitivity analysis, the model predicts high rates of N_2O emissions when high rates of N fertilizer (i.e., > 100 kg N ha^{-1}) are applied, regardless of other mitigation practices. This is in line with studies that have shown that rates of N_2O emission increase exponentially once the amount of N fertilizer exceeds the N requirements of the crops (Bouwman et al., 2002; Hoben et al., 2011; Shcherbak et al., 2014). The addition of crop residues, included as "additional C inputs" in the model, without the application of mineral N fertilizer did not result in higher modeled N_2O emissions, in line with observations (Abalos et al., 2013).

The three LTEs that reported on NO_3^- leaching assessed the effect of the incorporation of catch crops in the crop rotation cycle. The experiments by Hansen and Djurhuus (1997) were performed under similar environmental conditions and management practices, while soil texture differed between the experiments. Although the authors reported a decrease in NO_3^- leaching following the growth of catch crops, the model

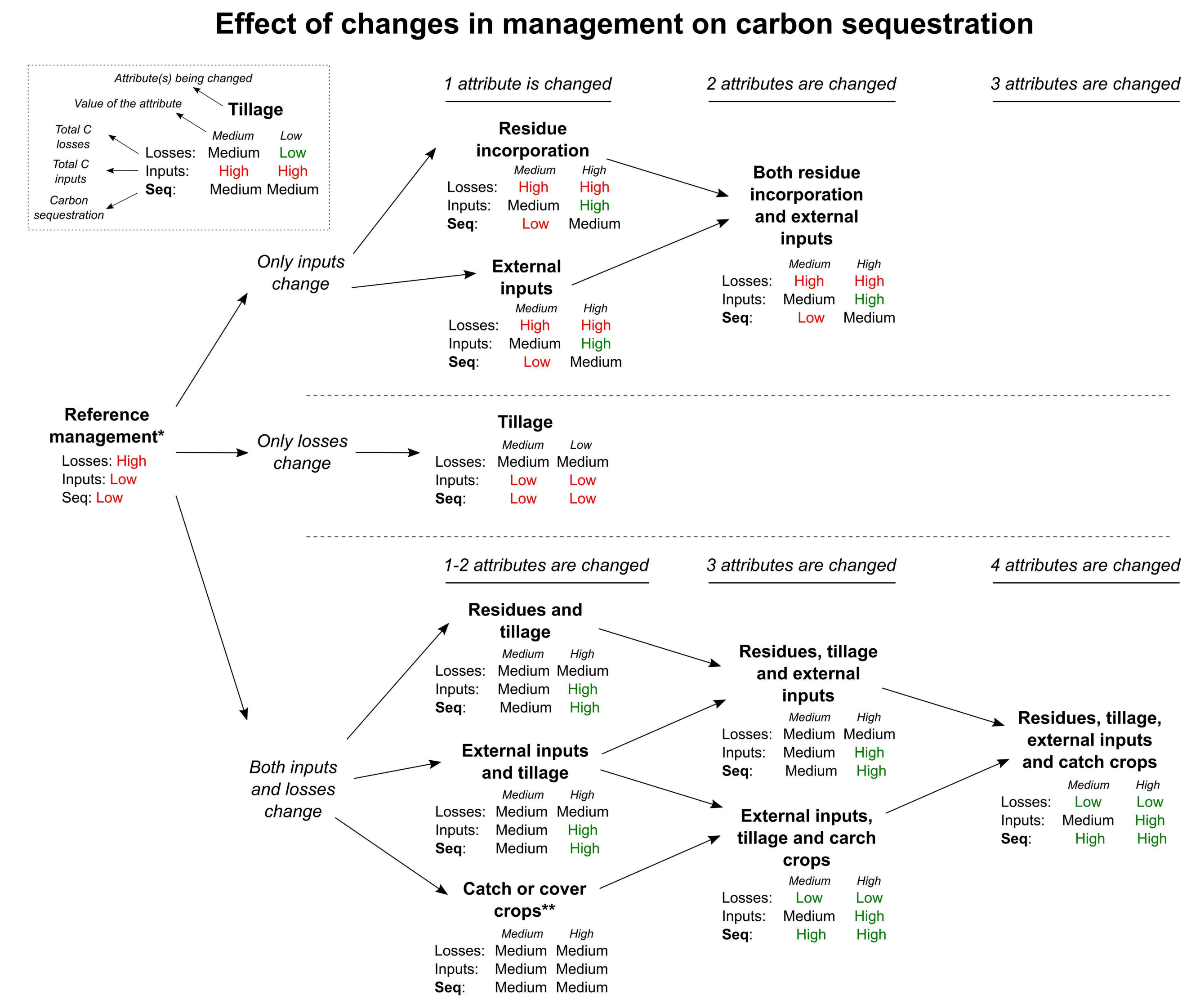

FIGURE 3 | Sensitivity analysis of the C sequestration part of the model (**Figure 1**), based on variations in management practices. The model outcomes are compared to a *reference management: a silty mineral soil with a low yield and medium values for temperature, precipitation and C content, no drainage and management practices that do not favor C sequestration, leading to low C inputs and high C losses. The inset in the upper left corner shows the legend. ** The effect of catch or cover crops is simulated by a reduction of C losses, while an increase in NPP accounts for increased C inputs.

predicted a decrease in NO_3^- leaching only for the silty soil, while no decrease for the sandy soil was predicted because of the high precipitation rate. Also the model predictions for another experiment, which measured the effect of catch crops on NO_3^- leaching in a silty soil, were in line with observations (Constantin et al., 2010).

The effect of different tillage practices on SOC sequestration and N_2O emissions has been studied in numerous long-term field experiments. Although it was initially assumed that the adoption of no-till or minimum tillage increases the SOC content, multiple studies and meta-analyses have shown that these practices generally only lead to a mere redistribution of OC in the topsoil, while not increasing the OC stock at the soil profile scale (Luo et al., 2010; Powlson et al., 2014; Haddaway et al., 2017). This effect is also simulated by the model, as shown in the sensitivity analysis (**Figure 3**). When reduced tillage or no-till is the only management practice that is changed, C outputs are reduced but C sequestration remains low when C inputs are low. When reduced tillage or no-till is combined with increased C inputs, e.g., the incorporation of crop residues, the model does predict a higher C sequestration. This is in line with field observations, which have shown that reduced tillage or no-till only lead to increased SOC stocks when combined with increased C inputs (Luo et al., 2010; Virto et al., 2012; Chowdhury et al., 2015).

Another management practice that has been studied intensively with respect to its effect on SOC stocks is the presence

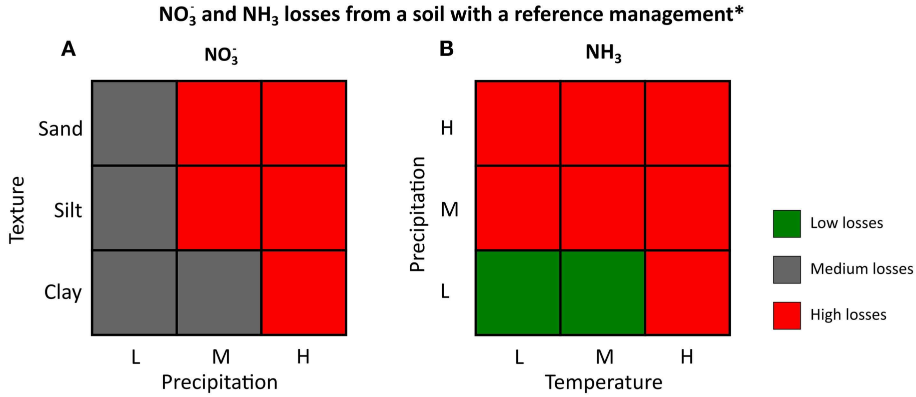

FIGURE 4 | (A) Example of the effect of combinations of texture and precipitation and **(B)** temperature and precipitation on NO_3^- and NH_3 losses respectively. *Reference management for NO_3^- losses: mineral soil without artificial drainage, medium N fertilizer application and no catch or cover crops. Reference management for NH_3 emissions: mineral soil with application of manure with a high NH_4^+ content.

of cover crops between the main crops. Based on data from 37 different sites, Poeplau and Don (2015) calculated that the inclusion of cover crops in the crop rotation cycle leads to a significant increase in topsoil OC stocks on a multi-decadal timescale. In the model, the effect of cover crops is represented in two different ways: (1) through an increase in crop yield, which increases C inputs, and (2) through a reduction in the magnitude of C losses during the time no cash crops are present. When both variables are improved compared to the reference management, similar to the sensitivity analyses (**Figure 3**), the predicted C sequestration increases from low to medium. This modeled increase in C sequestration after the inclusion of cover crops in the crop rotation cycle is thus in line with the results from Poeplau and Don (2015).

Another measure that has been proposed to increase the OC content of agricultural soils is the incorporation of crop residues in the soil (Paustian et al., 2016; Chenu et al., 2018). In an extensive review, Lehtinen et al. (2014) found that the incorporation of crop residues did not lead to a significant increase in the topsoil OC concentration when this practice was applied for <10 years, although the effect became apparent after > 10 years. When high rates of crop residue incorporation were considered in the sensitivity analysis (i.e., > 30 % of the yield), the predicted C sequestration increased from low to medium. This model outcome is thus in line with the results from Lehtinen et al. (2014), given that this management practice is maintained over a long period of time.

DISCUSSION

Designing a strategy to manage soils to mitigate climate change is not straightforward, as a thorough understanding of relevant processes at play is necessary. A change in soil management that increases the climate regulation function of soils can cause a decrease in another soil function, such as primary productivity (O'Sullivan et al., 2015; Schulte et al., 2015). Given the complexity of soil systems, models are often used to qualify or quantify the extent to which they perform different functions (Vogel et al., 2018), but the analysis of the multifunctional role of soils in society is still in its infancy. In this study, we presented a qualitative model to assess the climate regulation function of soils. This model has been coupled to similar models simulating other soil functions, in order to assess the trade-offs between these soil functions as a consequence of changes in management practices (Debeljak et al., 2019).

A sensitivity analysis has confirmed that changes in agricultural management practices have an effect on the predicted magnitude of C sequestration and N_2O emissions by the developed model. The predicted magnitude of C sequestration generally only increases from low to high when C inputs are increased while C losses are reduced. If only C inputs are increased, while C outputs remain high, a low predicted magnitude of C sequestration only increases to medium. When only C outputs are decreased, while C inputs remain low, no increase in the magnitude of C sequestration is predicted. This is in line with studies showing that only reducing C outputs, e.g., through the adoption of no-till, only leads to increases in SOC storage when being accompanied by increases in C inputs (e.g., Virto et al., 2012). In addition, the small predicted increase in C sequestration when C inputs are increased, while C outputs remain high, is in line with studies showing that only increasing C inputs can increase SOC concentrations (Lehtinen et al., 2014). Given the fact that the model has been developed for a timescale of several years, while increases in SOC stocks are generally a slow process [in the order of tens of g C m^{-2} yr^{-1} (Paustian et al., 2016; Minasny et al., 2017)], this model outcome is in line with current knowledge, and avoids an overestimation of the C sequestration potential of agricultural soils. With respect to N_2O emissions, the sensitivity analysis showed that the major factor determining the magnitude of predicted N_2O emissions is the rate at which N fertilizer (either mineral or organic) is applied. This is in line with multiple studies that have shown that the magnitude of direct N_2O emissions increases substantially

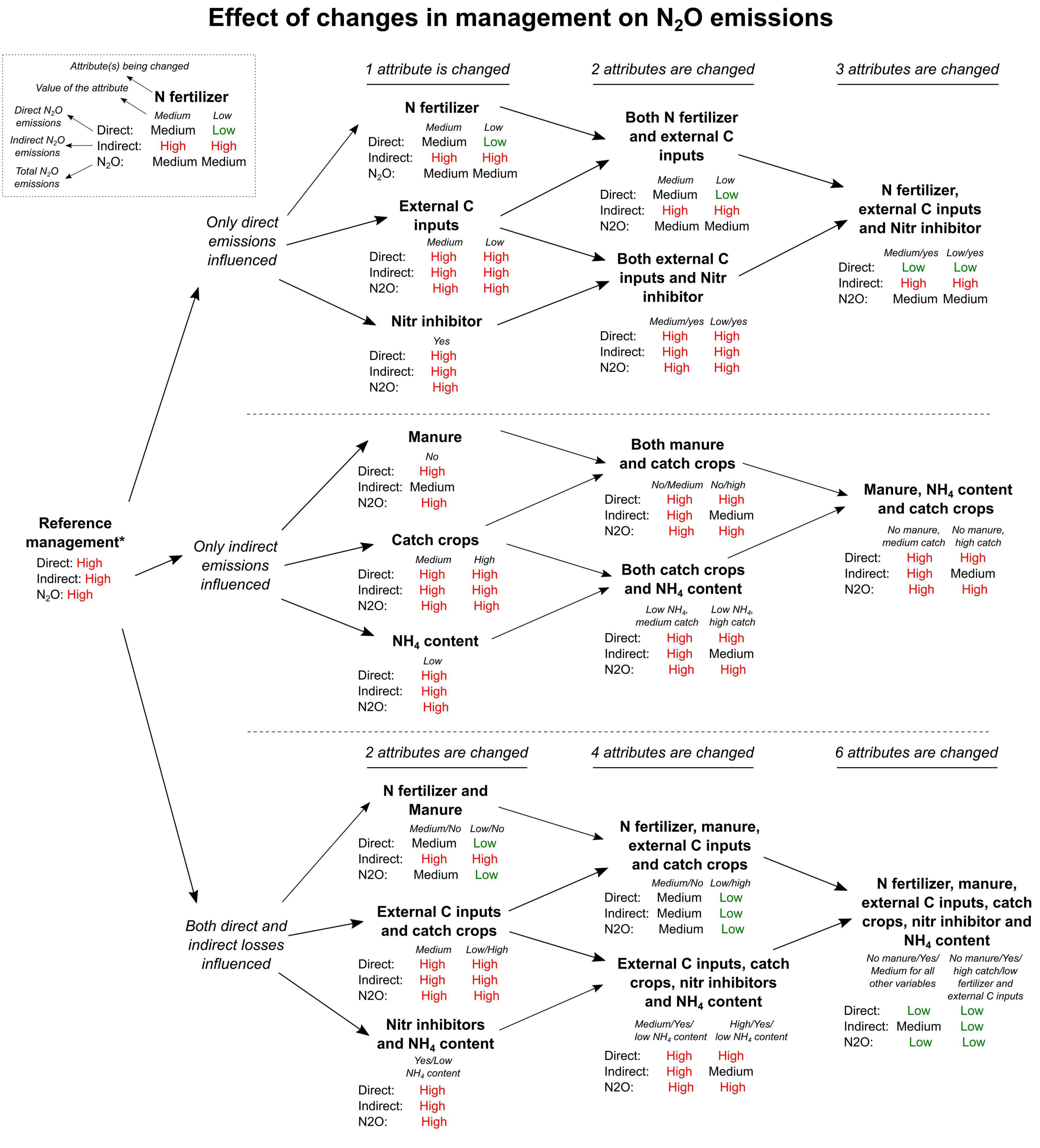

FIGURE 5 | Sensitivity analysis of the N_2O emissions part of the model (Figure 1), based on variations in management practices. The model outcomes are compared to a *reference management: a silty mineral soil with medium values for temperature, precipitation, OC content, no irrigation or artificial drainage and management practices that favor N_2O emissions.

when the plant demand for N is exceeded (Bouwman et al., 2002; Shcherbak et al., 2014).

The verification of the model performance has shown that the model is capable of correctly predicting the C sequestration function of soils that have received a constant management over the past decades (the control treatments). However, the model efficiency was lower for predictions of the alternative management practices that were applied in the LTEs. This was related to the fact that most LTEs assessed the effect of the addition of external C inputs on changes in SOC concentrations. While the model predicts that this has no effect, the majority of the LTEs reported an increase in SOC concentrations. The inability of the model to predict this change can be related to the combination of (i) the classification of inputs data and (ii) the small increase in SOC stocks that is generally observed when improved management practices are applied (10–100 g m^{-2} yr^{-1}; Paustian et al., 2016; Minasny et al., 2017). The effect of other management practices on changes in SOC concentrations (e.g., tillage and cover crops) was predicted adequately by the model. The evaluation of the model performance has thus shown that, in general, the model was able to satisfactorily predict the direction of the change in C sequestration for most of the assessed management practices. However, the effect of the addition of external C inputs on SOC stocks was generally underestimated. Also the effect of the application of N fertilizer on N_2O emissions was adequately assessed by the model in all cases. The magnitude of NO_3^- leaching was correctly predicted in 2 out of 3 cases, indicating that also this management practice is adequately simulated by the model.

The extent to which the model performance could be verified depended on the availability of data from LTEs. With respect to C, the majority of European LTEs evaluated the effect of tillage and the addition of different organic amendments on changes in SOC storage. Other management practices (e.g., the effect of grass in the crop rotation) were assessed in only a few experiments. The main focus of the assessment of the model performance was therefore on the former management practices, while also the effect of cover crops could be assessed based on a meta-analysis (Poeplau and Don, 2015). The performance of the C sequestration part of the model could thus be assessed fairly well. For N_2O emissions, the variation in available LTEs was substantially lower, as they mostly focused on the effect of the rate of N fertilizer application on direct N_2O emissions and the effect of catch crops on NO_3^- leaching. With respect to direct N_2O emissions, management practices that could not be assessed are the addition of external C inputs, irrigation, and artificial drainage. However, while the high rate of N fertilizer application generally has the greatest effect on direct N_2O emissions (Shcherbak et al., 2014), the uncertainties on the effect of the other variables will likely have a limited effect on the overall model uncertainty. The number of experiments used to test the NO_3^- part of the model was limited, but confirmed that the model correctly predicted lower NO_3^- losses as a consequence of the presence of catch crops. Furthermore, the structure of the NO_3^- part of the model is in line with evidence that the rate of NO_3^- losses is enhanced when high rates of N fertilizer are applied (Kirchmann et al., 2002) combined with a downward flux of water at high precipitation rates (Di and Cameron, 2002). In addition, NO_3^- losses were being reduced when catch crops were planted (Hansen and Djurhuus, 1997). In contrast, no experiments that assessed the effect of manure application on NH_3 losses were present. Therefore, this part of the model was constructed based on evidence that high rates of NH_3 emissions are enhanced by high rates of manure addition and a high NH_4^+ content of manure (Sommer and Hutchings, 2001). This part of the model is thus in line with knowledge of the main variables affecting NH_3 losses.

The available dataset allowed to evaluate the model for locations in all three temperature classes, but only for medium and high precipitation classes and silty and sandy soils. As a consequence, the model performance could not be assessed for clayey soils and environments with a mean annual precipitation below 400 mm. Future model evaluations should therefore focus on these environments in order to reduce uncertainties. The crops for which treatment effect were studied in the LTEs included mainly maize, winter wheat, barley and sugar beet, among other less-represented crops (**Table S1**). Some cropping systems, such as orchards, were thus not present in the validation dataset.

The effect of C sequestration and N_2O emissions on the overall climate regulation soil function could not be evaluated, as this soil function is difficult to quantify. In addition, this soil function as such is generally not evaluated in field experiments, but evaluated based on measurements of C sequestration or N_2O emissions separately. The combinations of both C sequestration and N_2O emissions into the climate regulation soil function (**Table 2**) are therefore an attempt to provide the user with an indication of this soil function. As this is an expert-based interpretation, model users are encouraged to look at the modeled magnitude of C sequestration and N_2O emissions to assess how management practices can be changed to improve the overall climate regulation soil function.

Although most of the generally applied management practices are represented in the model, some management practices are currently not included. For example, the effect of different types of compost on N_2O emissions is currently not represented in the model, although it has been shown that this has an important effect on N_2O emissions from agricultural soils (Zhou et al., 2017). However, it was chosen not to include this variable in the model since the effect is highly variable and greatly depends on soil type and climate (Zhou et al., 2017). Another treatment that has been the subject of multiple LTEs is the effect of mineral N fertilizer on C sequestration. Although generally no effect is observed (e.g., Nardi et al., 2004; Triberti et al., 2008; Poeplau et al., 2017), some authors report a small increase in SOC stocks after mineral N fertilization (Dersch and Böhm, 2001; Ladha et al., 2011). However, a potential increase in SOC stocks can be offset by the greenhouse gases produced during the manufacturing of mineral N fertilizer (Gao et al., 2018). Therefore, this has been omitted from the model. However, since the application of mineral N fertilizer generally leads to an increase in crop yields (Jiang et al., 2018), this effect can be included by increasing the NPP model input. Also the effect of cover crops on N_2O emissions was not included as an independent variable in the model. This is because it has been shown that the effect of cover crops on N_2O emissions greatly depends on factors other than the mere presence of cover crops, such as the rate of fertilizer application, the type of cover crop and the potential incorporation of the cover crop in the soil (Basche et al., 2014). Including all these interactions in the model would greatly increase model complexity and, as a consequence, model uncertainty. The addition of an additional C source, such as plowed-in residues of covers crops is, however, included in the model as a variable that stimulates direct N_2O emission. Also the effect of tillage on N_2O emissions was omitted from the model, as it has been shown that there is no significant difference in N_2O emissions under different magnitudes of tillage (no-till, reduced tillage, or inversion tillage) when a timescale more than 10 years is considered (Six et al., 2004; van Kessel et al., 2013). A last set of management practices that is not evaluated by the model to minimize model complexity include the application of different types of irrigation, e.g., drip-irrigation vs. furrow irrigation (Kennedy et al., 2013), biochar application, agroforestry and subsoil management. In addition to considering additional management practices, potential future model improvements may involve adapting the model to simulate (i) managed grassland systems, (ii) managed peatlands, including resulting methane emissions, (iii) the effect of soil pH on C sequestration and N_2O emissions and (iv) methane oxidation.

The model has been developed in the framework of the Horizon 2020 Landmark project, which aims to improve knowledge of the functions performed by European agricultural soils, while developing tools to assess the trade-offs between different soil functions. To achieve this, similar models have been developed for other soil functions: primary productivity (Sandén et al., 2019a), soil biodiversity and habitat provision (van Leeuwen et al., 2019), water regulation (Delgado et al., submitted) and nutrient recycling (Schröder et al., 2016). These separate models are brought together into a tool that assesses the extent to which agricultural soils perform these different soil functions (Debeljak et al., 2019). This allows to assess the win-wins and trade-offs between different soil functions as a consequence of management practices, and represents an important step forward in the quantification of different soil functions in agroecosystems across Europe in order to contribute to the understanding and management of soils to fulfill societal needs.

CONCLUSION

A qualitative decision support tool to assess the climate regulation soil function in European agroecosystems has been developed. This tool has been constructed based on the rationale that it should provide a reliable estimate of the magnitude of C sequestration and N_2O emissions of arable soils using data that is generally available. A sensitivity analysis and an assessment of the model performance based on European LTEs have shown that the model is generally able to correctly assess the effect of different management practices on C sequestration and N_2O emissions. However, the lack of validation data for agroecosystems in dry climates and on clayey soils prevented the model to be validated in these environments. This tool will be combined with similar models to assess trade-offs between different soil functions, in order to inform key stakeholders about the effect of different agricultural management practices on trade-offs between soil functions.

AUTHOR CONTRIBUTIONS

This article resulted from cooperation within the climate regulation task group in the LANDMARK H2020 project. CD, JS, MV, CH, EL, BG, AT, VK, and MD contributed to the development of the model. The validation dataset was constructed by MV, while the validation and interpretation of the results was done by MV, JS, CD, TS, and HS. MV did most of the writing, with major inputs from CD, AT, JS, TS, EL, HS, RC, and BG.

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SUPPLEMENTARY MATERIAL

The Supplementary Material for this article can be found online at: https://www.frontiersin.org/articles/10.3389/fenvs.2019.00131/full#supplementary-material

Table S1 | Detailed information about the input data used to validate the model and model outputs.

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Comparing Field Sampling and Soil Survey Database for Spatial Heterogeneity in Surface Soil Granulometry: Implications for Ecosystem Services Assessment

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Lithospheric-derived resources such as soil texture and coarse fragments are key soil physical properties that contribute to ecosystem services (ES), which can be valued based on "soil" or "mineral" stocks. Soil survey data provides an inexpensive alternative to detailed field measurements which are often labor-intensive, time-consuming, and costly to obtain. However, both field and soil survey data contain heterogeneous information with a certain level of variability and uncertainty in data. This study compares the potential of using field measurements and information from the Soil Survey Geographic database (SSURGO) for coarse fragments (CF), sand (S), silt (Si), clay (C), and texture class (TC) in the surface soil (Ap horizon) for the 147-hectare Cornell University Willsboro Research Farm, NY. Maps were created based on following methods: (a) utilizing data from the SSURGO database for individual soil map unit (SMU) at the field site and using representative or reported values across individual SMU; (b) averaging the field data within a specific SMU boundary and using the averaged value across the SMU; and (c) interpolating field data within the farm boundaries based on the individual soil cores. This study demonstrates the important distinction between mapping using the "crisp" boundaries of SSURGO databases compared to the actual spatial heterogeneity of field interpolated data. Maps of CF, S, Si, C, and TC values derived from interpolated field core samples were dissimilar to maps derived by using averaged core results or SSURGO values over the SMUs. Dissimilarities in the maps of CF, S, Si, C, and TC can be attributed to several factors (e.g., official soil series data being collected from "type locations" outside of the study areas). Correlation plot of clay estimates for each SMU showed statistically significant correlations between SSURGO and field-averaged ($r = 0.823$, $p = 0.003$) and field-interpolated clay ($r = 0.584$, $p = 0.028$) estimates, but no correlation was found for CF, S, and Si. Ecosystem services provided by quantitative data such as CF, S, Si, and C may not be independent from each other and other soil properties. Key soil properties should also include categorical data, such as texture class, which is used for another key soil property–available soil water ratings. Current valuation of soil texture is often linked to specific mineral commodities, which does not always address the issue of soil based valuation including indirect use value.

Keywords: geographic information systems (GIS), lithosphere, minerals, particle size, soil survey geographic database (SSURGO)

INTRODUCTION

Frameworks to assess ecosystem services (ES) are being developed in soil science to highlight key soil properties that provide previously unidentified (or unquantified) benefits to ecosystems (Turner and Daily, 2008). Soil texture (percent of sand, silt, and clay) and the presence of coarse fragments have been identified as key soil properties for provisioning, regulating, cultural, and supporting services in connection with the United Nations (UN) Sustainable Development Goals (SDGs) (**Table 1**; Adhikari and Hartemink, 2016; Wood et al., 2017). These soil physical properties are commonly used to describe and classify soils worldwide, but there is limited information on their actual use to assess ecosystem services.

Soil texture is an inherent soil property related to the mineral fraction (<2 mm in size), which is derived from lithosphere (**Figure 1**). Soil texture can be defined informally as the way the soil "feels" or using a more formal definition as the proportion of sand, silt, and clay (excluding organic matter and carbonates) in <2 mm particle fraction. Soil texture can be determined qualitatively (texture by feel analysis) or quantitatively (hydrometer, pipette methods, etc.; Gee and Bauder, 1986). There are various uses and interpretations of sand, silt, clay and coarse fragments, for example: name of soil separate with a specific diameter limit (e.g., clay is <0.002 mm in size, etc.), soil texture class (e.g., sandy clay, etc.), rock fragment (%) modifier of texture (e.g., gravelly, etc.; U.S. Department of Agriculture, 2017). The coarse fraction is not part of the formal definition of soil texture since texture applies to the particle fraction <2 mm in size. In addition to particle size separation, soil texture commonly implies a general relationship between particle size and kinds of minerals present (e.g., sand is primarily composed of quartz; clay is primarily composed of secondary silicate minerals, etc.; **Figure 2**).

Contribution of lithospheric resources (e.g., soil texture, etc.) to soil ES can be examined using a combined social-ecological system proposed by Jones et al. (2016) (**Table 2**). Based on this system, lithospheric capital can be "natural" (minimum human impact), "natural + human derived" (e.g., agricultural, peri-urban areas, etc.), and "human-derived" (e.g., urban areas, etc.). Lithospheric stocks are quantifiable amounts of material with units defined in a spatial context, and can be measured as separate pure constituent stocks (e.g., 100% sand, 100% silt, 100% clay) or as composite stock (e.g., loam with various proportions of sand, silt, and clay). Flows into or from stocks

TABLE 1 | Connection between ecosystem services and selected Sustainable Development Goals (SDGs) in relation to soil texture (adapted from Wood et al., 2017).

TEEB Ecosystem Service Categories (TEEB Typology)	Sustainable Development Goals (SDGs)
PROVISIONING (Food; water; raw materials; genetic resources; medicinal resources; ornamental resources)	SDG 2, 3, 13, 15
REGULATING (Air quality; regulation; waste treatment, water purification; moderation of extreme flows; erosion prevention; climate regulation; maintenance of soil fertility; pollination; biological control)	SDG 2, 3, 6, 13, 15
SUPPORTING (Maintenance of life cycles; maintenance of genetic diversity)	SDG 2, 3, 6, 13, 15
CULTURAL (Spiritual experience; aesthetic; information; inspiration for art, culture, design; recreation and tourism; information; cognitive; development)	SDG 3, 6, 13, 15

The Economics of Ecosystems and Biodiversity (TEEB). SDG 2, "Zero Hunger"; SDG 3, "Good Health and Well-Being"; SDG 6, "Clean Water and Sanitation"; SDG 13, "Climate Action"; SDG 15, "Life on Land".

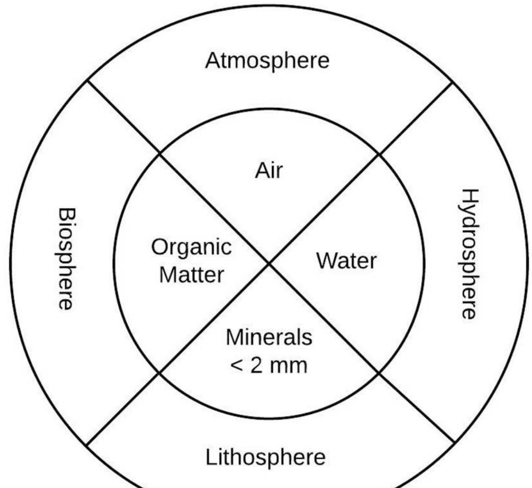

FIGURE 1 | Soil texture is an inherent soil property related to the mineral fraction (<2 mm in size), which is derived from lithosphere.

represent quantities or proportions per unit area per unit of time (e.g., illuvial accumulation of clay in the Bt horizon, etc.). Stocks are often examined on a mass basis, but soil texture is customarily expressed as proportions of the whole, therefore when discussing stocks and changes in stocks for soil texture, it is most useful to use proportions of a total. It is not clear that a mass basis would support a greater understanding of soil texture stocks.

Analysis of ecosystem services provided by sand, silt, clay, and coarse fragments should specify if these key soil properties

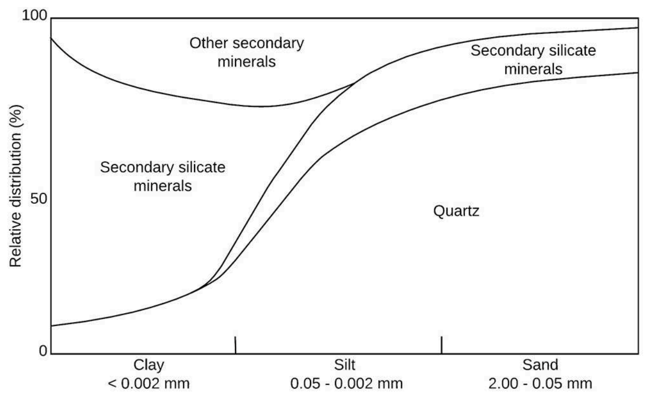

FIGURE 2 | General relationship between particle size and kinds of minerals present (adapted from Brady and Weil, 2002).

TABLE 2 | The building blocks of a systems approach to describing lithosphere and pedosphere ecosystem services exchange (modified from Jones et al., 2016).

	Pedosphere	
Natural Capital	Natural + Human-derived Capital	Human-derived Capital
Stocks	Stocks	Stocks
Flows	Flows	Flows
Stocks	Stocks	Stocks
Natural Capital	Natural + Human-derived Capital	Human-derived Capital
	Lithosphere	

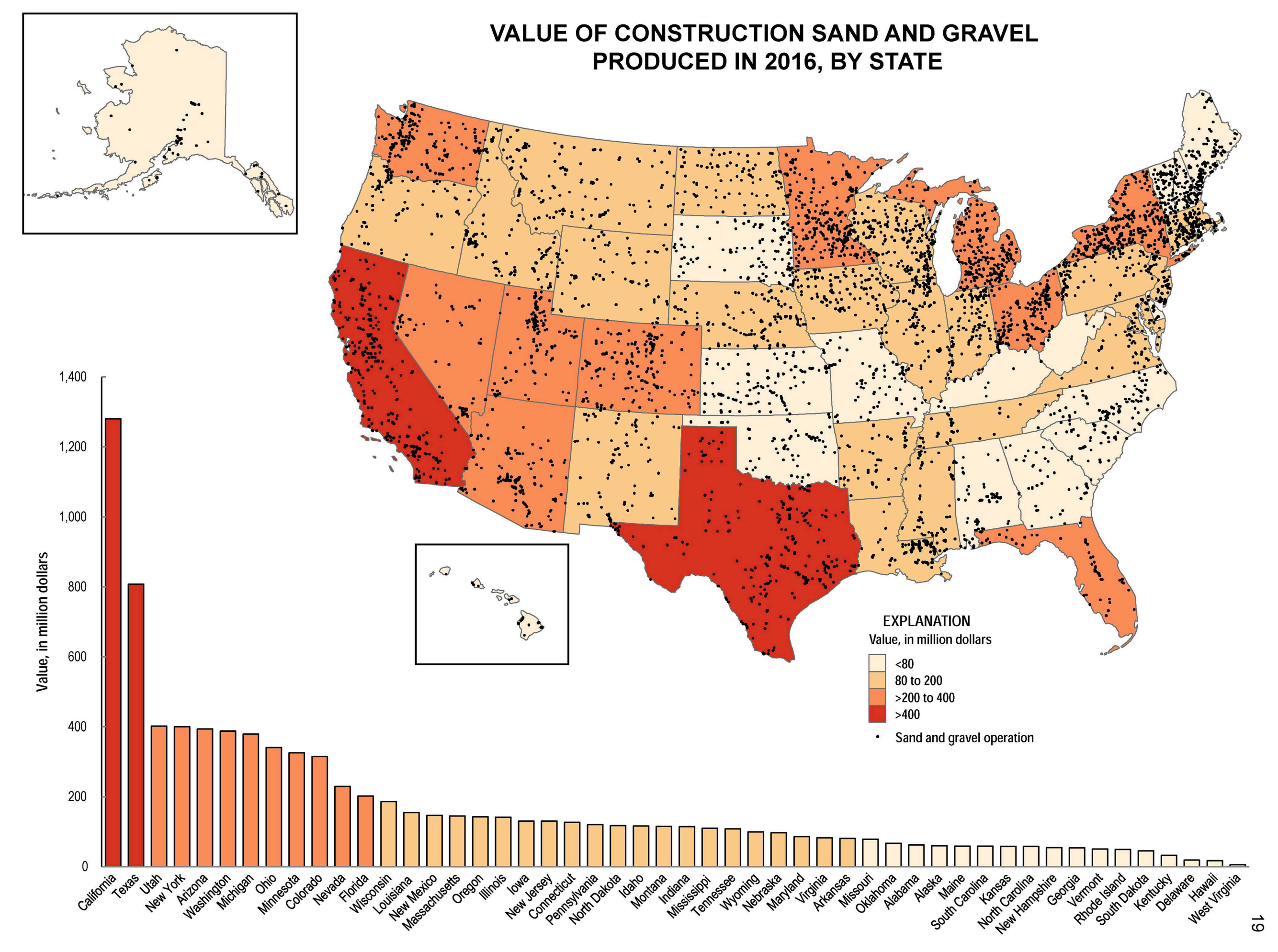

FIGURE 3 | Information about the value of construction sand and gravel from the Mineral Commodities Summary (U.S. Geological Survey, 2017).

TABLE 3 | Examples of "mineral" derived commodities in relation to sand, clay, and gravel (adapted from Comerford et al., 2013).

Use	Sub-use	Component	Purpose
Construction	Landfills	Clay	Landfill barriers
	Aquarium material	Sand and gravel	Base material and substrate
	Artificial reefs	Sand	Foundation for new reefs
	Beach renovation	Sand	Replace beach lost by erosion
	Road surfacing	Gravel	Road construction
	Walkways and driveways	Gravel	For homes and businesses
	Concrete	Sand and gravel	Making concrete
	Brick manufacturing	Sand	Home construction
	Cores of dams	Clay	Dam construction
Kitchenware	Dishes	Clay	Earthenware, stoneware, porcelain
Industrial	Paper coating	Clay	Paper making
	Heat shielding	Clay	Space shuttle
	Insulation	Clay	Temperature control
	Sand blasting	Sand	Cleaning surfaces
	Glass	Silica sand	Glass products
	Paint texture	Sand	Paints
	Foundry molds	Sand	Mold for products
	Toothpaste	Sand	Hygiene
	Filters	Sand/clay	Water and air purification
Medicinal	Sorption	Clay	Adsorbs bacteria to fight diarrhea

TABLE 4 | List of ecosystem services related to coarse fragments, sand, silt, clay, and texture class.

	Quantitative data (listed with ES)				Categorical data (not listed with ES)
Ecosystem services	**Coarse fragments**	**Sand**	**Silt**	**Clay**	**Rock fragment modifier, texture class**
		%			
Provisioning services:					
- Food, fuel, and fiber	x	x	x	x	x
- Raw materials	x	x	x	x	x
- Gene pool	–	–	–	–	–
- Fresh water/water retention	x	x	x	x	x
Regulating services:					
- Climate and gas regulation	x	x	x	x	x
- Water regulation	x	x	x	x	x
- Erosion and flood control	x	x	x	x	x
- Pollination/seed dispersal	–	–	–	–	–
- Pest and disease regulation	x	x	x	x	x
- Carbon sequestration	x	x	x	x	x
- Water purification	x	x	x	x	x
Cultural services:					
- Recreation/ecotourism	x	x	x	x	x
- Esthetic/sense of place	x	x	x	x	x
- Knowledge/ education/inspiration	x	x	x	x	x
- Cultural heritage	x	x	x	x	x
Supporting services:					
- Weathering/soil formation	x	x	x	x	x
- Nutrient cycling	x	x	x	x	x
- Provisioning of habitat	x	x	x	x	x

ES, Ecosystem Services.

are used as separate pure constituent stocks and/or as composite stocks, the context of use (e.g., size, mineralogy, etc.) and type of valuation (e.g., based on "soil" or "mineral" derived commodities, etc.). Mineral derived commodities related to texture (e.g., clays and their types: bentonite, kaolin, etc.) are commonly extracted from lithological, mineral deposits, which are tracked in terms of production and use (U.S. Geological Survey, 2017) (**Figure 3**). Current research often refers to these mineral derived commodities to represent soil ES (**Table 3**), but most likely these commodities were derived from mineral deposits.

Soil texture is quantified in the soil databases, but its monetary value is difficult to assess directly since its components (sand, silt, and clay) are not economical to extract as pure mineral commodities. The ES value of soil texture is recognized in the scientific sense and in association with other soil properties (e.g., available water, infiltration, hydraulic conductivity, etc.). Previous research has shown a wide use of soil texture and coarse fragments in agricultural research with specific benefits obtained from these properties by living organisms. The following examples represent some of the benefits living organisms obtain from texture and coarse fragments based on four categories of ES (Millennium Ecosystem Assessment, 2005) (**Table 4**):

Provisioning services are products derived from ecosystems (e.g., food, water, raw materials, etc.; Millennium Ecosystem Assessment, 2005). For example, soil texture influences food production because different crops prefer different soil textures (e.g., root vegetables prefer sandy soils; Gibberd et al., 2003); soil with specific texture can be used as raw materials (e.g., "fill" material in urban environments; Jim, 1998); soil texture influences water retention and plant available water (e.g., soil texture is used for soil water retention estimation; Martin et al., 2005; Mikhailova et al., 2018a). Tóth et al. (2013) mapped availability of coarse texture, stones, and gravel in the soils of the European Union (EU) for construction purposes.

Regulating services are benefits derived from the regulation of ecosystem processes (e.g., air quality, waste treatment, etc.; Millennium Ecosystem Assessment, 2005). For example, soil texture is important in climate and gas regulation (e.g., methane emissions in rice production; Brye et al., 2013); water regulation (e.g., water and salt movement under irrigation; Wang et al., 2016; Cole et al., 2017); erosion and flood control (e.g., vulnerability to water erosion; Bonilla and Johnson, 2012); carbon sequestration (Gami et al., 2009); water purification (Karathanasis et al., 2006); and overall soil health (Mikhailova et al., 2018b). Spatial analysis of soil texture can aide in guiding site-specific strategies for controlling pest populations (e.g., root nematode populations can be strongly influenced by sand, silt, and clay content, which may be spatially structured as indicated by soil map-units) (Avendano et al., 2004).

Cultural services are non-material enjoyment people obtain from ecosystems (e.g., spiritual experience, aesthetic, etc.; Millennium Ecosystem Assessment, 2005). A Japanese art form called Dorodango utilizes soils of different texture and mineralogy to form a moist ball of soil with the hand that slowly dries as more soil is added and eventually the surface is polished with a cloth. The final result is a nearly perfect sphere of shining soil. The process is often used as a form of self-reflection and meditation, though many have used the techniques to teach soil mineralogy and texture (Georgeson and Payler, 2013; Hartemink et al., 2014). Soil texture is important in the "rice culture" of South Carolina (Carney, 2000). Rice is one of the largest crops grown globally for consumption. For cultivation, the soil texture must be favorable for water retention and therefore the majority of rice crops are grown in soils with a clayey texture to limit the amount of water lost through percolation (Chapagain and Hoekstra, 2011).

Supporting services are services, which support all other ES (e.g., maintenance of life cycles and genetic diversity, etc.; Millennium Ecosystem Assessment, 2005). These include services such as weathering and soil formation (e.g., development of an argillic horizon; Phillips, 2007); nutrient cycling (e.g., total organic carbon and nitrogen; Bechtold and Naiman, 2006), and provisioning of habitat (e.g., abundance of the European earthworm is influenced by the clay content of the soil; Baker et al., 1998).

The SSURGO database is based on soil information gathered by the National Cooperative Soil Survey (NCSS) based on field estimates, ranges of properties that fit within the taxonomic class, and laboratory analyses compiled from USDA-NRCS and university (PEDON) databases (Soil Survey Staff, 2017). The data is displayed by soil map unit (SMU) for most areas in the United States (U.S.) and its Territories, Commonwealths, and Island Nations (Soil Survey Staff, 2017). Soil map units describe soils and other spatial components found in predictable locations across the landscape with unique properties, interpretations, and productivity (Soil Survey Staff, 2017). The SMUs are typically labeled based on the major component or components (Soil Survey Staff, 2017). Soil maps are available at scales ranging from 1:12,000 to 1:63,360 (Soil Survey Staff, 2017). Currently, the SSURGO database provides quantitative information for coarse fragments (CF), sand (S), silt (Si), and clay (C) by layers that must be correlated to describe soil horizons. SSURGO reports three related values for each attribute as "low," "representative value" (RV), and "high" values. The "low" and "high" values is the typical range of values of the attribute in the SMU, or soil horizon, while the RV is an average or expected value of the attribute in the SMU, or soil horizon (Soil Survey Staff, 2017) in the survey area. Another source of data for components of SSURGO map units is the Official Soil Series (OSD) database. The OSD database contains a description of each soil series. The typifying pedon for the series describes the amount of rock fragments and the texture class for each soil horizon, and the OSD also gives ranges of soil properties for each genetic horizon (e.g., A, E, Bt1, Bt2, etc.). Data in the OSD description are used to correlate the layers of SSURGO data and provide more specific horizon data than SSURGO. Both data sources are ubiquitous in extent for use anywhere in the U.S. with existing soil surveys, and contain data that can be substituted for on-site sampled data that is not always available.

The issue of soil heterogeneity has been extensively studied for various applications (e.g., geotechnical, agricultural fields, etc.), and it is commonly classified into two main categories: lithological and inherent spatial soil variability (Elkateb et al., 2003; Zhou et al., 2017). Lithological heterogeneity commonly relates to lithological inclusions within the soil in contrast to the inherent spatial soil variability, which is the variation of soil properties from one point (Elkateb et al., 2003).

This study compares mapping surface soil texture from SSURGO databases to actual field measurements within SMUs. Many farm and/or field-scale ES studies use SSURGO, but the error associated with this database is often not quantified or is simply unknown (Fortin and Moon, 1999; Jiang et al., 2007). The surface soil (Ap) horizon is particularly important in agriculture and the provisioning ES (Chandler et al., 2018; Mikhailova et al., 2018a). The aims of this study were to: (1) map averaged and interpolated values for CF, S, Si, and C resulting from soil core measurements taken within SSURGO SMU boundaries, (2) compare field estimates of CF, S, Si, and C with estimates based on existing SSURGO database information, and (3) discuss the potential of using soil texture in the ES framework evaluation at the farm scale.

MATERIALS AND METHODS

The Accounting Framework

Lithospheric-derived resources such as soil texture and coarse fragments can be valued as "soil" or "mineral" stocks (**Table 5**). Lithospheric stocks are quantifiable amounts of material with units defined in a spatial context, and can be measured as separate pure constituent stocks (e.g., 100 % sand, 100% silt, 100% clay) or as composite stock (e.g., loam with various proportions of sand, silt, and clay) with direct-use utilization. On the other hand, soil texture as a "soil" stock is commonly associated with indirect-use utilization (e.g., matrix for available water, soil infiltration, etc.). **Table 5** provides an accounting framework for valuation of soil texture.

TABLE 5 | Conceptual overview of the soil texture and coarse fragment accounting framework ("mineral" vs. "soil" stock) with examples related to the Willsboro farm, NY, United States.

Biophysical accounts (science-based)	Administrative accounts (boundary-based)	Monetary accounts	Benefit	Total value
Soil extent:	Administrative extent:	Ecosystem service(s):	Sector:	Types of value:
		"Mineral" stock		
- Soil map unit - Soil depth	- Farm	- Provisioning (e.g., raw materials) - Commodity	- Construction (e.g., sand, silt, clay, gravel, etc.)	Direct market valuation Market-based value (e.g., price of sand, silt, clay, gravel, etc.; U.S. Geological Survey, 2017)
		"Soil" stock		
		Example: Soil texture as a matrix for holding available water		
- Soil map unit - Soil depth (Ap-horizon)	- Farm	- Regulating (e.g., water regulation) - Potential flow	- Agriculture (e.g., matrix for holding water: soil texture class as it relates to available water storage)	Indirect use value - Potential for crop production

Study Area

The Willsboro Research Farm (located near Willsboro, NY, USA in the NE part of New York State) is maintained by the Cornell University Agricultural Experiment Station (Sogbedji et al., 2001). The 147-hectare site consists of relatively flat to rolling topography and is found on Willsboro point next to Lake Champlain (Mikhailova et al., 1996). The site has ∼150 days growing season with temperate climate (Mikhailova et al., 1996). Highly variable soils are found throughout the farm because of glacial deposits (e.g., sands, clays, and glacial till) which represent soil orders Inceptisols, Entisols, and Alfisols (**Table 6**).

Soil Sampling and Laboratory Analysis

A total of 54 soil cores were taken by laying out a surveyed grid sample pattern on the farm fields in the summer of 1995 where each grid was 137.16 m by 137.16 m (Cole et al., 2017). A professional land surveyor determined elevations for each sample location by using a Total Station (Set 2C SOKKISHA) tied to a local benchmark with a standard deviation of ±3 mm (Mikhailova et al., 1996). A Giddings hydraulic soil sampler (Model GSR-T-S) was used with plastic liners (4.5 cm diameter) to obtain undisturbed soil cores. The soil cores were of variable depth because of the available sample depth possible with the sampler (Mikhailova et al., 1996).

Soil cores were stored before processing by placing them vertically in a refrigerator at 1°C (Mikhailova et al., 1996). Soil cores were separated by horizons and coarse fragments (soil sample percent >2 mm) were measured. Soil samples were tested for an effervescence reaction using weak HCl. Soil samples consisting of the sectioned cores, with coarse fragments removed, were air-dried, and then ground and processed through a 2 mm sieve. The pipette method was used to determine particle-size distribution of this <2 mm fraction after first treating for removal of organic matter (using 30% H_2O_2) and carbonates and soluble salts (using 1 M NaOAc at a pH of 5; Gee and Bauder, 1986). This study only used the surface soil (Ap horizon) samples.

On-Line Soil Data and Spatial Analysis

Surface soil (Ap horizon) RV of S, Si and C (in %) were obtained directly from the SSURGO database (available from web browser search for "ssurgo data"). The soil texture class was determined from texture triangle (Cole et al., 2017). Content of CF (in %) for the surface soil were obtained from SSURGO or the OSD for the dominant soil in each SMU. Data from OSDs were found by web browser search for "official soil series database" or by typing the name of the soil series searched for in a web browser (e.g., "Bombay series").

Boundaries and composition of the SMUs were obtained from the online SSURGO source at scale of 1:12,000 and mapped in ArcGIS 10.4 (Environmental Systems Research Institute, 2016). The SMUs at the Willsboro Research Farm all had only one dominant soil. SSURGO and OSD values for each SMU were then applied to the corresponding SMU areas using ArcGIS 10.3 (Environmental Systems Research Institute, 2016). From the field measurements, the average CF (%), S (%), Si (%), and C (%) of soil cores taken from within each SMU were applied evenly across the SMU. In a similar fashion, CF (%), S (%), Si (%), and C (%) values were calculated by multiplying the SMU-averaged content values by the corresponding SMU area.

Inverse distance squared weighting (IDW) from the 12 nearest sampling points was utilized to interpolate results from the 54 soil cores across the study area using a 1 m grid cell size in ArcGIS 10.3 (Environmental Systems Research Institute, 2016). This resulted in maps that estimated CF (%), S (%), Si (%), and C (%) for each 1 m^2 of the field site. SSURGO SMU boundaries were used to assign the interpolated values to a SMU name. Inverse distance weighting (IDW) is a deterministic, spatial interpolation method, which is commonly used in many GIS software packages (Lu and Wong, 2008; Li and Heap, 2011, 2014). Although kriging methods generally are preferred over IDW when working with spatially clustered data, IDW methods tend to work well with regularly gridded data (e.g., Isaaks and Srivastava, 1989; Li and Heap, 2011, 2014). Inverse distance weighting is efficient

TABLE 6 | Soil types within Willsboro Farm with corresponding coarse fragments and particle size information included in map unit symbol and family category of taxonomic class.

Soil series (Map unit symbol)	Taxonomic class
Alfisols	
Bombay gravelly loam, 3–8% slopes (BoB)	Coarse-loamy, mixed, active, mesic Oxyaquic Hapludalfs
Howard gravelly loam, 2–8% slopes (HgB)	Loamy-skeletal, mixed, active, mesic Glossic Hapludalfs
Kingsbury silty clay loam, 0–3% slopes (KyA)	Very-fine, mixed, active, mesic Aeric Endoaqualfs
Kingsbury silty clay loam, 3–8% slopes (KyB)	Very-fine, mixed, active, mesic Aeric Endoaqualfs
Covington clay, 0–3% slopes (CvA)	Very-fine, mixed, active, mesic Mollic Endoaqualfs
Churchville loam, 2–8% slopes (CpB)	Fine, illitic, mesic Aeric Endoaqualfs
Entisols	
Claverack loamy fine sand, 3–8% slopes (CqB)	Sandy over clayey, mixed, superactive, non-acid, mesic Aquic Udorthents
Cosad loamy fine sand, 0–3% slopes (CuA)	Sandy over clayey, mixed, superactive, non-acid, mesic Aquic Udorthents
Deerfield loamy sand, 0–3% slopes (DeA)	Mixed, mesic Aquic Udipsamments
Stafford fine sandy loam, 0–3% slopes (StA)	Mixed, mesic Typic Psammaquents
Inceptisols	
Amenia fine sandy loam, 2–8% slopes (AmB)	Coarse-loamy, mixed, active, mesic Aquic Eutrudepts
Massena gravelly silt loam, 3–8% slopes (McB)	Coarse-loamy, mixed, active, non-acid, mesic Aeric Endoaquepts
Nellis fine sandy loam, 3–8% slopes (NeB)	Coarse-loamy, mixed, superactive, mesic Typic Eutrudepts
Nellis fine sandy loam, 8–15% slopes (NeC)	Coarse-loamy, mixed, superactive, mesic Typic Eutrudepts

Note: For example, gravelly is a rock fragment modifier with specific size and quantity: >15% but <35% gravel.

computationally and generally is considered to be highly suitable for sparse data collected on a regular grid (Li and Heap, 2014).

RESULTS AND DISCUSSION

Soils have been recognized as a key regulator of ecosystem functions but their value is rarely quantified. Quantitative assessment of soil ecosystem services and its value at various spatial scales requires use of soil survey databases and/or field data (Adewopo et al., 2014; Dominati et al., 2014). Shrinking financial resources dedicated to soil science research (Adewopo et al., 2014) require a close examination of utility of soil survey databases compared to field data, which is expensive to collect and analyze. There are advantages and disadvantages of using already existing soil survey databases for ecosystem services assessment. Advantages of using these databases include:

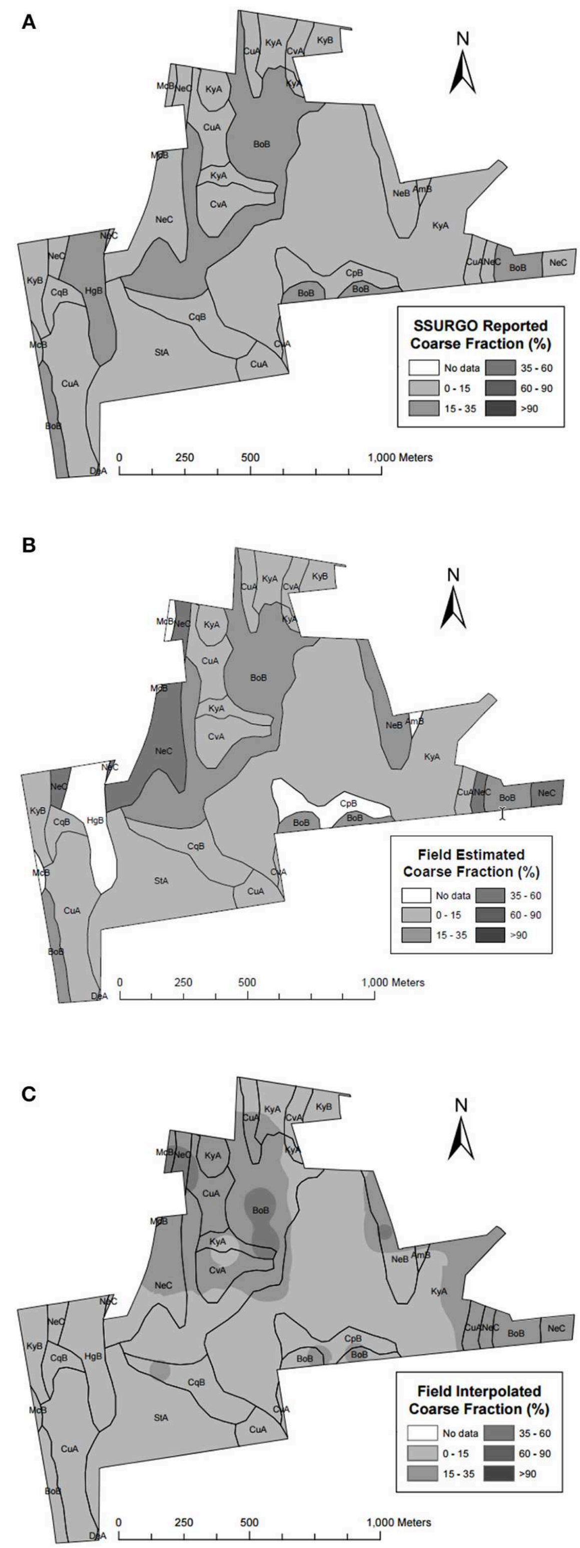

FIGURE 4 | Coarse fraction (CF) content (%): **(A)** from SSURGO representative values for each SMU, **(B)** from soil core sample results averaged over SMUs, and **(C)** interpolated from soil core sample results. In the middle figure only, some SMUs did not have soil cores taken from them and therefore appear as zero in the map.

(1) readily available at no cost, (2) soil data is collected and analyzed using standardized procedures, (3) soil maps are also created using standardized procedures at known scales, (4) soil databases and maps are often integrated with other spatial data sources related to land cover and use, and 5) represents a respected source of information. Disadvantages of using these soil databases include: (1) lack of detailed spatial resolution, (2) not designed for integration with ecosystem services, (3) crisp boundaries that do not necessarily represent natural conditions, (4) often created with limited field data, (5) focus on "shallow" soil, (6) data can be extrapolated instead of measured with depth, (7) static, and (8) not dynamic in temporal sense (Baveye et al., 2016; Small et al., 2017). Among soil properties, soil texture and mineralogy play a crucial role in the soil natural capital (Palm et al., 2007).

Coarse Fragments and Rock Modifiers

Coarse fragments (%) are important for ecosystem services assessment, and can be obtained from the OSD soil map unit name (e.g., Bombay gravelly loam contain >15% but <35% of coarse fragments of gravel size class), or from soil profile descriptions for individual soil horizons of each series (**Table 6**). For example, for the Bombay soil series description (Official Series Description database), the Ap horizon in the typifying pedon description has 20% gravel and 5% cobbles. The rock fragment (RF) texture modifiers based on size and shape class and quantity (e.g., gravelly, very cobbly, extremely stony, etc.) can be derived using the data from SSURGO map unit names (e.g., Bombay gravelly loam), or from the OSD typifying pedon, or from on-site field measurements (e.g., Bombay gravelly loam contain >15% but <35% of coarse fragments of gravel size class), or from soil profile descriptions. Coarse fraction (%) derived from SSURGO and obtained in the field did not agree. Field data CF values were higher for Entisols and Inceptisols than SSURGO values (**Figure 4**). Correlation plot of CF estimates for each SMU revealed no statistically significant correlations between SSURGO and field-averaged ($r = 0.466$, $p = 0.174$) and field-interpolated CF ($r = 0.146$, $p = 0.618$) estimates (**Figure 5A**).

In terms of ES, CF (%) is listed in ES framework as quantitative data. However, rock fragment (RF) texture modifiers are currently not included in the framework even though these data are available from SSURGO, OSD, and field measurements. Rock fragment modifiers play an important role in ES such as providing cultural services. For example, soils of the Willsboro farm formerly contained large amounts of stones, which were used to build typical "New England stone walls" and provide numerous cultural services (e.g., esthetic sense of place and cultural heritage, etc.; Thorson, 2004). According to Thorson (2004), stone walls were the biggest investment on a farm and became the "defining element" of the Northeast's landscape symbolizing the shift to an agricultural economy.

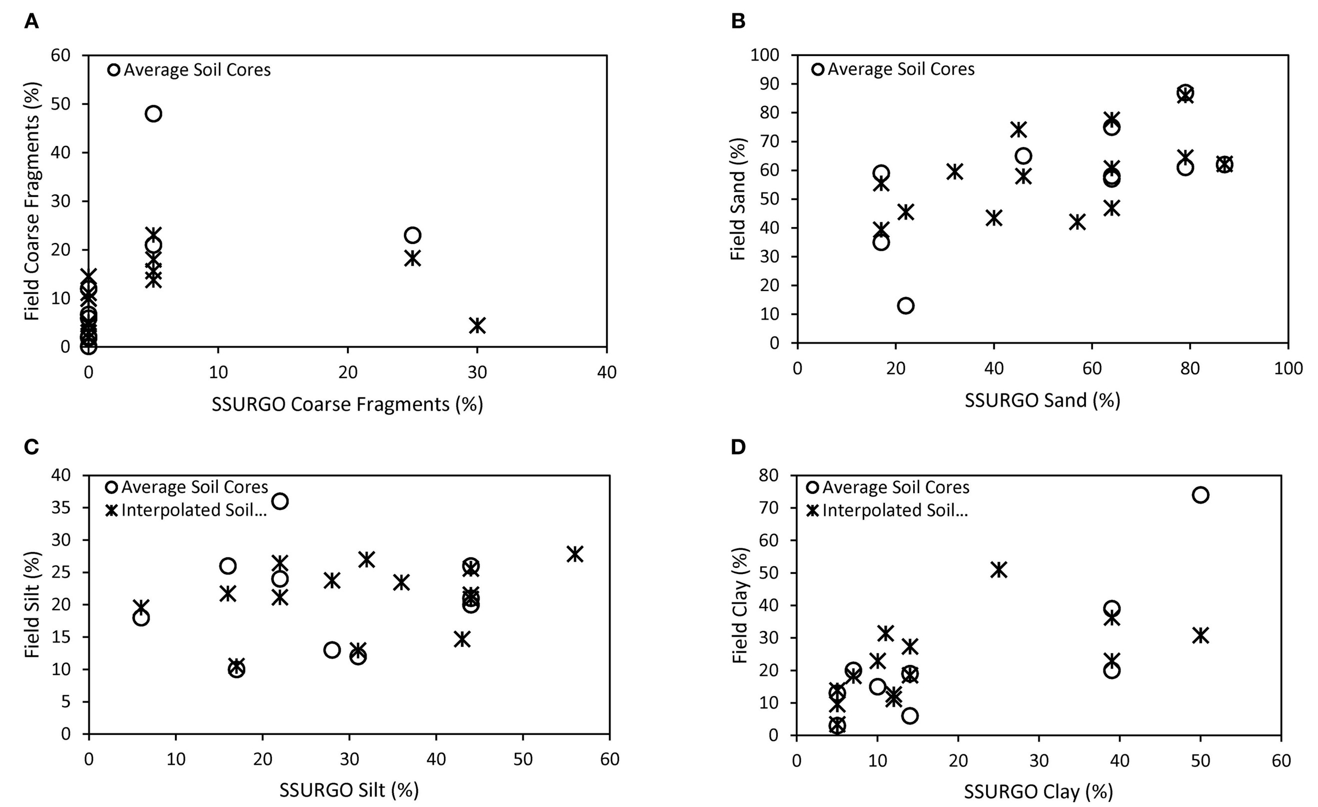

FIGURE 5 | Bivariate correlation plots of: **(A)** coarse fragments, **(B)** sand, **(C)** silt, and **(D)** clay for field results vs. SSURGO results for each SMU.

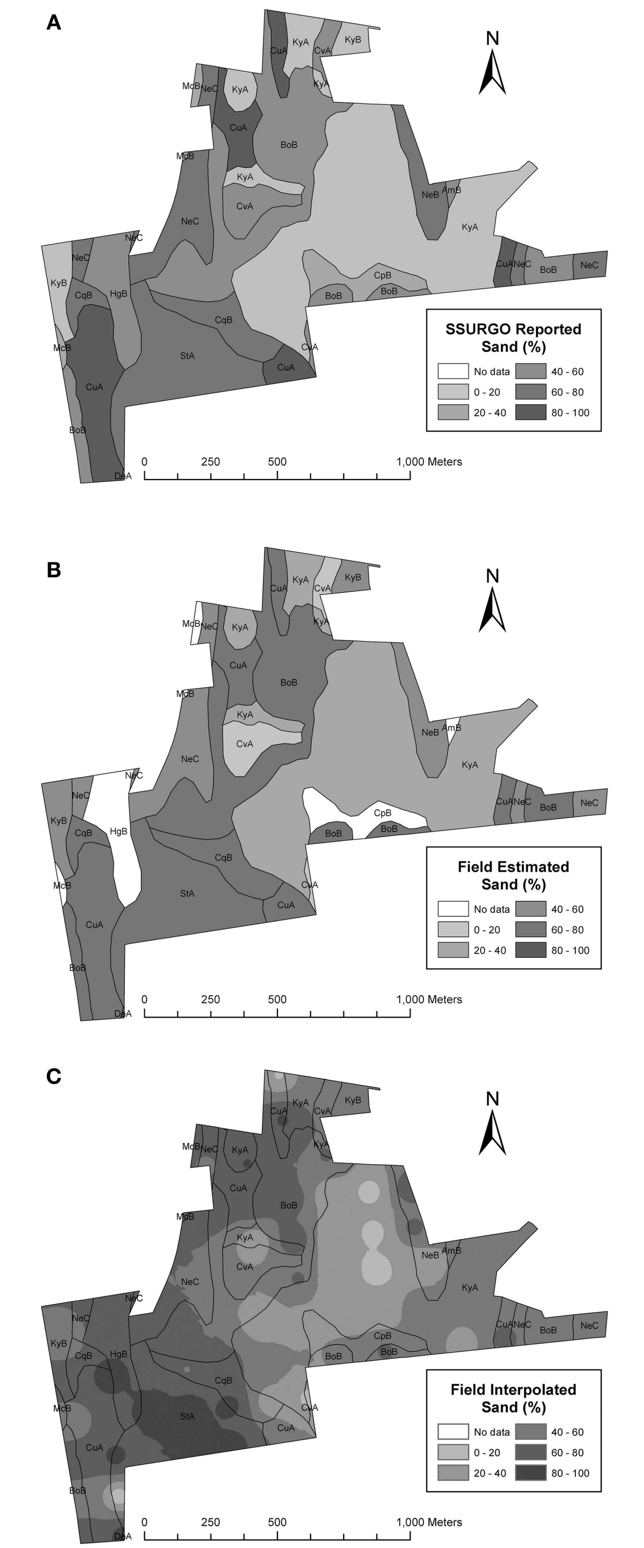

FIGURE 6 | Sand (S) fraction (%): **(A)** from SSURGO representative values for each SMU, **(B)** from soil core sample results averaged over SMUs, and **(C)** interpolated from soil core sample results. In the middle figure only, some SMUs did not have soil cores taken from them and therefore appear as zero in the map.

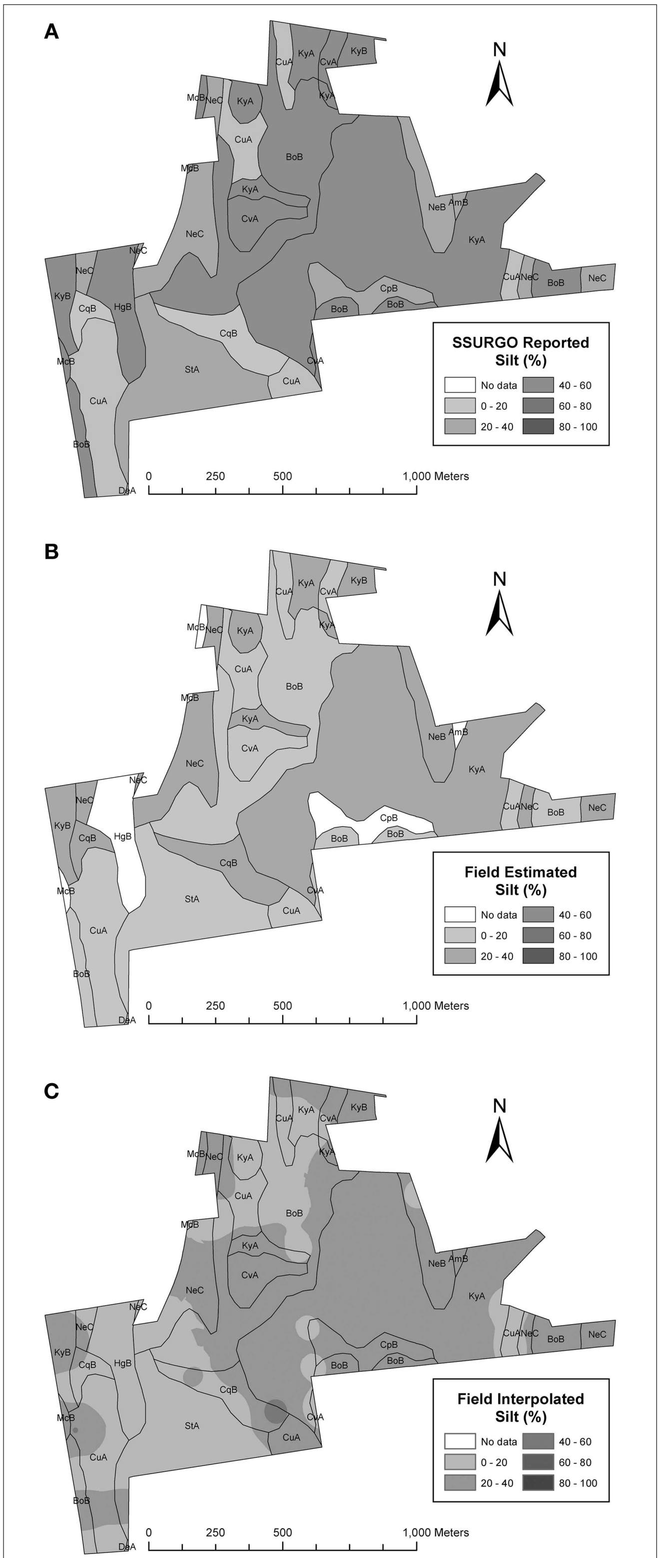

FIGURE 7 | Silt (Si) fraction (%): **(A)** from SSURGO representative values for each SMU, **(B)** from soil core sample results averaged over SMUs, and **(C)** interpolated from soil core sample results. In the middle figure only, some SMUs did not have soil cores taken from them and therefore appear as zero in the map.

Comparison of Field Sampling and Soil Survey Database for Sand, Silt, Clay, and Texture Class

Sand (%) is reported in SSURGO data and can be obtained from field measurements as well. Sand (%) derived from SSURGO and obtained in the field were both variable (**Figure 6**) with field data reporting values for sand within the ranges reported by SSURGO (**Figure 6**). Correlation plot of sand estimates for each SMU revealed statistically significant correlations between SSURGO and field-averaged ($r = 0.668$, $p = 0.035$) and field-interpolated sand ($r = 0.531$, $p = 0.051$) estimates (**Figure 5B**).

Silt (%) derived from SSURGO and obtained in the field were both variable (**Figure 7**) with field data reporting values for silt lower than values reported by SSURGO (**Figure 7**). Correlation plot of silt estimates for each SMU revealed no statistically significant correlations between SSURGO and field-averaged ($r = 0.057$, $p = 0.876$) and field-interpolated silt ($r = 0.304$, $p = 0.291$) estimates (**Figure 5C**).

Clay (%) derived from SSURGO and obtained in the field were both variable (**Figure 8**) with field data reporting values for clay higher than values reported by SSURGO for CvA soil map unit (**Figure 8**). Correlation plot of clay estimates for each SMU revealed statistically significant correlations between SSURGO and field-averaged ($r = 0.823$, $p = 0.003$) and field-interpolated clay ($r = 0.584$, $p = 0.028$) estimates (**Figure 5D**).

Soil texture class (categorical data) is currently not included in the ecosystem services framework, but it is commonly used by soil scientists and provided in SSURGO when there is only one dominant soil in the SMU, in OSD, and in field soil descriptions. Texture classes for many of the soil map units on the farm were different based on SSURGO data vs. field-measured estimates (**Figure 9**).

Soil texture determines the surface area, porosity, nutrient, and water holding capacity, water infiltration, etc., necessary for ecosystem processes (Parton et al., 1987; Palm et al., 2007; Cole et al., 2017). Several experiments conducted at the Willsboro Research Farm demonstrate the significance of soil texture in providing ecosystem services. For example, the grass biomass yields of Switchgrass ("Cave-in-Rock") and cool-season grasses (CSG) tall fescue (endophyte-infected, "KY-31") and reed canarygrass ("Rival") were higher on the clay than the sandy soils at the Cornell Baker Research Farm at Willsboro, NY (Cherney et al., 2013). Soil texture was a significant factor in nitrogen transformation rates with the cropping history of alfalfa (*Medicago sativa*), grass sod (primarily fescue *Festuca rubra*) with denitrification rates higher for the clay site compared to the sand site (Sogbedji et al., 2001). Soil texture class is also important in field assessments of infiltration rate, hydraulic conductivity, available water, soil interpretations (e.g., construction limitations, etc.), erosion potential (Karathanasis et al., 2013), and merits inclusion in the ecosystem services framework (Mikhailova et al., 2018a).

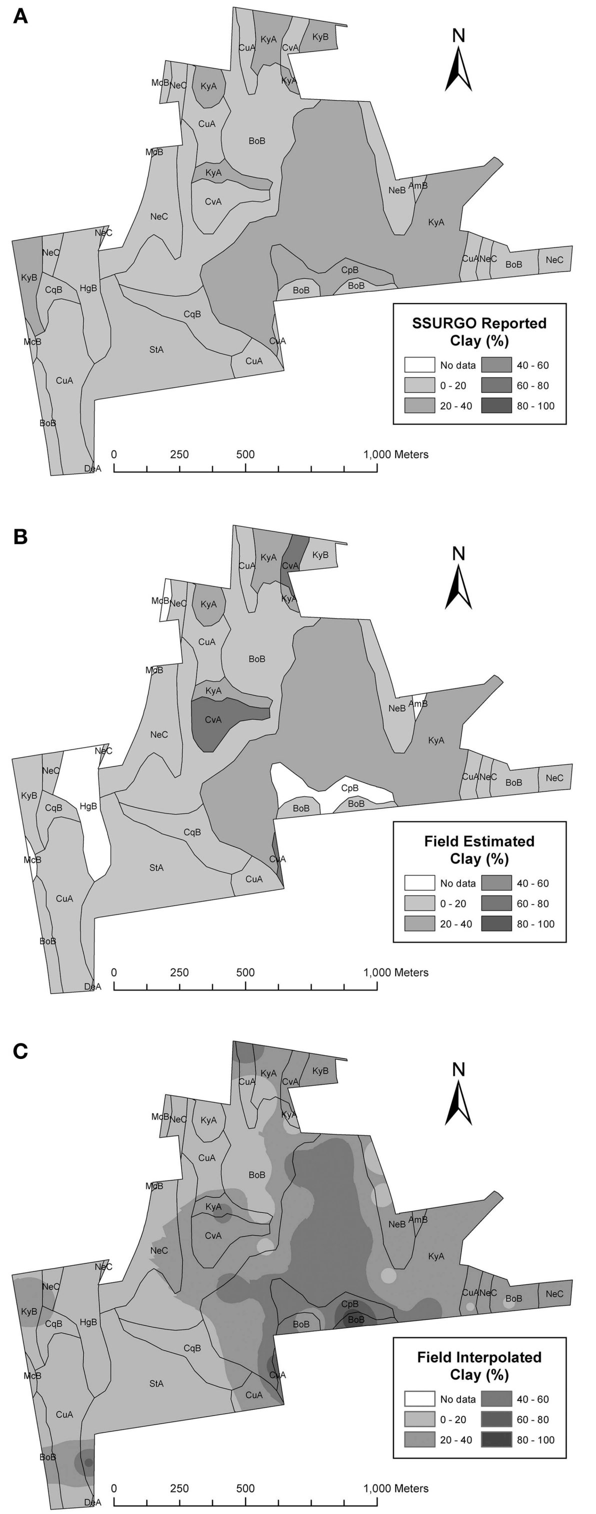

FIGURE 8 | Clay (C) fraction (%): **(A)** from SSURGO representative values for each SMU, **(B)** from soil core sample results averaged over SMUs, and **(C)** interpolated from soil core sample results. In the middle figure only, some SMUs did not have soil cores taken from them and therefore appear as zero in the map.

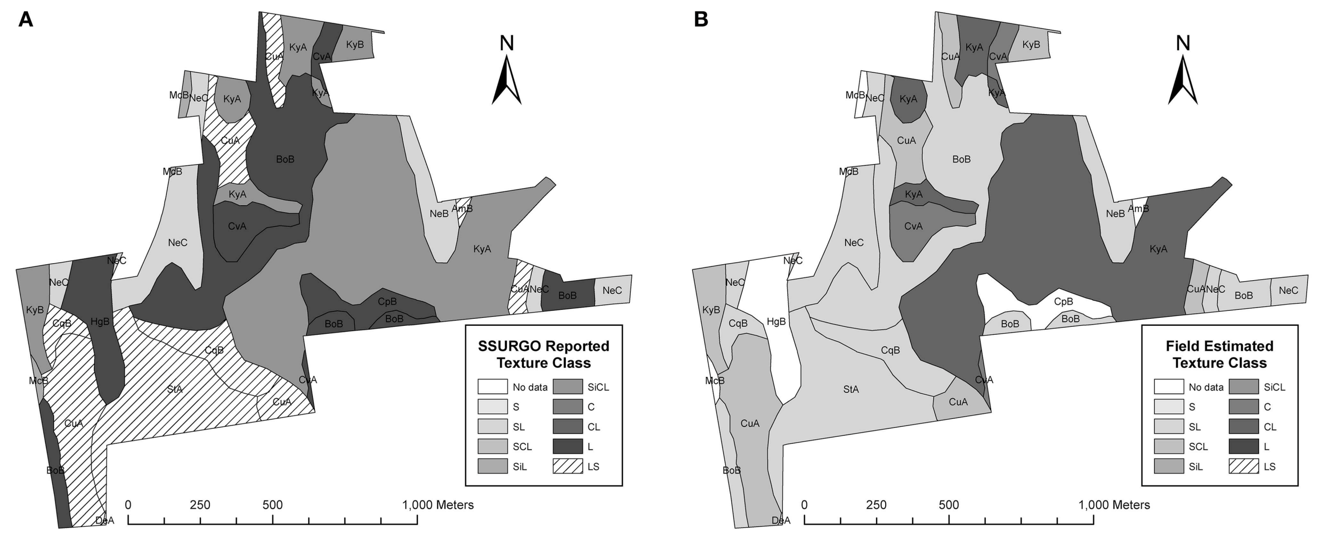

FIGURE 9 | Soil texture class: **(A)** from SSURGO representative values for each SMU, **(B)** from soil core sample results averaged over SMUs. S, sand; LS, loamy sand; SL, sandy loam; L, loam; SiL, silt loam; SCL, sandy clay loam; CL, clay loam; SiCL, silty clay loam; C, clay.

Challenges in Assessing Ecosystem Services of Sand, Silt, Clay, Coarse Fragments, and Soil Texture

Soil texture often relates to the mineral composition of soil. For example, sand is composed primarily of quartz, SiO_2, which provides limited plant nutrients in contrast to clay which can be a significant source of various nutrients as a result of weathering. Assessing ecosystem services of sand, silt, clay, coarse fragments, and texture is a challenging and complex task, because it can be “soil” or “mineral” stocks. Although these soil properties are extensively described and quantified in the existing soil databases they are often linked to the “mineral” commodities instead of “soil” stocks. For example, Comerford et al. (2013) list numerous uses of soil materials/particles derived from “shallow to deep subsoils” (**Table 3**), but most likely these materials/particles are mined from mineral deposits (e.g., sand and gravel deposits are found on beaches, rivers, and streams). These “mineral” commodities are often monitored and valued on a regular basis in contrast to the “soil” commodities. For example, Mineral Commodities Summaries (U.S. Geological Survey, 2017) provide annual reports for clays, sand and gravel (construction, industrial), stone (crushed, dimension) mined from specific operations, and used primarily for industrial and constructions purposes (**Figure 3**). For example, New York ranked 14th in 2016 in terms of value of non-fuel mineral production in the United States with stone (crushed), sand and gravel (construction), and clays (common) listed as some principle minerals mined from various operations. The “soil” derived material/particles commodities are often not economical to “mine” as “mineral” commodities from the soil and that is why they are not included in the standard Mineral Commodities Summaries (U.S. Geological Survey, 2017). Soil mineral particles as “soil” stocks can be used/mined over and over (e.g., as a matrix for plant growth) in contrast to “mineral” commodities, which are often used as one-time use commodities with the exception when they are recycled. The difference between soil texture as a “mineral” or “soil” stock can be incorporated into the accounting framework (**Table 5**). For example, surface soil texture at the Willsboro Farm can be a source of sand for construction purposes, which can be valued based on available commodity prices for construction sand (U.S. Geological Survey, 2017). On the other hand, the value of soil texture at the Willsboro Farm in relation to plant available water (Mikhailova et al., 2018a), and infiltration rate (Cole et al., 2017) is linked to indirect use value (**Table 7**). **Table 8** demonstrates the lithosphere-pedosphere-hydrosphere ecosystem services exchange, stocks, goods, flows, and ownership at the farm scale. Lithosphere provides pedosphere with mineral fraction (<2 mm in size) which serves as a matrix for holding available water provided by hydrosphere via ecosystem services flow. Since this study is conducted at the farm scale it creates an intricate ownership interplay since both lithospheric and pedospheric stocks are private within the farm boundaries, and hydrospheric resources are common-pool resources since they are not restricted by the farm boundaries. In this case available water attached to the soil particles is a tangible source of water (benefit obtained from regulation of hydrospheric ecosystem services) that can be consumed by crops (Ban et al., 2015). Su et al. (2018) stressed the important of “disentangling” the intricate links and processes essential to ES.

According to Grunwald et al. (2011), there are numerous limitations in using existing soil survey databases (including SSURGO). Soils are commonly mapped based on a typical pedon physical and chemical description and by identifying boundaries between different soil types. Grunwald et al. (2011)

TABLE 7 | Example of the effect of spatial heterogeneity of soil texture on the available water for the Ap horizon (AW_{Ap}) by soil type and soil order from SSURGO and detailed field study (modified from Mikhailova et al., 2018a).

Soil order/Soil series (Map unit symbol)	SSURGO			Detailed field study		
	Total area	Reported Ap thickness	AW_{Ap} from texture	Number of soil cores	Measured Ap thickness	AW_{Ap} from texture (interpolated)
	m^2	cm			cm	
Alfisols (total)	**937,923**	**23.7 ± 1.3***	**3.58**	**32**	**23 ± 6**	**2.75**
Bombay gravelly loam, 3–8% slopes (BoB)	270,606	25.40	2.86	10	21 ± 5	2.39
Churchville loam, 2–8% slopes (CpB)	36,898	22.86	4.11	n/a**	n/a	3.34
Covington clay, 0–3% slopes (CvA)	49,074	22.86	3.66	1	26	2.78
Howard gravelly loam, 2–8% slopes (HgB)	58,680	25.40	1.78	n/a	n/a	1.95
Kingsbury silty clay loam, 0–3% slopes (KyA)	480,680	22.86	4.11	19	23 ± 6	2.94
Kingsbury silty clay loam, 3–8% slopes (KyB)	41,985	22.86	4.11	2	30 ± 14	3.38
Entisols (total)	**378,719**	**27.9 ± 2.9**	**2.74**	**18**	**24 ± 7**	**2.13**
Claverack loamy fine sand, 3–8% slopes (CqB)	64,231	30.48	3.05	4	28 ± 10	3.06
Cosad loamy fine sand, 0–3% slopes (CuA)	168,536	30.48	2.13	6	19 ± 7	2.17
Deerfield loamy sand, 0–3% slopes (DeA)	331	25.40	2.03	1	22	1.10
Stafford fine sandy loam, 0–3% slopes (StA)	145,621	25.40	3.30	7	26 ± 4	1.69
Inceptisols (total)	**157,753**	**22.9±0.0**	**3.28**	**4**	**22 ± 8**	**2.37**
Amenia fine sandy loam, 2–8% slopes (AmB)	3,185	22.86	3.26	n/a	n/a	2.41
Massena gravelly silt loam, 3–8% slopes (McB)	8,479	22.86	3.69	n/a	n/a	2.48
Nellis fine sandy loam, 3–8% slopes (NeB)	39,027	22.86	3.26	3	19 ± 6	2.31
Nellis fine sandy loam, 8–15% slopes (NeC)	107,062	22.86	3.26	1	30	2.38

**Means ± standard deviations, unless only a single value was available.*
***n/a: not applicable. No soil core was taken from the specific SMU.*

TABLE 8 | Lithosphere-pedosphere-hydrosphere ecosystem services exchange, stocks, goods, flows (represented by arrows), and ownership at the farm scale in relation to soil texture and available water.

Lithosphere ⟷	**Pedosphere** ⟷	**Hydrosphere**
Mineral stock	Soil texture as a matrix for holding available water	Water stock
	Ownership at the farm scale	
Private within the farm	Private within the farm	Common-pool resource
	Types of utilization (valuation)	
Direct use (market-value): Mineral resources	Indirect use: Potential for crop production	Direct use (market value): Water

refers to these boundaries as "double crisp" because this spatial soil data is categorized by "crisp" map unit boundaries and "crisp" soil classes which do not represent soil physical and chemical property variation or allow for error assessment or uncertainty evaluation. Our study demonstrates the important distinction between mapping using the "crisp" boundary soil SSURGO databases (**Figures 4A**, **6A**, **7A**, **8A**) compared to the actual spatial heterogeneity of field interpolated data (**Figures 4C**, **6C**, **7C**, **8C**). Because of how the SSURGO databases were constructed at a typical scale of 1:12,000 using the polygon soil boundaries, they fail to represent actual field-scale variation in soil texture and coarse fraction which is clearly evident when the SSURGO and field interpolated maps are compared. This may affect both spatial and overall estimates of these soil physical properties as they relate to ecosystem services.

CONCLUSIONS

Lithospheric-derived resources such as soil texture and coarse fragments are key soil physical properties that contribute to ecosystem services (ES), which can be valued based on "soil" or "mineral" stocks. These stocks can be measured and valued as separate constituent stocks (e.g., % sand, % silt, % clay) or as composite (total) stocks: sand (%) + silt (%) + clay (%) = 100% (e.g., soil texture classes: loam, silty clay loam, etc.). For soil texture as a "mineral" stock, government Mineral Commodities Summaries provide annual reports for clays, sand and gravel (construction, industrial), stone (crushed, dimension) mined from specific operations, and used primarily for industrial and construction purposes. For soil texture as a "soil" stock, SSURGO data of CF (%), S (%), Si (%), and C (%) at the SMU can be used for soil ecosystem framework assessment, especially regarding sand and clay fractions. Categorical data (rock fragment, and texture class) are not currently included in the ecosystem services framework, but provide important information commonly used in agriculture and environmental science and therefore should be incorporated. Visual comparison shows that the SSURGO data differs from the higher resolution interpolated soil property maps based on field data. Care needs to be taken when deriving ecosystem services from existing soil databases (e.g., SSURGO) because they often provide limited information on both the physical property variability and spatial variability. The resolution of soil data needed to accurately estimate soil ecosystem services depends on the type of service and its relation to other environmental attributes. Soil maps in the future need to be represented at the same spatial resolution as the related land cover which is often mapped at a higher spatial resolution (e.g., 30 m pixel) with a known accuracy. Soil texture is often linked to other soil properties, which are valued based on indirect-use opposed to direct-use valuation.

AUTHOR CONTRIBUTIONS

EM: conceptualization. EM and MS: methodology. MC and HZ: visualization, EM, CP, MS, PG, GG, RS, and JG: writing–review and editing.

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Quantitative Evaluation of Soil Functions: Potential and State

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Soils play a key role for the functioning of terrestrial ecosystems. Thus, soils are essential for human society not only because they form the basis for the production of food. This has long been recognized, and during the last three decades the need to establish methods to evaluate the ability of soils to provide soil functions has moved toward the top of the agenda in soil science. Quantitative evaluation schemes are indispensable to adequately include soils into strategies to reach sustainable development targets. In this paper we build upon existing approaches and propose a concept to evaluate individual soil functions with respect to the soil's intrinsic potential in contrast to its actual state. This leads to a separation of indicator variables and allows for conclusions on the structure of appropriate models that are required to predict the dynamics of soil functions in response to external perturbation. This concept is demonstrated for the production function, carbon storage and water storage which are evaluated exemplarily for different plots of a long-term field experiment. It is discussed for nutrient cycling and habitat function, where evaluation schemes are still less obvious.

Keywords: soil functions, ecosystem services, soil indicators, modeling soil functions, soil evaluation

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1. INTRODUCTION

The wish and need to evaluate soil functions is probably as old as agriculture. Until the 1990s, the focus was mainly on the evaluation of soil fertility and its suitability for growing different crops. Since then, the perspective on soil functions has increasingly moved beyond the agricultural potential reflecting the fact that soils are essential for the functioning of terrestrial ecosystems in many different ways (Doran and Parkin, 1994; Larson and Pierce, 1994; Blum, 2005) including climate control, water quantity and quality, nutrient cycling and being the habitat of an overwhelming biodiversity. These four additional aspects are critical for the earth system and are the subject of this paper along with the production function of soils, which is still of central importance for human societies. These 1 + 4 soil functions also play an important role in realizing the UN Sustainable Development Goals related to food, water, climate health and biodiversity (Bouma and Montanarella, 2016; Keesstra et al., 2016). They are directly linked to soil ecosystem services which account for the immediate benefits that human societies derive from soils (Spangenberg et al., 2014; Hauck et al., 2013). Similarly, this was also addressed by the soil "natural capital" (Robinson et al., 2009; Costanza et al., 1997). Here we focus on soil functions as generated by interacting soil processes without any socioeconomic evaluation as implied by the notion of ecosystem services. Nonetheless, such an evaluation of soil functions is prerequisite for the derivation of ecosystem services.

Being aware of the multifaceted nature of soil functions, their evaluation is increasingly summarized under the terms of soil health and soil quality (Doran and Parkin, 1994; Karlen et al., 1997; Kibblewhite et al., 2008), and the need to maintain soil multifunctionality has been emphasized by the term soil security (McBratney et al., 2014) in analogy to food security and water security. Today, how to actually quantify soil functions (Andrews et al., 2004; Schulte et al., 2014, 2015; Greiner et al., 2017; Bünemann et al., 2018) is a very active field of research. This is a formidable research challenge since soil functions are not well-defined soil properties measurable using some specific sensor but are considered to be integral properties emerging from a multitude of complex interactions between physical, chemical and biological processes in soil (Vogel et al., 2018). Hence, the evaluation of soil functions needs to be based on measurable soil properties, in the following referred to as soil attributes. Such a quantitative evaluation is not only highly required for decision makers including politicians, administrators and farmers to monitor positive or negative changes in soil functions. It is also a prerequisite for modeling the change of soil functions, which is essential to predict the (positive or negative) effects of external perturbations brought about mainly by agricultural soil management and not least climate change. This is one of today's most critical challenges in soil science.

In light of this general evidence and because of different motivations for soil function evaluation, there are different concepts available and applied. The main differences originate from four dimensions of consideration: (i) the target functions (i.e., which soil functions are in the focus and how are they defined), (ii) the general purpose of evaluation (i.e., are we interested in the actual state of a soil or its potential to fulfill some function), (iii) the spatial scale (i.e., evaluation of a local soil or mapping of soil functions across landscapes) and (iv) the target group (i.e., farmers, authorities, environmental agencies and the public). The common baseline of all concepts is that soil functions are estimated based on observable soil attributes used as indicators. Useful indicators are soil attributes that provide substantial information on soil functions such as soil bulk density or water capacity. The choice of indicators, however, depends on the context with respect to the four dimensions of consideration mentioned above: should they address the potential of soil to provide a distinct soil function or its current state in relation to its potential? Or should they be observable in the field, measurable in the lab or available through soil maps?

Recently, very valuable reviews on the various approaches have been provided by Bünemann et al. (2018) and Greiner et al. (2017) which will not be repeated here. A major conclusion of Bünemann et al. (2018) was that there are only a few approaches that provide clear interpretation schemes for the measured indicator values and that often clear conceptual or mechanistic relationships between indicators and soil functions are missing. With respect to modeling the dynamics of soil functions, such clear relationships are essential. The identification of soil attributes as valuable indicators should not only be based on pure statistical correlations. It should be based on our understanding of how soil functions are generated through the complex interactions of soil processes. Such an approach can open an avenue to model the dynamics of soil functions in response to external perturbations—be it agricultural management or climate change—using process-based models that focus on the dynamics of the soil attributes identified as valuable indicators (Vogel et al., 2018).

The aim of this paper is to synthesize available knowledge and concepts with the focus on mineral soils under agricultural use and humid temperate climate as typical for Central Europe. A crucial question is how to separate the evaluation of the soils' potential and the soils' actual state to fulfill soil functions. The discrepancy between both indicates the room for improving soil management for a specific soil with respect to its soil functions. Moreover, we treat the 1 + 4 soil functions separately, which was recently suggested also by several authors (Bouma, 2014; Baveye et al., 2016; Bünemann et al., 2018). In this way, tradeoffs between soil functions can become visible, and the fact that different soils provide different contributions to the ensemble of soil functions is accounted for. This finally allows the development of soil- and site-specific management options. The evaluation of individual soil functions might be integrated under the roof of soil quality or soil health. However, we agree with Sojka and Upchurch (1999) that a general soil quality index entails a substantial loss of information. Evaluating the different soil functions separately allows for multicriterial optimizations of soil management strategies.

In the following, we first suggest a general concept of how to separate between the intrinsic potential of soil to fulfill the 1 + 4 functions and the soil's actual state. For doing both, we follow the approach of dimensionless scoring functions as already introduced by others (Andrews et al., 2004; Mueller et al., 2007). These scoring functions need to integrate our current process understanding. They are ideally formulated on continuum scales in contrast to ordinal scales provided by scoring tables to better address dynamic changes. This concept is then demonstrated for a set of different soil functions, i.e., production, carbon storage and water storage, and we discuss how this could be extended to other soil functions, such as nutrient cycling and habitat for biological activity. Finally, we discuss how this could help in modeling soil functions and where to get the required data to make this concept operational.

2. EVALUATION OF SOIL FUNCTIONS—SEPARATING POTENTIAL AND STATE

When evaluating soil functions, the motivation is either to estimate the intrinsic potential of soil to fulfill various functions or to evaluate its actual state for doing so. The intrinsic potential of a soil is considered to be the maximum a soil can offer based on its inherent properties with respect to the various individual soil functions. This implies that all soil properties that can be affected by soil management within the limits of a good agricultural practice are in some optimum state. This intrinsic potential needs to be distinguished from the soils' actual state since the analysis has to be based on different soil attributes depending on these two different perspectives as we will explain in the following.

The evaluation of the soils intrinsic potential should be related to inherent soil properties and site conditions (i.e., texture, mineralogy, soil depth, climate) since all that can be affected by soil management is only relevant for reaching this potential and, thus, cannot be part of its definition. For example, a silty loam soil from Loess has the potential to produce much higher yields as compared to a sandy soil even if the silty loam might perform as badly as the sandy soil due to insufficient management. Hence, when evaluating the potential of soil, we implicitly assume that all soil attributes that can be affected by soil management (e.g., bulk density, pH, organic matter content) are in some optimum state. This is in fact an intuitive assumption for the evaluation of the soils potential being defined as, what could be achieved by some optimal soil management? In contrast, the evaluation of the actual state needs to be based on the manageable soil attributes, which was also referred to as dynamic soil quality (Karlen et al., 2003). Indeed, the evaluation of the actual state of soil is currently the major focus of soil quality rating (Mueller et al., 2007) because of its practical meaning for local soil management by farmers. In principle, the actual state can be compared to the soils' potential to quantify the room for improvement for an individual soil with respect to the individual soil functions. It should be noted that climate may change as well and consequently also the intrinsic potential as defined here might change. However, in the context of evaluating soil functions in response to soil management we consider time scales of not more than a decade and we assume that climate is stable.

In **Table 1**, the set of soil and site attributes that we consider important and that are typically used to estimate the state and potential of the different soil functions are summarized. Thereby, we distinguish three different categories: those related to the local climate (C), to inherent soil properties and site conditions (S) and soil attributes which are affected by soil management (M). The categories C and S are used to evaluate the soils' potential while the evaluation of the actual state is based on category M. For each soil function, the soil attributes that are typically used as indicator variables are marked by colored boxes. The distinction of inherent and manageable properties was also introduced by Dominati et al. (2010) to demonstrate which properties can be affected by external drivers. Here we use this distinction to separate soils' potential from their actual state. It might be astonishing that among the inherent soil properties that determine the soils' potential there are no biological factors, although we are well aware that the vast majority of soil processes are biologically driven. The reason for this is that the development of biological communities and their activities depend on the abiotic boundary conditions. This has been reflected by an in-depth discussion of the meaning of organisms in soil formation by Jenny (1941). Hence, biological processes are included in the evaluation of soils' potential only implicitly in that e.g., a silty loam textured soil under humid conditions provides substantial capacity to store water and organic matter so that a rich biological community can evolve to ensure soil structure stabilization and nutrient cycling.

A technical challenge is how to combine properties with very different physical units as listed in **Table 1**. This is required to come up with some suitable estimator for each soil function. To do so, we build upon the concept of scoring functions for individual soil attributes or suitable combinations of them. This is common practice in soil quality rating (Karlen et al., 2003; Mueller et al., 2007; Moebius-Clune, 2017). The basic idea is that observable soil attributes which are used to build indicators have some optimum range where the considered soil function is not impaired, while there are critical threshold values beyond which the soil functions start to be compromised. This can be expressed by dimensionless scoring functions that take values, e.g., between zero and unity, depending on the indicator value. Such scoring functions are required since the renormalization of the indicator values to a dimensionless scale allows the combination of different qualities of indicators. Moreover, if these scoring functions are continuous in contrast to ordinal scales based on lookup tables, this allows researchers to better evaluate dynamic changes and to better address uncertainties (Greiner et al., 2017).

As is clearly shown in **Table 1**, there are many attributes which are relevant for more than one soil function. In contrast to the approach proposed by Andrews et al. (2004), who combined the relevance of a given attribute for the various soil functions into one single scoring function, we define individual scoring functions for each indicator and for each individual soil function (i.e., for each colored box in **Table 1**). This means that attributes, which are relevant for different soil functions, are described by different scoring functions related to the specific soil function. For example, the scoring function of air capacity with respect to water storage might be different from that with respect to the production function. The separation of scoring functions for individual soil functions facilitates their definition and finally allows us to quantitatively address tradeoffs between soil functions. The challenge is to find and combine the optimal set of soil attributes which would allow us to effectively integrate our current knowledge of soil processes and how they affect the individual soil functions. Basically, the definition of the scoring functions integrates our actual knowledge on soil processes and how soil attributes affect the individual soil function. This knowledge is certainly incomplete. In this paper, we focus on the concept of how to apply and combine scoring functions while the detailed definition of these functions remains open for discussion and might be different for different crops and climatic regions.

To come up with a unique quantification of the individual soil functions, the rating with respect to the relevant attributes needs to be combined in a suitable way. This can be done at two levels. First, different soil attributes can be combined to generate a meaningful indicator. For example, the water capacity obtained from soil porosity along the soil profile can be added to the climatic water balance during the vegetation period to generate a meaningful indicator for the water deficit as critical for the production function. At the next level, the multiple dimensionless values of the various scoring functions need to be combined in a reasonable way. We suggest to use the harmonic mean in case the various indicators cannot compensate each other with respect to their impact on the given soil function. As demonstrated further below, this is typically the case. If there are compensatory effects, an arithmetic mean might be more appropriate.

TABLE 1 | Inherent and manageable soil and site attributes which might be used as indicators to estimate the potential and the actual state of a soil to fulfill its functions.

		inherent soil & site conditions										affected by soil management							
		hydrol		site			soil					physics				chem.		biol.	
	SOIL & SITE ATTRIBUTES	water balance (vegetation period)	depth to groundwater	temperature	slope aspect	slope gradient	soil depth (rootable)	texture	mineralogy	$CaCO_3$	coarse fragments	bulk density	air capacity	plant available water	hydraulic conductivity	SOC	pH	earthworm abundance	species diversity
SOIL FUNCTIONS																			
Production (fertility)																			
Nutrient cycling – mobilization & buffering																			
Carbon storage																X			
Water storage & filtering												X							
Habitat for biological activity																			X

We distinguish the categories climate (C, blue), soil and site (S, yellow) and soil attributes affected by management (M, green). Lower color intensity indicates that the relation between property and function is not yet well established. Boxes marked by X provide the most direct measure for the corresponding function state.

In the following we demonstrate this concept for the evaluation of the potential and actual state of soil with respect to the production function, carbon storage and water storage. The proposed scoring functions are introduced to demonstrate the concept, being aware that they might require adaptation for different crops. For other soil functions, where the state of knowledge on suitable evaluation concepts is even more vague (e.g., nutrient cycling and habitat for biological activity), we restrict the discussion to the current understanding of suitable indicators and how they could be quantified without suggesting specific scoring functions.

3. EVALUATION OF SOIL FUNCTIONS—EXAMPLES

3.1. Production Function

3.1.1. Potential

The evaluation of the soils' potential to produce biomass has been on the agenda of soil science for centuries. A powerful and frequently applied approach in Germany today is the Soil Quality Rating (SQR) (Mueller et al., 2007). This approach uses scoring tables at ordinal scales for the combination of selected soil attributes and is in principle equivalent to our approach based on continuous scoring functions. Evidently, the production of biomass depends on the grown crop. Like for most rating systems, we refer to wheat as an indicator crop and a site-specific climate. To evaluate the soils' potential for biomass production, we need to define an indicator I_{prod} as a function of the inherent soil properties and site conditions, and we propose the following general form:

$$I_{\text{prod}} = f(I_{\text{soil}}, I_{\text{water}}, I_{\text{energy}}) \tag{1}$$

where I_{prod} is a function of water availability depending on the local water deficit, $I_{\text{water}}(W_{\text{def}})$ and the capacity to provide rooting space for the exchange of water and nutrients, which is a function of soil texture $I_{\text{soil}}(\text{texture})$. The supply of energy is a third criterion I_{energy}, depending on photosynthetic active radiation, which is further modified by temperature and the length of the frost-free period. Together, this determines the intensity of physiologic processes. For our indicator plant wheat, it is less limiting under conditions in central Europe, whereas it is crucial for other crops (as e.g., wine). This is why we only focus on the first two criteria in the following.

The local water deficit is obtained from the climatic water balance

$$W_{\text{bal}} = P - ET_{\text{pot}} \tag{2}$$

during the vegetation period (March - August) with P being the cumulative precipitation and ET_{pot} the potential evapotranspiration (Allen et al., 1998). This is added to the plant available water capacity estimated from soil texture, AWC_{texture} [vol %], of the soil in the upper 100 cm. The soil profile can be composed of different soil horizons having different vertical extensions d_i [mm] and different soil textures, so that the water deficit is calculated as:

$$W_{\text{def}} = \sum_i AWC_{\text{texture}}\ d_i + W_{\text{bal}} \quad (3)$$

This approach implicitly assumes that the soil is at field capacity in spring. It requires estimating field capacity from soil texture assuming some optimum state of the soil attributes in category M as e.g., bulk density. To do so, we refer to pedotransfer functions as proposed by the German soil mapping guideline (Ad-hoc-Arbeitsgruppe Boden, 2005) assuming a bulk density of 1.3 g/cm^3 in the topsoil and 1.5 g/cm^3 in the subsoil. The scoring function for water availability is defined as a partial linear function in which the threshold for the critical water deficit where yields are expected to decrease is chosen to be 0 mm and a lower threshold of −200 mm, below which no substantial yield can be expected anymore. This approach can be applied for soils with deep groundwater level where capillary rise is negligible. It is illustrated in **Figure 1**.

The potential of soil to provide rooting space for plants for the uptake of water and nutrients, I_{soil}, is expressed as a function of soil texture. This is also done in the SQR approach (Mueller et al., 2007) where soil texture is segmented into five classes which are rated by different scores. We follow a similar approach but on a continuum scale. It is based on the understanding that both high sand contents and high clay contents diminish soil fertility. For sand, this is due to limited supply and buffer capacity for nutrients and for clay, due to limited accessibility for plant roots and reduced water availability. Additionally, we account for the volume fraction of stones V_s. Combining scoring functions for sand and clay (**Figure 2**, right) leads to

$$I_{\text{soil}} = \sum_i I_{\text{texture}}\ (1 - V_{s,i})\ \omega_i \ \mid\ I_{\text{texture}} = \bar{x}_{\text{harm}}(I_{\text{sand}}, I_{\text{clay}}) \quad (4)$$

as a dimensionless indicator for soil fertility based on the substrate (i.e., texture) as illustrated in **Figure 2**. The results for different horizons are summed up while the different horizons are weighed by the assumed depth distribution of roots described by ω_i with $\sum_{d_i} \omega_i = 1$ and $\omega_i = 0$ if the horizon is not rootable due to water logging or limited depth of the soil profile. In this example an exponential decline with depth was assumed as typical for cereals.

Finally, we end up with the evaluation of the soil's potential for biomass production by combining the indicators for water availability and soil substrate by calculating the harmonic mean (since both aspects can hardly compensate each other).

$$I_{\text{prod}} = \bar{x}_{\text{harm}}(I_{\text{water}}, I_{\text{soil}}) \quad (5)$$

3.1.2. Actual State

For the evaluation of the actual state, all the actually observable soil attributes of category M that are deemed to be relevant need to be addressed (**Table 1**). In principle, all of them are observable and measurable. For the production function we suggest the following attributes: pH, SOC, bulk density and air capacity. The individual scoring functions should reflect if the optimum states depend on other soil properties. For example, the optimum SOC content depends on soil texture since coarse textured soils have a reduced capacity for stabilizing soil carbon. This can be accounted for by evaluating the clay/SOC ratio which was found by Johannes et al. (2017) to be optimal in terms of soil structural properties below a value of 8 while it becomes critical above a value of 13 in cropland soils of Western Switzerland. Considering the yields in long-term field experiments in Eastern Germany (unpublished data), we shifted these thresholds toward slightly higher values (10 and 18). They can be considered in the corresponding scoring function as illustrated in **Figure 3** where other scoring functions are plotted as well.

The scoring functions provide indicator values for each individual soil attribute based on thresholds defined for optimal and critical states. These thresholds might be adapted for different crops. The example given in **Figure 3** is assumed to be appropriate for wheat. The threshold values delimiting the range of optimal values with respect to the individual soil attributes are given on the individual x-axis in **Figure 3**. For air capacity we assume a step function at 1.0 vol% assuming that for higher values the soil is sufficiently aerated while this reduces abruptly below this value. The minimum values of the scoring functions are assumed to be different for the different soil attributes. While plant growth below pH 1 is hardly possible (min = 0.0), this is not the case for critical values of SOC. The minimum values given in **Figure 3** are our suggestions for a silty loam soil and are not based on any rigorous analysis.

It should be noted that all threshold values provided in **Figure 3** have no general validity in any way. They are plausible values to demonstrate the proposed concept and certainly need to be adapted for specific crops. But more generally, they can be easily adapted into our steadily improving understanding fed by ongoing research as documented by an enormous body of publications on the relation between soil attributes and soil functions. Thus, the scoring functions are a means for synthesizing the existing knowledge. They allow for including uncertainties in that the punctual kinks of the scoring function can be replaced by a fuzzy region which will directly translate to some uncertainty range for the evaluation of the result.

Finally, all indicators are combined to evaluate the actual state of a soil layer *i* based on manageable soil attributes relative to the site-specific optimum value:

$$\hat{I}_{\text{prod,i}} = \bar{x}_{\text{harm}}(I_{\text{pH}}, I_{\text{Clay/SOC}}, I_{\rho_b}, I_{\text{AC}}, \ldots) \quad (6)$$

The dots in Equation (6) indicate that other attributes might be considered in addition. In this example, not all soil attributes that are deemed to be relevant according to **Table 1** are considered. This is mainly because quantitative concepts are yet to be developed (topsoil structure, earthworm abundance, biodiversity).

The harmonic mean is defined such that its value tends toward zero if one of the elements is zero. The evaluation of the actual state of a soil profile is finally obtained by summation over the different horizons including a weighing function as introduced in **Figure 2**:

$$\hat{I}_{\text{prod}} = \sum_i \hat{I}_{\text{prod,i}}\ \omega_i \quad (7)$$

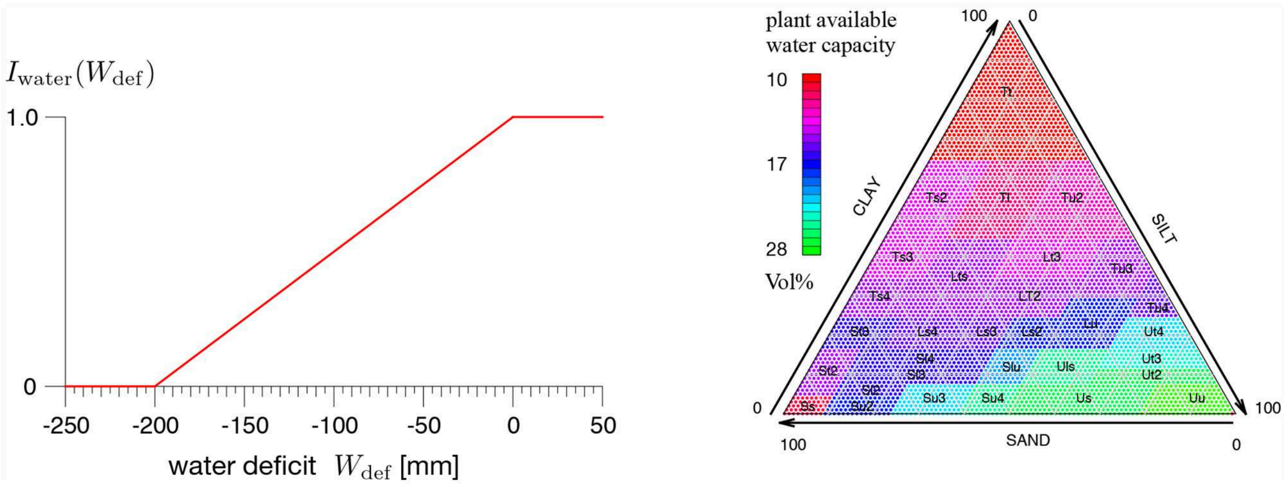

FIGURE 1 | **(Left)** Scoring function to get a dimensionless indicator for the water availability. **(Right)** Pedotransfer function to determine plant available water capacity, *AWC*, from soil texture to calculate the water deficit according to Equation 3. Maximum (28%) in green, minimum (10%) red.

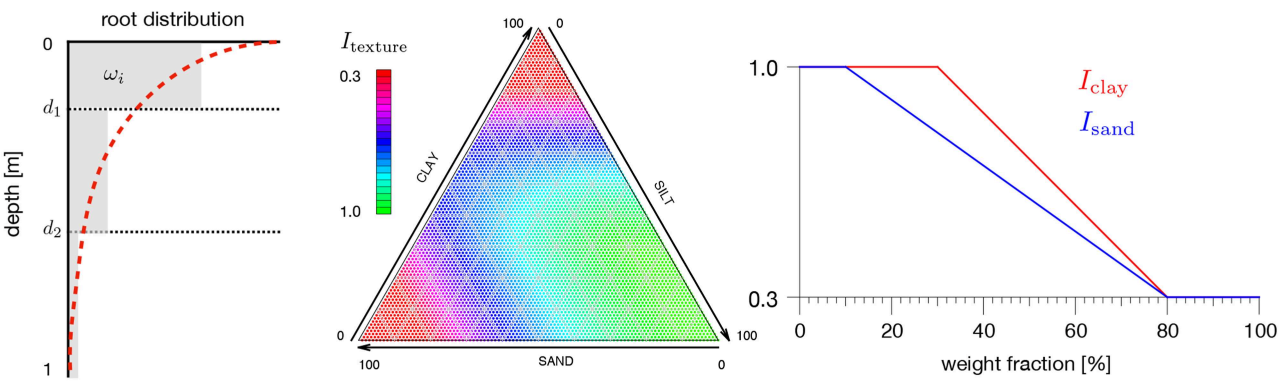

FIGURE 2 | Scoring functions for sand and clay content **(Right)** combined by their harmonic mean according to Equation (4) to get a dimensionless indicator for soil fertility based on soil texture (Middle, green is maximum) which is combined to an indicator for the entire soil profile by weighing the results for the different horizons based on the depth distribution of root length density **(Left)**.

The Clay/SOC ratio is especially relevant for the topsoil, which is assumed to be well mixed by tillage and natural structure dynamics. It is ignored in the subsoil while attributes relevant for root growth and water uptake need to be considered there. The evaluation of the actual state, $\hat{I}_{prod}$, quantifies the degree of fulfillment of the soil's potential I_{prod} (Equation 5) at a scale between 0 and 1.

3.2. Water Storage

3.2.1. Potential

The storage function for water is considered here as an important factor to retain precipitation water from fast transport toward groundwater and surface waters. The importance for plant production was considered in the context of the production function. Water storage is directly related to the available pore volume within the soil profile. Assuming an optimal bulk density of 1.3 g/cm^3 in the topsoil and 1.5 g/cm^3 in the subsoil, this pore volume can be estimated from soil texture along the soil profile. Following the approach of Danner et al. (2003), the large pores addressed by the air capacity contribute to water storage in flat areas while on slopes >9% this pore volume is assumed to be drained very fast. Hence, the potential for water storage in soil (upper 100 cm) is estimated by

$$I_{\text{water storage}} = \frac{1}{WC_{\max}} \sum_i (FC_{\text{texture}} + a\, AC_{\text{texture}})\,(1 - V_s)\, d_i \qquad (8)$$

where FC_{texture} [vol %] and AC_{texture} [vol %] are field capacity and air capacity at optimal pore volume, respectively, as estimated from soil texture (**Figure 4**) for i soil layers and $a = 1 - S/9$ for slopes S [%] <9% and $a = 0$ for steeper slopes where the term including air capacity is omitted. V_s [vol %] is the volumetric fraction of stones. $WC_{\max} = 450$ mm is the maximum water capacity of a 1 m deep soil profile as referred to a loamy clay soil.

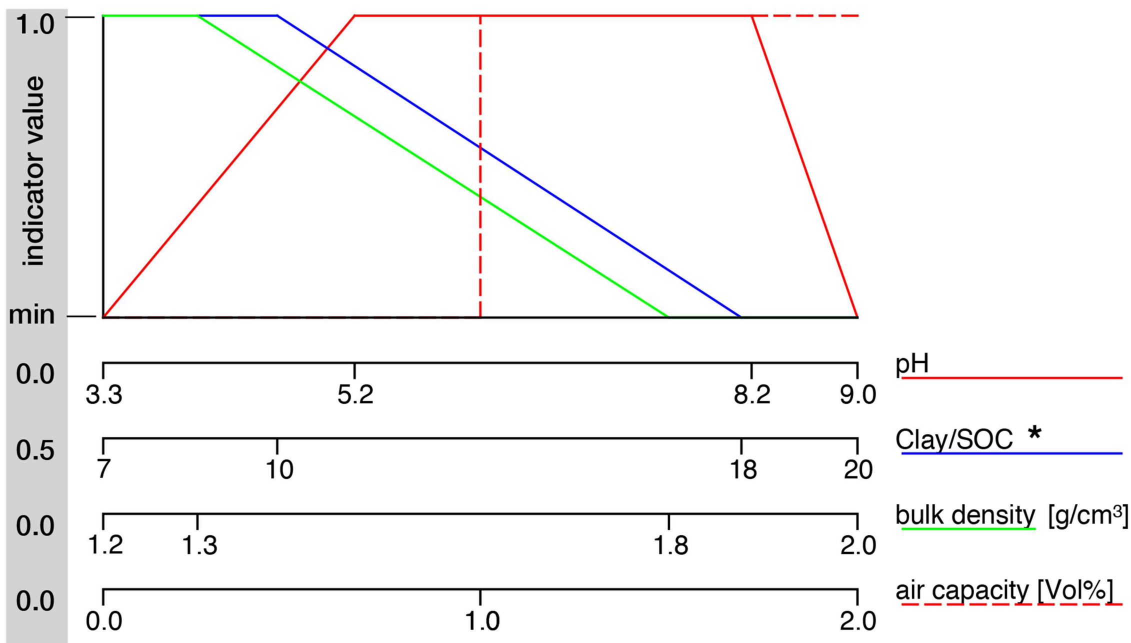

FIGURE 3 | Possible scoring functions for manageable soil attributes to evaluate the actual state with respect to the production function. The Clay/SOC ratio marked by * is only evaluated in the topsoil. Threshold values for optimal and critical states are given on the individual x-axis.

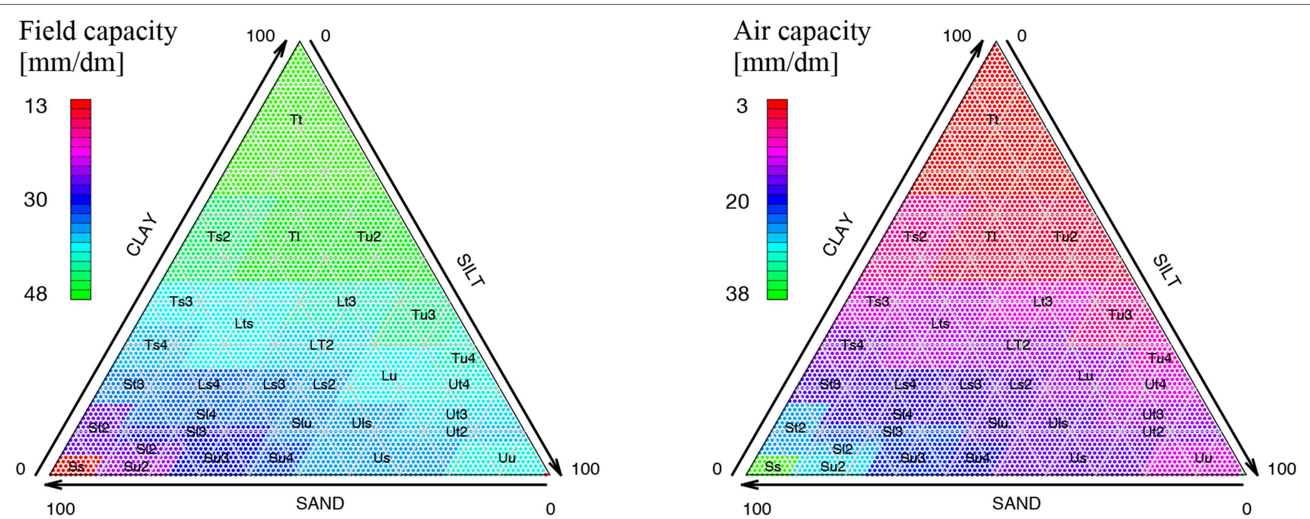

FIGURE 4 | Field capacity **(Left)** and air capacity **(Right)** as derived from soil textural classes according to the German soil classification (Ad-hoc-Arbeitsgruppe Boden, 2005). The range of values from low (red) to high (green) assuming a bulk density of 1.3 g/cm^3 is given in brackets.

3.2.2. Actual State

The estimation of the storage potential (Equation 8) implicitly assumes that field capacity is in some optimum state depending on soil texture. The actual state might be altered by soil compaction and can be measured directly by soil porosity. The degree of fulfillment of the water storage function is then provided by

$$\hat{I}_{\text{water storage}} = \frac{1}{\sum_i d_i} \sum_i \frac{FC_{\text{measured},i} + a\, AC_{\text{measured},i}}{FC_{\text{texture}} + a\, AC_{\text{texture}}}\, d_i \quad (9)$$

in analogy to Equation (8) assuming a constant fraction of stones.

3.3. Carbon Storage

3.3.1. Potential

The potential of soils to store carbon depends on a variety of pedogenic, biological, topographic and climatic properties. In a recent review, the suitability of various factors (clay mineralogy, specific surface area, metal oxides, Ca and Mg cations, microorganisms, soil fauna, aggregation, texture, soil type, natural vegetation, land use and management, topography, parent material and climate) as indicators for actual and potential carbon storage in temperate agricultural soils was assessed with regard to different spatial scales (Wiesmeier et al., 2019).

For an estimation of the SOC storage potential, different approaches have been proposed related to the C saturation of the fine mineral fraction (Hassink, 1997) as well as "data-driven" and "model-driven" approaches (Barré et al., 2017; Chen et al., 2019a). We follow the C saturation approach that was frequently used to quantify the potential of (agricultural) soils to store carbon (Angers et al., 2011; Chan, 2001; Carter et al., 2003; Conant et al., 2003; Sparrow et al., 2006; Stewart et al., 2008; Zhao et al., 2006; Wiesmeier et al., 2014a; Chen et al., 2018, 2019b). This approach is based on the observation that the amount of SOC in most soils in temperate environments is strongly correlated with silt/clay contents (Arrouays et al., 2006; Hassink, 1997), pointing toward the importance of organo-mineral associations as quantitatively the most important SOC stabilization mechanism (von Lützow et al., 2006). The stabilizing capacity of silt and clay-sized particles was used to delineate regression models for the estimation of the SOC storage potential related to the fine mineral fraction of different soils, land uses and climatic regions (Hassink, 1997; Six et al., 2002; Zhao et al., 2006; Feng et al., 2013; Beare et al., 2014; Wiesmeier et al., 2015). As size thresholds for the fine mineral fraction, both 20 and 50 μm were proposed. It is important to note that the C saturation approach only allows a quantification of the storage potential of C that is temporarily stabilized in the fine fraction. The amount of (labile) C in the coarse fraction which is controlled by actual C input cannot be quantified. However, given the fact that agriculturally used soils contain a relatively large proportion of stable C, the C saturation approach can be regarded as a useful method to quantify the C storage potential (Chen et al., 2019b; Beare et al., 2014; Wiesmeier et al., 2014b). Among the different approaches, the specific regression models proposed by Six et al. (2002) for different land uses (cropland, grassland) and size ranges of the fine mineral fraction (<20 μm, <50 μm) are most suitable for our approach. Following this approach, the C storage potential of topsoils under cropland (C_p [kg/m^2]) can be calculated by

$$C_p = (4.38 + 0.26\ T)\ \rho_b\ d\ (1 - V_s) \tag{10}$$

or

$$C_p = (7.18 + 0.20\ T)\ \rho_b\ d\ (1 - V_s) \tag{11}$$

where T is the percentage of particles $<20\,\mu$m [%] in Equation (10) and of particles $< 50\,\mu$m in Equation (11). The expression in the first brackets is the estimated C content [mg/g], ρ_b is the bulk density [g/cm^3], d is the thickness of the topsoil [dm] and V_s is the volume of rock fragments >2 mm [%]. As the content of particles $<20\,\mu$m (medium silt, fine silt and clay) is rarely reported in studies (although the information is available in most common methods for soil texture determination), the respective equations related to particles $<50\,\mu$m (total silt and clay content) may be used alternatively—taking into account the different classification approaches for silt. Following the C saturation approach, the potential of soil to store stabilized carbon is a direct function of soil texture. If the fraction of particles $<20\,\mu$m is considered, we relate the C_p amount to the theoretical maximum of 30.38 for $T = 100$ (Equation 10) and calculate the storage potential I_{SOC} as

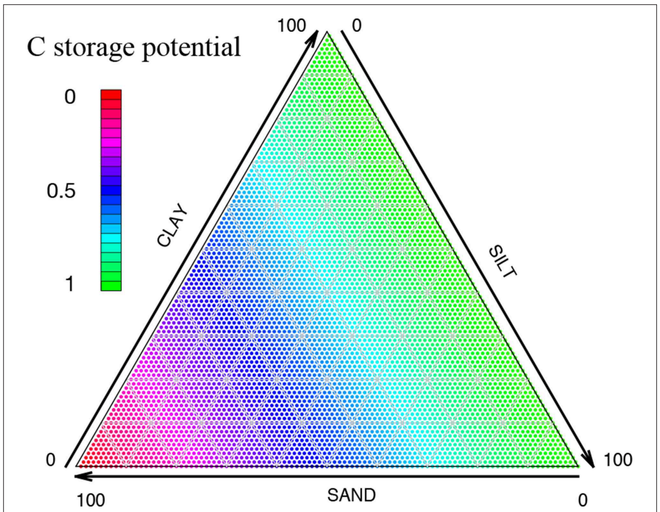

FIGURE 5 | Storage potential I_{SOC} for organic carbon is a direct function of soil texture according to Equation (12).

$$I_{\text{SOC}} = \frac{1}{30.38}(4.38 + 0.26T)(1 - V_s) \tag{12}$$

as illustrated in **Figure 5**.

Although the C saturation approach is a promising method to estimate the C storage capacity of agricultural soils, there are several limitations. To date, only C saturation of topsoils was studied, neglecting the fact that subsoils store considerable amounts of C and may contain a huge C storage potential (Lal, 2018; Rumpel and Kögel-Knabner, 2011). Studies are needed that determine the potential C saturation of subsoils under different land uses in a comprehensive way in order to derive a reliable estimate of the C storage capacity of subsoils. The method was further criticized as it does not allow a quantification of the total SOC storage potential but only refers to the stable C in the fine mineral fraction (Barré et al., 2017; Chen et al., 2018). Despite these limitations, the C saturation concept seems to be suitable to estimate the C storage potential at the plot scale with a limited data set of widely available soil properties.

3.3.2. Actual State

The actual state of SOC can be quantified directly using

$$C_s = \sum_i \text{SOC}_i\ \ \rho_{b,i}\ d_i(1 - V_{s,i}) \tag{13}$$

where C_s [kg/m^2] is the stock of soil organic carbon, SOC_i [mg/g soil] its concentration in soil horizon i, $\rho_{b,i}$ [g/cm^3] is the bulk density, d_i [dm] is the thickness of the horizon and $V_{s,i}$ is the volume of rock fragments >2mm [%]. This includes the stable and the labile C fractions. As the quantification of the stable fraction requires laborious and time-consuming soil fractionation, the amount of stable C can be estimated by assuming it is a constant proportion of total SOC (C_s). For temperate cropland soils, a proportion of stable C of approximately 80% of total SOC was determined (Chen et al., 2019b; Di et al., 2017; Wiesmeier et al., 2014b). The evaluation of the actual state of C storage can thus be calculated by

$$\hat{I}_{\mathrm{SOC}} = \frac{0.8\ C_s}{C_p} \tag{14}$$

to quantify the degree of fulfillment of the soil's potential to store organic carbon.

3.4. Nutrient Cycling

The provision of nutrients for plants and to fuel the ensemble of biological processes in soil is one of the key functions of soil. This is why "nutrient cycling" is almost always addressed explicitly in today's approaches of soil function evaluation (Greiner et al., 2017; Bünemann et al., 2018). The most important macronutrients are N, P, and S together with the cations K, Ca, and Mg. The absolute quantity of nutrients in arable soil is typically adjusted by fertilization, and the uptake by plants and the immobilization through biological processes and sorption are highly dynamic processes. Consequently, the actual concentration of available nutrients is highly variable and, thus, this concentration is difficult to interpret as an indicator for the processes of nutrient cycling. We consider this function to be mainly related to two different aspects: (i) the capacity of soil to provide nutrients from the mineral and organic soil resources in available form and (ii) the capacity to store mobile nutrients within the root zone to avoid losses by leaching and gaseous emissions.

The first aspect relates to the *nutrient mobilization capacity*, the second to the *nutrient buffering capacity*. Both aspects depend more on inherent soil properties such as texture, mineral composition and temperature as well as dynamic soil properties such as soil organic matter, soil water capacity, aeration and pH rather than on the actual concentration of nutrients in the soil solution. This is why nutrient concentrations are not part of the list of indicators in **Table 1**.

The processes responsible for nutrient mobilization and buffering are rather different for the various nutrients and cannot be described adequately by some general function or set of indicators. For example N, P, and S are mainly recycled from soil organic matter by the activity of various soil organisms, and the buffer capacity for these nutrients is mainly provided by the dynamic mass of the soil biome. In contrast, cations are released from the mineral phases along with slow weathering processes, and the buffer capacity is brought about by the capacity of sorption sites expressed by the cation exchange capacity (CEC), which is closely related to soil texture and organic matter.

An evaluation of nutrient cycling, on one hand, needs to address mineralization of soil organic matter and buffering of nutrients by soil organisms. Both features can be directly linked to the overall potential of soil to allow for biological activity as a lumped effective description. This implicitly assumes that the overwhelming diversity of soil biota provides the required functional traits for mineralization and the dynamic adaption in terms of active biomass. On the other hand, such an evaluation needs to include the extent of mineral surfaces acting as sorption sites.

All these features are implicitly included in the evaluation of the production function described above. Hence, we suggest that the soil's potential for nutrient cycling is approximated by I_{prod} (Equation 5) considering soil texture as an indicator for the quality of soil as habitat for organisms and the availability of water. In analogy, the soil's actual state in terms of nutrient cycling can be approximated by $\hat{I}_{\mathrm{prod}}$ as a function of pH, organic carbon, soil bulk density and soil air capacity. This accounts for the general understanding that soil fertility (i.e., the production function) and nutrient cycling are two sides of the same coin and hardly separable.

3.5. Habitat for Biological Activity

Soil biota and their interactions are both directly and indirectly responsible for delivering a number of soil functions, thus, the provision of a habitat for biological activity is an important prerequisite for other soil functions. We here perceive the function "habitat for biological activity" as the provision of a species (gene) pool that can buffer ecosystem functions against species extinction (Hooper et al., 2005) and assume that systems with low species diversity contain fewer species within each functional group, and are thus more susceptible to losing entire ecosystem functions (Bardgett and Van Der Putten, 2014). Hence, the habitat function addresses the diversity in terms of species and functions, which is in contrast to the biological activity in terms of mineralization rate and nutrient buffering as discussed in the previous section.

3.5.1. Potential

As with the other soil functions, the soil's potential to harbor a diverse community of soil biota depends on inherent soil properties and site conditions listed in **Table 1**. Soil organisms are affected by the local climate in terms of the local moisture and temperature regime. This effect is both direct (e.g., on the physiology) and indirect (e.g., by changes in carbon resources) (Turbé et al., 2010). Latitudinal and altitudinal gradients of biodiversity with increasing species richness toward the equator and decreasing soil biodiversity with altitude are shown for some soil faunal groups (Decaëns, 2010). Furthermore, soil texture affects soil biodiversity with e.g., lower earthworm or microbial biomasses in sandy soils (Turbé et al., 2010; Griffiths et al., 2016; Aksoy et al., 2017).

3.5.2. Actual State

Land use and soil management practices are known to affect soil faunal communities with different responses depending on taxonomic or functional groups (Sánchez-Moreno et al., 2011; van Capelle et al., 2012; Cluzeau et al., 2012). Agricultural intensification was shown to decrease functional diversity or even result in the loss of entire functional groups (Tsiafouli et al., 2015). Abundance, species richness and diversity of soil biota are affected by pH, bulk density and SOC content (see **Table 1**). Species abundance and diversity can furthermore be affected by vegetation composition and diversity in grasslands (Sabais et al., 2011) or the type of crop species in agriculture (Scheunemann et al., 2015).

To evaluate the actual state of the habitat for biological activity, soil biodiversity can be directly measured. Measures of soil biodiversity include species richness, diversity indices (e.g., shannon index, simpson index), the presence of keystone species and functional diversity. This requires extensive fieldwork and is done by a number of national monitoring programs, but methods vary and standardized indicators are not available (see Pulleman et al., 2012 for an overview of European approaches). To standardize indicators for soil biodiversity monitoring across Europe, the Envasso (ENVironmental ASsessment of Soil for mOnitoring) project proposed a minimum set of indicators comprising (a) earthworm diversity, abundance and biomass (or enchytraeids if earthworms are absent), (b) springtail diversity and abundance and c) microbial respiration (Huber et al., 2008; Bispo et al., 2009). Additional measurements of the diversity of macrofauna, mites, nematodes and microflora, as well as microflora activity, are recommended (Huber et al., 2008). The prediction and mapping of soil biodiversity based on inherent and manageable soil and site attributes is considered as currently not feasible by the LANDMARK project due to the lack of indicators and specific reference values with respect to soil types, climate and land use, as well as models (Staes et al., 2018). However, there are some recent approaches to assess the actual state of the habitat for biological activity based on, e.g., geographic location, soil pH, soil organic matter content, texture, land use and climate (Aksoy et al., 2017; Rutgers et al., 2016, 2019) or by using the QBS index (Qualità Biologica del Suolo), which assumes that the habitat function of soils is reflected by a higher number of microarthropods well adapted to soil habitats (Parisi et al., 2005), in combination with SOC content and bulk density (Calzolari et al., 2016).

According to our approach, comprehensive data on soil biodiversity in dependence of site-specific characteristics are needed to develop appropriate models and scoring functions relating soil properties to biodiversity measures. As a basis for model development, databases such as the soil zoological information system Edaphobase (www.edaphobase.org) (Burkhardt et al., 2014), which links data from collections, scientific literature and reports to soil and site conditions, or the Land Use/Cover Area frame statistical Survey Soil (LUCAS Soil), which included soil biodiversity in its 2018 soil sampling campaign (Orgiazzi et al., 2018), can be used.

4. EXAMPLE FROM A LONG-TERM FIELD EXPERIMENT

As an example to demonstrate our approach, we evaluate the production function, the C storage function and the water storage function for a Chernozem soil at the agricultural long-term field experiment in Bad Lauchstädt (51°23′24.93″N, 11°52′49.93″E). This soil from Loess deposits over glacial drift belongs to the most productive soils in Germany. The texture in the topsoil is silt loam with 22.2% clay, 72.2% silt (6.9% fine, 23.3% medium, 42% coarse) and 5.6% sand which corresponds to the class Ut4 in German soil classification (Ad-hoc-Arbeitsgruppe Boden, 2005). The long-term field experiment with different levels of organic and mineral fertilizers has been running since 1902, and we use some of the experimental plots to evaluate the actual state of the soil with respect to a number of manageable soil attributes which have been measured in the past. The inherent soil and site characteristics together with the manageable soil attributes measured in 1 year (1998) for a selection of different experimental plots are given in **Table 2**.

4.1. Production Function

There is no limitation for soil productivity based on the silty loam texture (**Figure 2**) so that $I_{\text{soil}} = 1$. Bad Lauchstädt is located in a relatively dry region of Germany with 8.9°C annual mean temperature and annual mean precipitation of 498 mm. The climatic water balance during the growth period (March-August) according to Equation (2) is 228 mm 412 mm = -194 mm (5 years average for 2013–2017). Because of the high water capacity of 370 mm, the water deficit (Equation 3) was positive (176 mm), meaning there is no water deficit, so that $I_{\text{water}} = 1$. Hence, the soil's potential in terms of productivity was equal to unity and herewith maximal. However, during the exceptionally dry year of 2018, the precipitation from March to August was reduced to 40 mm, ET_P was increased to 435 mm and, consequently, the water balance became negative (-25 mm) so that $I_{\text{water}} = 0.9$ according to **Figure 1**. In fact, the yield of wheat in 2018 was decreased to 75% as compared to the 5-year average before.

The evaluation of the actual state for the different experimental plots is restricted to the topsoil (0–25 cm) since measurements were available only for this layer. Bulk density is almost the same in all plots (1.4 g/cm^3), which is somewhat denser as compared to what was considered as optimum (1.3 g/cm^3). Thus, the corresponding scoring function (**Figure 3**) yields values for I_{ρ_b} below unity. Because of the differences in fertilization, the plots differ in SOC content, and this is reflected by the scoring function (**Figure 3**) for the clay/SOC ratio. This indicator ranges from 15.1 in the non-fertilized plot to 9.5 in the fully fertilized plot (NPK /manure) so that the optimum value, $I_{\text{clay/SOC}} = 1$ is reached only for the latter but decreases according to the scoring function (**Figure 3**) to 0.68 for the non-fertilized plot. This suggests that the level of soil organic matter is considered to be a limiting factor for biomass production. The pH is within the optimum range for all plots so that $I_{pH} = 1$.

Finally, the overall evaluation of the actual state for the different experimental plots is obtained by the harmonic mean according to Equation (6). The resulting values for $\hat{I}_{\text{prod}}$ as listed in **Table 2** suggest that the fully fertilized plot is close to its potential. In the non-fertilized plot, I_{prod} reaches 84%, suggesting that the impact of SOC on crop yield is not very high. Actually, the wheat yield was only 35% of the fully fertilized plot. At first glance, this looks like a complete failure of our indicator. However, this discrepancy is due to the fact that the indicator assumes some "good agricultural practice" including the provisioning of nutrients according to the expected yield. The nitrogen level of soil, though highly important for yield,

TABLE 2 | Inherent soil and site properties for the Chernozem in Bad Lauchstädt together with manageable soil attributes and related indicator values according to **Figure 3** for four experimental plots which received different amounts of fertilizers (NPK/manure) over a period of more than 100 years.

		inherent soil & site conditions					affected by soil management									
							physics			chemistry						
	SOIL & SITE ATTRIBUTES	water balance [m]	slope [%]	soil depth (rootable) [m]	texture	coarse fragments [%]	bulk density	I_{Pb}	$I_{\text{water storage}}$	SOC [%]	$I_{\text{Clay/SOC}}$	I_{SOC}	pH	I_{pH}	$\hat{I}_{\text{prod}}$	**yield [dt/ha]**
SOIL FUNCTIONS																
production (fertility)																
C-pool																
water storage																
Bad Lauchstädt		0.17	0	>1	Ut4	0										
	0/0						1.4	0.8	0.92	1.47	0.68	0.65	7.0	1	**0.84**	**32.3**
	NPK/0						1.4	0.8	0.92	1.68	0.80	0.75	6.2	1	**0.89**	**81.6**
	0/manure						1.41	0.78	0.91	2.14	0.98	0.95	6.8	1	**0.93**	**71.2**
	NPK/manure						1.39	0.82	0.93	2.33	1	1.04	6.2	1	**0.95**	**91.3**

*All manageable soil properties including yield of wheat were measured in 1 year (1998). In contrast to **Table 1**, only those attributes are included which are relevant for the three considered functions and which were available.*

is not considered in the evaluation of the soils' status because it is highly dynamic and can easily be adjusted by fertilization. On the non-fertilized plot, no fertilizer was applied so that the missing nitrogen especially led to a much more dramatic decline in yield as compared to the indicator. In other words, this suggests that we expect a decline in yield only to 84% if this plot is fertilized according to common practice and that this decline is mainly caused by the decrease in soil organic matter as a consequence of the management during the past decades. This seems to be plausible and, hence, we think that our concept provides useful results.

4.2. C-storage Function

The potential of the Bad Lauchstädt soil for carbon storage in association with fine particles is calculated to be 18.0 mg/g (Equation 10). Due to the fraction of particles $<20\,\mu$m (52.4%), this leads the relative potential of the Bad Lauchstädt soil to store stable carbon to be $I_{\text{SOC}} = 0.59$ (Equation 12). The actual state for the different experimental plots fulfills this potential to very different degrees reflecting the different fertilizing regimes. While in the non-fertilized plot the potential for C storage is reached only by a factor of 0.65 (Equation 14), it is considerably higher for the plots that received either mineral fertilizer or manure (0.75 and 0.95, respectively) and is completely reached in the plot that received mineral fertilizer plus manure (1.04). Again, it has to be considered that the chosen approach quantifies the potential for C stabilization associated with fine particles and not the total C storage. Experimental results from Bad Lauchstädt show that C storage in the plots with high addition of organic material is still increasing (unpublished data).

4.3. Water Storage

As already mentioned for the production function, the bulk density of all plots is somewhat higher as compared to the suggested optimal value for this silt loam soil (1.3 g/cm^3). Since the field is not inclined, the water capacity was measured by the total porosity calculated from the measured bulk density and assuming a particle density of 2.65 g/cm^3. Because of the elevated bulk density, the score for water storage $I_{\text{water storage}}$ was slightly below 1.0 for all plots.

5. DISCUSSION

5.1. General Concept

Our approach to evaluate soil functions is in line with other concepts that have been developed during the last three decades (Doran and Parkin, 1994; Karlen et al., 2003; Mueller et al., 2007). One common line is the identification of suitable and observable indicators that are related to the soil function to be evaluated and to use such indicators as proxies for soil functions. Another common feature is the use of scoring functions to map indicator values to a dimensionless scale reflecting their contribution with respect to the considered soil function, which allows the combination of a variety of relevant indicators.

The approach suggested in this paper was motivated by the wish to clearly distinguish between the intrinsic potential of some soil to provide various soil functions and its actual state, as recently suggested by Bünemann et al. (2018). This opens a clear perspective to come up with local options for actions toward sustainable management. This discrimination also leads to a clear identification of different types of soil properties (i.e., inherent vs. manageable) and provides a clear structure of what needs to be considered for modeling the dynamics of soil functions in response to soil management. Another motivation was to evaluate the various soil functions separately. In contrast to a general soil quality index, this allows for a differentiated analysis and a balancing between the different functions which are not necessarily synergistic. Moreover, the focus on individual soil functions can be based on more specific indicators so that the choice of soil properties used as indicator variables to quantify these functions can be more targeted.

At present, the proposed approach is in a conceptual stage and not yet fully developed for the entire spectrum of soil functions. For some of the soil functions it is not obvious what the most sensitive indicators should be. This is true for nutrient cycling having many different aspects (reactivity, sorption, buffering) depending on which nutrients are considered. For the habitat function, it is even not obvious what should be addressed, i.e., the diversity of the gene pool or the functional diversity of organisms, let alone the suitable indicators that could provide useful information. This is why we demonstrated the proposed approach in more detail only for those soil functions for which the current knowledge provides more solid grounds. It should be noted, however, that the proposed parametrizations of the various scoring functions are far from being rigorously tested (if this will be ever possible). They merely reflect our current understanding and certainly need to be adapted to different climatic regions, cropping systems or even soil types. However, this is not necessarily a shortcoming. In contrast, this provides the required flexibility to optimize the general concept for local applications. Overall, we believe that the proposed concept will be useful in the future. Our knowledge on soil processes is steadily growing, and this concept provides a framework where new insight can easily be included.

5.2. Implications for Modeling

Besides the evaluation of soils' potential and their actual state with respect to different functions, it is one of the most critical challenges in soil science today to understand the stability and resilience of soil functions and how they change in response to external forcing (e.g., through agriculture or climate change). The change in the state of soil functions can be assessed by evaluating time series of the related manageable attributes. Another important aspect is to identify critical thresholds in terms of forcing beyond which irreversible changes are expected. This has been investigated for example for critical mechanical loads that lead to irreversible soil compaction as a function of some critical water content in dependence of soil texture (Keller et al., 2012). Other examples, though less well understood, are how to reduce soil compaction through adaption of tillage and crop rotation or how to substantially increase stable soil organic matter by suitable management practices.

The key question is, are we able to model the dynamics of soil functions in response to external perturbations in quantitative terms? The previous analysis of how to evaluate the soil functions and especially their actual state provides a valuable basis for the development of the required models. In **Table 1**, the relevant soil attributes are listed for each soil function, separating inherent soil properties and those which are sensitive to soil management. Modeling the dynamics of an individual soil function needs to address the dynamics of all manageable soil attributes (marked green in **Table 1**) under the condition of the inherent soil properties. This implies that any model approach needs to be site-specific as, for example, the impact of tillage practices or the application of manure is different for different soil types and soil textures. Such a systemic model concept was recently suggested by Vogel et al. (2018).

An illustrative example is the dynamics of soil organic matter. To model the change in SOC stocks in response to some measures of soil management such as the quantity and quality of C inputs or the choice of the tillage system it is not sufficient to know the actual carbon content and the actual carbon saturation (Equation 14). Based on our current understanding and indicated in **Table 1**, we also need to address soil structural properties and their temporal dynamics induced by bioturbation and tillage. Earthworms enclose organic matter within relatively compacted casts, and in doing so, they protect organic matter from rapid decomposition and bring it in close connection to mineral surfaces for increased stabilization. In contrast, soil tillage tends to break open existing structures and expose stable carbon to further decomposition. Such feedback processes are currently not considered in classical soil carbon models (Dignac et al., 2017). For the other soil functions, the required modeling of their dynamics can be done analogously while the blueprint which soil attributes need to be considered is provided by the analysis of how to evaluate the soil's potential and its current state. This may open the possibility to come up with a scientifically sound impact assessment for selected practices of agricultural soil management with respect to individual soil functions.

For the evaluation of soil functions, process-oriented modeling would allow for a more direct assessment. For example, production can be estimated based on various crop growth models (Martre et al., 2015) so that the soils' actual state with respect to the production function could be quantified in absolute values of yield. Moreover, the soils' potential could be defined by choosing some optimal values for all the manageable properties and modeling crop yields for an ensemble of representative weather scenarios. One advantage of such a modeling approach is that the models can be calibrated on available data sets from Long Term Field Sites, including the not optimally fertilized sites as in the example of Bad Lauchstädt. Another perspective is that the model results can be used as a quantitative base for the formulation of appropriate, crop- and site-specific scoring functions. A major deficiency is that the required systemic models including the required dynamics and feedbacks of soil processes and properties are not yet available (Vogel et al., 2018).

5.3. Data Requirements

Once the required set of indicators and suitable scoring schemes for the evaluation of the single soil functions are identified, a crucial question is where to get the required data. The evaluation of soils potential for the various soil functions is based on inherent soil properties and site conditions (**Table 1**), which are typically available from classical soil profile descriptions and from meteorological data bases. The evaluation of the soils actual state is in most cases a local problem, and a typical question of farmers is, what is the state of my field with respect to its potential? In addition to the inherent soil properties, this evaluation is based on soil attributes that are affected by soil management, which needs to be addressed locally. In principle, this can be done at each location; however, it would be helpful to develop standardized protocols for both lab and field measurements or estimations of texture, bulk density, macro porosity, pH, SOC, biodiversity and abundance of organisms (Schindelbeck et al., 2008). Ideally, this type of analysis should be doable by each farmer on his field. For some properties, as e.g., the characterization of soil structure in the field, no clear protocols exist at all (Rabot et al., 2018) and new approaches are required along these lines. In principle, however, the estimation of all attributes that are suggested here to evaluate the actual state of soil with respect to the different functions is possible. In doing so, it is possible to directly identify which soil function is critically below its optimum and, moreover, which are the soil attributes that could be improved by appropriate soil management to most efficiently improve this function. For example, the production function of the soil in Bad Lauchstädt could be increased by decreasing the soil bulk density in the fully fertilized plot and by increasing the soil organic matter content in the non-fertilized plot. Another advantage of the assessment of the individual soil functions is that decision makers can make site-specific decisions on which soil function is most valuable to be optimized, i.e., whether optimization is aimed at productivity, nitrate reduction in groundwater, carbon storage or the quality of soil as habitat for organisms.

For some applications, the evaluation of soils potentials is required at the scale of landscapes, for example to support decision-making in landscape planning and to address the question of which soil function we lose when abandoning soils in a certain area in favor of some other purpose. In this case, the information on inherent soil properties (marked yellow in **Table 1**) should ideally be obtained from soil maps. However, available soil maps typically provide some characteristic soil types for each mapping unit and, hence, provide somewhat fuzzy information for specific locations. A rough estimation of the spatial distribution of soil functions within landscapes should nonetheless be possible. In any case, the proposed approach allows translating the uncertainties in soil information to uncertainties in the evaluation of soil functions. For example, if we know the confidence limits of soil texture analysis this can be directly translated to confidence limits for C storage potential (Equation 12), water storage (Equation 8) or the rating of the production function (Equation 4). This also demonstrates the advantage of continuous scoring functions as compared to discrete classified scores.

To further develop scoring functions and to validate concepts to evaluate soil functions, highly valuable data are provided by long-term agricultural field experiments and other long-term soil monitoring sites. They also allow evaluating the dynamics of the state of soil functions in response to soil management and variations in climate.

6. CONCLUSIONS

Building upon existing concepts for the evaluation of soil functions, we propose an approach to quantitatively evaluate soil functions while separating the intrinsic potential of soil and its actual state. This is done for each function separately so that the different contributions of a given soil to the individual soil functions can be accounted for. The concept is demonstrated for those functions where appropriate indicator variables are already well established (i.e., production, C storage and water storage). While the concept of using dimensionless scoring functions seems to be generally useful, we conclude that the parametrization of these functions needs more comprehensive data bases, especially since it needs to be sensitive to site conditions, crops and cropping systems. There are indicator variables such as soil structure including its stability and temporal dynamics, which are known to be essential for various soil functions but difficult to quantify. For other important soil functions the formulation of evaluation schemes still needs to be done. This is true for nutrient cycling due to the complexity of interacting processes and for the habitat function, which is still not clearly defined, and suitable indicators are missing. However, we believe that the presented approach is generally useful and can provide valuable input to modeling soil functions since it provides a blueprint of the type of soil variables and their interactions, which should be represented by some systemic modeling of the dynamics of soil functions.

DATA AVAILABILITY STATEMENT

All datasets generated for this study are included in the manuscript/supplementary files.

AUTHOR CONTRIBUTIONS

H-JV and UWo developed the concept of the presented approach. EE provided contributions to link the evaluation approach to available soil data handling. UF provided data and interpretation for the long-term field experiment in Bad Lauchstädt and contributed to the formulation of the scoring functions. BL reviewed literature on the habitat function of soil and wrote the corresponding text. ML critically reviewed the manuscript and improved the consistency. MW reviewed literature on the C storage function and wrote the corresponding text. UWe provided some links to modeling.

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frontiers in Environmental Science

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Primer and Database Choice Affect Fungal Functional but Not Biological Diversity Findings in a National Soil Survey

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The internal transcribed spacer (ITS) region is the accepted DNA barcode of fungi. Its use has led to a step-change in the assessment and characterisation of fungal communities from environmental samples by precluding the need to isolate, culture, and identify individuals. However, certain functionally important groups, such as the arbuscular mycorrhizas (Glomeromycetes), are better characterised by alternative markers such as the 18S rRNA region. Previous use of an ITS primer set in a nationwide metabarcoding soil biodiversity survey revealed that fungal richness declined along a gradient of productivity and management intensity. Here, we wanted to discern whether this trend was also present in data generated from universal 18S primers. Furthermore, we wanted to extend this comparison to include measures of functional diversity and establish trends with soil types and soil organic matter (SOM) content. Over the 413 individual sites examined (arable, grassland, woodland, moorland, heathland), we found congruent trends of total fungal richness and β-diversity across land uses, SOM class, and soil type with both ITS and 18S primer sets. A total of 24 fungal classes were shared between datasets, in addition to 15 unique to ITS1 and 12 unique to 18S. However, using FUNGUILD, divergent trends of functional group richness became apparent, especially for symbiotrophic fungi, likely driven by an increased detection rate of Glomeromycetes in the 18S dataset. The disparate trends were also apparent when richness and β-diversity were compared to soil properties. Additionally, we found SOM class to be a more meaningful variable than soil type biodiversity for predicting biodiversity analyses because organic matter was calculated for each sample whereas soil type was assigned from a national soil map. We advocate that a combination of fungal primers should be used in large-scale soil biodiversity surveys to capture important groups that can be underrepresented by universal barcodes. Utilising such an approach can prevent the oversight of ubiquitous but poorly described species as well as critically important functional groups.

Keywords: UNITE, SILVA, identification bias, high-throughput sequencing, arbuscular mycorrhizal fungi, Archaeorhizomycetes

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INTRODUCTION

Soil fungi are the dominant eukaryotic component of soil communities and are known to perform crucial ecosystem functions (Peay et al., 2008). Characterising the diversity of fungi within the landscape and their response to anthropogenic perturbation therefore represents an important topic within ecology. High-throughput sequencing has allowed the rapid estimation and identification of fungi by overcoming historical limitations of culture isolation and classifying fruiting bodies (Tedersoo et al., 2015). Using these DNA-based approaches it has been estimated that global fungal diversity in soil ranges from 3.5 to 5 million species. Yet at the beginning of the present decade, only around one-tenth of fungal diversity was thought to have been described (Rosling et al., 2011). In terms of ecosystem function, the majority of fungi are important in organic matter turnover and nutrient recycling as they facilitate the conversion of complex organic polymers into forms more readily accessible to other organisms (Peay et al., 2008; Nguyen et al., 2016). Consequently, they play a crucial role in regulating both below- and above-ground productivity (Peay et al., 2008). Many soil fungi also form important interactions with plants. Some form mutualistic relationships, best exemplified by the wide range of mycorrhizas (Wang and Qui, 2006; Smith and Read, 2008; Nguyen et al., 2016), whereas others are pathogens, responsible for numerous plant and animal diseases within agriculture and forestry (Fisher et al., 2012; Nguyen et al., 2016). Depending on environmental conditions or life stage, fungi are capable of taking on some or all of these roles (i.e., saprotroph, symbiotroph, pathotroph; Fisher et al., 2012). Despite the recognition that fungi are extremely important in soil ecosystems, characterising fungal communities has remained a challenge, exemplified by the numerous studies on soil bacteria in comparison to fungi.

Fungal barcode sequences are found within the ubiquitous, multicopy ribosomal RNA gene. Within this, the internal transcribed spacer (ITS) region has been accepted as a universal barcode for fungi (Schoch et al., 2012). Recent development of ITS-based databases such as UNITE (Kõljalg et al., 2013) and Warcup (Deshpande et al., 2016) have overcome limitations in collecting and assigning taxonomic identities to unknown sequences, though database selection may introduce bias into results (Tedersoo et al., 2015; Xue et al., 2019). Yet ITS barcodes exhibit some limitations when dealing with unknown or environmental samples. Generally, the ITS region cannot be aligned above the family-level (Cavender-Bares et al., 2009), making phylogenies based on ITS sequence data unreliable. Importantly, the ITS region has proven unreliable at distinguishing certain fungal groups at the species-level, such as Glomeromycetes (Stockinger et al., 2010). Such inconsistencies mean that ITS primers may not accurately detect target organisms. For instance, Berruti et al. (2017), found that ITS primers underestimated Glomeromycetes in bulk soil. Such uncertainty may confound experimental results and lead to erroneous conclusions.

Despite the widespread use of ITS barcodes, other markers may better capture the diversity of some fungal taxa. Primers targeting the small and large subunits as well as the ITS regions of the rRNA gene have all been applied to fungi (Tedersoo et al., 2015; Xue et al., 2019). For example, early diverging lineages such as Chytridiomycota (Schoch et al., 2012; Tedersoo et al., 2015) and Glomeromycetes (Tedersoo et al., 2015) are poorly represented in ITS sequencing. Additionally, advancements in classification have highlighted the shortcomings of environmental DNA barcoding. For example, the Archaeorhizomycetes are a poorly understood but ubiquitous class of soil fungi and their previously unidentifiable sequences have been major components of past soil biodiversity assessments (Anderson et al., 2003; Rosling et al., 2011). Overlooking these lineages may potentially lead to erroneous assumptions of biological and functional diversity in soils.

Underrepresentation of Glomeromycetes in particular exemplifies this issue. Arbuscular mycorrhizal fungi (AMF) form symbiotic relationships with more than 80% of vascular plant families and have been categorised into the monophyletic Glomeromycetes (Schüβler et al., 2001). Unlike most fungi, the ITS region has consistently demonstrated poor resolution in some closely related AMF species (Stockinger et al., 2010) as it is too hyper-variable (Thiéry et al., 2016). As mentioned previously, the ITS region underestimates Glomeromycetes in bulk soil (Berruti et al., 2017). Instead, the 18S region is more commonly used for barcoding AMF, especially in ecological studies (Öpik et al., 2014). Therefore, it is important to recognise biases inherent even in supposedly universal barcodes.

We previously undertook a nation-wide assessment of soil biodiversity across Wales, representing a breadth of heterogeneous land uses, which included agricultural land, grasslands, woodlands, and upland bogs. In this case, fungal richness and β-diversity were assessed using soil environmental DNA, utilising ITS1 primers (George et al., 2019). Yet, from the earliest stages of experimental design, we were cognisant that the ITS1 universal primer choice may not account for numerous functionally important fungal groups, particularly AMF. Thus, the primary objective of the present study was to assess whether observed fungal biodiversity (richness and β-diversity) across contrasting land uses from the ITS1 dataset would differ when compared to a dataset derived from an alternative choice of primer and database. We therefore sought to assess if primer choice influenced fungal biodiversity across land use, soil type, and soil organic matter (SOM) class. Our next aim was to critically evaluate the influence of climatic and edaphic factors [e.g., soil pH, total carbon (C), nitrogen (N), phosphorus (P)] on fungal diversity arising from the use of the two different primer sets. Our final aim was to look for differences in coverage of taxonomic and functional diversity between the two primer sets across the broad range of land uses and soil types evaluated.

MATERIALS AND METHODS

Study Design

Data were collected as part of the Glastir Monitoring & Evaluation Programme (GMEP). The GMEP initiative was established by Welsh Government to monitor their most recent agri-environment scheme, Glastir, which involved 4,911

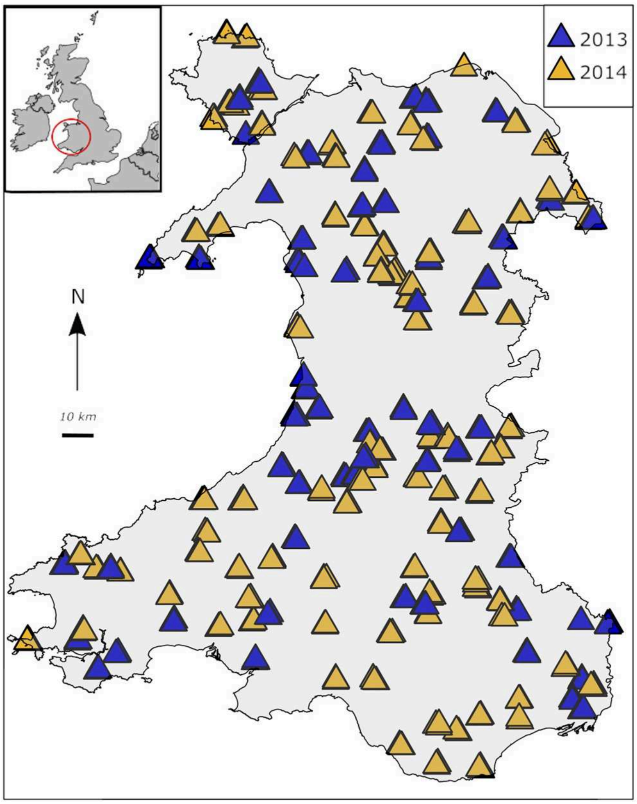

FIGURE 1 | Map of sites selected for GMEP monitoring. To protect landowner anonymity, each triangle gives an approximate location of every 1 km^2 plot from which samples were taken.

landowners over an area of 3,263 km^2 (**Figure 1**). Through the GMEP framework, survey teams collected samples in 2013 and 2014 between April and October in each year (Emmett and the GMEP Team, 2017). Sampling protocols were based on those of the UK-wide ecosystem monitoring programme, Countryside Survey (Emmett et al., 2010). The survey design randomly located 300, 1 km squares across 26 land classes in Wales which survey teams sampled with 5 plots in each square. A subset of samples were then randomly chosen from squares with a maximum of 3 selected in an individual square. A total of 437 samples were collected for biodiversity analyses.

At each sampling location, 2 cores were collected. One was a 15 cm deep by 4 cm diameter core from which measurements of soil physical and chemical properties were taken, including total C (%), N (%), P (mg/kg), organic matter (% loss-on-ignition), pH (measured in 0.01 M $CaCl_2$), mean soil water repellency (water drop penetration time in seconds), bulk density (g/cm^3), volume of rocks (cm^3), volumetric water content (m^3/m^3), as well as percentage sand and clay. For complete details on chemical analyses methodology, see Emmett et al. (2010). Soil texture data were measured by laser granulometry with a LS320 13 analyser (Beckman-Coulter) as described in George et al. (2019). The cut-off points for clay, silt, and sand were: 2.2, 63, and 2,000 μm, respectively. Clay and sand percentages were selected for subsequent analyses and normalised using Aitchison's $\log_{10}$-ratio transformation. Further geographic data including grid eastings, northings, and elevation were also collected. Mean temperature (°C) on date of sample collection and annual precipitation (mL) data were extracted from the Climate Hydrology and Ecology research Support System dataset (Robinson et al., 2017). Environmental variables were normalised (by $\log_{10}$ or square root transformation) where appropriate (see **Table 1**).

Each sampling site was assigned to a land use category, soil type, and SOM class (based on percentage organic matter). The land use classification used in this study was originally developed for the UK Countryside Survey in 1990 (Bunce et al., 1999). Briefly, vegetation was recorded by surveyors and used to classify each site into one of the 8 Aggregate Vegetation Classes (AVCs) as described in Bunce et al. (1999; for further details please see **Supplementary Material**). The AVCs have been shown to follow a gradient of soil nutrient content from which productivity and management intensity can also be inferred (see **Supplementary Material** and Bunce et al., 1999). There were 7 AVCs identified in the present study. The AVCs in descending order of productivity are: Crops/weeds (including arable land), Fertile grassland, Infertile grassland, Lowland woodland, Upland woodland, Moorland grass-mosaic, Heath/bog (**Supplementary Table 1**). Soil type based on the predominant major soil group classification was extracted from the National Soil Map (**Supplementary Material**; Avery, 1980). Additionally, we classified soils on a per sample basis by organic matter content. Each sample was grouped into one of four organic matter classes based on percent loss-on-ignition (LOI) following the protocols of the 2007 Countryside Survey (Emmett et al., 2010): mineral (0–8% LOI), humus-mineral (8–30% LOI), organo-mineral (30–60% LOI), and organic (60–100% LOI). Mean values for each environmental variable were recorded for each land use, soil organic matter class, and soil type.

DNA Extraction

Soils used in DNA extraction were collected from 15 cm deep by 8 cm diameter cores. Soil samples were transported in refrigerated boxes; samples were received at Environment Centre Wales, Bangor within an average of 48 h post-extraction and frozen at −80°C upon arrival. Soils were then thawed and homogenised as they passed through a sterilised 2 mm stainless steel sieve after which they were returned to a −80°C freezer until DNA extraction. Sieves were sterilised between samples by rinsing with tap water at high pressure and an application of Vircon® laboratory disinfectant followed by UV-treating each side for 5 min. DNA was extracted by mechanical lysis from 0.25 g of soil per sample using a PowerLyzer PowerSoil DNA Isolation Kit (MO-BIO Inc.). Soils were pre-treated with 750 μL of a suspension of $CaCO_3$ (1 M) following Sagova-Mareckova et al. (2008) to improve PCR performances, especially for acidic soils. Extracted DNA was stored at −20°C until amplicon library preparation began. The extractions and homogenisation steps were performed in triplicate. To check for contamination in sieves, 3 negative control DNA extractions were completed as well as 2 negative control kit extractions using the same technique

TABLE 1 | Mean values (± SE) of soil physical and chemical variables for each Aggregate Vegetation Class.

Environmental variable	Crops/weeds	Fertile grassland	Infertile grassland	Lowland wood	Upland wood	Moorland grass-mosaic	Heath/bog
Total C (%)^L	3.87 (± 0.83)d	4.75 (± 0.2)d	5.85 (± 0.33)d	5.78 (± 1.07)d	9.7 (± 2.25)c	12.19 (± 2.07)b	23.57 (± 1.88)a
Total N (%)^L	0.32 (± 0.05)d	0.45 (± 0.02)d	0.49 (± 0.02)d	0.4 (± 0.06)d	0.58 (± 0.1)c	0.83 (± 0.11)b	1.05 (± 0.09)a
C:N ratio^S	11.44 (± 0.81)cd	10.49 (± 0.13)d	11.62 (± 0.27)cd	13.92 (± 0.75)bc	15.86 (± 0.7)b	14.41 (± 0.42)b	20.65 (± 0.94)a
Total P (mg/kg)^S	1103.44 (± 145.47)ab	1194.9 (± 45.53)a	1045.5 (± 43.3)ab	601.68 (± 77.68)c	762.45 (± 61.95)bc	930.49 (± 57.5)ab	769.63 (± 50.04)ab
Organic matter (% LOI)^L	7.53 (± 1.62)d	9.39 (± 0.34)d	11.25 (± 0.55)d	10.71 (± 1.7)d	18.79 (± 4.16)c	22.99 (± 3.72)b	39.26 (± 3.6)a
pH ($CaCl_2$)	4.73 (± 0.26)b	5.2 (± 0.08)a	4.73 (± 0.05)b	4.31 (± 0.26)b	3.57 (± 0.1)cd	3.85 (± 0.09)c	3.84 (± 0.1)d
Soil water repellency*	4077.56 (± 3990.72)abc	264.01 (± 73.28)c	781.68 (± 137.58)b	2975.47 (± 2108.12)abc	1965.87 (± 698.61)a	4186.13 (± 798.48)a	3186.4 (± 812.15)a
Volumetric water content (m^3/m^3)	0.23 (± 0.03)bc	0.35 (± 0.01)b	0.34 (± 0.01)b	0.22 (± 0.02)c	0.36 (± 0.03)b	0.46 (± 0.02)a	0.52 (± 0.02)a
Rock volume (mL)	3.95 (± 1.11)abc	5.25 (± 0.45)b	5.44 (± 0.42)b	9.13 (± 2.49)a	4.41 (± 0.57)ab	3.25 (± 0.39)c	1.87 (± 0.21)c
Bulk density (g/cm^3)	1.03 (± 0.09)a	0.9 (± 0.02)a	0.8 (± 0.02)b	0.71 (± 0.08)b	0.56 (± 0.04)c	0.5 (± 0.04)c	0.47 (± 0.03)d
Clay content (%)^A	22.25 (± 1.85)ab	25.46 (± 0.65)a	23.18 (± 0.64)ab	17.47 (± 1.34)ab	17.82 (± 1.82)ab	18.12 (± 1.27)c	11.76 (± 2.24)d
Sand content (%)^A	30.97 (± 4.66)ad	24.88 (± 1.25)d	29.21 (± 1.44)bd	42.99 (± 4.01)ac	40.23 (± 4.15)abc	29.5 (± 3.0)b	45.15 (± 7.61)a
Elevation (m)	88.71 (± 47.69)cd	109.38 (± 8.62)d	167.28 (± 8.65)c	119.06 (± 16.38)cd	297.83 (± 20.62)b	406.63 (± 19.22)a	380.55 (± 19.7)a
Mean annual precipitation (mL)	968.44 (± 69.01)c	1078.19 (± 24.71)c	1177.05 (± 18.91)c	1100.12 (± 52.28)c	1405.33 (± 65.35)b	2027.23 (± 74.39)a	1771.2 (± 58.19)a
Temperature (°C)	12.64 (± 1.18)ab	12.09 (± 0.41)b	13.44 (± 0.29)a	15.80 (± 0.87)a	14.53 (± 0.53)a	14.51 (± 0.36)a	13.87 (± 0.29)a

*Following normalisation on selected variables, ANOVAs and Tukey's post-hoc tests were performed. Numbers followed by the same letter within each row are not statistically different. ^{A}denotes Aitchison's log_{10}-ratio transformation; ^{L}denotes log_{10}-transformation; square-root-transformation; *Soil water repellency was derived from median water drop penetration times (s) and log_{10} transformed.*

but without the $CaCO_3$ pre-treatment. Aliquots of the resultant DNA were used to create amplicon libraries for sequencing with each primer set.

Primer Selection and PCR Protocols for Library Preparation

Amplicon libraries were created using primers for the ITS1 (ITS5/5.8S_fungi) area to specifically target fungi (Epp et al., 2012) and the V4 region of the 18S gene (TAReuk454FWD1/TAReukREV3; Behnke et al., 2011) targeting a wide range of, but not all, eukaryotic organisms, including fungi. A two-step PCR following protocols devised in conjunction with the Liverpool Centre for Genome Research was used as described in George et al. (2019). Amplification of amplicon libraries was run in triplicate on DNA Engine Tetrad® 2 Peltier Thermal Cycler (BIO-RAD Laboratories Inc.) and thermocycling parameters for both PCR protocols started with 98°C for 30 s and terminated with 72°C for 10 min for final extension and held at 4°C for a final 10 min. For the ITS1 locus, there were 15 cycles of 98°C for 10 s; 58°C for 30 s; 72°C for 30 s. For the 18S locus there were 15 cycles at 98°C for 10 s; 50°C for 30 s; 72°C for 30 s. Twelve microliters of each first-round PCR product were mixed with 0.1 μL of exonuclease I, 0.2 of μL thermosensitive alkaline phosphatase, and 0.7 μL of water and cleaned in the thermocycler with a programme of 37°C for 15 min and 74°C for 15 min and held at 4°C. Addition of Illumina Nextera XT 384-way indexing primers to the cleaned first round PCR products were amplified following a single protocol which started with initial denaturation at 98°C for 3 min; 15 cycles of 95°C for 30 s; 55°C for 30 s; 72°C for 30 s; final extension at 72°C for 5 min and held at 4°C. Twenty-five microliters of second-round PCR products were purified with an equal amount of AMPure XP beads (Beckman Coulter). Library preparation for the 2013 samples was conducted at Bangor University. Illumina sequencing for both years and library preparation for 2014 samples were conducted at the Liverpool Centre for Genome Research.

Bioinformatics

Bioinformatics analyses were performed on the Supercomputing Wales cluster as previously described in George et al. (2019). A total of 104,276,828, and 98,999,009 raw reads were recovered from the ITS1 and 18S sequences, respectively. Illumina adapters were trimmed from sequences using Cutadapt (Martin, 2011) with 10% level mismatch for removal. Sequences were then de-multiplexed, filtered, quality-checked, and clustered using a combination of USEARCH v. 7.0 (Edgar, 2010) and VSEARCH v. 2.3.2 (Rognes et al., 2016). Open-reference clustering (97% sequence similarity) of operational taxonomic units (OTUs) was performed using VSEARCH; all other steps were conducted with USEARCH. Sequences with a maximum error greater than 1 and shorter than 200 bp were removed following the merging of forward and reverse reads for ITS1 sequences. A cut-off of 250 bp was used for 18S sequences, according to higher quality scores. There were 7,242,508 (ITS1) and 9,163,754 (18S) cleaned reads following these steps. Sequences were sorted and those that only appeared once in each dataset were removed.

Remaining sequences were matched first against the UNITE 7.2 (Kõljalg et al., 2013) and SILVA 128 (Quast et al., 2013) databases for the ITS1 and 18S sequences, respectively. Ten per cent of sequences that failed to match were clustered *de novo* and used as a new reference database for failed sequences. Sequences that failed to match with the *de novo* database were subsequently also clustered *de novo*. All clusters were collated and chimeras were removed using the uchime_ref command in VSEARCH. Chimera-free clusters and taxonomy assignment summarised in an OTU table with QIIME v. 1.9.1 (Caporaso et al., 2010) using RDP (Wang et al., 2007) methodology with the UNITE database for ITS1 data. Taxonomy was assigned to the 18S OTU table using BLAST (Altschul et al., 1990) against the SILVA database and OTUs appearing only once or in only 1 sample were removed from each OTU table. Based on DNA quality and read counts, 413 samples were used for analyses of the ITS1 data and 422 for 18S data (from the total of 438).

A Newick tree was constructed for the 18S tables using 80% identity thresholds and was paired with the 18S OTU table as part of analyses using the R package phyloseq (McMurdie and Holmes, 2013). Non-fungi OTUs were removed from both OTU tables. Read counts from each group were rarefied 100 times using phyloseq (as justified by Weiss et al., 2017) and the resulting mean richness was calculated for each sample. The ITS1 table was rarefied at a depth of 4,000 reads whereas the 18S table was rarefied to 10,000 reads. A subset of the 18S data was rarefied to 400 reads across 398 samples to analyse Glomeromycetes OTUs separately. Samples with observed lower read counts were removed before rarefaction. To assess functional diversity, both OTU tables were processed using FUNGUILD (Nguyen et al., 2016) and the resulting matched OTU tables were used to investigate functional roles based on trophic mode. Sequences have been uploaded to The European Nucleotide Archive and can be accessed with the following primary accession codes after the end of the data embargo: PRJEB28028 (ITS1), and PRJEB28067 (18S).

Statistical Analysis

All statistical analyses were run using R v. 3.3.3 (R Core Team, 2017) following rarefaction. For each data set, NMDS ordinations using Bray-Curtis dissimilarity were created with the vegan package (Oksanen et al., 2016) to assess β-diversity. Environmental data was fitted linearly onto each ordination of AVCs using the envfit function. NMDS scores were plotted against these values for each variable to determine the direction of associations. Differences in β-diversity amongst AVCs were calculated with PERMANOVA and homogeneity of dispersion was also assessed.

Linear mixed models were constructed using package nlme (Pinheiro et al., 2016) to show the differences in α-diversity amongst AVCs, soil types, and LOI classification, for both ITS1 and 18S fungal data sets. Sample year as fixed factors; sample square identity was the random factor. This methodology was also used for the subsets of data that matched to the FUNGUILD database. For each model, significant differences were assessed by ANOVA and pairwise differences were identified using Tukey's *post-hoc* tests from the multcomp package (Hothorn et al., 2008).

Partial least squares regressions from the pls package (Mevik et al., 2016) were used with the variable importance in projection (VIP) approach (Chong and Jun, 2005) to sort the original explanatory variables by order of importance to identify the most important environmental variables for richness. Such analysis is ideal for data where there are many more explanatory variables than sample numbers or where extreme multicollinearity is present (Lallias et al., 2015; George et al., 2019). Variables with VIP values > 1 were considered most important. Relationships between important variables and richness values for each group of organisms were investigated by linear regression. Richness was normalised before regression when necessary.

RESULTS

Soil Properties

Soil properties displayed a range of changes across land uses (**Table 1**). Notably, total C [$F_{(6, 427)} = 89.13$ $p < 0.001$], total N [$F_{(6, 427)} = 61.03$, $p < 0.001$], C:N ratio [$F_{(6, 427)} = 94.41$, $p < 0.001$], organic matter content [$F_{(6, 428)} = 107.02$, $p < 0.001$], elevation [$F_{(6, 429)} = 78.42$, $p < 0.001$], and mean annual precipitation [$F_{(6, 429)} = 72.6$, $p < 0.001$], and moisture [$F_{(6, 427)} = 33.74$, $p < 0.001$] increased with declining land use productivity. We also observed a reduction in pH [$F_{(6, 428)} = 69.56$, $p < 0.001$], bulk density [$F_{(6, 428)} = 79.87$, $p < 0.001$], and clay content [$F_{(6, 344)} = 19.54$, $p < 0.001$] across the land use productivity gradient. Trends in other variables such as soil water repellency [$F_{(6, 428)} = 22.08$, $p < 0.001$], total P [$F_{(6, 424)} = 7.1$, $p < 0.001$], sand content [$F_{(6, 344)} = 5.71$, $p < 0.001$], stone content [$F_{(6, 427)} = 10.4$, $p < 0.001$], and temperature at time of sampling [$F_{(6, 429)} = 4.4$, $p < 0.001$], though significant, were less clear across land uses however. These findings were also apparent when samples were grouped from low-to-high organic matter content by organic matter class (**Supplementary Table 2**). Overall, no clear trends were evident across the different soil types (**Supplementary Table 3**).

Sequencing Data

A total of 7,582 and 4,408 fungal OTUs were recovered using the ITS1 and 18S primer sets, respectively. Of these, 5,666 were assigned an identifier at the class-level in the ITS1 dataset while 4,367 were assigned an identifier in the 18S dataset. There were 15 classes that were only found in the ITS1 dataset and 12 unique to the 18S data. Endogonomycetes was the most abundant class found only in the ITS dataset (19 OTUs), whereas Laboulbeniomycetes (17 OTUs) was the most abundant fungal class unique to the 18S data. A total of 24 classes were present in both ITS1 and 18S data (**Figure 2A**).

As reported in George et al. (2019), Agaricomycetes were the most abundant class of fungi in the ITS1 dataset overall. There were also a large proportion of Sordariomycetes (**Figure 2B**). Archaeorhizomycetes was the most abundant class in the 18S dataset (**Figure 2C**). Proportionate abundances of Sordariomycetes and Agaricomycetes followed contrasting

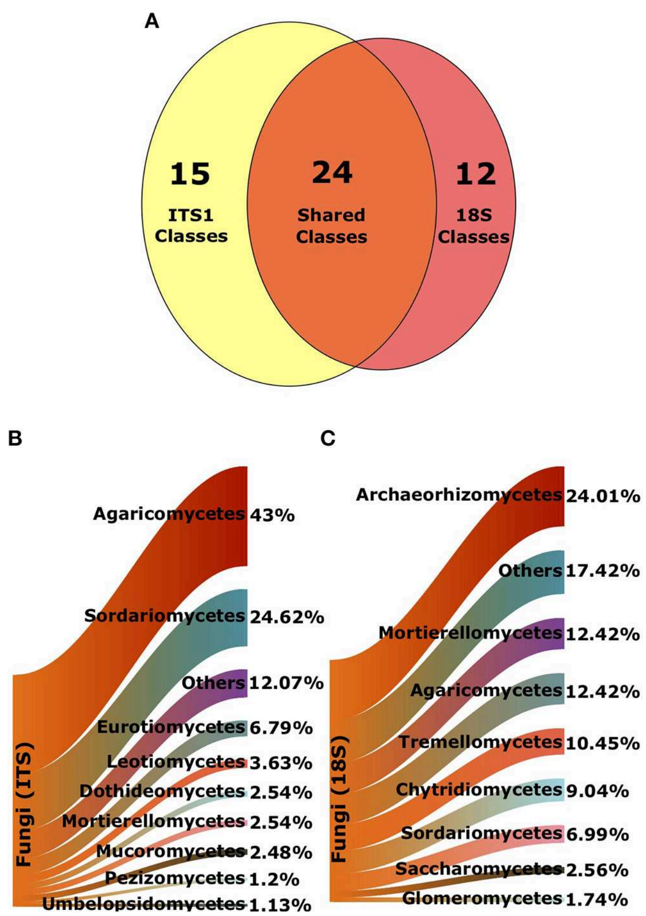

FIGURE 2 | Composition of fungal classes from ITS1 and 18S datasets. **(A)** Venn diagram denoting total number of shared and unique classes in each data set, following exclusion of unknown sequences. Sankey diagrams of proportional abundances of fungal OTUs from all samples from **(B)** ITS1 data and **(C)** 18S data. Arms denote proportions of OTUs of the most populous classes.

trends, with the dominance of the former replaced by the latter in lower productivity AVCs in the ITS1 data, as described previously (**Figure 3A**). Although Agaricomycetes and Sordariomycetes comprised smaller fractions of the 18S dataset (**Figure 2C**), this trend was still apparent (**Figure 3B**). Additionally, the Archaeorhiozmycetes from 18S data generally followed the same trend as the Sordariomycetes (**Figure 3B**). The preceding trends observed across land uses are also evident across organic matter classes (**Figure S1**) but are not as clear across soil types (**Figure S2**).

When a class was present in both datasets, it was usually much more prevalent in one than the other (**Supplementary Table 4**). For example, there were 1858 Agaricomycetes and 915 Sordariomycetes OTUs in the ITS1, yet these numbers dropped to 646 and 417 OTUs in the 18S dataset. Similarly, Glomeromycetes accounted for 162 of the OTUs in the 18S data, but only 6 OTUs in the ITS1 dataset. Abundances of classes unique to the ITS1 and 18S datasets can be found in **Supplementary Tables 5, 6**, respectively.

Fungal Richness and β-Diversity From ITS1 and 18S Data

We found that fungal richness followed the same trends across land use, irrespective of primer set. As previously demonstrated in George et al. (2019), fungal OTU richness from ITS1 metabarcoding significantly declined [$F_{(6,\ 258)} = 39.87, p < 0.001$; **Figure 4A**] from high to low productivity/management intensity. Richness in Fertile grasslands was significantly greater than all other AVCs ($p < 0.001$) except Crops/weeds. In the 18S dataset, richness was also significantly higher [$F_{(6,\ 267)} = 82.73, p < 0.001$] in more productive/managed land uses and declined along this gradient. However, richness in grasslands was highest in this dataset (**Figure 4B**). For complete pairwise differences between land uses see **Supplementary Material**.

The trend of declining richness with productivity was also apparent when samples were categorised by organic matter content (**Figure 5**). In both datasets, richness was significantly greater [$F_{(3,\ 259)} = 48.13, p < 0.001$; $F_{(3,\ 269)} = 46.71, p < 0.001$; for ITS1 and 18S, respectively] in mineral and humus-mineral than all other classifications (ITS1, **Figure 5A**; 18S, **Figure 5B**). There was no consistent pattern of richness when soils were categorised by soil type (**Figure S3**). Again pairwise differences between organic matter classes and soil types are described in the **Supplementary Material**.

Community composition based on non-metric multidimensional scaling of Bray-Curtis distances also showed consistent trends between the datasets. Plots demonstrate tight clustering of Crops/weeds, and grassland AVCs in both ITS1 (**Figure 6A**) and 18S (**Figure 6B**) compared to the wide dispersal of other AVCs. Such results are supported by PERMANOVAs, which show significant differences [$F_{(6,\ 406)} = 10.74, p = 0.001$; $F_{(6,\ 415)} = 15.65, p = 0.001$]; however, analyses of dispersion were also significant [$F_{(6,\ 406)} = 41.30, p = 0.001$; $F_{(6,\ 415)} = 10.69, p = 0.001$] as a result of the large disparity in replicates between land uses.

When these results are visualised by organic matter classification, the tight clusters are populated by mineral and humus-mineral samples, whereas organo-mineral and organic samples are more common in the widely dispersed areas of the plots (**Figures S4, S5**). Soil types are more widely dispersed but Brown and Surface-water gley soils are more common in the tightly grouped area (**Figures S6, S7**). Again, significant results were observed for both PERMANOVA and dispersion of variance across organic matter classes and soil types in both datasets.

Relationships Between Soil Properties and Fungal Biodiversity

Fungal richness showed similar relationships to soil properties in both datasets. Across samples, PLS and VIP analyses highlighted strong correlations between fungal richness and soil properties. There were significant, positive relationships of richness with pH and bulk density; and significant, negative correlations between richness and C:N ratio, organic matter, elevation, and mean annual precipitation (**Table 2**). Although these results followed the same trend in ITS1 and 18S data, however, their

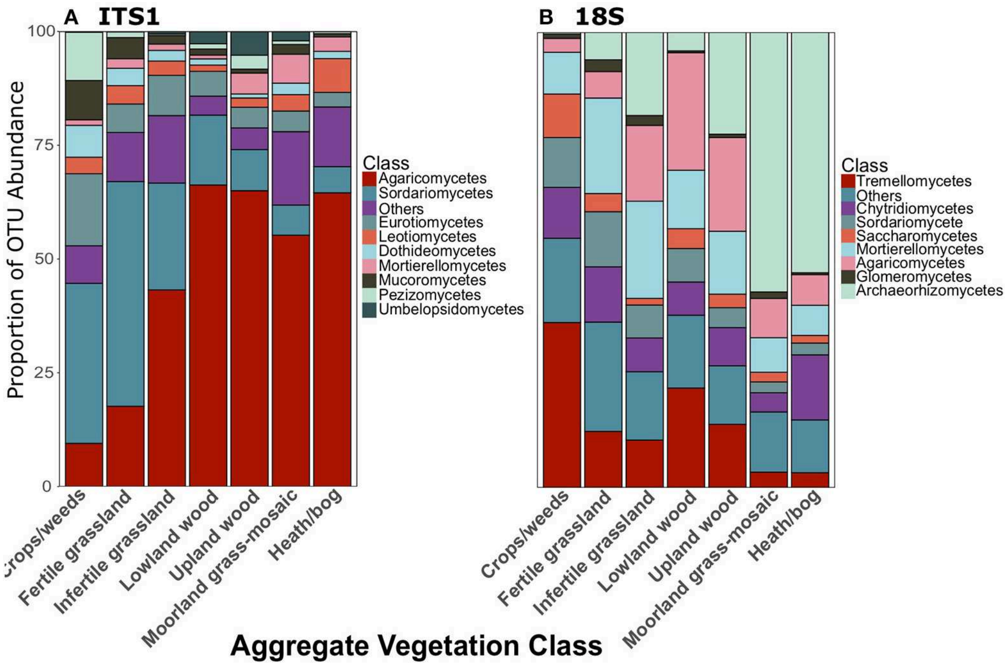

FIGURE 3 | Proportionate abundances of fungal OTUs for **(A)** ITS1 and **(B)** 18S data across Aggregate Vegetation Class. Aggregate Vegetation Classes are ordered from most (Crops/weeds) to least (Heath/bog) productive.

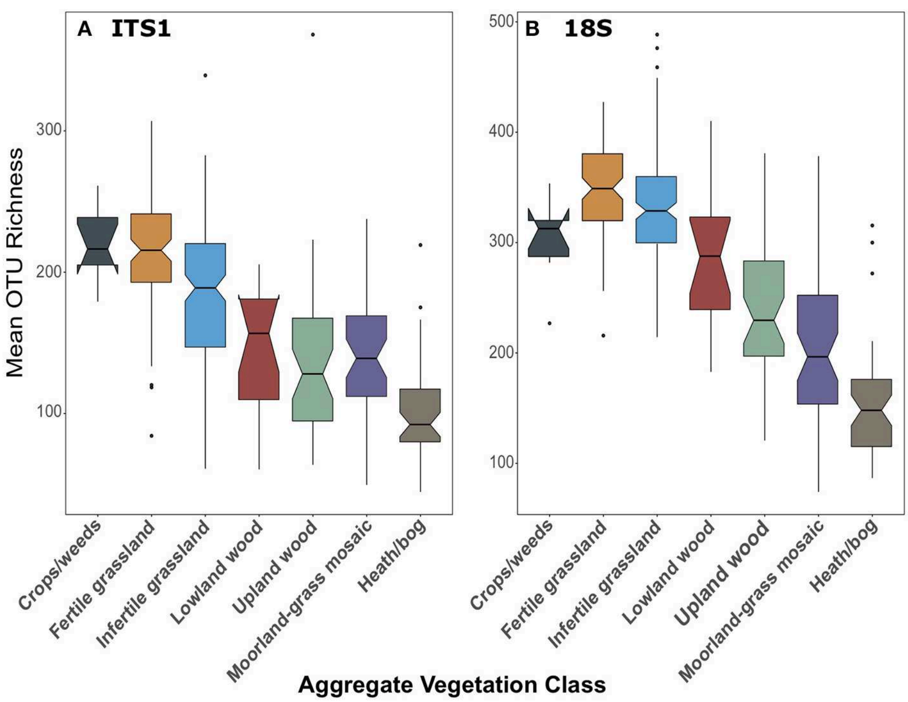

FIGURE 4 | Boxplots of fungal OTU richness for **(A)** ITS1 and **(B)** 18S datasets plotted against Aggregate Vegetation Class. Aggregate Vegetation Classes are ordered from most (Crops/weeds) to least (Heath/bog) productive. Boxes cover the first and third quartiles and horizontal lines denote the median. Black dots represent outliers beyond the whiskers, which cover 1.5X the interquartile range. Notches indicate confidence interval around the median. Overlapping notches are a proxy for non-significant differences between medians. Black dots are outliers.

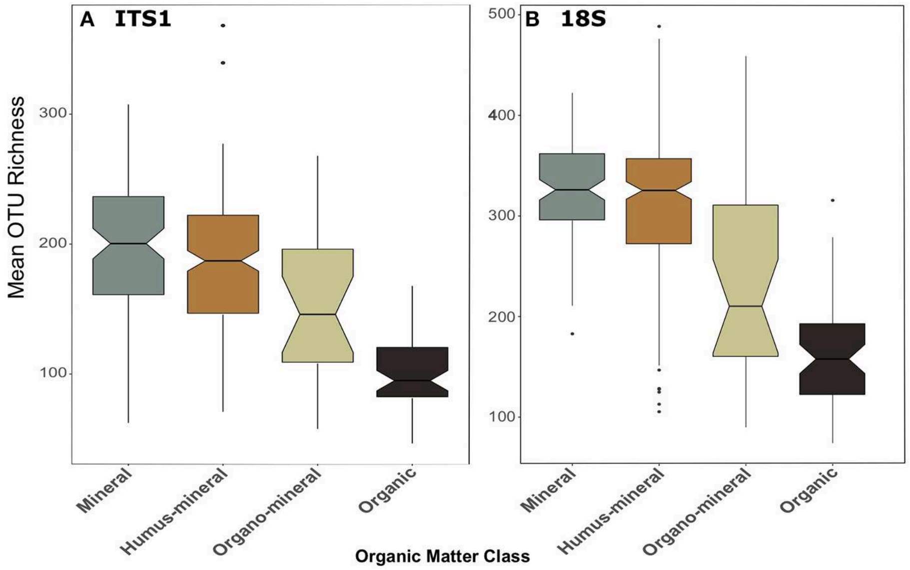

FIGURE 5 | Boxplots of fungal OTU richness for **(A)** ITS1 and **(B)** 18S datasets plotted against organic matter class. Organic matter classes are listed in order of increasing percent organic matter. Boxes cover the first and third quartiles and horizontal lines denote the median. Black dots represent outliers beyond the whiskers, which cover 1.5X the interquartile range. Notches indicate confidence interval around the median. Overlapping notches are a proxy for non-significant differences between medians. Black dots are outliers.

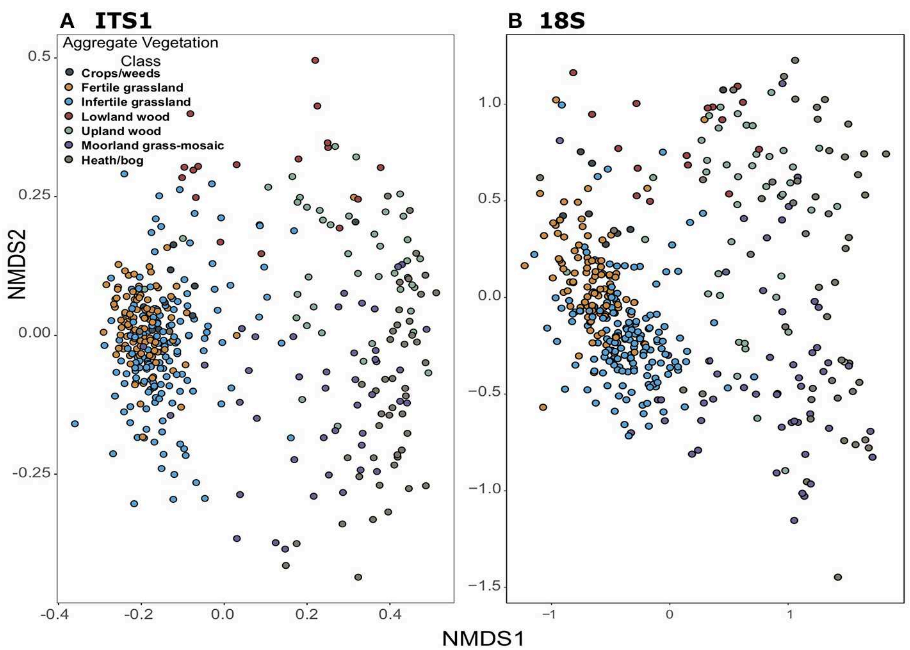

FIGURE 6 | Non-metric dimensional scaling ordinations of fungal community composition across GMEP sites. Samples are coloured by Aggregate Vegetation Class. Data from ITS1 (stress = 0.13) is shown in **(A)**; data from 18S (stress = 0.11) is shown in **(B)**.

relative rankings varied. For example, fungal richness from ITS1 data was most strongly correlated with bulk density and organic matter, while richness from 18S data was more strongly correlated to C:N ratio and elevation in addition to bulk density (**Table 2**). Furthermore, there were some relationships unique to each dataset. Significant negative relationships were observed between richness and soil water repellency. Similarly, richness derived from 18S data was negatively related to total

TABLE 2 | Results of partial least squares regressions for fungal richness against environmental variables.

Soil and environmental variables	Fungi (ITS)	Fungi (18S)
Total C^L	0.44	*1.03 ($R^2 = 0.38^{***}$)*
Total N^L	0.93	0.56
C:N ratio^S	*1.64 ($R^2 = 0.28^{***}$)*	*1.71 ($R^2 = 0.41^{***}$)*
Total P^S	0.70	0.87
Organic matter (% LOI)^L	*1.13 ($R^2 = 0.29^{***}$)*	*1.17 ($R^2 = 0.38^{***}$)*
pH ($CaCl_2$)	$\underline{1.52\ (R^2 = 0.23^{***})}$	$\underline{1.55\ (R^2 = 0.37^{***})}$
Soil water repellency^L	*1.23 ($R^2 = 0.13^{***}$)*	0.82
Volumetric water content (m^3/m^3)	0.60	0.70
Rock volume (mL)	0.64	0.43
Bulk density (g/cm^3)	$\underline{1.41\ (R^2 = 0.29^{***})}$	$\underline{1.33\ (R^2 = 0.41^{***})}$
Clay content (%)^A	0.84	$\underline{1.19\ (R^2 = 0.11^{***})}$
Sand content (%)^A	0.6	*1.11 ($R^2 = 0.1^{***}$)*
Elevation (m)	*1.68 ($R^2 = 0.22^{***}$)*	*1.83 ($R^2 = 0.41^{***}$)*
Mean annual precipitation (mL)	*1.44 ($R^2 = 0.18^{***}$)*	*1.52 ($R^2 = 0.27^{***}$)*
Temperature (°C)	0.56	0.52

*Positive relationships are underlined; negative relationships are written in italics. ***indicates P < 0.001, blank indicates P > 0.05. ^{A}denotes Aitchison's log_{10}-ratio transformation; ^{L}denotes log_{10}-transformation; ^{S}denotes square-root-transformation.*

TABLE 3 | Summary of relationships amongst environmental factors and fungal communities based on ITS data.

Variable		Correlation	
	R^2	Axis1	Axis2
pH ($CaCl_2$)	0.6***	−	+
C:N ratio^S	0.47***	+	−
Elevation (m)	0.41***	+	−
Volumetric water content (m^3/m^3)	0.41***	+	−
Mean annual precipitation (mL)	0.39***	+	−
Bulk density (g/cm^3)	0.38***	−	+
Organic matter (% LOI)^L	0.37***	+	−
Total C^L	0.31***	+	−
Clay content (%)^A	0.28***	−	+
Soil water repellency^L	0.24***	+	−
Total N (%)^L	0.21***	+	−
Sand content (%)^A	0.19***	+	+
Total P (mg/kg)^S	0.11***	−	−
Rock volume (mL)	0.07***	−	+
Temperature (°C)	0.04***	−	+

*+/− signify the direction of association between each variable and respective NMDS axes. ***indicates P < 0.001, blank indicates P > 0.05. ^{A}denotes Aitchison's log_{10}-ratio transformation; ^{L}denotes log_{10}-transformation; ^{S}denotes square-root-transformation.*

TABLE 4 | Summary of relationships amongst environmental factors and fungal communities based on 18S data.

Variable		Correlation	
	R^2	Axis1	Axis2
pH ($CaCl_2$)	0.61***	−	+
Elevation (m)	0.50***	+	−
Mean annual precipitation (mL)	0.46***	+	−
Volumetric water content (m^3/m^3)	0.45***	+	−
C:N ratio^S	0.43***	+	+
Organic matter (% LOI)^L	0.43***	+	+
Bulk density (g/cm^3)	0.39***	−	−
Total C^L	0.34***	+	+
Clay content (%)^A	0.30***	−	+
Total N (%)^L	0.28***	+	−
Soil water repellency^L	0.21***	+	−
Sand content (%)^A	0.14***	+	+
Total P (mg/kg)^S	0.10***	−	−
Rock volume (mL)	0.06***	−	+
Temperature (°C)	0.05***	−	+

*+/− signify the direction of association between each variable and respective NMDS axes. ***indicates P < 0.001, blank indicates P > 0.05. ^{A}denotes Aitchison's log_{10}-ratio transformation; ^{L}denotes log_{10}-transformation; ^{S}denotes square-root-transformation.*

C and sand content of soil but also positively related to clay content.

We found pH was the best predictor of β-diversity from linear fitting for fungi no matter what gene region is amplified (**Tables 3**, **4**). All fitted variables were significantly correlated to β-diversity, though most of these only weakly. It is likely that they did not strongly influence the fungal communities. Variables followed similar rankings in both the ITS1 and 18S data. Elevation, annual precipitation, soil moisture, C:N ratio, organic matter, and bulk density all had R^2 values greater than 0.35, but their relative order differed between datasets (**Tables 3**, **4**).

Effect of Land Use on Functional Diversity

There was a distinct difference in trophic modes of OTUs that were successfully matched to the FUNGUILD database between ITS1 and 18S datasets. In total, 3,402 and 1,783 OTUs from the ITS1 and 18S datasets, respectively were matched to the FUNGUILD database. Overall, saprotrophs were the most abundant trophic mode in both datasets (**Figure 6**); however, pathotrophs ranked second in ITS1 (**Figure 6A**) data while the pathotroph-saprotroph-symbiotroph multi-trophic group was second-most abundant in 18S data (**Figure 6B**). Across land uses, proportions of pathotrophs and pathotroph-saprotroph-symbiotrophs fell with declining productivity (**Figure 7**). In matches from the ITS1 data, pathotroph-saprotrophs increased across the productivity gradient (**Figure 7A**), as did saprotrophs in the 18S data (**Figure 7B**). The aforementioned trend in proportional abundance of pathotrophs and pathotroph-saprotroph-symbiotrophs was also present across organic matter classes (**Figure S8**). Symbiotrophs appeared to follow an opposite trend, increasing as productivity fell. Interestingly, this was the case for saprotrophs in the 18S (**Figure S8B**) but not the ITS1 (**Figure S8A**) dataset. Proportional abundances of fungal OTUs grouped by trophic modes did not follow a discernable pattern across changing soil types (**Figure S9**). For simplicity, we focused further analyses only on the broadly defined saprotroph,

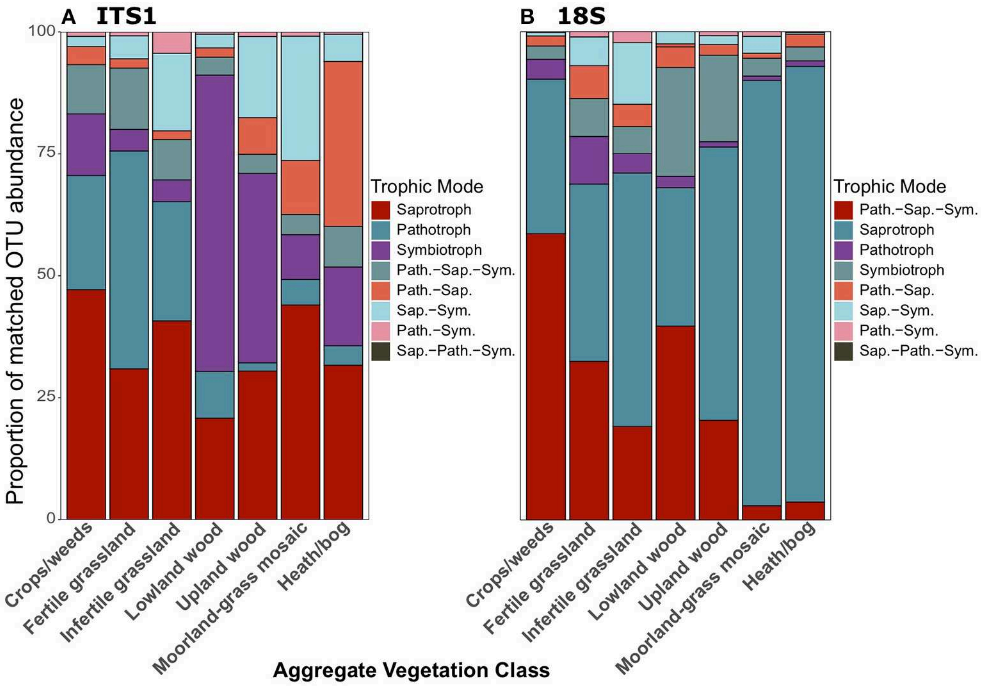

FIGURE 7 | Proportionate abundances of fungal OTUs matched to FUNGuild trophic groups for **(A)** ITS1 and (**B)** 18S data across Aggregate Vegetation Classes. Aggregate Vegetation Classes are ordered from most (Crops/weeds) to least (Heath/bog) productive. Abbreviations for multi-trophic mode groups are as follows: Path.-Sap. (Pathotroph-Saprotroph); Path.-Sap.-Sym. (Pathotroph-Saprotroph-Symbiotroph); Path.-Sym. (Pathotroph-Symbiotroph); Sap.-Path.-Sym (Saprotroph-Pathotroph-Symbiotroph); Sap.-Sym. (Saprotroph-Symbiotroph).

pathotroph, and symbiotroph groups, ignoring all combination groups; pairwise differences for all of the following comparisons are described in the **Supplementary Material**.

Across land uses, significant differences were observed in the richness of saprotrophic fungi in both the ITS1 [$F_{(6,\ 258)} = 25.14$, $p < 0.001$] and 18S [$F_{(6,\ 267)} = 31.10$, $p < 0.001$] data; however, there were differences between datasets (**Figure 8**). In the ITS1 dataset, richness followed the same trend as overall fungal richness, with the highest and lowest values in the Crops/weeds and Heath/bog AVCs respectively (**Figure 8A**). Although this pattern was preserved in the 18S data (**Figure 8B**), richness of saprotrophs was much more even across AVCs in this case. Indeed, rather than the linear decline of richness along the productivity gradient, there appeared to be 3 distinct levels in the data affiliated with (i) grassland/agricultural sites, (ii) woodlands, and (iii) bogs.

The same pattern was also apparent across organic matter classifications in both datasets [ITS1: $F_{(3,\ 260)} = 32.86$, $p < 0.001$; 18S: $F_{(3,\ 269)} = 41.13$, $p < 0.001$; **Figure 9**]. In the ITS1 dataset, each class was significantly different from the others (**Figure 9A**). In the 18S data, saprotroph richness was significantly higher in mineral and humus-mineral soils than organo-mineral and organic soils (all $p < 0.001$ except mineral—organo-mineral $p = 0.02$) (**Figure 9B**). Again, the overarching trend of fungal richness was not apparent when samples were grouped by soil type. Although there were significant differences across soil types in both the ITS1 [$F_{(5,\ 259)} = 9.7$, $p < 0.001$] and 18S [$F_{(5,\ 268)} = 10.73$, $p < 0.001$] datasets, these differences did demonstrate consistent patterns across soil types (**Figure S10**).

In the case of pathotrophic fungi, richness also followed a similar trend to the saprotrophs across both datasets. In the ITS1 data, significantly [$F_{(6,\ 258)} = 26.11$, $p < 0.001$] greater richness values were observed in Crops/weeds and grassland samples (**Figure 8A**). Richness of pathotrophs was significantly highest in Crops/weeds sites. Again, this trend was present, though not as clear, in the 18S dataset (**Figure 8B**). Significant differences [$F_{(6,\ 267)} = 52.26$, $p < 0.001$] were observed between AVCs, with the highest richness of pathotrophs occurring in the Fertile grassland and Crop/weeds land uses.

Across organic matter classes, significant differences were also observed in pathotroph richness in the ITS1 [$F_{(3,\ 250)} = 24.91$, $p < 0.001$] and 18S [$F_{(3,\ 269)} = 30.49$, $p < 0.001$] datasets. However, in this case the trends were more apparent in the 18S data than the ITS1 data (**Figure 9**). Pathotroph richness was highest in mineral soils and lowest in organic soils when compared to all other classes in the ITS1 data (**Figure 9A**). However, all organic matter classifications were statistically different from each other in the 18S data (**Figure 9B**), in descending order from mineral to peat soils. Again, trends were less clear across soil types (**Figure S10**). Significant differences were observed in the ITS1 data [$F_{(5,\ 259)} = 6.93$, $p < 0.001$] with the lowest pathotroph richness found in peat soils (**Figure S10A**). In the 18S data, differences between pathotrophic fungi across soil types were more similar to those observed in other groups (**Figure S10B**).

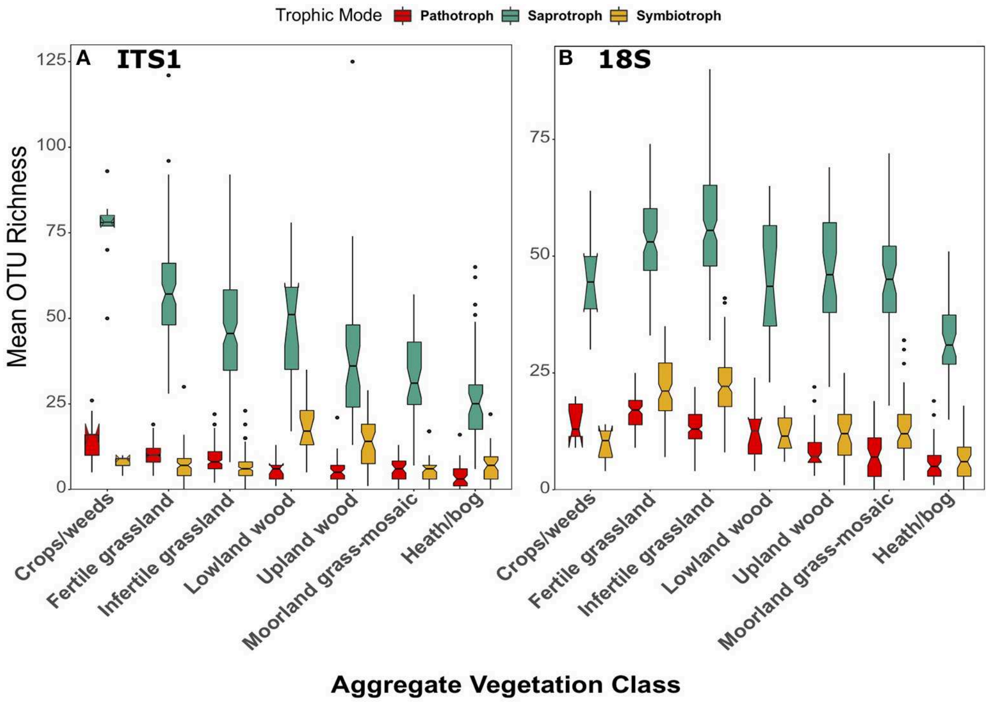

FIGURE 8 | Boxplots of richness of fungal OTUs matched to the pathotrophic, saprotroph, and symbiotroph trophic modes in FUNGuild for **(A)** ITS1 and **(B)** 18S datasets plotted against Aggregate Vegetation Class. Aggregate Vegetation Classes are ordered from most (Crops/weeds) to least (Heath/bog) productive. Boxes cover the first and third quartiles and horizontal lines denote the median. Black dots represent outliers beyond the whiskers, which cover 1.5X the interquartile range. Notches indicate confidence interval around the median. Overlapping notches are a proxy for non-significant differences between medians. Black dots are outliers.

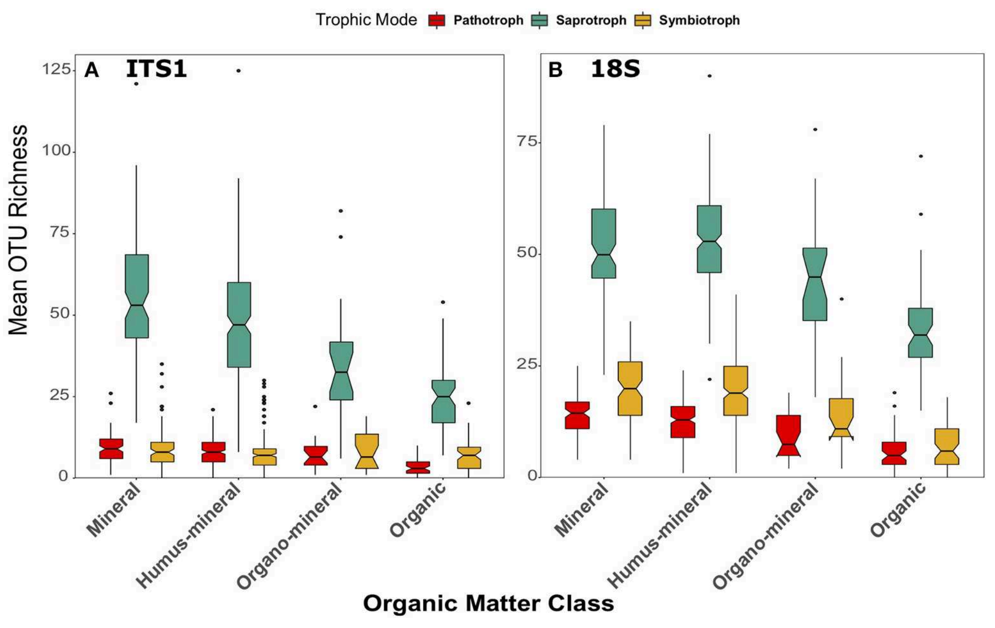

FIGURE 9 | Boxplots of richness of fungal OTUs matched to the pathotrophic, saprotroph, and symbiotroph trophic modes in FUNGuild for **(A)** ITS1 and **(B)** 18S datasets plotted against organic matter class. Organic matter classes are listed in order of increasing percent organic matter. Boxes cover the first and third quartiles and horizontal lines denote the median. Black dots represent outliers beyond the whiskers, which cover 1.5X the interquartile range. Notches indicate confidence interval around the median. Overlapping notches are a proxy for non-significant differences between medians. Black dots are outliers.

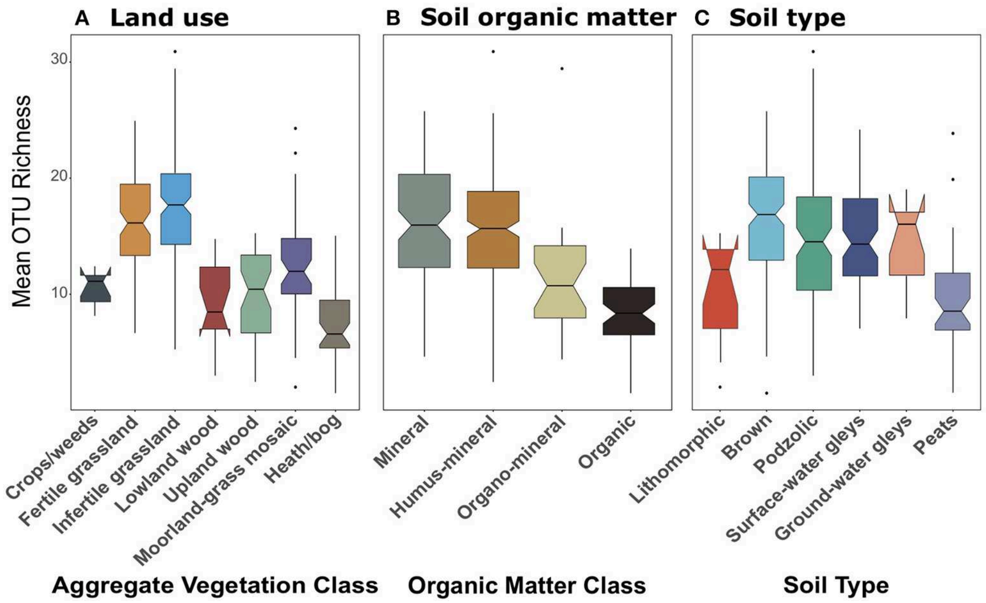

FIGURE 10 | Boxplots of richness of Glomeromycetes OTUs plotted against **(A)** Aggregate Vegetation Class; **(B)** organic matter class; **(C)** soil type. Aggregate Vegetation Classes are ordered from most (Crops/weeds) to least (Heath/bog) productive. Organic matter classes are listed in order of increasing percent organic matter. Soils are listed in increasing order of moisture retention. Boxes cover the first and third quartiles and horizontal lines denote the median. Black dots represent outliers beyond the whiskers, which cover 1.5X the interquartile range. Notches indicate confidence interval around the median. Overlapping notches are a proxy for non-significant differences between medians. Black dots are outliers.

Pathotroph richness was significantly [$F_{(5,\ 268)} = 13.6, p < 0.001$] different across soil types with the highest values found in brown soils and the lowest in peats.

The previously described trend of declining richness across the land use productivity gradient (i.e., **Figure 4**) was not apparent when considering symbiotrophs. Furthermore, although significant differences were apparent in both the ITS1 [$F_{(6,\ 258)} = 14.88$, $p < 0.001$] and 18S [$F_{(6,\ 267)} = 55.13$, $p < 0.001$] datasets they were by no means identical (**Figure 8**). Symbiotroph richness was highest in Lowland wood sites followed by Upland wood. This trend was not apparent in the 18S dataset, however (**Figure 8B**). Here richness of symbiotrophs was greatest in grassland AVCs and lowest in Heath/bog sites much like the overarching trend of total fungal OTU richness.

When samples were grouped by organic matter class, further discrepancies became apparent between the datasets. Whereas, the previously described trend of decreasing richness with increasing organic matter content held true in the 18S data [$F_{(3,\ 269)} = 36.28$, $p < 0.001$; **Figure 9B**], no significant differences were observed in the ITS1 dataset [$F_{(3,\ 260)} = 1.88$, $p = 0.13$; **Figure 9A**]. In the 18S data, richness of symbiotrophs was greater in mineral and humus-mineral soils when compared to organo-mineral ($p = 0.002$, $p = 0.04$, respectively) and organic ($p < 0.001$) soils (**Figure 9B**). There were also no significant differences [$F_{(5,\ 259)} = 1.43$, $p = 0.21$] in symbiotroph richness across soil types in ITS1 data (**Figure S10A**), though there were in 18S data [$F_{(5,\ 259)} = 12.52$, $p < 0.001$; **Figure S10B**]. As described previously, richness was lowest in peat soils and highest in brown soils.

We suspected that the differences in functional diversity observed between datasets might be a result of differential coverage of important groups. We were able to confirm this when we analysed the richness of OTUs identified as Glomeromycetes present in the 18S dataset (**Figure 10**). All of the 162 Glomeromycetes OTUs were assigned as highly-probable symbiotrophs through FUNGUILD. Across land uses, richness of Glomeromycetes followed similar trends to those of symbiotrophs and saprotrophs from 18S data. There were significant [$F_{(6,\ 244)} = 33.47$, $p < 0.001$] differences across land uses, though they appeared, like the saprotroph richness to be tiered between grasslands, woods, and bogs (**Figure 10A**). Richness of Glomeromycetes was higher in grasslands than all other AVCs except Crops/weeds and lowest in Heath/bog sites. Again, when grouped by organic matter class (**Figure 10B**) and soil type (**Figure 10C**), Glomeromycetes richness followed the same trend as saprotrophs and symbiotrophs from the 18S dataset. Richness was significantly [$F_{(3,\ 246)} = 37.65$, $p < 0.001$] greater in mineral and humus-mineral soils than all others. Across soil types, richness of Glomeromycetes was significantly [$F_{(5,\ 245)} = 8.65$, $p < 0.001$] lower in peat soils when compared to most other soil types.

Relationships Between Soil Properties and Fungal Functional Diversity

Across all samples, PLS and VIP analyses highlighted strong correlations between fungal richness and soil properties by trophic groups. Richness of pathotrophs showed similar relationships to soil properties in both datasets. There were significant, positive relationships of richness with pH and bulk density; and significant negative correlations between richness and total C, C:N ratio, organic matter, elevation, and mean annual precipitation (**Table 5**). As with the total fungal data, the relative rankings of the strength of relationships between pathotroph and each property varied between datasets. Organic matter was most strongly correlated with pathotroph richness from ITS1 data whereas pH was most strongly correlated with pathotroph richness in the 18S data (**Table 5**). Also soil moisture content was also negatively correlated with pathotroph richness in the ITS1 dataset only.

Organic matter, elevation (both negative), pH, and bulk density (both positive) all showed significant relationships with saprotroph richness in both datasets (**Table 5**). The correlations between richness of saprotrophs and both bulk density and pH were the strongest observed in the ITS1 data. There were also negative correlations between saprotroph richness and total C, mean annual precipitation, soil moisture, soil water repellency, and mite abundance in the ITS1 data. However, it again should be noted that the correlation with mites was extremely weak. C:N ratio was strongly and positively correlated with saprotroph richness in the 18S data. Similarly, richness from 18S data was negatively related to total C and sand content of soil but also positively related to clay content. In addition, there was a significant, positive, but weak correlation between sand content and saprotroph richness.

In both datasets, symbiotroph richness was significantly correlated with pH and C:N ratio (**Table 5**). Interestingly, the relationships were positive in the case of C:N ratio and negative for pH in ITS1 data but the opposite was apparent in the 18S data. There were also many more relationships unique to each dataset. Weak but significant positive relationships were observed between symbiotroph richness and rock volume, Collembola abundance, and temperature as well as a negative correlation to soil moisture. In the 18S data, stronger relationships were observed between symbiotroph richness and bulk density (positive) and elevation (negative). Furthermore, a weakly negative correlation was observed with sand content in addition to weak positive correlations with clay content and total P.

DISCUSSION

Primer Choice and the Total Fungal Community

We observed congruent patterns in total fungal OTU richness across land uses, organic matter classes and soil type when measured with either ITS1 or 18S primer sets. Richness was greater in arable and grassland land uses, which are highly productive, intensively managed and declined in the less productive, largely unmanaged bogs. Although these findings had been previously known from the ITS1 dataset (George et al., 2019), it is important to note that the trend was also present in the fungal OTUs identified from 18S sequencing. A similar trend was observed across organic matter classes. Here, fungal richness fell as organic matter increased. Fungal α-diversity is known to be greater in arable soils than in grasslands or

TABLE 5 | Results of partial least squares regressions for richness of OTUs classified by trophic mode from FUNGUILD analyses against environmental variables.

Soil and environmental variables	Saprotrophs (ITS)	Saprotrophs (18S)	Pathotrophs (ITS)	Pathotrophs (18S)	Symbiotrophs (ITS)	Symbiotrophs (18S)
Total C (%)^{L}	*1.1 ($R^2 = 0.24^{***}$)*	0.89	*1.07 ($R^2 = 0.17^{***}$)*	*1.0 ($R^2 = 0.25^{***}$)*	0.24	0.99
Total N (%)^{L}	0.99	0.10	0.82	0.64	*1.17 ($R^2 = 0.02^{*}$)*	0.10
C:N ratio^{S}	0.95	*2.31 ($R^2 = 0.28^{***}$)*	*1.22 ($R^2 = 0.16^{***}$)*	*1.41 ($R^2 = 0.25^{***}$)*	<u>1.69 ($R^2 = 0.01^{*}$)</u>	*2.47 ($R^2 = 0.34^{***}$)*
Total P (mg/kg)^{S}	0.07	0.86	0.75	0.75	1.38	<u>1.31 ($R^2 = 0.02^{*}$)</u>
Organic matter (% LOI)^{L}	*1.36 ($R^2 = 0.28^{***}$)*	*1.02 ($R^2 = 0.24^{***}$)*	*1.38 ($R^2 = 0.21^{***}$)*	*1.16 ($R^2 = 0.28^{***}$)*	0.37	0.92
pH ($CaCl_2$)	<u>1.34 ($R^2 = 0.21^{***}$)</u>	<u>1.27 ($R^2 = 0.14^{***}$)</u>	<u>1.4 ($R^2 = 0.16^{***}$)</u>	<u>1.98 ($R^2 = 0.4^{***}$)</u>	*2.35 ($R^2 = 0.05^{***}$)*	<u>1.45 ($R^2 = 0.2^{***}$)</u>
Soil water repellency^{L}	*1.28 ($R^2 = 0.15^{***}$)*	0.36	0.84	0.98	0.3	0.62
Volumetric water content (m^3/m^3)	*1.46 ($R^2 = 0.22^{***}$)*	0.56	*1.38 ($R^2 = 0.17^{***}$)*	0.99	*1.42 ($R^2 = 0.05^{***}$)*	0.40
Rock volume (mL)	0.68	0.06	0.8	0.59	<u>1.09 ($R^2 = 0.02^{**}$)</u>	0.10
Bulk density (g/cm^3)	<u>1.42 ($R^2 = 0.28^{***}$)</u>	<u>1.23 ($R^2 = 0.2^{***}$)</u>	<u>1.71 ($R^2 = 0.12^{***}$)</u>	<u>1.29 ($R^2 = 0.27^{***}$)</u>	0.51	<u>1.48 ($R^2 = 0.26^{***}$)</u>
Clay content (%)^{A}	0.71	0.74	0.90	<u>1.17 ($R^2 = 0.1^{***}$)</u>	0.49	<u>1.05 ($R^2 = 0.03^{**}$)</u>
Sand content (%)^{A}	0.18	*1.71 ($R^2 = 0.05^{***}$)*	0.05	0.32	0.21	<u>1.63 ($R^2 = 0.08^{***}$)</u>
Elevation (m)	*1.58 ($R^2 = 0.25^{***}$)*	*1.13 ($R^2 = 0.13^{***}$)*	*1.6 ($R^2 = 0.19^{***}$)*	*1.98 ($R^2 = 0.39^{***}$)*	0.37	<u>1.07 ($R^2 = 0.17^{***}$)</u>
Mean annual precipitation (mL)	*1.45 ($R^2 = 0.23^{***}$)*	0.81	*1.38 ($R^2 = 0.16^{***}$)*	*1.49 ($R^2 = 0.24^{***}$)*	0.00	0.69
Temperature (°C)	0.09	0.49	0.21	0.43	<u>1.17 ($R^2 = 0.01^{*}$)</u>	0.53

*Positive relationships are underlined; negative relationships are written in italics. ***indicates $P < 0.001$, **$0.001 > P < 0.01$, *$0.01 > P < 0.05$, blank indicates $P > 0.05$. ^{A}denotes Aitchison's log_{10}-ratio transformation; ^{L}denotes log_{10}-transformation; ^{S}denotes square-root-transformation.*

forests (Szoboszlay et al., 2017). Potential mechanisms for this include: (i) increased nutrient availability due to fertiliser input (Szoboszlay et al., 2017), and (ii) beneficial disturbance from tillage and other standard agricultural practices. The latter is consistent with the intermediate disturbance hypothesis whereby high levels of diversity are maintained by consistent interruption of successional processes (Connell, 1978).

Soils rich in organic matter, especially peats, found in upland moors, bogs, and other wetlands across harbour distinct fungal communities from neighbouring habitats (Anderson et al., 2003). Fungi dominate microbial communities in bogs (Thormann and Rice, 2007) although their proportional abundance drops sharply below the first 5 cm of bog habitats (Potter et al., 2017). Yet, richness in bogs is consistently low, perhaps due to environmental pressures such as high acidity, highly recalcitrant SOM, low nutrients, and oxygen levels (Rousk et al., 2010; Tedersoo et al., 2014) or reduced competition within the fungal community.

In comparison to AVC and SOM levels, differences in fungal communities were not as clear across soil types as defined by the National Soil Map (Avery, 1980), which is inline with previous work on microbial activity across the UK (Jones et al., 2014). Richness was highest in brown soils and was lowest in peats. Brown soils commonly support grassland communities across Wales (Avery, 1980; Rudeforth et al., 1984). Nearly half of the Fertile and Infertile grasslands surveyed in GMEP were categorised as brown soils. The absence of other major trends besides these may be due to the use of the dominant soil type and lack of resolution for the soil classification. The soils map used in this study simply does not provide enough resolution (1:63, 360; Avery, 1980) for soil type to be an effective category. Furthermore, this system heavily uses subsoil properties to determine soil type (Avery, 1980), while our work only involved the upper 15 cm. However, it is our opinion that the use of organic matter classification is more effective and simple metric that can be easily implemented in large-scale studies in lieu of fine-scale maps.

Results of PLS analyses demonstrates that soil properties and associated environmental factors influencing fungal richness are consistent across ITS1 and 18S datasets. Major drivers included pH, bulk density, C:N ratio, organic matter, elevation, and mean annual temperature (**Table 2**). Such results from 18S data are consistent with previous findings from the ITS1 data (George et al., 2019). However, there were certain properties that were significant in only one of the datasets and the relative importance of these properties does vary between the two datasets. There are several possible explanations for this. Firstly, 9 more samples were used in the 18S dataset ($n = 422$) than the ITS1 data ($n = 413$), which may have introduced the discrepancy in relative importance of the data. However, it is much more likely that a differential coverage of fungal groups between the two datasets caused these discrepancies.

Community composition showed consistent clustering across land uses, organic matter classes, and soil types in both data sets. As in George et al. (2019), communities were most similar in the grassland and arable sites and more spread out across woodlands and upland habitats. This was likely driven by environmental factors across Wales. In both datasets, pH was the most important environmental variable influencing community composition and although the remaining properties followed similar patterns, their relative importance again differed in the dataset. The importance of pH, elevation, C:N ratio, and precipitation in determining fungal community composition fits well in the wider context of soil fungi biogeography. Tedersoo et al. (2014) previously highlighted the importance of these variables in the distribution of fungi at the global scale. Furthermore, the strong positive correlation with C:N ratio is indicative of the expected fungal dominance (de Vries et al., 2006) of nutrient-poor, acidic soils (Bloem et al., 1997).

Primer Choice and Fungal Functional Diversity

Differences between richness of trophic modes of fungi, used here as a proxy for functional diversity, showed some discrepancies across land uses and soil classification between data sets. Saprotrophs made up the largest proportion of the 3 functional groups studied and generally exhibited the same trends as total richness across soils and land uses. This was also the case for pathotrophs. Indeed, correlations between environmental variables with pathotroph and saprotroph richness were largely consistent across datasets. However, we observed divergent trends in symbiotroph richness across land uses and soils. Symbiotroph richness was highest in woodlands in the ITS1 dataset whereas it was highest in grasslands according to the 18S data (**Figures 7A,B**). A similar increase in richness within grasslands in the 18S data is repeated when Glomeromycetes were considered on their own (**Figure 9**); AMF are the predominant mycorrhizal fungi in grassland systems (Smith and Read, 2008). The symbiotroph peak in the ITS1 data may be explained by an increase in coverage of ectomycorrhizas which are the most common group to associate with trees and shrubs (Smith and Read, 2008). Despite these differences, both datasets suggest that symbiotroph richness was low in arable land, which is in line with previous findings demonstrating high susceptibility of mycorrhizal fungi to disturbance, for example tillage (Schnoor et al., 2011; Säle et al., 2015), and the addition of fertilizers, which decreases the receptiveness of many agricultural plants to mycorrhizal infection (Smith and Read, 2008).

The divergent trend in symbiotroph richness and discrepancies in relationships between functional groups and environmental variables likely stem from primer biases. Primer biases have been well-recognised as a confounding factor in categorising communities from environmental DNA (Cai et al., 2013; Elbrecht and Leese, 2015; Tedersoo et al., 2015). Tedersoo et al. (2015) assessed the effectiveness of fungal barcodes from the ITS, 18S, and 28S rDNA regions and found that primer choice did not affect richness or β-diversity results of soil fungi communities from Papua New Guinea, although fewer OTUs were recovered by 18S primers than ITS primers. *In silico* analyses suggests such findings are the result of lumping of sequences in the 18S that may predominantly affect rare sequences, thereby strengthening community matrices. Similarly, results were similar enough for all primers to be suitable for analyses at the class-level (Tedersoo et al., 2015). Although the 18S primers used here were designed to cover the breadth of eukaryotes and may lack specificity to fungi (Behnke et al., 2011), our results show strong congruence to the ITS1 data across total richness and indeed most functional groups.

Unlike Tedersoo et al. (2015) we observed considerable differences in the proportions of fungal classes between the ITS1 and 18S data sets. We suspect that such differences stem from the need to use appropriate databases to assign taxonomy to OTUs to each dataset (Xue et al., 2019). Perhaps only 30–35% of Glomeromycetes are present in 18S and ITS databases, respectively (Hart et al., 2015), and although sequences are continuously being uploaded to such repositories, it is likely the majority of AMF are not identifiable from environmental samples (but see Öpik et al., 2014). Similarly we suspect that, although not studied in detail, primer choice may lead to biases in other groups. Archaeorhizomycetes accounted for nearly 25% of the 18S sequences but less than 1% from the ITS1 data (**Figure 2B**). Primer bias has been recognised for Archaeorhizomycetes even before the class' formal description; ∼19% of 18S sequences collected from Anderson et al. (2003), have been matched to Archaeorhizomycetes, whereas none were recovered from the same samples using ITS primers. Despite its recent description, Archaeorhizomycetes are ubiquitous components of soil communities. Strong associations have been observed with trees, yet precise functional roles of these fungi have yet to be determined (Rosling et al., 2011). Subsequently, such biases likely account for divergent relationships between functional group richness and environmental properties.

CONCLUSIONS

Our comparison of the use of ITS1 and 18S primers and their respective databases in a nationwide metabarcoding survey of fungi yielded 3 major findings. First, the congruent findings of total richness and β-diversity across land use and their relationships to environmental variables confirmed our previous research (George et al., 2019). Second, soil organic matter was found to be a more sensitive metric than soil type in our survey design. Third, biases from the combination of primer and database choice became apparent for certain classes of fungi, including Glomeromycetes and Archaeorhizomycetes, which strongly influenced functional group richness across land uses as well as their relationships with environmental variables. It is therefore important to recognise the sensitivity of metabarcoding to primer choice, even when using universal primers. Without simultaneous analyses of environmental DNA using both primers and databases, the presence of AM fungi as well as the newly characterised Archaeorhizomycetes would have been overlooked and unquantified in this survey. Furthermore, since the majority of soil biodiversity is undescribed (Ramirez et al., 2015), utilising multiple primers will elucidate a more complete picture of belowground biodiversity by revealing shortcomings in existing probes and revealing the presence of as yet undescribed organisms. We therefore advocate that future nation-wide surveys included both a sample-based metric of soil type (i.e., organic matter classification) and multiple primers for fungal biodiversity. Such measures should not be arduous to implement, especially if researchers can identify specific fungal groups of particular interest to accommodate.

DATA AVAILABILITY STATEMENT

Data associated with this paper will be publically published in the National Environment Research Council (NERC) Environmental Information Data Centre (EIDC). Currently, pH, bulk density, C, N, P, moisture, and water repellency data are available (Robinson et al., 2019). Data are also available from the authors upon reasonable request with permission from the Welsh Government. Sequences with limited sample metadata have been uploaded to the European Nucleotide Archive and can be accessed with the following primary accession codes: PRJEB28028 (ITS1) and PRJEB28067 (18S).

AUTHOR CONTRIBUTIONS

PG, DJ, DR, and SC conceived this project. BE and DR facilitated the use of GMEP data. Bioinformatics and statistical analyses were led by PG with assistance from SC and RG. PG wrote the first draft of the manuscript. SC, DR, and DJ contributed to subsequent revisions. All authors read and approved the final draft of the manuscript.

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SUPPLEMENTARY MATERIAL

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A Framework to Consider Soil Ecosystem Services in Territorial Planning

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As a critical interface in the environment, soils can provide a wide range of ecosystem services (ES). However, while there is growing demand to assess soil ES from agricultural systems, considering them in land management strategies remains a challenge. Indeed, because of the difficulty in relating soil properties to ES, soil ES are still not fully considered in the territorial planning decision process. Through a comprehensive approach based on soil processes, an assessment framework is proposed to make soil ES understandable and usable by actors of territorial planning. This assessment framework is based on a conceptual model that is then developed into an operational framework. The conceptual model, which is supported by a literature review, relates agricultural soil ES to common socio-economic development challenges. The operational framework is based on the development of soil ES modeling and enables comparison of soil management options, which provides information to help choose among planning scenarios. This soil ES assessment framework, relating soil science to territorial governance, should improve integration of soil ES into decision making in a territorial planning context and support sustainable socio-economic development.

Keywords: agricultural system, process-based approach, land management, territorial planning, decision support information

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INTRODUCTION

Since the seminal publication about the ecosystem services (ES) concept (Costanza et al., 1997) and its widespread expansion through the Millennium Ecosystem Assessment (MEA, 2005), the ES concept has continually evolved (Costanza et al., 2017). It is recognized that human activities such as agriculture depend on and strongly influence multiple ES (MEA, 2005; Therond et al., 2017; Bommarco et al., 2018). Several ES that influence human well-being (e.g., food production, water flow and/or quality regulation, climate mitigation) have been shown to be directly affected by soil-related ES (Bouma, 2014; McBratney et al., 2014; Adhikari and Hartemink, 2016), referred to here as soil ES. These results have increased policy makers' awareness that ES, especially those involving soil processes and functions, should be explicitly considered in territorial planning (Breure et al., 2012; Albert et al., 2016; Drobnik et al., 2018), i.e., the process developed by public and private entities to influence the distribution of people and activities within territories of various sizes (a city, a county, a watershed, a metropolitan area).

Due to its interest to research and policy communities, there has been much debate on certain critical conceptual and operational issues, such as the following:

1) defining the related key terms, such as ecosystem processes, functions vs. services, goods, benefits vs. contributions (Boyd and Banzhaf, 2007; Wallace, 2007; Fisher et al., 2009)
2) classifying ES through international initiatives (TEEB, 2012; CICES, 2018; IPBES, 2018)
3) understanding and representing relations between ES and human well-being (Dominati et al., 2010; Haines-Young and Potschin, 2010; Potschin-Young et al., 2018)
4) developing assessment methods (Jónsson and Davíðsdóttir, 2016; Burkhard and Maes, 2017; Englund et al., 2017)
5) exploring the accessibility and usefulness of the ES concept to better inform territorial planning policies (de Groot et al., 2010; Hatton MacDonald et al., 2014; Ruckelshaus et al., 2015; Albert et al., 2016; Posner et al., 2016).

As a critical interface in the environment, soils ensure the provision of a wide range of ES (see Adhikari and Hartemink, 2016 and Jónsson and Davíðsdóttir, 2016 for reviews) through complex and highly time- and space-dependent feedbacks and interconnections among above- and below-ground ecosystem components (Dominati et al., 2010; Birgé et al., 2016). The European Commission (EC) (2006) has recognized soils as crucial to support humanity's capacity "to produce food, prevent droughts and flooding, stop biodiversity loss, and tackle climate change." Nevertheless, soils are highly subject to degradation, including "erosion, organic matter decline, salinization, compaction and landslides." Among terrestrial ecosystems, agricultural systems are probably the most concerned by these threats. Indeed, they face major societal (e.g., food security) and environmental (e.g., soil security, water security, climate mitigation) pressures (McBratney et al., 2014; Bommarco et al., 2018; FAO, 2018). Human activities, particularly urban expansion and inadequate agricultural practices, negatively impact agricultural land, influencing not only the provisioning services but also the entire range of soil ES (which may include provisioning, regulating and cultural services) (MEA, 2005; Bommarco et al., 2018). As Swinton et al. (2007) discussed, consideration of ES (and by extension soil ES) provided by agricultural systems is dual and must be "viewed in the context of what they replace and what they might be replaced with." Indeed, while human needs cause either natural land to be transformed to agriculture or agricultural land to be urbanized, sustainably managing soil ES from agricultural systems could meet the objectives of food security, climate mitigation and environmental conservation. Thus, agricultural soils need to be addressed specifically as a critical resource and integrated in decision-support tools for sustainable planning strategies, as emphasized by Robinson et al. (2013) and McBratney et al. (2014).

Despite the recognition of soil management in agroecosystems as a powerful mechanism for addressing environmental challenges (Robertson et al., 2014; Schulte et al., 2014; Ruhl, 2016), few studies have focussed specifically on soil-centered assessment of ES within agroecosystems (Greiner et al., 2017; Vogel et al., 2019) or even in other ecosystems (Dominati et al., 2010; Breure et al., 2012; Bouma, 2014; Grêt-Regamey et al., 2017). Recent publications on soil ES (Dominati et al., 2014; Adhikari and Hartemink, 2016; Birgé et al., 2016; Jónsson and Davíðsdóttir, 2016) highlight the need to develop an assessment framework for soils to be integrated in ES assessment studies.

This article revisits definitions and concepts from both science- and policy-based perspectives to argue for a possible way forward, positing that relevant soil ES assessment needs its own defined framework. Based on well-established frameworks such as the "cascade model" of ES (Haines-Young and Potschin, 2010; Potschin-Young et al., 2018) and the "conceptual framework linking soil to human needs" of Dominati et al. (2010, 2014), the assessment framework we developed is adapted to the objective of enhancing operational implementation of soil ES in decision-making processes. To this end, we first discuss critical assumptions about the perception of soils in an ES assessment context and detail the conceptual model that forms the first part of the assessment framework. An operational model is then developed to assess soil ES, followed by discussion of the relevance and potential added value of this assessment framework in a territorial planning context.

A CONCEPTUAL MODEL TO CONSIDER SOIL ES: LITERATURE REVIEW AND DEVELOPMENT

Perception of Soils: From an Integrated Component to an Integral Component of Ecosystems

As discussed by Ponge (2012), applying the definition of "ecosystem" to soils is not new and remains an on-going debate. The issue of considering soils either as ecosystems in themselves or only as components of ecosystems needs to be addressed in ES assessment to develop a soil-centered assessment framework. Until recently, the MEA (2005) framework, distinguishing four categories of ES (i.e., provisioning, regulating, cultural and supporting), did not explicitly consider soils as providers of ES, recognizing them only as contributors to ES provision through the "supporting" category, which underlies the others. In contrast, the working group on Mapping and Assessment of Ecosystems and their Services (MAES) (Maes et al., 2018), in line with the CICES (2018) classification, tends to consider soils as providers of ES, merging the "supporting" and "regulating" categories into a "regulating and maintenance" category. Despite this increased consideration of soils in the ES approach, these frameworks still do not view soils as the subject of ES assessment but only as a component of the subject, which remains the ecosystem.

This under-consideration of soils in ES assessment could come from diverging perceptions of their place within ecosystems. To date in ES assessment (i.e., at the ecosystem scale), soils are commonly considered as a physical component that supports activities, which leads to their perception as only an "integrated component" of ecosystems (Ponge, 2012; Bouma, 2014). Otherwise, in line with the MEA (2005), ES are defined

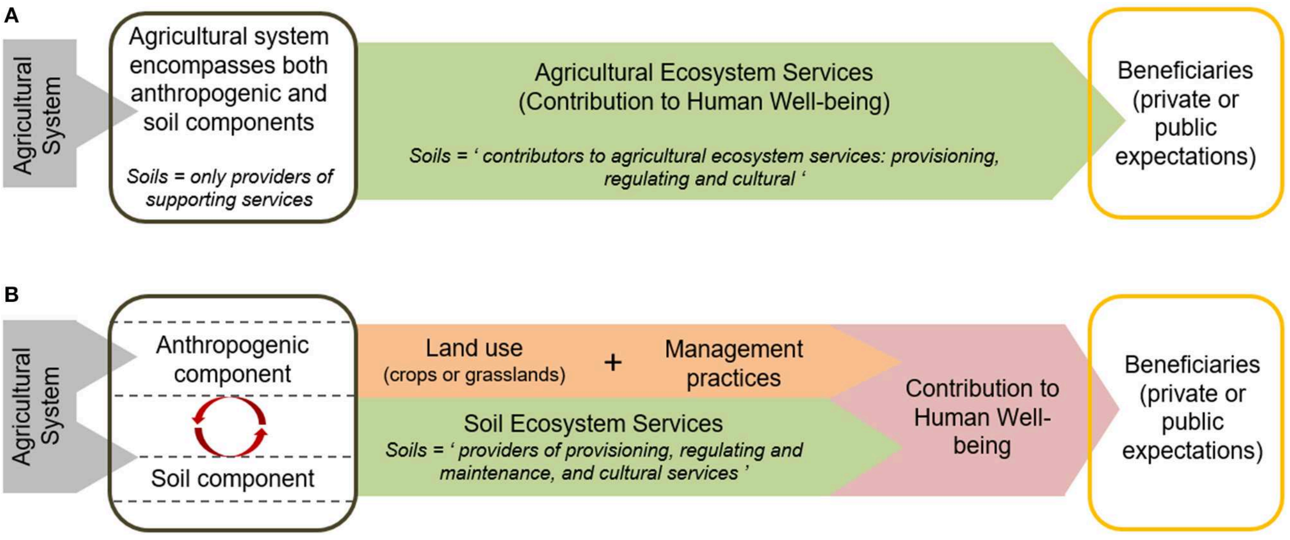

FIGURE 1 | Two alternative representations of soils in agricultural systems and their outcomes that regard soils as **(A)** contributors to agricultural ecosystem services or **(B)** providers of soil ecosystem services.

as "the goods and services from ecological systems that benefit people." Thus, for agricultural systems, soils are embedded in the definition of the system, and soil ES are not differentiated explicitly from agricultural ES. In this perception, agricultural ES resulting from both natural and anthropogenic components are aggregated into the contribution to human well-being (**Figure 1A**). This perception reduces soils to "contributors" rather than "providers" of ES (see Adhikari and Hartemink, 2016 and Greiner et al., 2017 for reviews), which relegates soil ES to the "supporting" category (MEA, 2005). This perception prevents soils from being captured specifically and explicitly (McBratney et al., 2014; Adhikari and Hartemink, 2016) in the complex chain connecting ES to human well-being (Costanza et al., 2017; Potschin-Young et al., 2018).

Ponge (2005, 2012) suggested applying to soils the assumption of interdependence with overlying activities. By assuming that soils interact with their overlying environment (i.e., both influencing their overlying environment and being influenced by it), they can be perceived as an "integral component" of the system considered. Thus, for agricultural systems, soils are one of the elements that define the system. In this perception, soil ES can be differentiated explicitly from agricultural ES and defined as the natural part of the contribution to human well-being, in contrast to the anthropogenic part that results from land use and management practices. In line with some recent literature (Costanza et al., 2017; Therond et al., 2017), the contribution to human well-being results from interactions between the soil component (and ultimately soil ES) and anthropogenic components (**Figure 1B**). This perception of soils as co-suppliers of the contribution to human well-being can be a solution to correcting the perception of soils by considering them as direct "providers" of ES and as an explicit subject in ES assessment. Furthermore, this perception is in line with recent classifications of ES (CICES, 2018; IPBES, 2018), which promote soil ES to the merged category "regulating and maintenance."

Finally, beyond these ecosystem concepts lies the need to clarify the perception of soils in ES assessment. Indeed, in line with the relatively recent reintroduction of the "geodiversity approach" [i.e., "the natural range (diversity) of geological, geomorphological and soil features" (Gray, 2008; Gray et al., 2013; Alahuhta et al., 2018)], which emphasizes the role of soil features in providing ES, the concept of soil ES is emerging (Birgé et al., 2016; Jónsson and Davíðsdóttir, 2016; Su et al., 2018). Thus, we suggest splitting the agricultural system into an anthropogenic component as an external driver (including both land use and management practices as land management, and policy action as a societal response) and a soil component as natural assets (including both inherent and dynamic properties) in order to highlight the proper role of soils in ES assessment (**Figures 1A,B**). This perception is more in line with the recent classification and provides the opportunity to (i) capture soil ES better in the complex chain connecting soil ES, contributions to human well-being and governance and (ii) better assess the role that soils can play in territorial planning processes.

A Common Language for Mutual Understanding

Soil ES Lexicon

Barnaud and Antona (2014) and Danley and Widmark (2016) reported that a broad range of stakeholders used the ES concept and argued that its wide adoption creates ambiguity in its meaning. Reporting stakeholders' feedback about operationalization of ES, Carmen et al. (2018) and Jax et al. (2018) identified the need to adapt language to each stakeholder as one of the crucial principles to frame and shape action on land management across scales of governance. Considering these

TABLE 1 | Definition of key terms used in this framework of soil ecosystem services assessment.

Key term	Definition
Soil Natural Assets	The physical, chemical and biological properties of soils, as natural assets (expressed as mass, energy and organization), that create the basis for supporting processes. These properties (inherent or dynamic) can be measured and used to qualify and compare soils
Inherent Properties	Intrinsic components of soils, derived from soil formation conditions, that are use- and time-invariant at the human time scale
Dynamic Properties	Components of soils, susceptible to change due to land use, agricultural practices and climate change, that are thus use- and time-variant at the human scale
Soil Processes	The complex interactions (physical, chemical or biological) among soil components underlying soil ecosystem services. These interactions include processes of cycling (decomposition, mineralization), storage (retention, buffering) and transfer (filtering, release) of nutrients, contaminants or water, as well as biotic support, and can be calculated to quantify soil ecosystem services
Soil Ecosystem Services	Contributions to human well-being resulting from direct expression of soil processes. These contributions cover several service categories such as regulating and provisioning, related to expectations of human well-being (e.g., climate, water, food, energy, biodiversity and soil itself)
Current Soil Ecosystem Service	The service representing the currently expressed conditions of a service obtained under the current context of soil, climate, land use and cropping system. The value of this service can, depending on the case, be measured, derived from databases or expressed relative to a maximum theoretical value defined by the potential service
Potential Soil Ecosystem Service	The maximum service that can be obtained under the current soil and climate context among all potential land uses and cropping systems. The value of this service is used as a reference and, depending on the case, can be predicted by modeling or derived from the literature
Contributions to Human Well-being	All perceived economic, social and health expectations (positive and negative) underpinned by soil ecosystem services and the anthropogenic component. These contributions may result from a monetary approach (economic goals) or policy approach (environmental goals). They can be viewed as the starting point of soil ecosystem services assessment as they represent a goal to meet
Governance Scale	Social and policy scales at which knowledge about soil ecosystem services can be integrated to support decisions and build specific support for land planning strategies

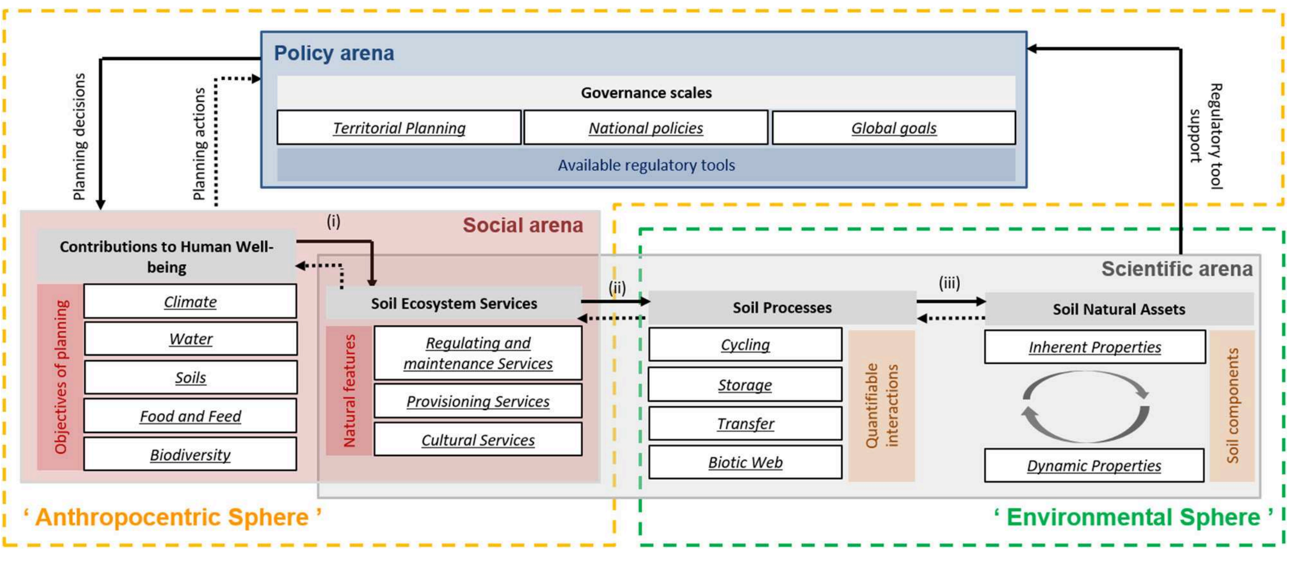

FIGURE 2 | Conceptual model connecting social, scientific and policy arenas, and anthropocentric and environmental spheres. Solid arrows indicate the effects of causal links and clarify the connections between the two terms "contributions" and "soil natural assets" (i, ii, iii); dotted arrows indicate the stepwise integration of soil ecosystem services in the decision-making process.

findings, we suggest a common lexicon for soil ES (**Table 1**) based on the ES literature.

Clearly distinguishing the terms "contributions" and "services" is necessary to (i) clarify relations between environmental and anthropocentric spheres and (ii) provide a common support bridging science, social and policy arenas (**Figure 2**), as emphasized by IPBES (2018) goals and Potschin-Young et al. (2018). First, unlike Potschin-Young et al. (2018), the term "contributions" is preferred to "benefits," as proposed in the latest discussions of IPBES (Díaz et al., 2018), thus avoiding the trend toward purely economic considerations. In this article, "contributions to human well-being" is defined as the perceived societal expectations (positive and negative) underpinned by soil ES and anthropogenic components when setting up territorial planning (**Table 1**). Second, in line with Costanza et al. (2017) and Therond et al. (2017), "soil ES" is considered as the share of soils in the "contributions to human well-being." Defined as contributions to human well-being resulting from direct expression of soil processes (**Table 1**), "soil ES" meets the need to match the social language with natural features that are usually studied in the research arena (scientific language) (**Table 1**). Among "soil ES," we distinguish "current" and "potential" soil ES. "Current soil ES" is defined as the current soil ES provision observed under current agricultural systems, while "potential soil ES" is defined as the potential soil ES provision that could be expected under alternative agricultural systems. Furthermore, according to territorial planning objectives (e.g., balance between urban development and protection of natural landscapes, maintaining human well-being) in a context of urbanization and limited land area, the objective of promoting high soil ES provision is crucial. Thus, to satisfy this need stated by stakeholders, "potential soil ES" is considered as the maximum soil ES that can be obtained in a given context.

As Díaz et al. (2018) discussed, the concepts of "services" and "contributions" can be seen from context-specific (i.e., local scale) to general (i.e., global scale) perspectives and aim to be incorporated into policy and practice. To this end, "governance scale" is defined as the policy scale at which "contributions" could be incorporated and considered in a regulatory way. "Governance" meets the need to match the planning objectives to be achieved (social language) with consistent policy tools at a given territorial scale (policy language).

The definition of soil ES retained (**Table 1**) and the use of the term "soil processes" is similar to Boyd and Banzhaf's (2007) perception of a service that contributes to human well-being and clarifies somewhat in a territorial planning context the concept of intermediate and final services discussed by Fisher et al. (2009) and Robinson et al. (2013). Thus, aligning largely with previous studies (Dominati et al., 2010; TEEB, 2012; Haines-Young and Potschin, 2013; Robinson et al., 2013), supporting services from the general ES assessment framework (MEA, 2005) are considered as "soil processes" rather than "soil ES." Consequently, "soil processes" are defined as interactions among soil natural assets underlying soil ES (**Table 1**). These interactions are classified into four processes (i.e., cycling, storage, transfer and biotic web) (**Figure 2**) and define the basis of our soil ES operational model, in which processes underlying soil ES are quantified by simulation models or pedotransfer functions. As soil ES can be supported by several soil processes (**Figure 2**), distinguishing the two terms avoids the problem of double counting (Fu et al., 2011) in subsequent economic valuations.

Finally, although the concept of soils as a natural capital initially defined by Costanza et al. (1997) is broadly embodied in the ES approaches that consider soils (Robinson et al., 2013; Dominati et al., 2014; Smith et al., 2017), the term "soil natural assets" (**Table 1**) is preferred to "soil natural capital." This asset also refers to intrinsic characteristics of soils derived from soil formation that are use- and time-invariant at the human scale and to characteristics of soils susceptible to change due to land use and climate change that are use- and time-variant at the human scale (**Table 1**, **Figure 2**). To define these soil characteristics, the terminology of Robinson and Lebron (2010) is retained, namely "inherent properties" and "dynamic properties," which Dominati et al. (2010, 2014) spread widely as a basis for defining "natural capital." Thus, "soil natural assets" are defined as both inherent and dynamic properties (**Table 1**), which refer to any soil properties used to define and compare soils.

A Conceptual Model to Bridge Science, Social, and Policy Arenas

The science-policy arena, through international initiatives (e.g., TEEB, IPBES, the Convention on Biological Diversity), recognizes the need to produce usable science-based knowledge to move toward sustainable governance of ecosystems (Díaz et al., 2015; Tengö et al., 2017). Despite the progress made on ES definitions and conceptualization, this knowledge still plays a limited role in decision making during planning (Carmen et al., 2018; Saarikoski et al., 2018). This suggests that simply increasing the amount of soil ES knowledge does not always improve understanding or integration of soil ES into decision-making processes. Thus, developing a conceptual model for using soil ES knowledge adapted to multi-stakeholder planning contexts is crucial to perform decision-relevant assessment and support sustainable regional governance at multiple scales.

The conceptual model proposed is divided into three components (or arenas). The policy arena (in the anthropocentric sphere), which refers to governance, includes considerations related to territorial, national or global policy and planning constraints. The social arena (in the anthropocentric sphere) refers to considerations related to human well-being and ES. Lastly, the scientific arena (in the environmental sphere) considers soil processes and soil natural assets. Using this structure as a basis, the model suggests a series of steps to integrate soil ES into the territorial planning process (**Figure 2**). This model can first be used as a basis for implementing soil ES in a regulatory context. The iterative step from "contributions" to "governance" allows evaluation of the potential to consider contributions by using currently available regulatory tools and thus determine the contributions that could be effectively implemented and the corresponding governance scale. The model can also be used as the basis of a soil ES assessment methodology. The steps from "contributions" to "soil natural assets" clarify the connections between the two terms by answering the following questions: (i) Which soil ES are related to the given "contributions"? (ii) Which model of soil processes can quantify the given soil ES? and (iii) Are the data required to model the steps from soil process to soil natural assets available? These connections constitute the steps to structure the soil ES assessment, thus putting theoretical concepts into operation.

This conceptual model is in accordance with the frameworks of Potschin and Haines-Young (2011, 2016) and Dominati et al. (2010, 2014), as they appear suitable for disentangling relations among soils, soil ES and human well-being. A stepwise "cascade model" is useful for supporting multi-stakeholder understanding of soil ES (Spangenberg et al., 2014) and using related knowledge, which builds an argument for using them in decision making in a structured way.

The conceptual model developed (**Figure 2**) shows interconnections between science, social and policy arenas, including causal effects among the main elements of our assessment framework (**Figure 2**). Although "soil ES" has progressively acquired status as a scientific concept (Barnaud and Antona, 2014), the language used is more a social language that places "soil ES" at the interface between the scientific and social arenas. The anthropocentric sphere includes both social and policy arenas, which are connected through "contributions." These "contributions" bridge a gap in implementation from the social to policy arenas, in line with other authors (Primmer et al., 2015; Bouwma et al., 2018; Dick et al., 2018; Saarikoski et al., 2018), through planning decisions. Also, through "soil ES," "contributions" bridge the gap in implementation from the social to scientific arenas, in line with reviews of Grêt-Regamey et al. (2017) and Dick et al. (2018). Thus, "contributions" connect, in a practical way, the soil ES concept to its potential degree of integration in planning strategies, defining which governance

TABLE 2 | Soil ecosystem services (soil ES) developed in the assessment framework, underpinning soil processes, indicators, governance scales, and parallels with common ecosystem services (ES) frameworks.

Challenge	Category of contributions (IPBES)	Class of ES (CICES 5.1)	Soil ecosystem service	Soil process	Indicators	Governance scales
Climate	Regulation of climate	Regulation of chemical composition of the atmosphere and oceans	Global warming attenuation	Storage (Soil capacity to sequester carbon)	Carbon pool sequestration capacity	Local planning, National policies, and Global goals
			Global warming attenuation	Storage (Soil capacity to maintain carbon pool)	Carbon pool lost	
	Regulation of hazards and extreme events	Regulation of temperature and humidity, including ventilation and transpiration	Peri-urban heat island attenuation	Transfer (Soil capacity to use latent heat energy)	Energy flow associated with soil evaporation	Local planning
Water	Regulation of freshwater quantity, location and timing	Ground (and subsurface) water for drinking and non-drinking purposes	Blue water provisioning	Transfer (Soil capacity to recharge groundwater)	Drained water yield	Local planning
	Regulation of hazards and extreme events	Hydrological cycle and water flow regulation (including flood control and coastal protection)	Base flow maintenance	Transfer (Soil capacity to regulate water flows)	Water storage content during dry periods	Local planning and National policies
			Flood risk regulation		Water storage content during wet periods	
	Regulation of freshwater and coastal water quality	Regulation of the chemical condition of freshwater by living processes	Water purification	Transfer (Soil capacity to filter water)	Nitrogen retention yield	Local planning and National policies
Soils	Formation, protection and decontamination of soils and sediments	Control of erosion rates	Erosion prevention	Storage (Soil capacity to maintain itself in the long term)	Number of days favorable for soil maintenance	Local planning, National policies and Global goals
Food and Energy	Regulation of detrimental organisms and biological processes	Pest control (including invasive species)	Biological control	Biotic web (Soil capacity to regulate pests)	Number of days unfavorable for biological development	Local planning
	Formation, protection and decontamination of soils and sediments	Decomposition and fixing processes and their effects on soil quality	Nutrient availability	Cycling (Soil capacity to supply nitrogen crop demand)	Soil content of available nitrogen	Local planning
	Regulation of freshwater quantity, location and timing	Ground (and subsurface) water used as a material (non-drinking purposes)	Green water availability	Storage (Soil capacity to supply water crop demand)	Crop transpiration	
Biodiversity	Habitat creation and maintenance	Maintaining nursery populations and habitats (including gene pool protection)	Genetic pool maintenance	Biotic web (Soil capacity to support biodiversity pool)	Number of days favorable for biological development	National policies and Global goals

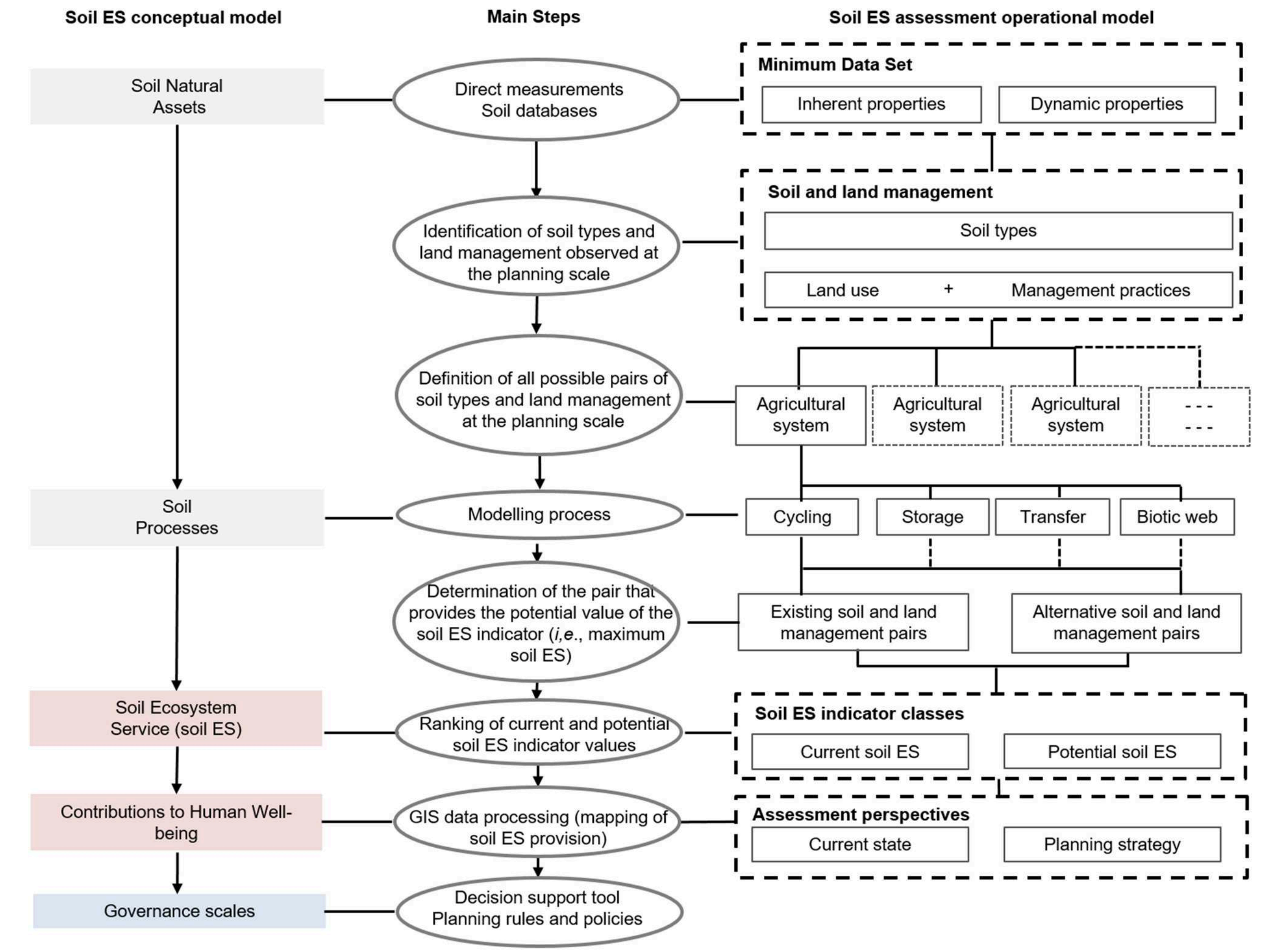

FIGURE 3 | Workflow of the operational model for assessing agricultural soil ecosystem services (ES).

scale corresponds to the planning objective and which policy tools integrate knowledge about soil ES. Finally, "driving forces," particularly through human-induced factors, connect the policy and scientific arenas through potential impacts on soil natural assets. "Driving forces" also connect the policy and social arenas as co-suppliers of "contributions" to soil ES (**Figure 1**). This connection bridges the two knowledge systems (i.e., science-based knowledge as a decision-support tool and policy-based knowledge as a tool to support policy instruments) described by Carmen et al. (2018).

PROPOSAL OF AN OPERATIONAL MODEL TO ASSESS AGRICULTURAL SOIL ES

Ecosystem Services Provided by Agricultural Soils

Soil ES that can be provided by agricultural soils were selected (**Table 2**) based on studies related to soil ES, including global reviews (Adhikari and Hartemink, 2016; Jónsson and Davíðsdóttir, 2016; Greiner et al., 2017), methodological frameworks (Robinson et al., 2013; Dominati et al., 2014; Lescourret et al., 2015; Birgé et al., 2016; Calzolari et al., 2016) and existing ES typologies (MEA, 2005; COM, 2006; Zhang et al., 2007; Ruhl, 2008; CICES, 2018; Díaz et al., 2018). Within agricultural systems, soils and their interactions with other ecosystem components (e.g., land use, management practices, climate, hydrology) can provide a set of ES, as conceptualized by Dominati et al. (2010, 2014).

Twelve soil ES (**Table 2**) were identified in seven IPBES (2018) ES categories (excluding cultural ES), corresponding to nine CICES (2018) ES classes. These soil ES support certain major challenges addressed in territorial planning and their scale of governance (i.e., local, national or global) (**Table 2**). This list relates soil ES to underlying soil processes and suggests indicators derived from model outputs used to quantify soil ES.

Agricultural Soil ES Assessment

We start from a conceptual model of soil ES (**Figure 2**) that focusses on agricultural systems and intends to estimate soil ES. The associated operational model to assess soil ES (**Figure 3**)

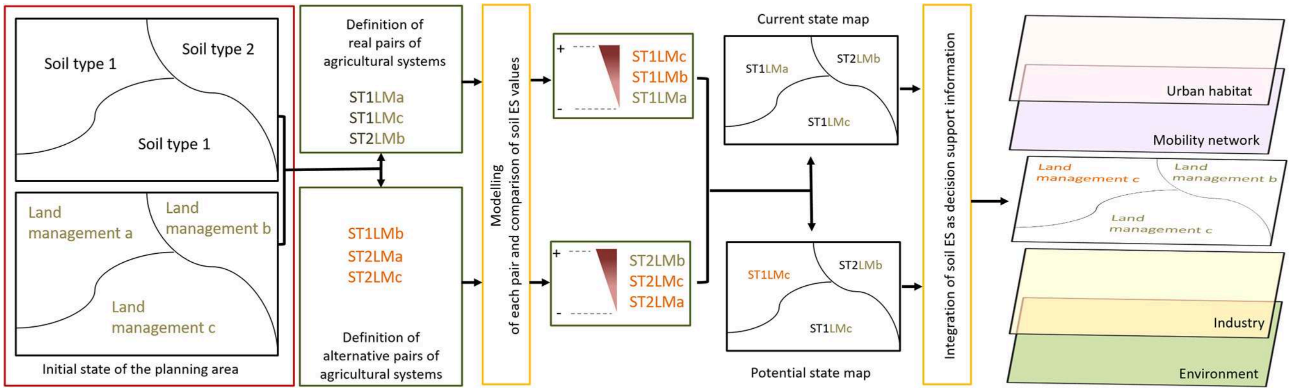

FIGURE 4 | An example of application of the operational model to consider soil ecosystem services (ES) as decision support information in territorial planning.

focusses on agricultural system management, particularly on the relation between soils and land management. This allows one, using dedicated models, to (i) estimate impacts of land management on soil processes and thus on soil ES and (ii) predict the evolution of multiple soil ES. Results from this modeling framework will indicate which agricultural system provides both the largest contribution to human well-being, given the objectives of territorial planning, and the lowest environmental impacts. Applying this operational model requires three successive steps and is illustrated by an example in which two soil types and three land management types are considered.

Define Agricultural Systems as a Combination of Soil and Land Management

As shown previously, the agricultural system is split into two components: (i) soils, with their physical, chemical and biological properties, and (ii) land management, which includes land use (i.e., cropping or grassland) and management practices (e.g., crop rotation, fertilization, grazing density, and timing) (**Figure 1**) observed at the spatial extent of the planning area. Soil natural assets (**Table 1**) have inherent properties, which may vary spatially, and dynamic properties, which vary greatly both spatially and temporally, due to disturbance or changes caused by agricultural land management, which modify soil processes and subsequently the soil ES they provide (Groffman et al., 2009; Burkhard et al., 2012; McFero Grace and Skaggs, 2013; Durán et al., 2017).

For the operational model, agricultural systems are described by all possible pairs of soil types (i.e., observed in the field or clustered into groups) and land management types (i.e., commonly observed in the field) in the planning area. Soil types and their associated properties (i.e., inherent and current dynamic properties, which are initial input data of the models considered) in the planning area are extracted from a soil database. Land management types may be (i) existing types, identified by analysis of agricultural censuses or specific surveys, or (ii) alternative types, selected or designed in the territorial planning procedure. Combinations of soil type and land use and management type define either existing or alternative agricultural systems (**Figure 4**).

Modeling and Comparison of Current and Potential Soil ES

To estimate the "current state" of soil ES provision, only currently existing agricultural systems are considered, and soil ES prediction models are selected to quantify them (**Figure 4**). The "potential state" of soil ES provision is estimated by the maximum of ES modeling predictions for all existing or alternative agricultural systems (**Figure 4**). This assessment enables evaluation of possible gains and/or losses in overall soil ES provision under several planning scenarios.

Models that simulate carbon, nitrogen, water and energy flows at the field scale (not described in this article) are used to predict soil ES values. Using agricultural system characteristics as inputs, model predictions are processed to calculate one indicator value per soil ES for each agricultural system. Two key classes of indicators can then be defined: "current soil ES" (soil ES indicator value provided by a real pair of soil type and land management type) and "potential soil ES" (maximum soil ES indicator value provided by a real pair or by an alternative pair corresponding to the same soil type combined with another land management type observed at the planning scale).

Subsequent analysis of these modeling results allows one to (i) determine potential soil ES, (ii) compare current and potential soil ES indicator values, (iii) evaluate the multiservice provision ability of each agricultural system defined and (iv) display these results in a map (GIS data processing).

Mapping Soil ES and Integrating Them Into Territorial Planning

Mapping ES can be a useful and powerful tool for raising awareness and support decision making (Grêt-Regamey et al., 2017; Maes et al., 2018). For territorial planning purposes, stakeholders may require both qualitative and quantitative knowledge: simple qualitative information may capture strengths and weaknesses of a given area better, while more quantitative information is needed to evaluate expected results from alternative agricultural systems.

The last step of the operational model is therefore to develop a sequential mapping approach that describes at the territory scale both current and potential soil ES states (**Figure 4**). First, a map showing the current soil ES value can be drawn using semi-quantitative classes to identify areas with low and high provision of soil ES. Second, a map showing the difference between the current soil ES value and the potential soil ES state may identify areas with high expectations of increased soil ES if actions are implemented. Finally, a map showing the potential soil ES enables the potential provision of soil ES and the existing soil ES demand to be compared within the territory.

Finally, full implementation of the operational model would enable two potential assessment perspectives:

- Assessment of the current state of provision of a given soil ES. Here, soil ES assessment aims to answer the following questions: What are the values of soil ES at various planning scales? How are these values spatially distributed (areas of low or high provision)? and How does this spatial distribution correspond to social needs?
- Assessment of different territorial planning scenarios in which gains or losses of soil ES are compared. Here, soil ES assessment aims to answer the following questions: Under different conditions (i.e., land-use change scenarios), what gains or losses of soil ES provision can be expected? and Which soils are best suited to provide a given soil ES and under which land management conditions?

TOWARD AN OPERATIONAL TOOL

In a planning context, the soil-centered assessment framework and the associated conceptual (**Figure 2**) and operational models (**Figure 3**) raise four key methodological issues:

- *Data availability*. Values of soil natural assets underpinning current and potential soil ES can be obtained in three ways: (i) direct measurements (if no data exist), (ii) soil databases (as minimum data set providers) and (iii) modeling (i.e., predicted from soil properties).
- *Data homogeneity*. As soil ES assessment is highly time dependent, it must consider both land management and climatic conditions. To do so, soil ES values must be integrated over cropping periods to consider interactions between land use and soils properly. If soil ES are modeled, simulation periods must capture climatic variability; so, simulations of several years or decades are recommended, depending on the agronomic and pedoclimatic contexts.
- *Data operability*. Fully integrating soil ES assessment in planning processes requires tools that are accessible and compatible. Mapping soil ES at the territory scale appears to be an appropriate tool that territorial planners and stakeholders can easily understand to help compare scenarios and identify land management that enhances soil ES.
- *Data transferability*. The range of potential soil ES values defines the validity domain (i.e., ranges of spatial scale and soil types) of the assessment. Depending mainly on the resolution of available data, transferability of one assessment to another also depends on boundary values of potential soil ES.

PERSPECTIVES AND CONCLUSION

There is growing demand to assess ES from agricultural systems for the purpose of territorial planning (Birgé et al., 2016; Ruhl, 2016). Planning strategies can involve spatial distribution of different land uses (e.g., definition of urban, agricultural or natural protection areas) and, for agricultural areas, be based on a variety of land management options, such as "land sparing" (separate areas of high-intensity agriculture and wilderness) or "land sharing" [low-intensity agriculture interspersed with natural features (e.g., hedgerows, ponds, wetlands)] (Legras et al., 2018). Consequently, the assessment framework proposed provides a basis for integrating the soil ES concept into the land management decision making process, mainly for the following points.

By combining biophysical approaches and connecting environmental and anthropocentric terms, the assessment framework tends to provide the holism required by Primmer et al. (2015), Schleyer et al. (2015), and Loft et al. (2015) in the ES approach, integrating multiple modes (i.e., hierarchical, scientific-technical and adaptive collaborative) and scales (i.e., vertical and horizontal knowledge production, sharing and policy integration) for governance of ES.

Because it is soil-based, the framework contributes to emerging knowledge about how ES provided by agricultural systems depend upon soil characteristics by assessing the testable hypothesis that optimal soil/land use combinations that maximize soil ES do exist. Scientific understanding of assessment framework components (**Table 1**, **Figure 2**) and how they emphasize soil ES may encourage decision makers to follow the soil ES approach in land planning (Swinton et al., 2007). In addition, its combined biophysical approach provides a decision-support tool that allows estimation of potential provision of soil ES due to land planning strategies and differentiation of land management options and the soil ES they may provide (i.e., trade-offs and synergies) (Loft et al., 2015; Ruhl, 2016; Bommarco et al., 2018; Kim and Arnhold, 2018).

As a process-based assessment, the workflow of the operational model (**Figure 3**), can help define a monitoring dataset that decision makers can use to assess the effectiveness of land management strategies on soil ES provision and thus the success or failure of policy instruments (Loft et al., 2015; Rabot et al., 2017). Feedback from this monitoring could help inform policy design and encourage decision makers to implement a particular land management option (Primmer et al., 2015; Baveye, 2017; Legras et al., 2018).

Finally, these insights address the new paradigm of a shift from conserving nature to using it sustainably (Loft et al., 2015; Legras et al., 2018). This change in perception involves considering both societal needs (i.e., demand for soil ES) and conservation of natural assets (i.e., supply of soil ES). Because it does so by producing knowledge, this soil ES assessment framework supports the nature-based solutions approach, which aims to conciliate socio-economic development goals with beneficial outcomes for both society and the environment (European Commission (EC), 2015; Faivre et al., 2017; Lafortezza et al., 2017). As an agricultural soil-based assessment, the framework includes a soil security dimension (McBratney et al., 2014) by considering the resilience and sustainable use of soils (i.e., conserving soil natural assets) and provides a tool that addresses soil ES trade-offs (Kim and Arnhold, 2018) through the ability to arbitrate land management strategies effectively (e.g., supply vs. demand, land sharing vs. land sparing).

Agroecosystems provide services that must respond to both human needs and environmental constraints. Because they lie at a critical interface in the biosphere, soils contribute greatly to provision of these services. To address the increasing demand for consideration of these services in territorial planning, the evaluation framework proposed takes into account scientific, social and policy considerations. This assessment framework is based on both a conceptual model and an operational model. In this framework, soils are considered as providers of ES, and are therefore better positioned in the chain of decision. On this basis, the operational framework proposed allows identification of land use and management practices that optimize soil ES. Further development and applications have already begun to (i) define soil-indicator thresholds using both empirical data and modeling and (ii) improve the soil ES model's operability (i.e., in its tool forms, as maps and matrices) to improve usability and acceptance through interdisciplinary work among soil scientists, urban planners, decision makers and economists.

DATA AVAILABILITY STATEMENT

All datasets generated for this study are included in the article/supplementary material.

AUTHOR CONTRIBUTIONS

MF: substantial contributions to the conception of the work and drafting the work. Agree to be accountable for all aspects of the work. DA, CC, CG-O, and CW: substantial contributions to the conception of the work and revising it critically for important intellectual content. CBu, CBe, PD, AJ, and GP: provide approval for publication of the content.

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