Authors response to referee and editor comments on the manuscript: Soil organic matter and labile fractions depend on specific local parameter combinations

Authors response to Reviewer 1 (RC 1) for soil-2021-81

Reviewer comments:
In their manuscript, 'Soil organic matter and labile fractions depend on specific local parameter combinations', Ortner et al. present their work on the analysis of factors controlling the soil organic carbon (SOC) concentration in topsoils of the region around Trier, Germany. The authors collected topsoil samples in arable land and grassland in 4 regions with different parent material, and determined the organic carbon (OC) concentration, hot water extractable carbon (HWEC), microbial biomass carbon (MBC) and multiple soil properties on these samples. They used PCA to cluster the soil samples based on parent material and soil texture into different clusters. The aim of their study was to assess the main factors controlling topsoil organic carbon concentration, HWEC and MBC using two modelling approaches: a bivariate model and mixed effects models. The main findings are that (i) mixed effect models outperformed bivariate (linear) models in predicting OC%, HWEC and MBC, (ii) at the local scale, site-specific parameters explained OC variability better than landscape-related variables and (iii) using the 'local' model resulted in better results when predicting the OC% of a specific cluster compared to the 'global' model.

The results of the present study help to improve our understanding of the factors controlling topsoil organic carbon concentrations at the landscape scale, which is needed e.g. in order to improve soil organic carbon models. The authors have constructed a valuable dataset which may benefit other researchers. I would therefore encourage the authors to make this data available through an online repository, instead of making it only available upon request.

We thank for this comment. The dataset was generated in the framework of a contract project of the UBA. We aim to clarify with UBA if the data can be fully published.

Overall, the manuscript is well-written. However, at multiple locations very long sentences are used, which does not benefit a smooth reading. Splitting those sentences and using more commas would improve the readability of the manuscript considerably. In addition, I would encourage the authors to use subsections in the Results and Discussion sections, which will provide a better overview to the reader of what is being presented and discussed.

Following the advice, we revised and split several of the longer sentences. Further, we took up the valuable hints regarding subsections for the results and discussion sections.

One of my main concerns about the present manuscript is related to the quantification of the goodness-of-fit of the different models, which is now done using R-square. This is a measure to quantify the proportion of variation in a dependent variable that is explained by an independent variable, but is not a measure for the goodness-of-fit of a model. For example, a very poor model can have a high R-square value, while a good model can have a relatively low R-square value. Therefore, the authors should use a different measure to quantify the goodness-of-fit of their model when comparing measured with modelled data, such as the (root) mean square error or similar.
We agree that R2 is good to show the percentage of explained variance but not fully sufficient to document the goodness-of-fit of a multivariate and/or non-linear model. Hence, the RMSE was added as a measure for the goodness-of-fit. The presentation of R2 was reduced to the bivariate linear models.

In addition, I missed a discussion about the broader implications of the results and the implications for future research. For example, do the authors suggest that researchers should use 'local' model whenever possible? And how about regions where local information is not present? It would also be very informative if the authors would quantify the difference in predicted SOC% when using a global versus local model. To how much of an over or underestimation would this lead? Is that difference significant enough to invest more resources in the collection of local data?
Statements about broader implications and some recommendations for further research were added to the conclusions.
The level of over- or underestimation is represented by the RMSE. We added the RMSE

Another concern is related to the title, which I find not very informative. For example, it will not be clear to someone who has not read the manuscript what 'specific local parameter combinations' are. Also, it would be good to be more specific about what they mean with ‘soil organic matter and labile fractions’. From the title it is not clear if the authors mean SOC concentrations, stock, spatial distribution etc. In addition, the manuscript discusses soil organic carbon, and not all soil organic matter, so would be good to change this in the title.

We changed the title in order to make it clearer: “Content of soil organic carbon and labile fractions depend on local combinations of mineral phase parameter”

Lastly, it would good if the authors specify in the beginning of the manuscript that they discuss SOC concentrations, and not stocks. Throughout the manuscript, the authors talk about ‘SOC’ without specifying that it concerns concentrations, not stocks. This is an important difference, which should be clear to the reader from the abstract onwards, and repeated throughout the manuscript. For example, the authors could change ‘SOC’ to ‘SOC%’ to make this clear.

In the text (e.g. Abstract) and title it is now explicitly mentioned that concentrations were investigated.

Answers to specific comments RC1

L18: Would be good to explain here what you mean with ‘global’ and ‘local’ clusters (and models).

Thank you for this hint, we added the definition for the investigated clusters. Further we decided to replace the term ‘global’ by ‘total’ to prevent any confusion regarding different scales (local vs. global scale). It should be now clearer that we talk about the total dataset encompassing the different local datasets.

L19: define that you assess SOC concentrations, and thus not stocks

See general comments. We added this information to the title, Abstract as well as in the Introduction and in Material and Methods. In Tables and Figures SOC is given in % as unit, indicating that we assessed concentrations.

L20: would be good to explain here which ‘labile fractions’ you study

Information regarding the labile fractions was added as requested. “… explaining SOC and its labile fractions hot water-extractable C (HWEC) and microbial biomass C (MBC)”.

L27: here you use the term ‘organic matter’, while until here you used ‘SOC’. Please be consistent with these terms, and only use one

It was changed to ‘organic carbon’.

L29-30: ‘showing that labile fractions depend less on soil properties than on organic matter input and turnover in soil’. The latter were not studied, so you cannot say this with certainty. Would be better to end the abstract with a statement about the broader implications of your results.

We thank for that comment. To avoid the impression that organic matter input and turnover were investigated in this study, we changed the sentence: “showing that labile fractions depend less on soil properties but presumably more on processes such as organic carbon input and turnover in soil.”

L41: another important labile fraction of SOC is particulate organic carbon. Would be good to justify why you did not study this fraction

The authors fully agree that particulate organic carbon (POC) is an important labile fraction. Due to trivial financial reasons we had to decide which fraction(s) we can study. We decided for hot water extractable carbon (HWEC) and microbial biomass carbon (MBC) because they are methodically clearly defined. Quite often it is stated in the literature that both are very closely correlated with each other, and thus deliver no different information. We hypothesized and aimed to show that this is not the case (which was confirmed in this study). Additionally, we decided against POC because it is not uniformly defined, either by size or by density. So we hope that HWEC and MBC are representative measures of labile SOC pools. Again, we fully agree that having additional data on POC would have been a perfect completion of the dataset.

L45: ‘MBC is expedient to explain SOC dynamics’: this is rather vague, please be more specific

To make the point more clear, we added the following sentence: “Additionally, labile carbon fractions such as MBC quantitatively dominate in short-term turnover processes, while changes in SOC will only become significant over periods of decades. Therefore, MBC is expedient to explain SOC dynamics”.

L45-46: ‘much less research and attempts for quantitative modelling of these labile fractions […]’: recently, multiple mechanistic models have been used to simulate labile carbon fraction such as MBC and POC, e.g. Ahrens et al. (2015), Wieder et al. (2015) and Zhang et al. (2021)

Thanks for this valuable comment. We changed the sentence and included some recent publications on modelling. We left the statement that SOC is mostly considered for such simulations, while there is still a need to take labile fractions more into account in order to gain a better understanding of SOC dynamics.

L58: ‘In addition or even instead of’: choose one

Ok, done.

L63: please clarify what you mean with parameters versus factors, as you use these terms throughout the manuscript

We added some examples. In general parameters include soil properties on a interval or ratio level of measurement while factors were applied on a nominal level of measurement.

L87: please define what you mean with 'global models'

To avoid confusion, we replaced both terms 'global dataset' and 'global model' with 'total dataset' and 'total model'. The total model is based on all data of the total dataset that encompasses all local datasets.

L99: the term 'sufficient quantification' is rather vague, please clarify this

The sentence was changed as follows: "It was aimed to determine the suitability of local models in comparison to total models to achieve an improved quantification of SOC, HWEC and MBC for local landscapes with distinct properties.".

L107: 'similar numbers of samples': how many per region?

Number of samples taken per region were shown in Table 1. Additionally, they were now added to the sentence in brackets for each sampling region.

L108-109: the use of the abbreviations throughout the manuscript is not intuitive and confusing for the reader, please use different names to identify the different regions, e.g. the parent material

We agree that abbreviations are a compromise between clarity and readability. Using the full terms or terms such as 'Muschelkalk' and 'Luxemburg sandstone' would have been too long, though. Shorter abbreviations were also inconclusive, e.g. schist and sandstone are both abbreviated 'S'. Hence, we plead for keeping the chosen abbreviations.

L119: why were some samples stored at -20 °C and others air-dried?

Samples were stored until they were analyzed. Storage was done in a uniform way for all samples. One part of each sample was air dried for subsequent chemical and physical soil analysis, another part was kept moist and was frozen for subsequent soil microbial analyses (MBC, MBN or respiration). This is now clarified in the text.

L134: was the chloroform fumigation extraction performed on samples freshly collected from the field?

Chloroform fumigation extraction was done on sieved material that was stored at -20°C before analysis. This was done to avoid changes until measurement was conducted. The suitability of this storage was proven in preliminary projects (data not shown).

L137-140: for how long were the samples incubated? How often was the CO2 measured?

Samples were preincubated at room temperature for one week (7 days), measurement was conducted for 24 hours at an interval of one hour. The information was added to the text.

L143: were all parameters log-transformed? Please clarify this

To conduct the principal component analysis all variables were log transformed to receive standardized and comparable variables. The information is contained in the text.

L146: please provide some examples of the 'mineral phase parameters'

We added two examples (Fe_o and fSilt+clay) into this sentence.

L146-147: please provide more information about the linear regressions that were performed

We added the information that we applied linear regressions using single predictors, and information that we checked the residuals for normality.

L156-157: Please provide information about which parameters were removed from the models

The non-significant parameter with the highest p-value was removed from the model. This was repeated until all remaining parameters were significantly contributing to SOC, HWEC or MBC. This information was added to the sentence.

L161: were all parameters checked for collinearity? Please clarify

We checked all mineral phase parameters for collinearity, which were used by the mixed effect models. Based on this, it was found that soil texture components (Sand, c+mSilt and fSilt+clay) showed collinearity as well as ECEC and $Ca+Mg_{ECEC}$.
We clarified this in the text.

L163: why a square root transformation? Please justify this
Square root transformation was selected as a common transformation and was suited to achieve normal distribution and heteroscedasticity of the residuals.

L163: Please clarify how the performance of the models was examined
Basically, we started by comparing the explained variance and, based on your valuable comments, now also added RMSE as indicator for performance.

L170: Please clarify the difference between 'soil' and 'topsoil' properties
Topsoil was separately mentioned due to the fact that our study focusses on agricultural topsoils. To avoid confusion or misunderstanding we decided to use only the term 'Soil properties'.

L177: are those differences statistically significant? What are the averages for the different parent materials?
There are some statistically significant differences, averages for the parent materials are given in Table 1 as mean ± sd.

L186: please provide examples for the 'parameters describing the composition of SOM'
We now mention some examples in the text, such as SOC, Nitrogen, hydrogen or oxygen, HWEC or MBC.

L191-194: this is not clear
We rephrased these sentences to make it clearer. Clusters identified by the PCA cover a different number of samples of the total dataset. Based on this clusters including the vast majority of samples were considered to represent the total dataset, while substantially distinct clusters, including only a part of all samples, were considered to represent local datasets.

L205-206: which 10 parameters?
Selected parameters were shown in Table 1 and in Table 3. Further we mention examples of these parameters in the Material and methods section. Examples of these parameters were added to the text in brackets.

L213: 'that largely matched with those found for the complete dataset': this is not clear
We adapted this sentence to make it clearer.

L224: what do you mean with 'sufficient extent'? Similar wording is used throughout the manuscript, but this is very subjective and should be clarified.
Thanks for this hint, we checked the manuscript and exchanged such phrasings by objective formulations using statistical parameters is applicable. See also L369

L240: please clarify what 'equal weight of samples' means
It means that both clusters (arable and grassland) contain a similar number of samples from each parent material resulting in a broad range for each soil property, catching up the properties from soils of each sampling region. We rephrased the sentence to clarify its meaning.

L237-242: please make clear that you are discussing the results of the bivariate models
We now mention that these lines address the bivariate regressions.

L241: what are the 'complex interactions of several different parameters'?
The term 'complex' was deleted. It makes sense concerning the environmental interaction of these parameters but not concerning the contribution to a mathematical model.

L243: please clarify what you mean with 'insufficient'. Which measure do you use to determine if a model performance is sufficient or not?
The authors thank for this hint, we changed such phrasings to objective formulations.

L249-251: R-square values are no measure for model performance, please provide the root mean square error (or a similar measure). Please show these results in a graph, perhaps in the supplement?
R-square is used to show the explained variance, this manuscript aims to show how much mineral phase parameters and their different combinations are able to explain the variance of SOC, HWEC and MBC. Notwithstanding, we fully agree that the root mean square error is a much better measure to determine the model performance. Therefore we added it to the text.

L273: do you mean the bivariate models with 'linear regressions' Please be consistent with this terminology
Yes, it means the bivariate models, we made it clearer.

L284: please replace R-square with a measure of model performance
See the above response. Further, as a measure for mixed effect models we added marginal and conditional R^2 to describe the R^2 directly related to these models.
R^2 based on predictions is only able to give a pseudo R^2 which is based on a linear regression between predicted vs measured. Such comparison between predicted vs measured and the received pseudo R^2 was technically the only option to test the performance of a total model, when applied on a local dataset. This information was added to the text.

L287: please provide the goodness-of-fit values before concluding that a certain model has an 'inferior performance'
We added this information, but we also kept the R^2 because it was aimed to investigate which model explained the variance to the highest extent.

L309-310: by saying 'Al- and Fe-oxides were shown to have a relevant influence on sequestration and stabilization of SOC', it seems like you explicitly studied this, while you only used a statistical model to assess this. Also, since you model SOC concentrations and not stocks, you cannot say anything about C sequestration, as this also depends on bulk density.
This sentence was linked to a reference and started with the term 'accordingly' in order to emphasize that this mechanistic interpretation of our statistical finding is not based on our study. We deleted the term 'sequestration' as requested since we do not address SOC stocks.

L342: please explain what you mean by 'multidimensional'
Multidimensional means that SOC is simultaneously affected by serval soil properties and factors which explain the overall accumulation and variability instead of single one to one interactions.

L348: 'to explain SOC': please clarify which aspect of SOC
The factors mentioned in the sentence were able to explain SOC under different scales and environmental conditions but in general, these factors enable to explain the accumulation and the variability of SOC.

L366: how do you conclude that sample size biased the results? Did you test for this?
It is true, randomly selecting a data subset from a total dataset does not necessarily lead to different (biased) modelling results. However, in this study total clusters including a larger number of samples showed a higher explained variance, which is a consequence of a broader variety of soil properties in the dataset. Local clusters with a smaller sample size also showed smaller ranges of the tested soil properties, leading to models with a lower explained variance.

L369: 'satisfying extent': how is it quantified that a model performs satisfying? Please be objective in deciding if a model is good or not
Thanks for this hint, we checked the manuscript and exchanged such phrasings by objective wordings.

L370: what do you mean with 'partially practicable'?
We replaced the term with 'less suitable', which is based on the lower statistical performance.

L374-375: 'sufficient quality level': same remark as L369
Similar to comment to L369, we changed the wording.

L380-381: by saying 'It became clear that […] with different annual dynamics', it seems like you tested annual dynamics. Please rephrase
We rephrased this sentence accordingly.

L281-382: You did not take SOC turnover into account, so how can you say that this is a reason for the lower explained variability by the different models?
An aim of this study was to investigate the linkage between mineral phase properties and labile fractions. Compared to SOC we found a lower explained variance for the labile fractions. Hence, we assume that – although we didn't explicitly investigate it - the known faster turnover of these fractions (depending, e.g. on land use management) will significantly contribute to the concentration of HWEC and SOC, thus explaining the gap in explained variance of HWEC and MBC.

L403-404: 'sufficient estimation': same remark as L369
Similar to comment to L369, we exchanged this formulation.

L405: would be good to end the Conclusions section with a statement about the broaderimplications of your results
We added the following statement: "Our research shows that local models, respecting site-specific parameter combinations, are superior to total models, although they are based on much smaller datasets. If available, they should be preferred."

Figures and tables

Fig. 2: the colours in B are difficult to distinguish
It was changed accordingly.

Table 3: please make clear in the caption that these are the result for the bivariate Regressions
It was changed accordingly.
Fig. 3: 'Predicted vs. measured': please clarify in the caption which model was used to make these predictions. Please provide a measure for the goodness of fit and remove the R-square values, as this is not measure for model performance
We now mention it in the caption and added RMSE as measure for model performance.

Table 5: please provide more information about the table in the caption, the table should be clear to the reader without having read the entire manuscript. It would be more informative to provide a table with e.g. root mean square errors instead of R-square
We added some information regarding the RMSE, but we also want to show how the models differ in their explained variance. So we kept R^2.

Figure 6: it would be informative to show the same graphs for other clusters in the supplement. Please remove the R-square values and replace them by a measure for the goodness-of-fit of the models
Fig. 6 shows the performance of the previously developed total model, when applied to a local dataset. The model was not fitted to the data of the local dataset (which would have yielded the local model). Consequently, pseudo R^2 is given as a measure to compare the agreement (or disagreement) of modelled vs. measured data. Additional, we also added the RMSE to this Figure.

Technical comments

L36: driver => drivers
Done

L57: expedient => suitable
Changed

L73: space between 'asCa2+'
Changed

L119: it's not clear what 'respectively' refers to
Removed due to changes in this sentence.

L170: it's not clear what 'respectively' refers to
Ok, rephrased

L172: it's not clear what 'thereby' and 'essentially' refer to

Ok, rephrased

L252: it's not clear what 'respectively' refers to
Ok, rephrased

L275: what do you mean with 'not last'?
We want to highlight that soil acidity and its describing parameter were also relevant. The typo, however, was corrected to 'not least'.
L304: 'the in total very sandy soils': please rephrase
Ok, rephrased
L320: what is 'circumneutral'?
Circumneutral means soil pH that is close to neutral or neutral having a pH between 6.5 and 7.5. It is an established term. See for example:
Carl O. Moses, Janet S. Herman, 1991, Pyrite oxidation at circumneutral pH, Geochimica et Cosmochimica Acta 55/2, 471-482.

L324: please remove 'respectively'
Done.

L343: please remove 'respectively'
Done.
L344: confirmed => is in line with
Done.

References

These references were chosen based on their scientific content. I leave it up to the authors to decide if they wish to include them in their manuscript.
Thanks for this valuable references, we added some of them to our manuscript.

Ahrens, B., Braakhekke, M.C., Guggenberger, G., Schrumpf, M., Reichstein, M., 2015.Contribution of sorption, DOC transport and microbial interactions to the 14C age of a soil organic carbon profile: Insights from a calibrated process model. Soil Biology and Biochemistry 88, 390–402. https://doi.org/10.1016/j.soilbio.2015.06.008

Wieder, W.R., Grandy, A.S., Kallenbach, C.M., Taylor, P.G., Bonan, G.B., 2015. Representing life in the Earth system with soil microbial functional traits in the MIMICS model. Geoscientific Model Development 8, 1789–1808. https://doi.org/10.5194/gmd-8-1789-2015

Zhang, Y., Lavallee, J.M., Robertson, A.D., Even, R., Ogle, S.M., Paustian, K., Cotrufo, M.F., 2021. Simulating measurable ecosystem carbon and nitrogen dynamics with the mechanistically defined MEMS 2.0 model. Biogeosciences 18, 3147–3171. https://doi.org/10.5194/bg-18-3147-2021

Authors response to Reviewer #2 (RC 2) for soil-2021-81

This manuscript presents the distribution of SOC and its labile fractions predicted using parent material, land use and soil properties in Southwest Germany. The results indicated that soil properties were clustered by parent materials and soil texture rather than land use. In general, mixed-effect model gave better predictions than bivariate regression. They compared "global model" with "local model" to show that the application of global model on local dataset introduced poorer predictions. Also, the explained variance generally decreased from bulk SOC to its labile fractions.

In general, the objectives were clear and relevant while the scientific value is sufficient. The large sample size contributes to a robust prediction. However, there are several concerns to be addressed.

One concern is the distribution of the sampling points. As mentioned in L47-48, soil formation is also controlled by climate and topography. The clustered locations of the four parent materials are likely to introduce differences in topographical and climate conditions. As climate and topography factors were not included in the models, their effects might be recognized as the effects of parent materials, texture or land use in the predictive models. (Details in comments for Fig. 1)

See answer to comment on Fig. 1

Another concern is that the usage of "global/local scale", "global/local model", "global/local cluster" and "global/local/entire dataset" may confuse readers because they were used without necessary explanations. In addition, the words "global" vs. "local" give the impression that the study aimed to compare SOC distribution on global vs. local scale, but no investigation on global scale was given in this study.

Thanks for your comments. We fully agree that the term 'global' may be confusing. Therefore, we decided to replace 'global' by 'total' to avoid this misunderstanding.

In addition, in some parts of the manuscript, R^2 was used to estimate whether models are well-fitted, which is not proper. Also, the Results and Discussion can be improved by splitting them into sub-sections and better re-organizing. Finally, the readability of the manuscript can be improved by revising long-complexed sentences and vague expressions.
As similar mentioned to Reviewer #1, R-square is used to show the explained variance, this manuscript aims to show how much mineral phase parameters and their different combinations are able to explain the variance of SOC, HWEC and MBC. Notwithstanding, we fully agree that the root mean square error is a much better measure to determine the model performance. Therefore we added it to the text.
Title: (1) Although "soil organic matter" is used in the title, the main part of this manuscript is mostly talking about "soil organic carbon". Please be consistent in using them because soil organic matter contains not only organic carbon but also other elements such as nitrogen.
We agree that a consequent use of the terminology is required. Therefore we changed the title to "soil organic carbon"

(2) It is advised to add restrictions on the area/location because the study was performed in western Germany and will not be necessarily applicable in other places.
We agree that local areas were sampled that were all located in the larger region of Trier in southwestern Germany. Anyhow, it was not our primary intention to characterize a specific region. Instead, the sampling region was selected because it covers soils with identical land use types (arable and grassland) and similar climatic/pedoclimatic conditions but substantially different parent material, and thus different soil mineral phase properties. Our prior aim was to show that SOC of local clusters is better assessed using local models. It is clear that at larger scales (nation-wide and larger) differences in pedoclimate add to the factors explaining SOC (and labile fractions). However, the climatic impact is generally not relevant for local areas independent of where they are. At the same time what the reviewer states is exactly would we found and suggest: A specific assessment of local areas with a local model is preferred. Such a local model is not transferable on to one to another local area.

L14, L18 and L21: It is confusing to mention "local scale", "global/local cluster" and "global/local dataset" in abstract without further explanation. The usage of "local" vs."global" gives me a feeling that this study compares SOC distribution on local vs. global scales. Apparently, the distribution of the sampling sites represents a local or sub-regional scale. It is suggested to either give them definitions when they are mentioned for the first time or replace them with more suitable words.
Thanks for your comment, we now define what is meant by local and total (previously global) cluster/dataset and we replaced the scale-related terminology.

L21: As only regressions were performed in this study, it is recommended not to use both correlation and regression in the text.
We revised the text accordingly.

L21-23: It is difficult to understand this sentence. It is not clear between which factors the correlations are significant. What does "partially low" mean? Splitting this sentence into simple ones may help.
For a better understanding of the sentence, we followed the advice to split it. 'Partially low' means that some of the correlation coefficients (R^2) only showed a small explained variance. Such vague terminology was replaced by more objective wordings.

L66: In general, organo-mineral associations are considered contributing to the formation of stabilized fractions (not labile fractions) and therefore the accumulation of SOC.
We agree that the formation of organo-mineral associations leads to the stabilization of SOC. Additionally, such accumulation of SOC goes along with increasing contents (not stabilization) of labile fractions such as DOC that are only weakly retained through other mechanisms in the presence of pedogenic oxides. This is what we wanted to say. We changed the sentence as follows to make it more clearer: "Organo-mineral associations are highly relevant for stabilization and accumulation of SOC and also for the accumulation of its labile fractions (Lützow et al., 2006)."

L72: …leading to SOC sequestration…
We adapted this line.

L85: Please check if surnames and given names are misplaced in this reference.
Checked, there is no misplacement of surname and given names. Surname is Jian-Bing, given name is Wei. See https://link.springer.com/article/10.1007/s10661-005-9158-5#article-info

L90: "Local vs. global models" are confusing. Do they mean models on local vs. global scales?
We wanted to indicate that it is necessary to apply models on local clusters/datasets instead of on one global (total) dataset to best explain SOC (more precisely its variance).

L102: Is the "entire dataset" equivalent to the "global dataset"?
A global (now total) dataset is defined as a dataset encompassing the large majority of the dataset. Therefore, next to the entire dataset, the clusters of arable, grassland and loam act as total (previously global) dataset.

Materials and Methods
L104: It is recommended to add more information about the study area. In general, most studies show readers climate factors (e.g. annual precipitation and average temperature), soil type/classification and composition of vegetation/crops.
We added additional information regarding the study area.

L119: Please explain why soil samples were stored either at -20 °C or air-dried. For different analyses?
Samples were stored until they were analyzed. Storage was done in a uniform way for all samples. One part of each sample was air dried for subsequent chemical and physical soil analysis, another part was kept moist and was frozen for subsequent soil microbial analyses (MBC, MBN or respiration). This is now clarified in the text.

L139: More information of the incubation is appreciated. How long the samples were incubated before sampling? What was the temperature? Did you sample for only once or multiple times?
Samples were preincubated at room temperature for one week (7 days), measurement was conducted for 24 hours at an interval of one hour. The information was added to the text..

L146: Please give more information of linear regressions. For example, indicate that they only have one predictor. Did you check the normality of residues?

We added respective information. Normality of residues was checked.

L147: and after: What are the reasons for performing mixed-effect models? Why parent materials, texture group and land use are selected as random effect variables? In general, random effects are used when samples are only a small subset of the group or when limited groups are included. Does it aim to make predictors on a larger scale using the limited dataset?

West, Welch, & Galecki suggest in their book "*Linear mixed models*" that such models can be applied to clustered data. We decided to use mixed effect models to capture the effect of soil properties applied as fixed effects. Developed on different parent material or under different land use management the soils showed a further source of variability. Furthermore, we selected these variables as random factors. It is aimed to remove their bias from the specific levels of the applied random factors. To this end, sampling sites were specifically selected that covered the factors parent materials, texture group and land use.

L162-163: Why was response variable transformed but not predictors?

Transformation of the response variable is common and was applied to achieve a normal distribution of the residues. The predictors of the mineral phase determine the variability of SOC and its labile fractions. Therefore we tried to keep them as they occur in the environment/our dataset. SOC (or its labile fractions) as variable part of the soil was consequently transformed to achieved normally distributed residues.

Result

Overall: The readability can be improved by dividing this section into a few subsections due to a large content in this section.
Thanks for this valuable advice, we divided the results in subsections.
3.1 Soil properties and cluster identification
3.2 Bivariate relationships of mineral phase and SOC and its labile fractions
3.3 Estimation of SOC and its labile fractions by mixed effect models
3.4 Comparison of total and local explained variability.

L170: What are “soils and topsoil properties”? Consider revising.
Line was revised. Topsoil was separately mentioned due to the fact that our study is focused on agricultural topsoils. To avoid confusion or misunderstanding we decided to use only the term ‘Soil properties’.

L177-178: Are they significantly different or different by looking at means/ranges?
Differences were mostly statistically significant differences. Here we solely wanted to mention that a higher proportion of organic substance was found in grassland soils compared to arable soils.

L190: “Somewhat different” is vague.
It was changed accordingly.

L205: and after: This paragraph is comprised of isolated points, which makes it difficult to follow. A suggestion is to describe Table 3 in a well-organized way to shorten this paragraph. For example, you can follow the order of entire dataset --> land use --> parent materials --> texture, or you can introduce them by the types of predictors. Also, focusing on your key findings helps.
We will try to rephrase it paragraph. Anyhow we include subsections.

L207-208: The items “global cluster” and “local cluster” are explained here but they appear in previous parts (e.g. L18 and L193). Please give explanations when they appear for the first time.

Thanks for this hint, we mention the definitions earlier.

L208 and L94: Please be consistent for “parent material” or “parent rock material”.
We changed it. Now it is consistent.

L224: What is “a sufficient extent”? Please specify.
Applying “sufficient” is not objective enough, therefore we rephrased this line and specified it by giving the respective level of R^2.

L237 -242: Please indicate that they are from Table 3.
The reference to Table 3 was added.

L240: How to know “weight of samples” is equal? Why does it act as global cluster?
We mean the statistical weight of the samples. We changed the sentence as follows: “The clusters of both land use types largely overlapped and contained a similar proportion of samples from each parent material. Therefore they can be regarded as total clusters.”.

L250: It is not clear how to compare R^2 between bivariate regression and mixed-linear model. By the means of each cluster?
Next to the comparison of the explained variance we showed the RMSE to give a measure for model performance. This is now better clarified in the revised text. ”By the mixed effect models, R^2_{cond} reach higher explained variance for SOC (R^2_{cond} = 0.39-0.89, RMSE = 0.21 – 0.42%) compared to the bivariate regressions (R^2 = 0.00-0.73, RMSE = 0.27-1.12%).” Further we added some information at section 2.3

L257-258: DCS sites look different from LBS and DLS.
We clarified it. “Models using parent material or texture as random effect mostly showed minor differences for predictions of SOC, HWEC or MBC. Anyhow, for some local clusters (e.g. DCS, LBS and DLS) distinct results were found. Models using land use as random effect were partly distinct, though, indicating the different influence of land use on SOC and its labile fractions (Table 4). “

L279-286: Please indicate related Tables and Figures. It is hard to follow.
We now refer to the considered Tables.

L282 & L287-288: This gives me a feeling that you are estimating whether the models were well-fitted. If this is true, comparing R^2 does not make sense. Large R^2 means more variation is explained by predictors. Instead, you have to look at the distribution of residue using e.g. root mean square error (RMSE).
It is aimed by this study to show how well the specific models with their specific parameter combination explained the variance of SOC, HWEC and MBC. Therefore, we rephrased this sentence. We agree that in order to show the goodness of the model fit RMSE is the correct measure. We added this information.

Discussion

L304-305: “for the in total very sandy soils …of LBS”. Try to revise this sentence.
Sentence was adapted.

L309: “…SOC in soil” --> “in soil”
It was changed accordingly.

L314-315: “ECEC, Ca and Mg are suitable predictors for SOC in this study”; L317-318: “The minor ability of ECEC (Ca+Mg) to explain SOC..” They look like contradictory. Also, I missed a point that whether you are talking about entire dataset or specified cluster. Table 3 showed that the predictions using ECEC and (Ca+Mg) are largely dependent on parent materials and texture cluster. A possible explanation is that DCS soils had more sands and lower pH, so that Ca and Mg do not contribute to SOC stabilization, whereas DLS and PSS soils had higher pH, so that Ca and Mg bridging play a role in SOC stabilization (see your cited paper). Please consider re-organizing this part.
We clarified these sentences. (L314-315)“The minor ability of ECEC and $(Ca+Mg)_{ECEC}$ and the higher ability of pedogenic oxides to explain variance of SOC and its labile fractions indicated in this study for several cluster (total and local) by bivariate regressions (Table 3), corresponds to findings of Rasmussen et al. (2018).”……
(L317-318)“ Ability of ECEC and $(Ca+Mg)_{ECEC}$ was further strongly dependent on the observed parent material or texture cluster. By the mixed effect models, $(Ca+Mg)_{ECEC}$ were more frequently identified as relevant to explain SOC and its labile fractions. Thereby it is shown that by a collective approach of several soil parameters more driver explain a larger part of the variability than by bivariate approaches. As example ECEC and $(Ca+Mg)_{ECEC}$ was found as relevant for the clusters of DLS and PSS, while for DCS it show a minor importance.”

L328-333; Grassland had higher SOC contents than arable land, but the PCA showed that they were largely overlapping. This is a good point for discussion. Some explanations will be appreciated.
We amended the Discussion accordingly. “In comparison, mineral phase soil properties clearly separate the dataset while composition of SOM was less enabled for this purpose. Consequently, a broad scatter of the land use clusters was obtained by PCA, suggesting to treat the land use clusters as total datasets as well.”

L334-336: “Several studies with…” has only one citation?
Thanks for this hint, we added further studies.

L351-352: Previous explanations are good reasons for using multiple parameter models. However, the reasons for using mixed-effect linear model are not well mentioned. For example, why not multiple fixed-effect model or partial least square regression? My recommendation is to stay in a safe way.
As mentioned above, West, Welch & Galecki suggest in their book “*Linear mixed models*” this type of model for clustered data. Soil parameters (e.g. pedogenic oxides, texture) have an influence (with differing strength) on SOC, HWEC or MBC. Furthermore, there is an effect by factors such as the parent material or land use. To further capture this effect, we decided to use mixed effect models.

L373-374: To be prudent, I would say models of parent materials explained more variation of SOC because we don’t if the model-fitting was better than others (see comments on L282). The same for L374-375.
We changed the sentences to highlight the explained variance.

L379 and after: A major finding of this study is that the overall explained variance decreased in the order SOC>HWEC>MBC. Some explanations for this would be appreciated.
Ok, we added further explanations.

L395: Please be consistent with “mixed effect model” and “mixed parameter model”.
Ok, thanks for this hint. The relevant line was changed to mixed effect model

Figures and Tables:
Fig. 1 The clustered locations of the four parent materials are likely to introduce

differences in topographical and climate conditions. For example, DCS and LBS sites are mostly located on the top of the mountain/hill, whereas PSS sites are located in a flatter area. The difference may affect soil formation and SOC accumulation. Also, the different altitudes between DCS and PSS sites may cause differences in climate conditions. Therefore, it is possible that the variation caused by climate and topography factors was explained by parent material or land use in this study. I just wonder whether something has been performed in experimental design, statistics or anything else to deal with this problem.

It was aimed by this study to estimate the effect of the mineral phase. Selected sampling region covers soils with identical land use and similar climatic/pedoclimatic condictions but the parent material is substantially different. Consequently soil mineral phase properties differ largely between the local sampling clusters. Our prior aim was to show that SOC of local cluster is better explained by local models, at larger scales we fully agree that differences in pedoclimatic conditions were factors needed to explain SOC (and its labile fractions). For local areas the climatic factors is generally not relevant independent of where they are.

Table 1: What does the unit for respiration mean? As suggested for L146, more information of the incubation is needed.
There was a typo in the unit. We corrected it: [µg CO_2-C/(g dry matter h)]
We added more information regarding the incubation.

A suggestion for Fig. 2: Why not combining Fig. 2 and Fig. S1 if you want to show the readers that parent material and soil texture make good separations while land use make an insufficient separation?
We tried this option. However, with three plots on one page the readability of the individual plots was poor. So we decided to leave it as is with a focus on the two plots showing differences between clusters

Fig. 2 and 5: The shape of the font might be improved as some of them are narrow but others are wide.

Ok, we adapted the fonts of these figures.

Fig. 3 It looks like that the residue of MBC is less normally distributed compared to SOC and HWEC. Particularly, MBC in grassland soils is underestimated. Also, HWEC has a similar but less obvious trend. My questions are: (1) Is the model prediction of MBC less reliable than others due to the skewed distribution of residue? (2) Are there any reasons for the underestimation of MBC in grassland soils?
For SOC, HWEC and MBC there is a trend of underestimation for grassland sites which increases from SOC to the labile fractions. We assume that additional soil properties (e.g. content of fine root biomass) affect the organic matter here. Since this study is focused on mineral phase parameters and did not consider further biological properties models were less suited to explain SOC and its labile fractions in grassland soils.

Fig. 4 What do “dataset”, “DCS”, “sand” and “arable” on the left mean?
It shows which cluster is shown there with its models. We added information to the figure in order to clarify it.

Table 5: Does the “model” before “global model to local cluster” mean local model?
Yes, this model means the R^2 which is received by the consideration of predicted vs measured data of the models for the specific clusters/datasets. We clarified it

Fig. 6: Is it a part of Table 5? Is there any reason to make it a new Figure? Maybe try to combine Table 5, Table S3 and Fig. 6 into a good shape, or move unnecessary information to supplementary.
Fig. 6 shows the performance of the total model and the respective local model, when both are applied to the same local dataset. This was tested by comparing measured and modelled data based on simple linear regression. This yielded a pseudo R^2. This information is contained in Table 5. We added information regarding RMSE at Table 5 and Figure 6.

Content of ~~S~~soil organic ~~matter~~ carbon and labile fractions depend on ~~specific~~ local combinations of mineral phase parameters ~~combinations~~

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Abstract. Soil organic matter (SOM) is an indispensable component of terrestrial ecosystems. Soil organic carbon (SOC) dynamics are influenced by a number of well-known abiotic factors such as clay content, soil pH or pedogenic oxides. These parameters interact with each other and vary in their influence on SOC depending on local conditions. To investigate the latter, the dependence of SOC accumulation on parameters and parameter combinations was statistically assessed that vary on a local scale depending on parent material, soil texture class and land use. To this end, topsoils were sampled from arable and grassland sites in southwestern Germany at four regions with different soil parent material. Principal component analysis (PCA) revealed a distinct clustering of data according to parent material and soil texture that varied largely between the local sampling regions, while land use explained PCA results only to a small extent. The ~~obtained~~ PCA clusters were differentiated into total~~global~~ clusters that contain the entire dataset or major~~large~~ proportions of it ~~the entire dataset~~ and local clusters ~~which only~~ representing only a smaller part of the dataset. ~~and the different local clusters of the dataset were further~~All clusters were analyzed for the relationships between SOC concentrations (SOC %) and mineral phase parameters in order to assess specific parameter combinations explaining SOC and its labile fractions hot water-extractable C (HWEC) and microbial biomass C (MBC). Analyses were focused on soil parameters that are known as possible predictors for the occurrence and stabilization of SOC (e.g. fine silt plus clay and pedogenic oxides). Regarding the total ~~global~~ clusters~~dataset~~, we found significant relationships,~~,~~ ~~correlations~~ by bivariate models, between SOC ~~and~~ , its labile fractions ~~hot water-extractable C (~~HWEC~~)~~ and ~~microbial biomass C (~~MBC~~), respectively~~ and the applied predictors~~,~~. Y~~y~~et ~~some correlation coefficients indicate a~~ partly~~were partially~~ low explained variances indicated the limited suitability of bivariate models. ~~Mixed~~ Hence, mixed effect models were used to identify specific parameter combinations that significantly explain SOC and its labile fractions of the different clusters. Comparing measured and mixed effect models-predicted SOC values revealed acceptable to very good regression coefficients ($R^2 = 0.41$-0.91) and low to acceptable root mean square error~~,~~ (RMSE = 0.20-0.42 %). Thereby, the predictors and predictor combinations clearly differed between models obtained for the whole data set and the different cluster groups. At a local scale site specific combinations of parameters explained the variability of organic ~~matter~~ carbon notably better, while the application of total~~global~~ models to local clusters resulted in less explained ~~variability~~variance and a higher RMSE~~sufficient performance~~. Independent from that, the ~~overall~~ explained variance by marginal fixed effects ~~generally~~ decreased in the order SOC > HWEC > MBC, showing that labile fractions depend less on soil properties but presumably more on processes such as ~~than presumeably on~~ organic carbon~~matter~~ input and turnover in soil.

1 Introduction

Soil as an inherent part of terrestrial ecosystems acts as a major regulator of the organic carbon (OC) cycle especially through the function of OC storage (Heimann and Reichstein, 2008; Scharlemann et al., 2014). Hence, it is of utmost relevance and a focus of ongoing research to define models and parameter sets that best describe and predict soil organic carbon (SOC) contents of soils. Further it is required to identify the drivers for SOC storage at different scales and sites to adapt the management of soils. Overall, the relevance of parameters for quantification of SOC is often described by bivariate relationships (Hassink et al., 1993; Barré et al., 2017). Yet, SOC and its potential sequestration by formation of organo-mineral associations depends on combinations and interactions of several environmental factors or soil properties, so that the number of multivariate applications to estimate the accumulation of SOC is increasing ~~-~~ (Hobley et al., 2015; Heinze et al., 2018).

In addition to total SOC, its labile subfractions such as hot water extractable carbon (HWEC) or microbial biomass carbon (MBC) are more and more recognized as fast reacting SOC pools in order to analyze carbon dynamics in soils (Weigel et al., 2011; Lal, 2016). The HWEC is known as a measure of the bioavailable and mineralizable fraction of SOC (Spohn and Giani, 2011; Heller and Zeitz, 2012). The MBC is a quantitative measure of the microbial community that plays an indispensable role for the turnover of SOC. Additionally, ~~Because of the faster turnover~~ labile carbon fractions such as MBC quantitatively dominate in short-term turnover processes, ~~should be considered more frequently to improve the understanding of~~while changes in SOC will only become significant over periods of decades~~dynamics in various regions.~~ Therefore, MBC is expedient to explain SOC dynamics (Liang et al., 2017). Determination of HWEC and MBC, allows to get a representative measure of the labile SOC pool. Labile carbon fractions were recently simulated (Wieder et al., 2015; Zhang et al., 2021) but ~~In contrast, much less research and attempts for quantitative modeling of these labile fractions~~ compared to SOC they were less considered~~have been done~~ in the past (Liddle et al., 2020). ~~Because of the faster turnover labile carbon fractions should be considered more frequently to improve the understanding of SOC dynamics in various regions.~~

It is well known that factors such as climate, topography, vegetation, parent material and time are major factors influencing contents and storage of SOC (Jenny, 1941). Accordingly, large scale (often national or continental) surveys often include geographical properties, vegetation types, general forms of land use as well as climatic site conditions to explain the variability of SOC (Wiesmeier et al., 2014; Gray et al., 2015). Consequently, vegetation and anthropogenic influence by land use and land use changes are essential factors to model SOC accumulation and dynamics (Poeplau and Don, 2013; Dignac et al., 2017). The relevance of the parent material for SOC sequestration and stocks was discussed for sites and small landscapes of a few km² (Barré et al., 2017; Angst et al., 2018) as well as for large areas on the scale of regions or countries (Wiesmeier et al., 2013; Vos et al., 2019). The potential influence of parent material on SOC is mostly considered by parameters of soil mineralogy and texture (Herold et al., 2014). Factors such as climate, topography, parent material, vegetation or land use are well suited to explain the variability of SOC at larger scales or at landscapes with a high variability concerning these factors. In contrast, for smaller, local study areas or rather uniform areas with a low factor variability an inclusion of these factors as variables is less suitable~~expedient~~ (Wiesmeier et al., 2019).

In addition to ~~or even instead of~~ these general factors, further parameters describing the soil composition in a more specific way, become relevant at regional or local scale setting boundaries for SOC accumulation, e.g. by the formation of organo-mineral associations. For an identification of SOC variations due to site specific characteristics selected parameters are used which are mostly known as indicators for stabilization of SOC such as content of fine silt, clay and pedogenic oxides or microbial parameters such as microbial biomass and amino sugars (Angst et al., 2018; Quesada et al., 2020). There are indications that for the explanation of SOC variability on a local to regional scale soil parameters (~~e.g.~~e.g., pedogenic oxides, texture fractions) instead of factors (e.g., parent material or climate) are especially suitable. Models based on soil parameters also allow to identify possible drivers of SOC stabilization while using the above mentioned general factors would not deliver a satisfying result (Wiesmeier et al., 2019; Adhikari et al., 2020).

Organo-mineral associations are highly relevant for stabilization and accumulation of SOC and its labile fractions (Lützow et al., 2006). It is well known that the different mineral particle size classes vary in their ability to interact with SOC, forming organo-mineral associations (Arrouays et al., 2006; Lützow et al., 2007). On one hand coarse particle size fractions such as sand, coarse silt (cSilt) and medium silt (mSilt) contribute less to interactions between SOC and the mineral phase while on the other hand fine silt (fSilt) and clay dominate such interactions (Ludwig et al., 2003). In addition, the mineral composition of the fine fraction, i.e. types of clay minerals and pedogenic oxides, is relevant for the interactions of SOC with the mineral phase (Kleber et al., 2015; Porras et al., 2017). Especially iron and aluminum oxides interact with SOC leading to its sequestration (Mikutta et al., 2006). Stabilization of SOC is further enhanced by multivalent cations such as Ca^{2+} and Mg^{2+} going along with higher soil pH (Kaiser et al., 2012; O'Brien et al., 2015). Covering on one hand all quantitative relevant cations and on the other hand being an overall measure of soils sorptive properties the effective cation exchange capacity (ECEC) provides an overall measure to model cation impact on SOC storage (Kaiser et al., 2012; O'Brien et al., 2015). Rock fragments (soil skeleton) contribute only little to SOC storage (Poeplau et al., 2017). Anyhow, the fraction of rock fragments is considered as a relevant parameter to assess SOC accumulation due to a potential saturation effect in soils with a high rock fragment content in consequence of a disproportionately high input of organic matter in the fine soil fraction (Bornemann et al., 2011).

Consequently, understanding SOC as a dynamic equilibrium of heterogeneous compounds with distinct relationships to various components of the soil mineral phase (Lehmann and Kleber, 2015) implements that SOC accumulation is best described and predicted by a variety of soil mineral phase parameters instead of a single predictor. Thereby combinations of parameters or factors can differ according to the considered scale. Consequently, multivariate approaches better explain the SOC variability (Heinze et al., 2018; Liddle et al., 2020) compared to bivariate linear regression~~correlation~~ models that are often unsuited at the level of local and regional soilscapes (Jian-Bing et al., 2006). The latter especially applies for studies that are limited to a single specific location or only contain a limited number of categorical variables or estimated soil parameters (Liddle et al., 2020). On the other hand, predictions based on total~~global~~ models, based on the ~~majority~~largest part of the dataset, are often less site-specific and thus can possibly lead to an insufficient quantification of SOC at certain sites.

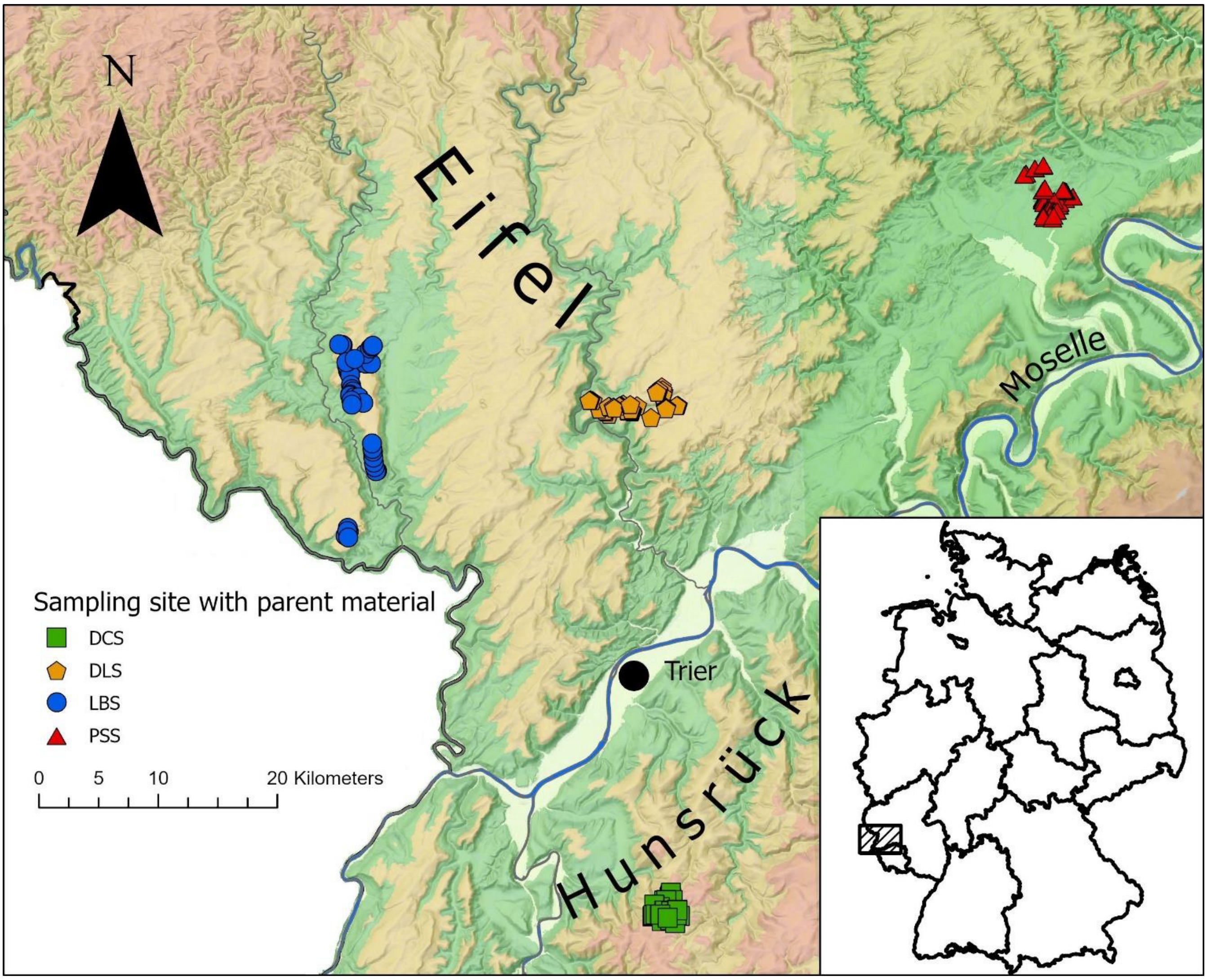
Consequently, it is required to determine parameter sets to estimate SOC and its labile fractions HWEC and MBC at a regional or landscape scale. It is necessary to identify predictor parameters and categorical environmental factors that are able to predict SOC as well as its labile fractions by using models based on local and total~~global~~ datasets~~models~~. Differences regarding the relevance of a predictor in local vs. total~~global~~ models have to be identified to boost model performance and to fit adequate datasets using the best set of parameters for the prediction of SOC at the investigated location. This overall aim was investigated in this study using a dataset from four local agricultural areas in the greater region of Trier (each with a size of 5-10 km²), thus with similarity in the global factors but distinct local properties such as parent ~~rock~~ material, soil texture and land use. Regarding the composition of the soil mineral phase the four local areas differ among each other, but as a total~~global~~ dataset they represent a broad range of soil properties typical for soils in temperate regions. Therefore, the dataset enables to verify whether the total~~global~~ dataset is able to cover the local variability of SOC and its labile fractions. Objectives of this study were, (i) ~~based on identified differences in soil properties~~ to determine best fitting factors and parameter combinations, based on identified differences in soil properties, that explain the variability in SOC and its labile fractions HWEC and MBC. (ii) It was aimed to determine the suitability~~relevance~~ of local models in comparison to total ~~global~~ models to achieve an improved ~~sufficient~~ quantification~~, on a comparablesimilar level,~~ of SOC, HWEC and MBC for local landscapes with distinct properties. To this end, bivariate linear regression, principal component analysis (PCA) and mixed effect models were used in order to find out whether total~~global~~ models or local models are better fitting. (iii) It was assessed if local datasets show a distinct combination of significantly contributing predictor parameters compared to other local datasets and the entire dataset.

2 Material and Methods

2.1 Study area

The study was conducted in the greater area of Trier in southwestern Germany (Fig. 1). Bulk samples from topsoil horizons, i.e. 0-25 cm for arable and 0-15 cm for grassland soils, were taken in spring 2017 and 2018 from 199 agricultural sites used as arable land (150) and grassland (49). Similar numbers of samples were taken from four regional areas with different parent materials. Parent materials were Devonian clay schist (DCS, n= 50), Luxemburg sandstone (LBS, n= 50), sandy dolomitic limestone (DLS, n= 50) from the Muschelkalk, and Permian siltstone and fine sandstone (PSS, n= 49) from the Rotliegend (Wagner et al., 2011). Across the different parent materials, a similar proportion of samples were taken at sites under arable or grassland management. Climatic conditions in the greater area of Trier are classified as warm-temperate, fully humid with warm summer temperate (Cfb) (Kottek et al., 2006). According to the German Weather service (DWD) mean annual precipitation is 784 mm and mean annual temperature is 9.8°C. Investigated sites were dominated by the soil groups Regosol and Cambisol. The main cultivated crop plants are wheat, barley, triticale, maize ~~or~~and rapeseed.

Fig. 1. Study area in the greater Trier region; sampling sites at the four regions with different parent material are indicated, i.e. Devonian clay schist (DCS), sandy dolomitic limestone (DLS) from the Muschelkalk, Luxemburg sandstone (LBS), and Permian siltstone and fine sandstone (PSS) from the Rotliegend (©GeoBasis-DE).



2.2 Analysis of soil properties

Samples were sieved < 2 mm and the stone content (> 2 mm) was determined gravimetrically. ~~For further analysis,~~ Each sample~~s~~ ~~were divided~~was split and stored at -20°C on one hand and~~or~~ air-dried on the other hand~~,~~ for subsequent~~ly~~ biological and chemical soil analysis, respectively. Soil pH was measured in 0.01 M $CaCl_2$ solution using a pH/Con 340i glass electrode (WTW GmbH, Weilheim). Particle size distribution was determined by a combination of wet sieving and pipette method according to Blume et al. (2011). Dithionite-citrate extractable Fe (Fe_d) was measured according to Mehra and Jackson (1958). To this end, 2 g air-dry soil were extracted with a mixture of 1 g sodium dithionite, 40 ml sodium citrate and 10 ml $NaHCO_3$. Oxalate extractable Fe and Al (Fe_o, Al_o) were determined according to~~-~~ Schwertmann (1964). For extraction, 1 g air-dry soil was shaken for 2 h in the dark in 50 ml NH_4^+-oxalate (pH 3) and filtered afterwards. Extraction for the determination of the effective cation exchange capacity (ECEC) was conducted using 1 M NH_4Cl. Elemental analyses for pedogenic oxides and ECEC (Na, K, Fe, Mn, Al, Ca, Mg) were done using atomic absorption spectrometry (Varian AA240 FS Fast Sequential Atomic Absorption Spectrometer; Darmstadt, Germany).
For estimation of total carbon (TC) and nitrogen soil was dried at 105°C, grinded and measured by an Elemental ~~Analyzer~~ Analyser EA3000 Series (HEKAtech GmbH, Wegberg). For carbonate containing soils the inorganic carbon (IC) was determined following carbonate destruction using phosphoric acid at a temperature of 100°C (IC Kit combined with Elemental ~~Analyzer~~ Analyser EA3000 Series, HEKAtech GmbH, Wegberg). SOC content was calculated as the difference of TC and IC. HWEC and hot water extractable nitrogen (HWEN) were determined following Körschens et al. (1990), using a Gerhardt Turbotherm TT 125 (Gerhardt, Bonn, Germany) for extraction of 10 g soil with distilled water (50 ml) at 100°C for 1 h. After extracts cooled down 1 ml of 0.2 M $MgSO_4$ was added and samples were centrifuged at 1476 g for 10 minutes. Microbial biomass was estimated by using chloroform fumigation extraction according to Joergensen (1995) with 0.01 M $CaCl_2$. Extracts of HWEC, HWEN, microbial biomass carbon (MBC) and nitrogen (MBN) were ~~analyzed~~ analysed with a TOC-VCPN ~~analyzer~~ analyser (Shimadzu, Duisburg, Germany). For MBC and MBN correction factors kEC = 0.45 and kEN = 0.4 respectively, were used (Joergensen, 1996; Joergensen and Mueller, 1996). Soil respiration was measured according to Heinemeyer et al. (1989)~~-~~. Following a week of incubation at room temperature (20 °C)~~Therefore~~, 25 g dry matter equivalent of sieved field moist soil were weighted in a tube that was flushed with 200 mL min^{-1} of CO_2-free, humid air for 24 hours. Evolved CO_2 was determined ~~by a~~in one-hour intervals after the soil passage using an infrared gas ~~analyzer~~ analyser (ADC 225 MK3, The Analytical Development, Hoddesdon, England).

2.3 Data analysis

Principal component analysis (PCA) was carried out to identify clusters within the dataset. For that purpose, 24 parameters describing the mineral phase as well as SOM were included (Table 1). To conduct the PCA applied variables were log transformed, centered and scaled to achieve standardized and comparable variables. Ellipses were defined by 95 % of the confidence interval according to Fox and Weisberg (2019), The cluster of clayey soils was not included in the analysis due to a small number of samples (n = 5). Using single predictors, ~~L~~linear regressions were performed to identify significant impact of mineral phase parameters (e.g. Fe_o [g kg^{-1}] or fSilt plus clay [%])~~–~~ on SOC, HWEC and MBC for the entire dataset as well as for the identified clusters. Residues of the bivariate linear regressions were checked for normality.~~.~~ Mixed effect models were determined for the entire dataset and for identified clusters. To this end, selected soil properties of the mineral phase (Fe_{d-o} [g ~~/~~kg^{-1}], Fe_o [g~~/~~ kg^{-1}], Al_o [g~~/~~ kg^{-1}], sand [%], cSilt plus mSilt [%], fSilt plus clay [%], $(Ca + Mg)_{ECEC}$ [mmolc~~/~~ kg^{-1}], stones [%] and pH) were used as fixed effect while, 'parent material', 'soil texture group' or 'land use' were used as random effect. In general, as random effects only categorical variables were selected, while for the fixed effects variable mineral phase parameters were selected. Parent material as a random effect includes the four different soil parent materials that dominate at the four sampling sites. For the soil texture group as random effect four levels were applied (sandy, silty, clayey and loamy soils). The additional implementation of the soil texture groups was done to consider the potential different intercepts of the specific groups. Land use as random effect comprised the two management practices arable and grassland. Restricted ~~M~~maximum likelihood was applied as estimation procedure for the mixed effect models. At the beginning, all selected soil properties were included in each model. Stepwise removal of ~~the most~~ the least significant parameters ~~–~~was conducted until all properties included in the models significantly contributed to SOC, HWEC or MBC~~,~~ ~~respectively~~. ~~Additional~~ Additionally, the relevance of variables was visualized by the mean values of the clusters multiplied with their coefficient received from the mixed effect models. All parameters involved as fixed parameter in the mixed effect models were checked for collinearity. To avoid collinear behaviour of the soil texture related parameters either 'sand' or 'coarse silt plus medium silt' (cSilt plus mSilt) were used for model development. The two models received were compared by their Akaike information criterion (AIC) using ANOVA to identify the best model. Furthermore, ECEC was excluded from mixed effect models to avoid overfitting due to collinearity with $(Ca+Mg)_{ECEC}$. Residuals of models were examined for homoscedasticity and normality. In case these criteria were not fulfilled, the response variable was square root transformed to achieve variance homogeneity and normality. For the mixed effect models a marginal R^2 (R^2_{marg}) and conditional R^2 (R^2_{con}) coefficient~~s~~ was estimated according to Nakagawa and Schielzeth (2013). Thereby R^2_{marg} examines~~a~~ the explained variance of the fixed effects while R^2_{cond} ~~also include~~tests the variance including the effect ~~i~~of the random effects. ~~Next to this,~~The root mean square~~d~~ error (RMSE) was estimated as a measure ~~for~~of the model performance. For the mixed effect models, RMSE was estimated based on the comparison of predicted and measured values. To transfer the mixed effect models of a total dataset to a local dataset, predictions were conducted ~~us~~applying ~~the~~ total ~~dataset~~ models ~~on~~to ~~a~~ local datasets. ~~Measures to inspect these results (R² and RMSE) were~~ The ~~received from comparisons of~~ predicted values of SOC; HWEC and MBC received from the different mixed effect models were compared with the~~vs. M~~measured values using bivariate linear regressions. This yielded ~~of SOC; HWEC and MBC~~R^2 and RMSE as measures of goodness. ~~To examine performance of mixed effect models, predicted values were tested against measured values of SOC, HWEC and MBC, respectively using bivariate linear regressions. Data~~ All data are shown as mean (± SE) if not indicated otherwise. Statistical significance ~~was~~ is indicated with *$p < 0.05$, **$p < 0.01$ and ***$p < 0.001$. Statistical analyses were carried out using the R statistical package version 4.1.1~~3.6.2~~ (R Core Team, 2021).

Table 1. Soil properties in agricultural topsoils for the complete dataset and defined group levels according to parent material, land use and soil texture class. Values are means ± SD.

	Dataset (n=199)	DCS (n= 50)	LBS (n=50)	DLS (n=50)	PSS (n=49)	Sandy soils (n=54)	Loamy soils (n=98)	Silty soils (n=42)	Arable (n=150)	Grassland (n=49)
SOC [%]	1.94 ± 0.87	3.03 ± 0.78	1.61 ± 0.39	1.92 ± 0.49	1.17 ± 0.33	1.41 ± 0.45	2.08 ± 0.87	2.08 ± 0.76	1.82 ± 0.73	2.29 ± 1.11
Nitrogen [%]	0.20 ± 0 10	0.33 ± 0.08	0.14 ± 0.03	0.19 ± 0.04	0.13 ± 0.04	0.13 ± 0.03	0.22 ± 0.10	0.21 ± 0.08	0.19 ± 0.08	0.23 ± 0.12
Hydrogen [%]	0.56 ± 0.29	0.94 ± 0.25	0.33 ± 0.07	0.59 ± 0.15	0.38 ± 0.12	0.33 ± 0.08	0.64 ± 0.31	0.63 ± 0.22	0.57 ± 0.29	0.54 ± 0.27
Oxygen [%]	3.77 ± 1.93	6.15 ± 0.97	2.45 ± 0.63	3.87 ± 2.00	2.56 ± 0.70	2.18 ± 0.53	4.23 ± 1.63	4.67 ± 2.46	3.62 ± 1.82	4.24 ± 2.14
HWEC [µg ~~/~~g^{-1}]	753 ± 322	1071 ± 353	661 ± 163	732 ± 214	545 ± 252	570 ± 199	813 ± 319	782 ± 276	669 ± 231	1010 ± 410
HWEN [µg ~~/~~g^{-1}]	99.4 ± 42.0	130 ±35.5	78.9 ± 28.2	107 ± 37.2	80.4 ± 43.8	70.4 ± 31.0	106 ± 39.9	116 ± 40.3	93.8 ± 39.9	116 ± 43.5
MBC [µg ~~/~~g^{-1}]	247 ± 143	325 ± 159	130 ± 42.1	320 ± 118	209 ± 117	123 ± 47.2	271 ± 132	322 ± 119	205 ± 93.0	377 ± 186
MBN [µg ~~/~~g^{-1}]	41.2 ± 23.5	53.5 ± 25.3	22.6 ± 8.78	50.8 ± 23.2	37.1 ± 17.7	22.9 ± 10.2	44.5 ± 22.1	52.3 ± 21.7	35.5 ± 18.3	58.5 ± 28.5
Respiration [µg CO_2-C ~~/~~ (g^{-1} dry matter h^{-1})]	0.26 ± 0.11	0.29 ± 0.11	0.21 ± 0.05	0.30 ± 0.12	0.22 ± 0.10	0.20 ± 0.07	0.27 ± 0.11	0.28 ± 0.10	0.23 ± 0.09	0.32 ± 0.13
MBC/SOC	1.36 ± 0.71	1.05 ± 0.31	0.89 ± 0.61	1.75 ± 0.72	1.73 ± 0.62	0.97 ± 0.51	1.42 ± 0.67	1.71 ± 0.82	1.23 ± 0.66	1.74 ± 0.70
SOC/N	11.7 ± 2.13	10.5 ± 0.98	13.7 ± 2.20	11.9 ± 2.11	10.7 ± 1.25	12.9 ± 2.58	11.1 ± 1.55	11.5 ± 2.06	11.6 ± 2.24	12.0 ± 1.76
HWE-C/N	9.90 ± 4.98	9.76 ± 2.33	11.1 ± 5.02	8.60 ± 2.85	10.2 ± 7.61	11.64 ± 6.77	9.66 ± 4.45	8.20 ± 2.15	9.80 ± 5.64	13.3 ± 6.40
MB-C/N	7.41 ± 2.57	7.62 ± 2.66	7.54 ± 3.36	7.83 ± 2.00	6.66 ± 1.81	7.02 ± 3.17	7.57 ± 2.44	7.55 ± 2.01	7.36 ± 2.79	7.55 ± 1.68
IC [%]	0.37 ± 1.18	-	-	1.43 ± 1.98	-	-	0.12 ± 0.62	1.36 ± 2.04	0.39 ± 1.24	0.29 ± 0.98
pH	4.98 ± 0.89	4.78 ± 0.61	4.70 ± 0.72	5.89 ± 0.77	5.47 ± 0.57	4.79 ± 0.73	5.02 ± 0.76	5.46 ± 0.90	5.02 ± 0.87	4.88 ± 0.87
ECEC [mmolc ~~/~~kg^{-1}]	65.6 ± 29.2	66.8 ± 21.0	38.8 ± 14.4	96.7 ± 26.3	58.6 ± 15.2	40.1 ± 12.9	66.6 ± 21.6	94.7 ± 28.5	65.6 ± 28.6	65.5± 31.1
Ca + Mg_{ECEC} [mmolc ~~/~~kg^{-1}]	55.7 ± 28.5	54.2 ± 21.2	30.8 ± 14.3	86.4 ± 26.6	50.0 ± 13.6	32.4 ± 12.9	55.5 ± 21.1	84.9 ± 28.5	54.9 ± 27.6	58.3 ± 31.0
Fe_o [g ~~/~~ kg^{-1}]	2.34 ± 1.18	3.95 ± 0.72	1.40 ± 0.40	2.24 ± 0.80	1.77 ± 0.66	1.32 ± 0.32	2.69 ± 1.12	2.66 ± 1.05	2.30 ± 1.14	2.49 ± 1.27
Fe_d-Fe_o [g ~~/~~kg^{-1}]	4.57 ± 2.18	6.92 ± 2.00	3.27 ± 1.18	4.50 ± 1.48	3.54 ± 1.74	2.91 ± 1.15	5.22 ± 2.20	5.10 ± 2.04	4.67 ± 2.23	4.27 ± 1.97
Al_o [g ~~/~~kg^{-1}]	1.26 ± 1.13	2.98 ± 0.89	0.84 ± 0.44	0.62 ± 0.30	0.61 ± 0.21	0.77 ± 0.45	1.53 ± 1.25	1.10 ± 0.98	1.21 ± 1.07	1.42 ± 1.28
Sand [%]	44.2 ± 23.1	26.8 ± 5.80	69.1 ± 17.9	24.6 ± 8.71	57.6 ± 13.5	75.1 ± 10.8	38.4 ± 13.5	21.0 ± 5.09	44.8 ± 23.8	42.3 ± 20.9
cSilt+ mSilt [%]	29.1 ± 13.3	30.8 ± 4.53	17.6 ± 13.6	43.7 ± 6.67	23.4 ± 7.97	13.5 ± 8.39	30.5 ± 7.11	45.1 ± 6.59	28.8 ± 13.5	29.9 ± 12.8
fSilt + clay [%]	26.8 ± 12.7	42.4 ± 4.95	13.2 ± 4.75	31.7 ± 5.74	19.0 ± 7.01	11.5 ± 3.22	31.1 ± 10.6	33.9 ± 6.67	26.4 ± 13.0	27.8 ± 11.7
Stones [%]	14.3 ± 12.3	29.3 ± 8.91	6.70 ± 6.51	13.1 ± 8.99	7.59 ± 8.29	6.88 ± 4.52	18.0 ± 14.0	14.5 ± 10.1	15.0 ± 12.7	11.9 ± 10.7

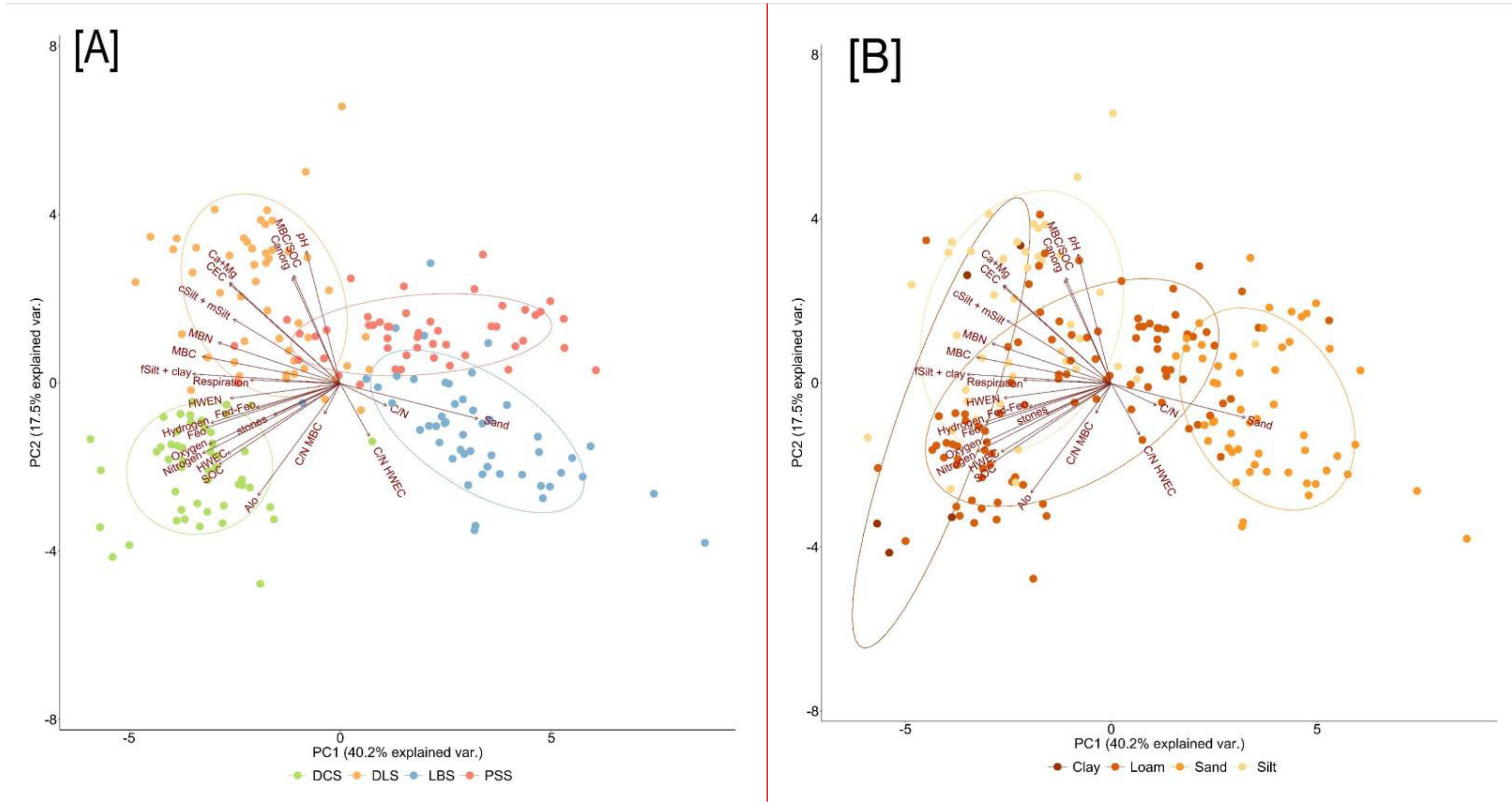
3 Results

3.1 Soil properties and cluster identification

The dataset covers soils~~s~~ ~~and topsoil~~ ~~properties~~ with broad ranges of 24 parameters and parameter ratios ~~, respectively,~~ of SOM, soil mineral phase and microbial biomass (Table 1). For example, soil pH ranged from very strongly acidic (pH 3.8) to slightly alkaline (pH 7.4); soil texture varied from sandy to clayey texture. ~~Thereby,~~ Parent materials essentially influenced characteristics of the mineral phase related parameters such as texture.~~, e.g.~~ ~~As~~For example soils developed from sandy parent material such as LBS had a sandy texture with sand content of up to 91.9 %. Soils developed from DCS and DLS parent material had elevated contents of fine silt plus clay (33.4-53.3 % and 16.7-44.8 %, respectively). Additionally, high contents of pedogenic oxides were found in soils from DCS while ECEC and especially the contents of the polyvalent cations $(Ca+Mg)_{ECEC}$ were high in soils developed from DLS (Table 1). Higher contents of SOC, HWEC and MBC were found for all parent material substrates in grassland soils compared to arable soils (Table 1 and ~~S1~~ Table S1~~A~~). For the entire dataset, SOC ranged from 0.38 to 5.32 %, while ranges from 237 to 1889 µg/g and 52.4 to 810 µg/g were determined for HWEC and MBC, respectively. SOC was strongly correlated with HWEC ($R^2 = 0.75$) while the regression~~correlation~~ with MBC was substantially lower ($R^2 = 0.40$). The dissimilar regressions~~correlations~~ of SOC with the two labile fractions indicate differences between HWEC and MBC, which was further confirmed by the mediocre ~~correlation~~ regressions between HWEC and MBC ($R^2 = 0.55$).

To identify possible local clusters due to different sampling sites, parent material or land use systems within the dataset, PCA was conducted including all 24 soil parameters and parameter ratios (Fig. 2). Principal component (PC) 1 to 3 explained 65 % of the variance and had eigenvalues > 1 (Table 2). Parameters related to the soil mineral phase loaded on all three PCs. Additionally, highest loadings on PC 1 were found for parameters describing the composition of SOM such as content of SOC, nitrogen, hydrogen or oxygen as well as HWEC or MBC. For PC 2 high loadings were further found for parameters related to soil acidity (pH, IC, ECEC, $(Ca+Mg)_{ECEC}$), as well as for SOC and the microbial ratio MBC/SOC. ~~The~~ HWEC and respiration further loaded on PC 3 (Table 2). A plot of the first two PCs shows clear clusters that were strongly related to the parent materials according to the different sampling sites (Fig. 2 A). In addition, samples clustered ~~somewhat~~ differently when assigned to different soil texture classes (Fig. 2 B). Land use, however, was insufficient to explain separation into different local clusters (Fig. S1). Instead, the land use clusters~~it~~ ~~represent~~~~could be used as a~~ total~~global~~ ~~clusters~~ ~~covering~~ covered soils from all sampling regions and property combinations, and thus represented total clusters~~with a differentiation according to its~~~~with separated effects due to land use management~~. Compared to the entire dataset or the land use clusters, the identified clusters based on parent material and soil texture ~~showed~~ covered distinct property ranges~~ies~~ of ~~the SOM~~ SOC and the mineral phase (Table 1). In contrast to the local clusters, the total~~global~~ cluster according to land use classes showed mostly properties quite similar to the entire dataset. Overall, identified clusters strongly depended on the composition of SOM as well as on specific properties of the soil mineral phase, e.g. texture or soil pH related properties. With a smaller relevance, parameters regarding the characteristics of soil microorganisms separated the dataset into clusters (Table 2).

Fig. 2. Principal components 1 and 2 with loadings of the variables indicating the clustering of the dataset according to parent material [A] and soil texture [B]. Parent materials are Devonian clay schist (DCS), sandy dolomitic limestone (DLS), Luxemburg sandstone (LBS), and Permian siltstone and fine sandstone (PSS).



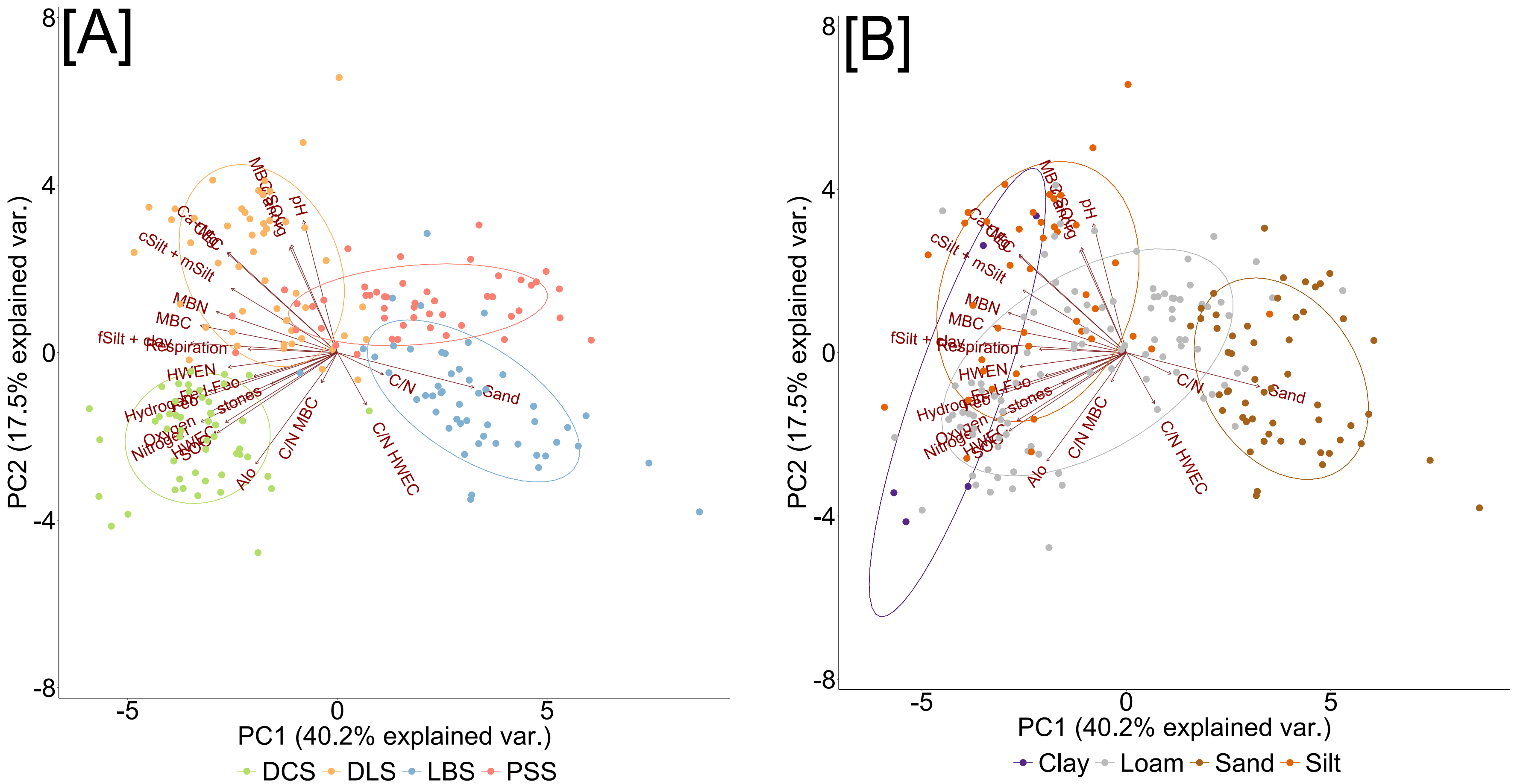

[A]
[B]
PC2 (17.5% explained var.)
PC1 (40.2% explained var.)
DCS
DLS
LBS
PSS
Clay
Loam
Sand
Silt
pH
cSilt + mSilt
MBN
MBC
fSilt + clay
Respiration
HWEN
stones
C/N MBC
Alo
C/N
C/N HWEC
HWEC
SOC
Oxygen
Nitrogen

Table 2. Loadings of the variables on the first three principal components.

	PC1	PC2	PC3
SOC	-0.24	-0.24	-0.19
Nitrogen	-0.27	-0.21	-0.04
Hydrogen	-0.26	-0.12	0.17
Oxygen	-0.26	-0.18	0.07
HWEC	-0.22	-0.21	-0.36
HWEN	-0.22	-0.04	-0.19
MBC	-0.27	0.08	-0.26
MBN	-0.24	0.12	-0.26
Respiration	-0.18	0.01	-0.36
MBC/SOC	-0.09	0.33	-0.12
C/N SOM	0.09	-0.07	-0.36
C/N HWEC	0.06	-0.16	-0.13
C/N MB	-0.03	-0.09	0.04
IC	-0.09	0.32	-0.09
pH	-0.07	0.4	0.03
ECEC	-0.22	0.3	0.07
$(Ca+Mg)_{ECEC}$	-0.22	0.3	0.06
Feo	-0.27	-0.13	0.12
Fed-Feo	-0.17	-0.07	0.37
Alo	-0.16	-0.34	0.14
Sand	0.27	-0.11	-0.11
cSilt + mSilt	-0.21	0.19	0.12
fSilt + clay	-0.29	0.03	0.18
Stones	-0.13	-0.09	0.29
Proportion of Variance	40.2	17.5	7.47
Cumulative Proportion	40.2	57.8	65.23
Eigenvalue	9.66	4.21	1.79

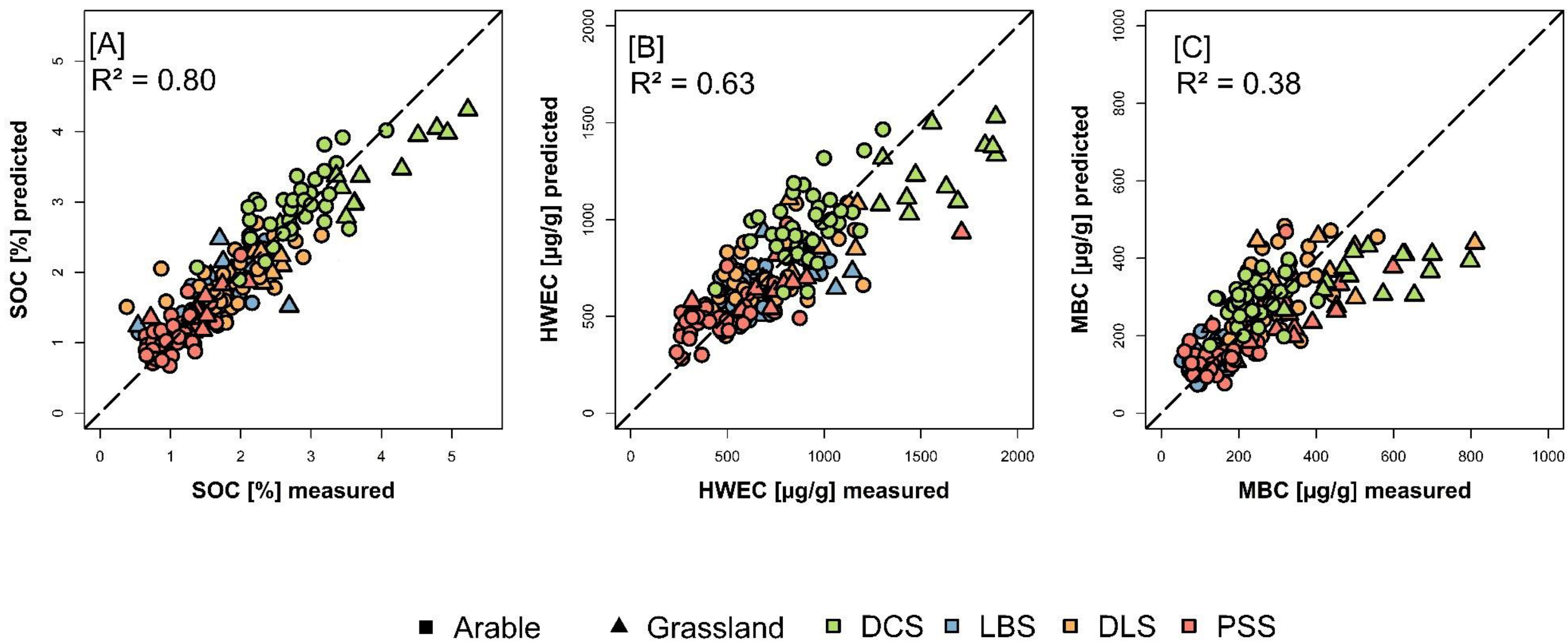
3.2 Bivariate relationships of mineral phase and SOC and its labile fractions

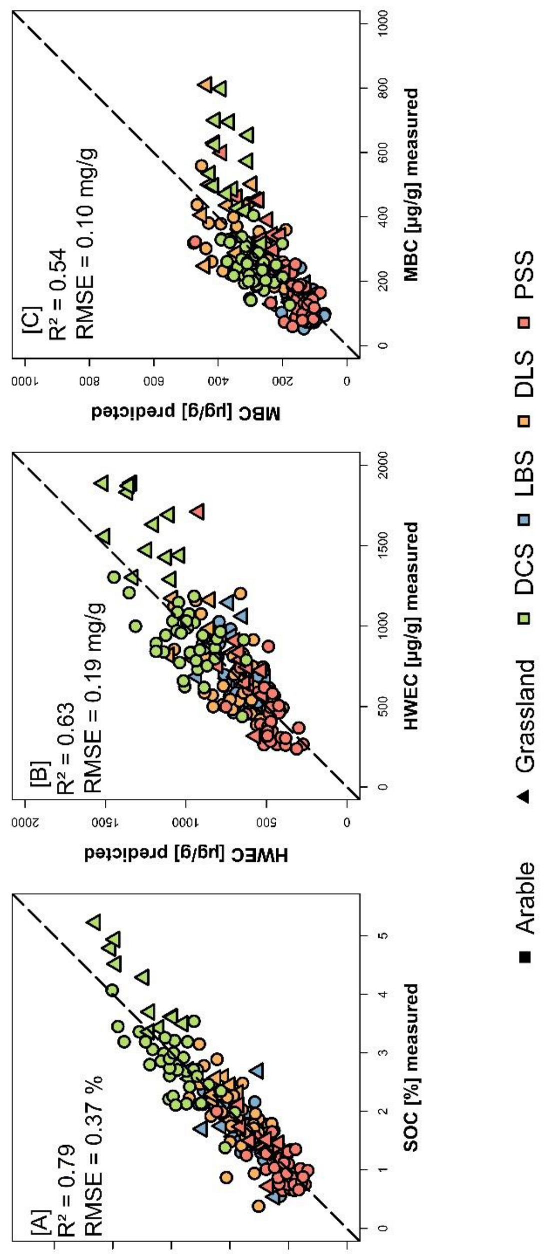
In order to test whether single parameters are suitable predictors of SOC, HWEC and MBC ten independent parameters describing the properties of the soil mineral phase were selected from the dataset (Table 1, Table 3). Bivariate linear ~~R~~regressions were calculated based on the total dataset (n = 199), for further total~~global~~ clusters (e.g. arable or grassland soils) and the local clusters that were identified in PCA, i.e. subgroups based on the four parent ~~rock~~ materials and major texture classes (Table 3). Using the complete dataset, highly significant regressions of SOC, HWEC and MBC to most soil mineral phase parameters were found, yet predominantly at a low level of explained variance (Table 3). Compared to the complete dataset substantially different soil parameters explained SOC, HWEC and MBC especially for smaller clusters such as soils from the parent materials DCS or LBS. Yet, clusters comprising large sample numbers, where soil parameters cover broad ranges such as the clusters of loamy, arable or grassland soils, showed significantly contributing parameters that were largely in line with~~matched with~~ those found as significant for the complete dataset. All clusters differed in their pattern of significant parameters. However, for the complete dataset as well as for the clusters the explained variance decreased from SOC to the labile fractions HWEC and MBC (Fig. 3 and Table 3). Only some properties such as sand. ECEC or $(Ca+Mg)_{ECEC}$ showed for MBC ~~–~~a higher explained variance compared to SOC and HWEC (Table 3). For the entire dataset the content of SOC was best explained by Al_o and Fe_o as predictor parameter (R^2 = 0.~~63~~ 58 and 0.56, respectively) while soil texture related properties such as sand or fSilt plus clay explained SOC on a lower level (Table 3). Other determined mineral phase parameters such as cSilt plus mSilt or ECEC explained variance to a negligible extent (Table 3). With lower values for R^2, HWEC was explained by similar soil mineral phase parameters, as it was the case for SOC. With R^2 of 0.39 and a variance of 0.38 HWEC was best explained by pedogenic oxides (Fe_o and Al_o, Table 3). In contrast, the predictors for MBC were quite distinct. Especially parameters related to soil texture such as fSilt plus clay (R^2 = 0.43) or sand (R^2 = 0.45) better explained the variance of MBC compared to HWEC (R^2 = 0.27 and 0.16, respectively). Nevertheless, none of the applied parameters could explain in all cases the complete variance of SOC, HWEC or MBC to a higher~~sufficient~~ extent ($R^2 > 0.75$). Explained variance of SOC and its labile fractions varied strongly between the parent material clusters. In general, the variance in these clusters was explained to a substantially lower extent compared to the whole dataset (Table 3). In most cases, parameters of soil texture and pedogenic oxides correlated significantly with SOC, HWEC and MBC. Additional to these parameters, $(Ca+Mg)_{ECEC}$ was useful to predict SOC and MBC for some parent material clusters (Table 3). Highest values of R^2 were reached for the regression between SOC and Al_o and Fe_o (0.47, 0.42) in the cluster DCS and fSilt plus clay (0.37) in the cluster PSS. R^2 was even lower in the clusters LBS and DLS with maximum values of 0.21 and 0.20 respectively. Further, the cluster of loamy soils was also best described by parameters representing pedogenic oxides and texture. Much lower R^2 were found for the sandy and silty soil clusters with Al_o and texture parameters (sandy) and additionally Fe_o (silty) as best descriptors. While for SOC, HWEC and MBC mostly the same descriptors were found (yet on different level of R^2), they were partially different for MBC of the clusters silty and loamy soils.

Table 3. Bivariate ~~L~~linear regression coefficient R^2 for parameters explaining the variance of SOC [%], HWEC and MBC [µg kg^{-1}] respectively, for soils groups of different parent material, major textural class and land use

		Fe_o [g kg^{-1}]	Fe_d-Fe_o [g kg^{-1}]	Al_o [g kg^{-1}]	Sand [%]	cSilt + mSilt [%]	fSilt + clay [%]	Stones [%]	ECEC [mmolc kg^{-1}]	$(Ca+Mg)_{ECEC}$ [mmolc kg^{-1}]	pH
All samples											
Dataset n = 199	SOC	0.56***	0.16***	0.58***	0.23***	0.04**	0.46***	0.24***	0.07***	0.05**	0.02
	HWEC	0.39***	0.05**	0.38***	0.16***	0.04**	0.27***	0.11***	0.03*	0.02*	0.06***
	MBC	0.29***	0.07***	0.10***	0.45***	0.29**	0.43***	0.06***	0.29***	0.28***	0.04**
Land use											
Arable n = 150	SOC	0.51***	0.25***	0.61***	0.23***	0.05**	0.46***	0.29***	0.09***	0.05**	0.02
	HWEC	0.37***	0.11***	0.37***	0.18***	0.06**	0.28***	0.17***	0.08***	0.04*	0.03*
	MBC	0.25***	0.15***	0.06**	0.64***	0.52***	0.51***	0.12***	0.61***	0.53***	0.21***
Grassland n = 49	SOC	0.73***	0.08*	0.73***	0.25***	0.02	0.59***	0.44***	0.04	0.04	0.00
	HWEC	0.67***	0.03	0.59***	0.21***	0.02	0.47***	0.30***	0.00	0.00	0.05
	MBC	0.54***	0.07	0.24***	0.41***	0.13**	0.67***	0.15**	0.11*	0.11*	0.00
Parent material											
DCS n = 50	SOC	0.42***	0.25***	0.47***	0.00	0.04	0.03	0.00	0.00	0.00	0.02
	HWEC	0.17**	0.24***	0.17**	0.00	0.01	0.00	0.03	0.00	0.00	0.04
	MBC	0.14**	0.18**	0.06	0.00	0.03	0.01	0.06	0.00	0.00	0.01
LBS n = 50	SOC	0.01	0.11*	0.18**	0.11*	0.11*	0.08*	0.00	0.10*	0.11*	0.10*
	HWEC	0.03	0.03	0.06	0.01	0.01	0.01	0.00	0.05	0.04	0.00
	MBC	0.16**	0.04	0.00	0.21***	0.19**	0.21***	0.00	0.20**	0.17**	0.06
DLS n = 50	SOC	0.03	0.03	0.00	0.02	0.00	0.08*	0.20**	0.20**	0.20**	0.03
	HWEC	0.07	0.05	0.00	0.00	0.00	0.00	0.06	0.04	0.04	0.02
	MBC	0.02	0.00	0.03	0.05	0.00	0.11*	0.08*	0.19**	0.19**	0.06
PSS n = 49	SOC	0.35***	0.00	0.28***	0.36***	0.23***	0.37***	0.04	0.30***	0.27***	0.02
	HWEC	0.20**	0.03	0.21***	0.30***	0.29***	0.20**	0.12*	0.10*	0.09*	0.08*
	MBC	0.15**	0.00	0.28***	0.44***	0.37***	0.35***	0.02	0.16**	0.17**	0.10*
Texture											
Sandy n = 54	SOC	0.00	0.01	0.40***	0.18**	0.19***	0.07	0.01	0.02	0.02	0.04
	HWEC	0.00	0.06	0.29***	0.08*	0.06	0.08*	0.03	0.03	0.04	0.11*
	MBC	0.13**	0.08*	0.04	0.08*	0.12*	0.00	0.00	0.07	0.05	0.01
Silty n = 42	SOC	0.25***	0.02	0.33***	0.01	0.22***	0.27***	0.00	0.03	0.03	0.01
	HWEC	0.20**	0.00	0.12*	0.00	0.08	0.08	0.04	0.01	0.02	0.04
	MBC	0.01	0.06	0.00	0.16**	0.00	0.07	0.05	0.17**	0.19**	0.06
Loamy n = 89	SOC	0.63***	0.16***	0.70***	0.41***	0.01	0.56***	0.36***	0.04*	0.02	0.10**
	HWEC	0.36***	0.02	0.36***	0.20***	0.01	0.24***	0.13***	0.00	0.00	0.15***
	MBC	0.08**	0.00	0.04*	0.12***	0.02	0.13***	0.00	0.14***	0.15***	0.00

Fig. 3. Predicted vs. measured content of SOC [A], HWEC [B] and MBC [C] for the global (complete) dataset, based on mixed effect models. Parent materials are Devonian clay schist (DCS), sandy dolomitic limestone (DLS), Luxemburg sandstone (LBS), and Permian siltstone and fine sandstone (PSS).




[A]
R² = 0.79
RMSE = 0.37 %
SOC [%] predicted
SOC [%] measured
[B]
R² = 0.63
RMSE = 0.19 mg/g
HWEC [µg/g] predicted
HWEC [µg/g] measured
[C]
R² = 0.54
RMSE = 0.10 mg/g
MBC [µg/g] predicted
MBC [µg/g] measured
Arable
Grassland
DCS
LBS
DLS
PSS

Comprising soils from all identified clusters, the sets of descriptor parameters of the land use clusters were comparable to those of the total~~global~~ dataset (Table 3). Yet, the variance of SOC and its labile fractions were explained~~,~~ by bivariate linear regressions~~,~~ to a much higher extent for the total~~global~~ dataset and the clusters of arable soils and especially grassland soils compared to the clusters based on parent material and texture (Table 3). ~~Both~~ The clusters of both land use types largely overlapped and contained a similar proportion of samples from each parent material.~~include an equal weight of samples from each parent material~~ Therefore they can ~~be regarded~~act as total~~global~~ clusters. While SOC was explained by ~~complex~~ interactions of ~~several~~ numerous different parameters (up to eight) for the distinct ~~fractions~~factors, less variables showed a significant contribution to explain the variability of HWEC and MBC (Table 3).

3.3 Estimation of SOC and its labile fractions by mixed effect models

Since bivariate linear models insufficiently explained SOC, HWEC and MBC, respectively, mixed effect models were developed. In these models, mineral phase parameters were applied as fixed effects, and land use, parent material and texture were used as random effects (Table 4, Fig. 4 and Fig. 5). Variability of SOC, HWEC and MBC were much better explained than by linear regressions indicating that organic matter depends on complex interactions of several components of the mineral phase. ~~In general,~~ Based on marginal effects~~, of~~ the mixed effect models ~~mostly~~ explained the variance in most cases in the order SOC > HWEC > MBC (Fig. 3~~, and~~ Table 4 and Table 5). ~~By t~~The mixed effect models~~, R^2_{cond}~~ reached a higher explained variance and mostly lower RMSE for SOC (R^2_{cond} = 0.39-0.89, RMSE = 0.21 – 0.42 %) compared to the bivariate regressions (R^2 = 0.00-0.73, RMSE = 0.27-1.12 %). Data for RMSE are listed in Table SI3. ~~Also~~Accordingly, the mixed effect models ~~for HWEC and MBC~~ yielded a~~nd~~ higher explained variance for HWEC and MBC~~was estimated by the mixed effect models~~. Representing the explained variance of the fixed effects, the R^2_{marg} revealed~~,~~ for the majority of the clusters~~,~~ a large~~r parts of the~~ explained variance. ~~Anyhow,~~But even in the cases ~~-~~of low R^2_{marg} several of that clusters ~~provide~~had a high R^2_{con} ~~even if R^2_{marg} was low~~. This highlights the ~~overall importance~~relevance of the random effects (Table 4). ~~By a~~Applying different random effects resulted in large differences ~~, explained variance~~in ~~(~~R^2_{cond}~~) differed larger~~ for some clusters (e.g., 'sandy soils'). In particular, modelling the labile fractions w~~ere~~as more affected by the different random effects, showing ~~in majority~~mostly highest R^2_{cond} values if land use was applied as random effect. ~~RMSE of the mixed effect models was mostly lower compared to the bivariate linear regression (Table SI3).~~

Independent from the applied random effect, explained variance increased with sample number and width of the data range of parameters. Consequently, best model performance was achieved for the complete dataset as well as for the total clusters. Similar model performance was only found for some local clusters (e.g. DCS), while models for other local clusters such as LBS, DLS or sandy soils revealed the poorest, yet still sufficient (R_{cond} ≥ 0.39, RMSE ≤ 0.40 %) estimates of SOC (Table 4). In general, applying random effects such as parent material, land use or texture for mixed effect models led to distinct results for the prediction of SOC, HWEC or MBC (Table 4). For clusters according to land use variance was explained to a high extent (mean R^2_{con} of 0.66 and 0.77 for cluster of arable soils and grassland, respectively). Models using parent material or texture as random effect mostly showed minor differences for predictions of SOC, HWEC or MBC. Anyhow for some local clusters (e.g. DCS, LBS and DLS) distinct results were found. Models using land use as random effect were partly distinct, though, indicating the different influence of land use on SOC and its labile fractions (Table 4).

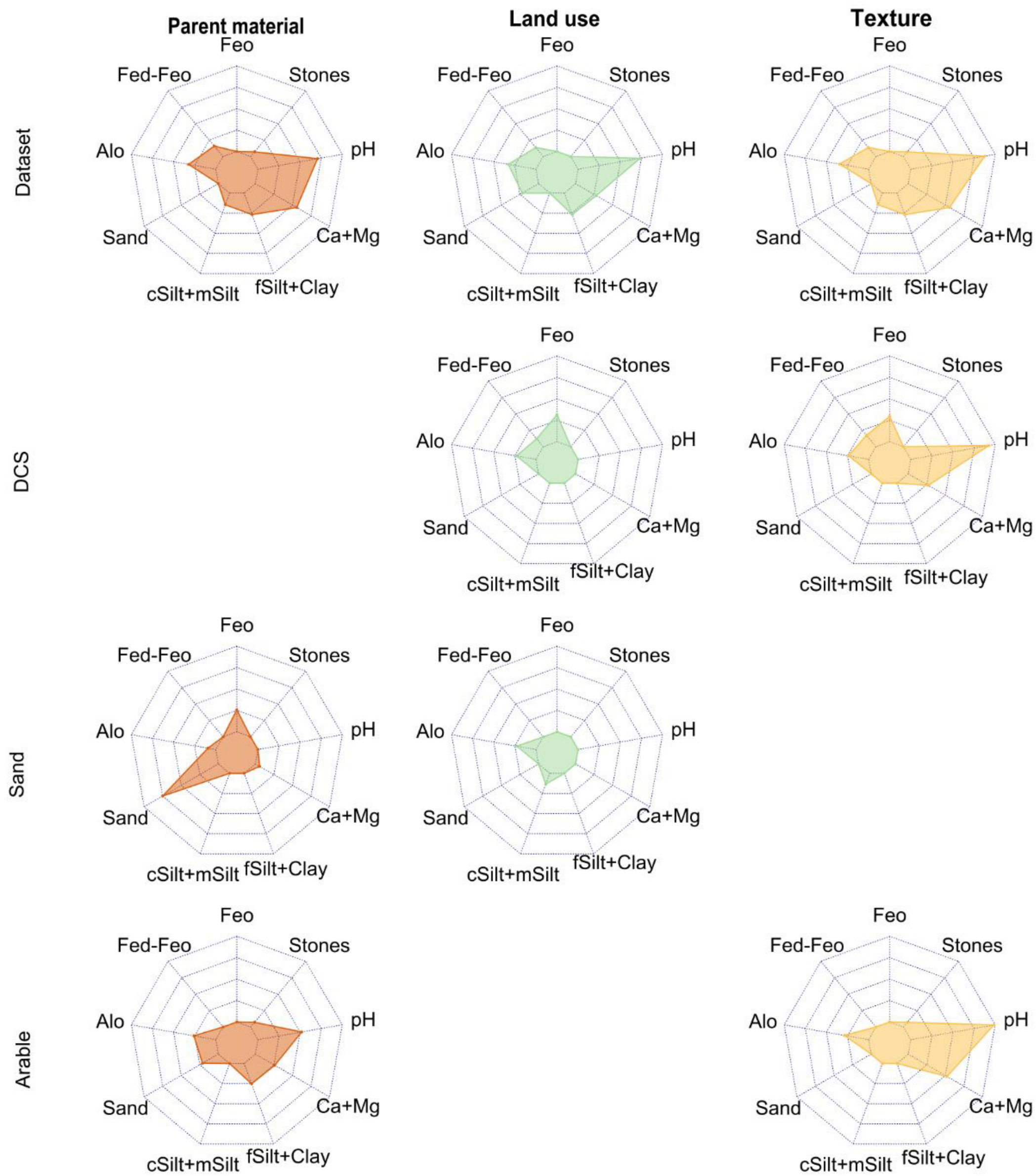
The different mixed effects models particularly comprised variables (Fig. 4, Fig. 5) that also proved significant in the bivariate linear regressions (Table 3). Mineral phase parameters contributed with different significance to the models for SOC, HWEC and MBC. The SOC and HWEC were primarily explained by pedogenic oxides followed by soil texture related parameters. Not least, soil acidity specified by pH and $(Ca+Mg)_{ECEC}$ was also relevant. MBC, compared to SOC or HWEC, was better explained by parameters linked to soil texture. Contribution of the variables, on SOC and its labile fraction was visualized using the mean values multiplied with their coefficients (Fig. 4, Fig 5). Distinct significant parameter combinations explaining SOC, HWEC and MBC were also found between the total data set and local clusters (Table 3, Fig. 4 and Fig. 5, SI Table 2). For example, within the soil texture related clusters pedogenic oxides, $(Ca+Mg)_{ECEC}$, pH and texture parameters were relevant to estimate SOC, HWEC and MBC (Table 3, Fig. 4 and Fig. 5). Regarding the random effects, applied mixed effect models using parent material as random effect explained variability of SOC best (Table 4). For MBC and HWEC, however, highest explained variance were mostly obtained with land use as random effect (Table 4). Only estimates of HWEC for the texture clusters were better when parent material was used as random effect.

~~Measured and predicted data using the mixed effect models showed a close relationship along the 1:1 prediction line while scatter increased at higher contents of HWEC and especially of MBC, showing that estimates for grassland soils were inferior. Anyhow,~~ bivariate linear regression~~correlations between measured data and predictions~~ predicted data from~~of the mixed effect models (R^2 = 0.29-0.91) were mostly higher than for bivariate linear regressions (R^2 = 0.00 – 0.73). Independent from the applied random effect, precision of prediction results increased with sample number and data range of parameters, respectively. Consequently, best model performance was achieved for the complete dataset as well as for some of the local clusters (e.g. DCS, loamy soils), while models for other local clusters such as LBS, DLS or sandy soils revealed the poorest estimates of SOC (Table 4). In general, applying random effects such as parent material, land use or texture for mixed effect models led to distinct results for the prediction of SOC, HWEC or MBC (Table 4). For clusters according to land use variance was explained to a high extent (mean R^2 of 0.68 and 0.80 for cluster of arable and grassland respectively). Models using parent material or texture as random effect mostly showed minor differences for predictions of SOC, HWEC or MBC. Models using land use as random effect were partly distinct, though, indicating the different influence of land use on SOC and its labile fractions (Table 4).~~

Table 4. R^2_{marg} and R^2_{con} of the models for SOC, HWEC, and MBC based on the results of mixed effect models.

	Land use						Parent material						Texture					
	SOC		HWEC		MBC		SOC		HWEC		MBC		SOC		HWEC		MBC	
	R^2_{marg}	R^2_{con}	R^2_{marg}	R^2_{con}	R^2_{marg}	R^2_{con}	R^2_{marg}	R^2_{con}	R^2_{marg}	R^2_{con}	R^2_{marg}	R^2_{con}	R^2_{marg}	R^2_{con}	R^2_{marg}	R^2_{con}	R^2_{marg}	R^2_{con}
Data	0.74	0.76	0.48	0.65	0.39	0.78	0.65	0.78	0.47	0.59	0.57	0.59	0.76	0.76	0.56	0.59	0.51	0.57
Arable							0.62	0.77	0.37	0.55	0.72	0.72	0.71	0.71	0.5	0.51	0.69	0.71
Grassland							0.85	0.89	0.43	0.71	0.72	0.74	0.88	0.88	0.65	0.65	0.72	0.77
DCS	0.38	0.82	0.10	0.84	0.03	0.89							0.52	0.73	0.31	0.68	0.17	0.72
LBS	0.40	0.43	0.13	0.36	0.21	0.57							0.39	0.39	0.27	0.27	0.1	0.46
DLS	0.48	0.48	0.33	0.34	0.14	0.42							0.48	0.48	0.35	0.37	0.25	0.25
PSS	0.57	0.58	0.31	0.61	0.09	0.86							0.50	0.59	0.54	0.56	0.42	0.56
Sandy soils	0.52	0.52	0.45	0.48	0.15	0.75	0.13	0.85	0.29	0.61	0.21	0.35						
Silty soil	0.69	0.69	0.65	0.65	0.39	0.47	0.43	0.73	0.33	0.86	0.45	0.45						
Loamy soils	0.75	0.81	0.47	0.67	0.19	0.75	0.55	0.76	0.49	0.56	0.41	0.41						
Mean	0.57	0.65	0.36	0.57	0.20	0.69	0.54	0.80	0.40	0.65	0.52	0.54	0.61	0.65	0.45	0.52	0.41	0.58

Fig. 4. Coefficients of the mixed effect models to predict SOC, multiplied with the mean values of the specific cluster indicating the impact of the applied variables. Differentiation into clusters and used random factors. Variables are scaled from 0 to 1.


Parent material
Land use
Texture
Dataset
DCS
Sand
Arable
Feo
Stones
pH
Ca+Mg
fSilt+Clay
cSilt+mSilt
Sand
Alo
Fed-Feo

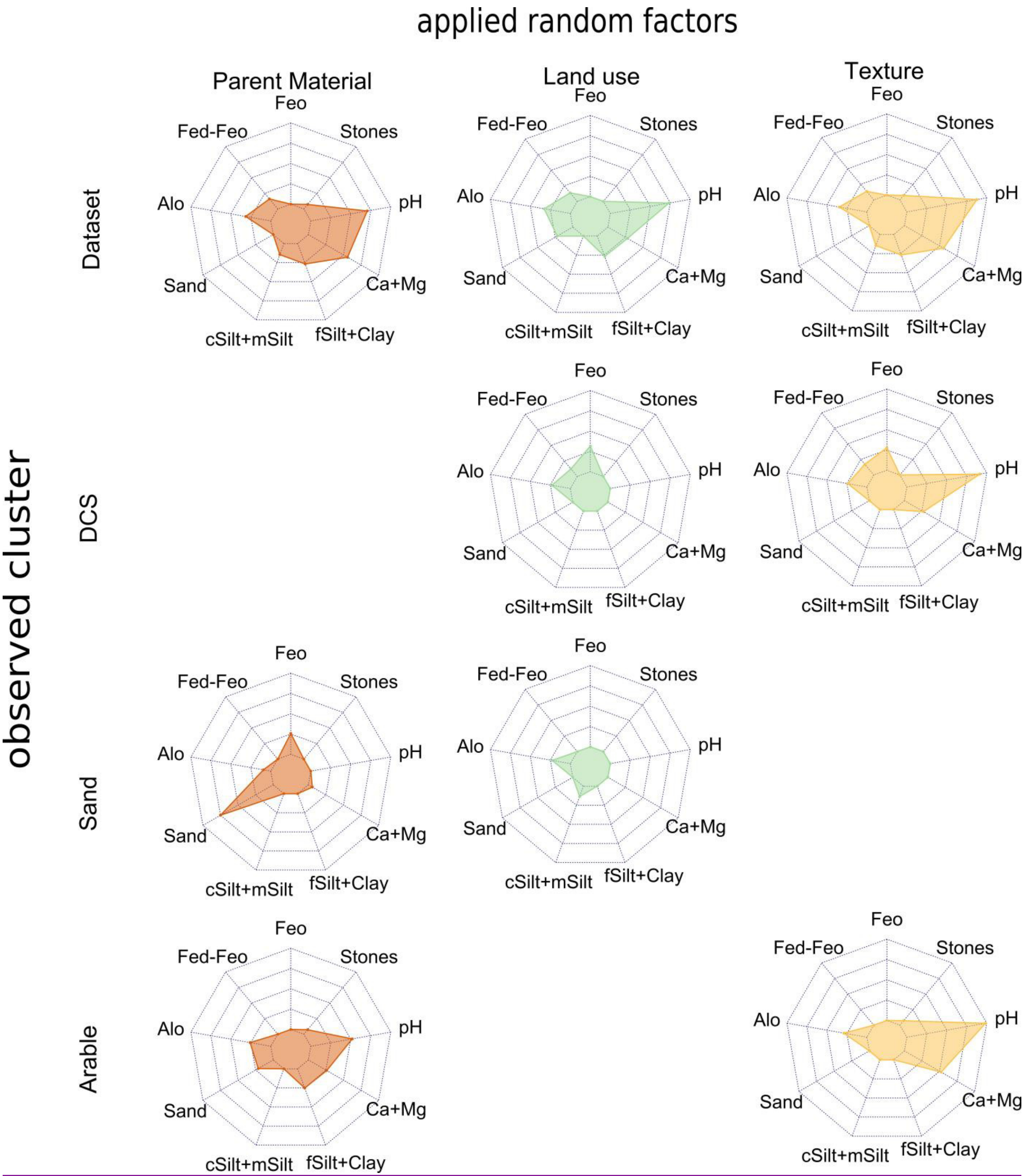
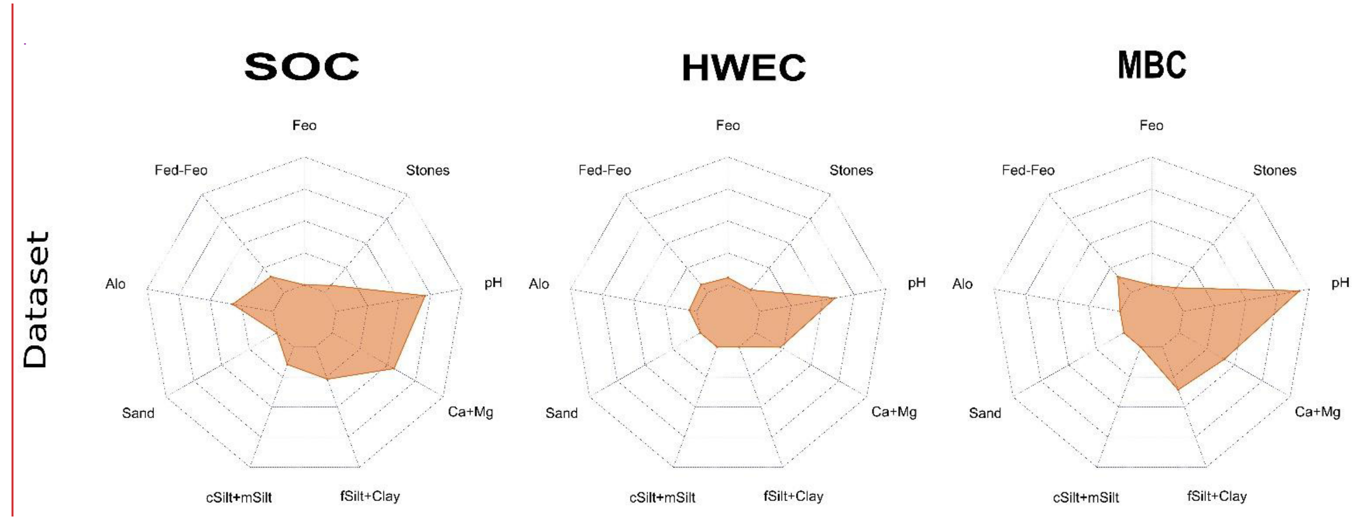
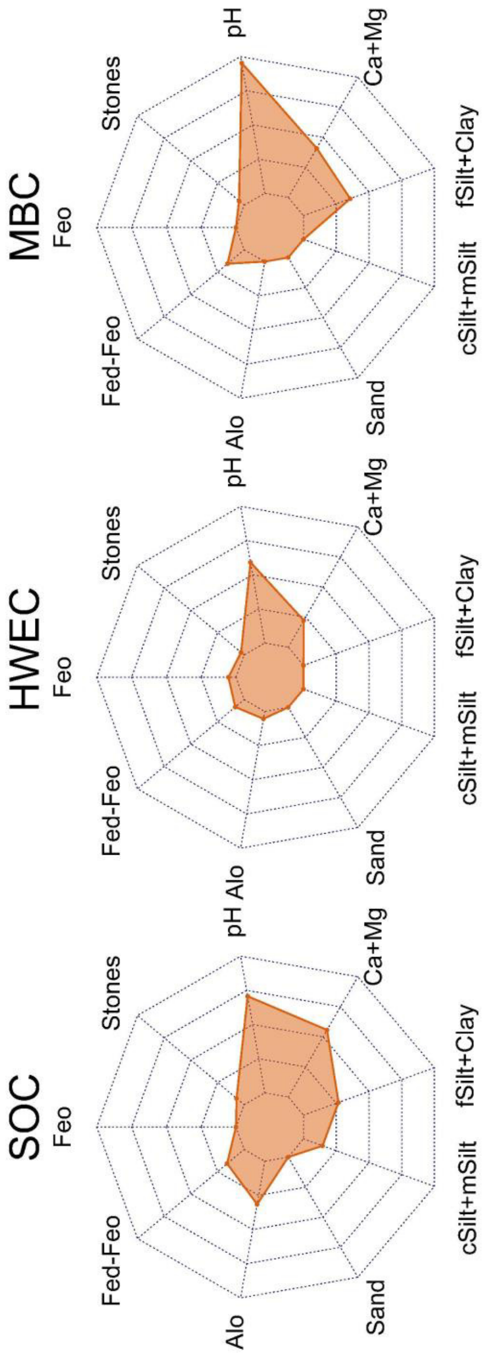

applied random factors
Parent Material
Land use
Texture
observed cluster
Dataset
DCS
Sand
Arable
Feo
Stones
pH
Ca+Mg
fSilt+Clay
cSilt+mSilt
Sand
Alo
Fed-Feo

Fig. 5. Comparison of the coefficient impact for mixed effect models to predict SOC, HWEC and MBC for the entire dataset by using parent material as random factor. Variables are scaled from 0 to 1.




SOC
Feo
Fed-Feo
Alo
Stones
pH Alo
Sand
Ca+Mg
cSilt+mSilt
fSilt+Clay
HWEC
Feo
Fed-Feo
Stones
pH Alo
Sand
Ca+Mg
cSilt+mSilt
fSilt+Clay
MBC
Feo
Fed-Feo
Stones
pH
Sand
Ca+Mg
cSilt+mSilt
fSilt+Clay

3.4 Comparison of total and local explained variability.

~~The different mixed effects models particularly comprised variables (Fig. 4, Fig. 5) that also proved significant in linear regressions (Table 3). Mineral phase parameters contributed with different significance to the models for SOC, HWEC and MBC. The SOC and HWEC were primarily explained by pedogenic oxides followed by soil texture related parameters. Not last, soil acidity indicated by pH and $(Ca+Mg)_{ECEC}$ was also relevant. MBC, compared to SOC or HWEC, was better explained by parameters linked to soil texture. Contribution of the variables, on SOC and its labile fraction was visualized using the mean values multiplied with their coefficients (Fig. 4, Fig 5). Distinct significant parameter combinations explaining SOC, HWEC and MBC were also found between the global data set and local clusters (Table 3,Fig. 4 and Fig. 5, SI Table 2). For example, within the soil texture related clusters pedogenic oxides, $(Ca+Mg)_{ECEC}$, pH and texture parameters were relevant to estimate SOC, HWEC and MBC~~ (Table 3, Fig. 4 and Fig. 5)~~. Regarding the random effects, applied mixed effect models using parent material as random effect explained variability of SOC best~~ (Table 4)~~. For MBC and HWEC, however, best model fits were mostly obtained with land use as random effect~~ (Table 4)~~. Only estimates of HWEC for the texture clusters were better when parent material was used as random effect.~~

Predictions for SOC, HWEC and MBC were conducted based on the mixed effects models. Subsequent linear regression between measured and predicted data showed a close relationship along the 1:1 prediction line leading to a high explained variance (Fig. 3, Table 5). For these regressions the explained variance was mostly ~~comparable~~similar to R^2_{con}. Especially for the total clusters, i.e. ~~all~~ the total dataset and data clustered according to arable or grassland land use, best results were ~~found~~obtained.

~~The R^2 of model predictions was best for the global clusters tested in this study, i.e. all data and data clustered according to arable or grassland land use.~~ Yet, this was at least partly due to a larger sample size and a broader range of parameter values compared to the various local clusters. Applying a~~the~~ total~~global~~ model for SOC estimation to a smaller local cluster data set clearly revealed an inferior explained variance~~performance~~ of the total~~global~~ compared to the local model (Fig. 6). Alongside with decreasing explained variance, RMSE values were mostly increasing if a total model ~~of a total dataset~~ was applied to a local dataset. The higher explained variance~~better performance~~ of specific local models and parameter combinations was also found for other local clusters (Table 6~~5~~ and SI Table ~~3~~4).

By transferring a total model to local clusters, the explained variance differed~~s~~ for SOC by up to 20 % while RMSE differed by up to 0.25 %. ~~mlocal~~ ~~Even if~~Also in case a total model was transferred to a local dataset to estimate HWEC or MBC, the explained variance decreased ~~and RMSE mostly increased. Thereby, explained variance decreased~~ by up to 17 % for HWEC and MBC. The RMSE increased by up to 0.07 ~~or~~and 0.06 mg g^{-1} for HWEC and MBC, respectively.

Table 5. R^2 and RMSE of the models for prediction of SOC, HWEC, and MBC based on the results of mixed effect models. RMSE is given in % for SOC and in ~~µ~~mg/g for HWEC and MBC.

		Parent material$^+$			Land use$^+$			Texture$^+$			Mean model prediction
Sample		SOC	HWEC	MBC	SOC	HWEC	MBC	SOC	HWEC	MBC	R^2
Dataset	R^2	0.79*	0.63*	0.55*	0.77*	0.68*	0.71*	0.77*	0.61*	0.56*	0.67*
	RMSE	0.37	0.19	0.10	0.41	0.18	0.08	0.42	0.20	0.10	0.40 % / 0.14 mg g^{-1}
Land use											
Arable	R^2	0.80*	0.59*	0.70*				0.72*	0.53*	0.71*	0.68*
	RMSE	0.33	0.15	0.05				0.39	0.16	0.05	0.36 % / 0.10 mg~~/~~ g^{-1}
Grassland	R^2	0.91*	0.78*	0.76*				0.89*	0.67*	0.76*	0.80*
	RMSE	0.33	0.19	0.09				0.36	0.24	0.09	0.35 % / 0.15 mg~~/~~ g^{-1}
Parent Material											
DCS	R^2				0.81*	0.78*	0.79*	0.74*	0.62*	0.55*	0.72
	RMSE				0.34	0.17	0.07	0.40	0.22	0.11	0.37 % / 0.14 mg~~/~~ g^{-1}

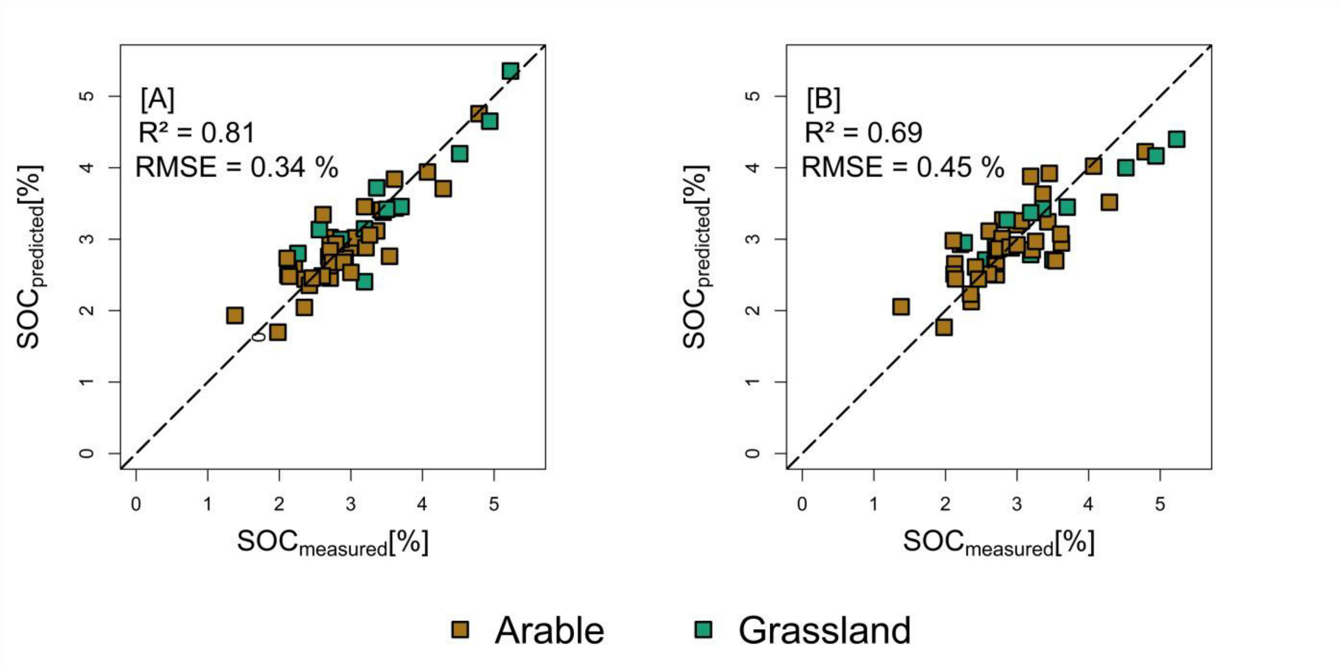
LBS	R^2				0.43*	0.27*	0.48*	0.41*	0.29*	0.41*	0.38
	RMSE				0.30	0.14	0.03	0.30	0.14	0.03	0.30 % / 0.09 mg~~/~~ g^{-1}
DLS	R^2				0.50*	0.36*	0.32*	0.50*	0.37*	0.26*	0.39
	RMSE				0.35	0.17	0.10	0.35	0.17	0.10	0.35 % / 0.13 mg~~/~~ g^{-1}
PSS	R^2				0.61*	0.62*	0.74*	0.63*	0.56*	0.60*	0.62
	RMSE				0.21	0.16	0.06	0.20	0.16	0.07	0.21 % / 0.11 mg~~/~~ g^{-1}
Texture											
Sandy	R^2	0.79*	0.61*	0.28*	0.54*	0.51*	0.58*	-	-	-	0.55
	RMSE	0.21	0.12	0.04	0.31	0.14	0.03				0.26 % / 0.08 mg~~/~~ g^{-1}
Silty soils	R^2	0.74*	0.75*	0.48*	0.72*	0.66*	0.50*	-	-	-	0.64
	RMSE	0.39	0.14	0.09	0.40	0.16	0.08				0.40 % / 0.12 mg~~/~~ g^{-1}
Loamy	R^2	0.83*	0.59*	0.41*	0.81*	0.66*	0.64*	-	-	-	0.66
	RMSE	0.35	0.20	0.10	0.38	0.19	0.08				0.37 % / 0.14 mg~~/~~ g^{-1}
Mean model prediction											
Mean	R^2	0.81	0.66	0.53	0.65	0.57	0.59	0.67	0.52	0.55	
	RMSE	0.33	0.17	0.08	0.34	0.16	0.07	0.35	0.18	0.08	

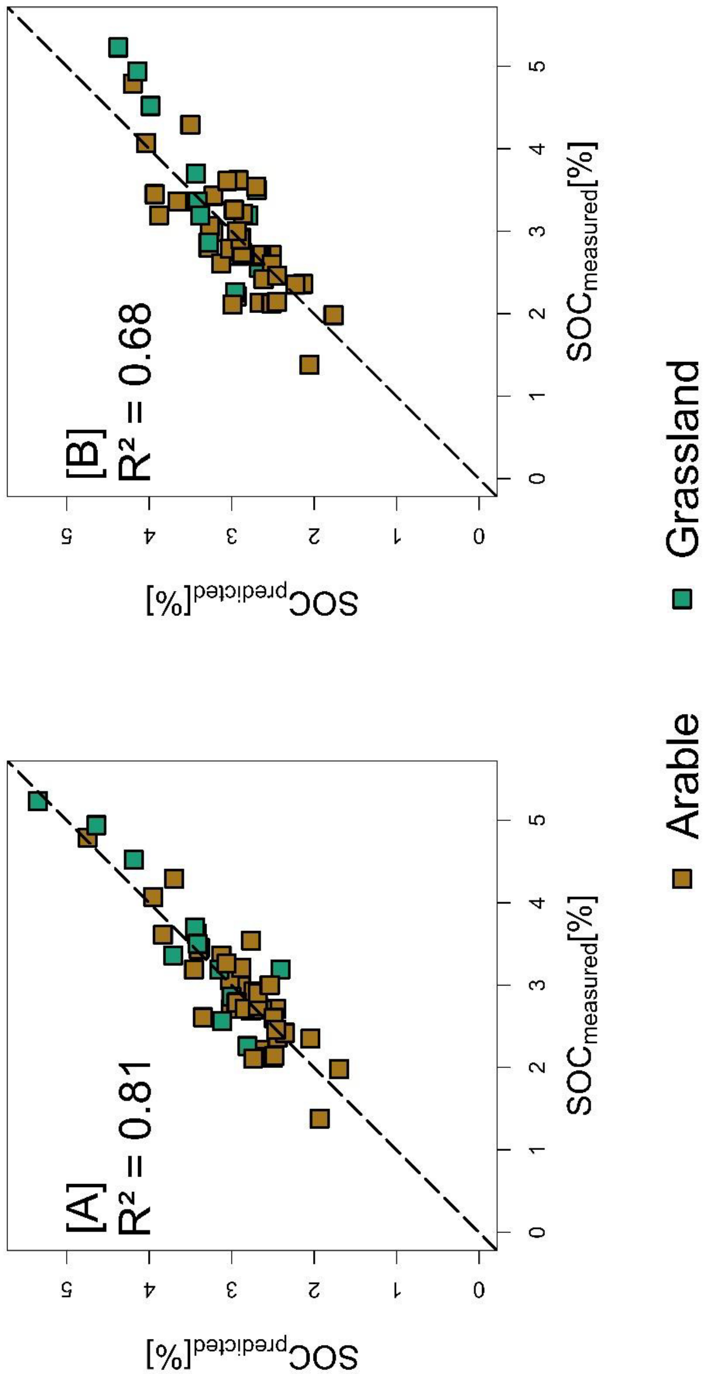
+Applied random effect; ˜Not all random effects could applied to this group of clusters because of missing factor levels. *Significant on a level of <0.05

Table ~~5~~6. R^2 and RMSE for implementation of the total~~global~~ dataset to local clusters to estimate SOC.

SOC							
		Parent material		Land use		Texture	
Sample subgroups		Cluster specific ~~M~~model	total~~Global~~ model to local cluster	Cluster specific m~~M~~odel	total~~Global~~ model to local cluster	Cluster specific m~~M~~odel	total~~Global~~ model to local cluster
Dataset	R^2	0.79		0.77		0.77	
	RMSE	0.37		0.41		0.42	
DCS	R^2	-		0.81	0.69	0.74	0.65
	RMSE			0.34	0.44	0.40	0.47
LBS	R^2	-		0.43	0.23	0.41	0.24
	RMSE			0.30	0.41	0.30	0.40
DLS	R^2	-		0.50	0.30	0.50	0.35
	RMSE			0.35	0.42	0.35	0.41
PSS	R^2	-		0.61	0.57	0.63	0.57
	RMSE			0.21	0.38	0.20	0.38
Sandy soils	R^2	0.79	0.68	0.54	0.37	-	
	RMSE	0.21	0.26	0.31	0.36		
Silty soils	R^2	0.74	0.65	0.72	0.60	-	
	RMSE	0.39	0.45	0.40	0.48		
Loamy soils	R^2	0.83	0.83	0.81	0.79	-	
	RMSE	0.35	0.36	0.38	0.40		
Arable	R^2	0.80	0.80			0.72	0.73
	RMSE	0.33	0.34			0.39	0.39
Grassland	R^2	0.91	0.87			0.89	0.87
	RMSE	0.33	0.44			0.36	0.47

Fig. 6. Predicted vs. measured content of SOC of soil samples from the DCS cluster; predictions based on the local model [A] and the global model [B].




[A]
R² = 0.81
[B]
R² = 0.68
SOC predicted [%]
SOC measured [%]
Arable
Grassland

4 Discussion

Our study showed that interactions of SOC with the mineral phase are highly relevant for the content of SOC as well as of its labile fractions HWEC and MBC in soils. High ~~correlations~~ regression coefficients of SOC to fSilt plus clay (Table 3) agree with reports on the relevance of organo-mineral associations for the stabilization of SOC and related to this the accumulation of the labile fraction HWEC and MBC (Lützow et al., 2006). Furthermore, sandy soils contained the lowest content of SOC while loamy and silty soils had an equally higher content of SOC (Table 1). This is typically expected and confirms numerous previous reports, e.g. Ludwig et al. (2003) and Vos et al. (2018). In contrast, for the LBS cluster with its very sandy soils~~,~~ a slightly positive effect of sand on SOC was found. ~~for the in total very sandy soils in the parent material cluster of LBS.~~ This, however, is most likely a consequence of agricultural practice, with high manure application to the LBS soils in the sampled area. This was further confirmed by a factor of 1.2 higher ratios of SOC/N and HWEC/N as well as by a lower oxygen content of SOM compared to soils of the other parent material clusters (factor of 0.6; Table 1). Besides parameters directly related to soil texture, pedogenic Al- and Fe-oxides were found to be strong predictors of SOC in soils. Accordingly, Al- and Fe-oxides were shown to have a relevant influence on the accumulation ~~the sequestration~~ and stabilization of SOC (Kaiser and Guggenberger, 2000; Lützow et al., 2006) as well as to have a high affinity to retain components of the labile SOC fractions (Kaiser and Zech, 1998; Kaiser et al., 2002). Although soil acidity strongly affects soil processes such as microbial activity and turnover that are relevant for SOC accumulation (Kemmitt et al., 2006), no clear ~~regression~~relation ~~coefficients~~~~correlation~~ between pH and SOC or its labile fractions was found by bivariate linear regression. Yet, soil parameters that are strongly related to soil acidity, i.e. ECEC as well as the content of exchangeable polyvalent cations such as Ca^{2+} and Mg^{2+}, were suitable predictors for SOC and its labile fractions in this and previous studies (O'Brien et al., 2015; Rasmussen et al., 2018). This is causally explained by the stabilization of SOC in organo-mineral associations and the contribution of multivalent cation bridges (Ca^{2+} and Mg^{2+}) to it (Kaiser et al., 2012). The ~~minor ability of ECEC and (Ca+Mg)$_{ECEC}$ and the~~even higher ability of the content of pedogenic oxides to explain variance of SOC and its labile fractions was indicated in this study for several clusters (total and local) by bivariate regressions (Table 3~~),~~). This corresponds to findings of Rasmussen et al. (2018). They found a prevalence of pedogenic oxides in humid areas with moderately acidic soils, while exchangeable Ca and clay ~~prevealed~~ prevailed in soils of dry climates with circumneutral to alkaline pH. Such a case-specific prevalence of parameters to predict SOC, HWEC or MBC demonstrates that it is preferred to use specific parameter sets when it is aimed to focus on local areas. In this study~~Ability of~~ ECEC and (Ca+Mg)$_{ECEC}$ were not generally applicable as predictors but it ~~was further~~ strongly depende~~nt~~d on the ~~observed~~ parent material ~~or~~and texture cluster. For example, ECEC and (Ca+Mg)$_{ECEC}$ were found to be relevant for the clusters of DLS and PSS, while for DCS they were of minor importance. ~~More often than ECEC the was in mixed effect modelsThis showsn using combined snce ofSOC, HWEC or MBC better~~. ~~As example ECEC and (Ca+Mg)$_{ECEC}$ was found as relevant for the clusters of DLS and PSS, while for DCS it show a minor importance.~~ The bivariate models revealed that the stone content had only a small impact on SOC, HWEC and MBC. Hence, a funnel effect of the stone content, by funneling more SOC into the remaining fine textured soil (Bornemann et al., 2011) was irrelevant. The combinations of factors and soil properties affecting SOC and SOC fractions, respectively, were dissimilar between the different local areas investigated in this study. The PCA revealed that differences according to parent material and soil texture were most relevant to separate the dataset into various local clusters based on different factors (Fig. 2 A and B; Table 2). At the same time, this illustrates the importance of the mineral composition (parent material) and grain size (soil texture) for the accumulation of SOC as well as its labile fractions HWEC and MBC. In contrast, land use was not useful for a separation into clusters. This was unexpected because typically topsoils under grassland have higher SOC contents compared to arable soils (Poeplau et al., 2020), which was largely confirmed for the samples investigated in this study (Table 1). This went along with differences in the composition of SOM (Table 1 and Table SI). However, data ranges of SOC, HWEC and MBC contents were largely overlapping and similarities even increased in PCA when further soil properties were included. In comparison, mineral phase soil properties clearly separated the dataset~~ while composition of SOM was less enabled for this purpose~~. Consequently, a broad scatter of the land use clusters was obtained by PCA, suggesting to treat the land use clusters as total~~global~~ datasets as well.

Several studies with large datasets covering national or continental scales, e.g. soil inventories, pointed out the relevance of combinations of multiple factors and parameters instead of using single predictors to estimate SOC or its labile fractions (Wieder et al., 2015; Vos et al., 2018; Gray et al., 2019)~~ (Vos et al., 2018)~~. Furthermore, local studies covering small areas with narrow ranges of soil properties often show weak bivariate relationships between SOC and components of the mineral phase or environmental factors (Jian-Bing et al., 2006; Liddle et al., 2020). Accordingly, models focused on specific local clusters and combined with multiple parameter sets were superior compared to the total~~global~~ model that was developed for the total~~global~~ ~~(complete)~~(entire) dataset to estimate SOC, HWEC or MBC (Fig. 6). The different parameter combinations indicate that distinct properties of the mineral phase control SOC, HWEC and MBC in the soils of the different clusters.

Understanding SOC as continuum (Lehmann and Kleber, 2015) implies that accumulation of SOC is a multidimensional process with various interacting factors and soil properties, respectively. The substantially lower ability of bivariate models to estimate SOC compared to multiple parameter models is in line with~~confirmed~~ this assumption. Accordingly, it was superior to use multiparameter mixed effect models to estimate SOC and the two labile fractions. Especially parameter combinations within the land use clusters gained a high-explained variance (Table 3, Table 4). A comparison with studies on regional or national scale (Vos et al., 2018; Mayer et al., 2019) suggests that the importance of factors such as land use, soil texture or parent material varies with the observed scale. Wiesmeier et al. (2019) reported that soil texture, land use and land management are relevant to explain SOC variability at all scales. On regional or larger scale, also environmental factors such as climate, geology, soil use, topography are relevant for SOC. Yet, at a local or smaller scale factors such as climate become less important, while parameters representing small-scale soil physico-chemical properties gain importance for explaining the variability of SOC. Thereby, different factor and parameter combinations were identified for the different local clusters by mixed effect modelling. The prevalence of a parameter for quantification of SOC can differ dependent on environmental factors (Rasmussen et al., 2018).

Consequently, the quality of the multiparameter models was further improved by the implementation of local specific random effects such as parent material or land use. Dependent on the random factors parent material, soil texture class and land use different parameter combinations explained SOC, HWEC or MBC (Fig. 4 and Fig. 5). For the total~~global (complete)~~ dataset, nearly all predictor parameters showed a significant contribution to the explanation of SOC. Most of these soil mineral phase parameters were also significant in linear regression. In contrast to the bivariate models, most mixed effect models revealed parameters related to soil acidity as significantly important to estimate SOC, HWEC and MBC. This highlights the importance of soil acidity on SOC dynamics due to its effects on the reactivity of the mineral phase and the activity of microorganisms (Hillel, 2004). In order to explain the variability of HWEC and MBC for the various local clusters, different combinations of mineral phase parameters were required that also clearly differed from the parameter combinations used in the models for SOC (Fig. 4 and Fig. 5). Such differences concerning significantly contributing parameters were also found by other studies for specific clusters or local sampling sites (Heinze et al., 2018; Quesada et al., 2020). This emphasizes that local models are required and superior when it is the aim to estimate SOC and SOC fractions on a local scale. The total~~global~~ models used for the total~~global~~ datasets in this study reached the best predictions for SOC, HWEC and MBC. ~~Nevertheless some local cluster revealed a smaller RMSe than the total clusters.~~ Yet, this was largely biased by the large samples size; applying the same total~~global~~ models to local samples sets produced clearly poorer estimates compared to the more specific local models as indicated by the explained variance and the RMSE (Fig. 6; Table 4~~5~~ and Table 6~~5~~). ~~This was found even for the explained~~

~~variance as well as for the RMSE.~~ Consequently, aggregation of smaller datasets, e.g. from a local scale, to a larger dataset enables to predict SOC and its labile fractions to a ~~satisfying~~ higher extent. In opposite a model that was derived from a total~~global~~ dataset and is applied to ~~the~~ a local ~~area and its~~ dataset with ~~defined~~ smaller ranges of properties is ~~partially practicable~~less suitable, resulting in a variance explained on a lower level. ~~Dependend~~Depend~~ent~~ing on the properties of the soil mineral phase, each specific cluster was controlled by other properties, which best explain the accumulation of SOC and its labile fractions. This implies the importance for analysis of local clusters to avoid a subordination by models of total~~global~~ datasets.

Comparing the results of mixed effect models using the different random effects (parent material, soil texture, land use), the models using parent material yielded highest explained variance~~best results~~ for the estimation of SOC. For HWEC and MBC best predictions at a high ~~sufficient quality~~ level of explained variance were obtained by models using land use as random effect (Table 4). ~~RMSE was mostly in line with founding concerning explained variance.~~ High explained variance ~~resulted~~ mostly ~~in~~went along with smaller RMSE values. The parent material predefines the boundaries for accumulation and stabilization of organic matter (Gray et al., 2015). The importance of land use as random effect especially for the labile fractions results from the fact that these are especially influenced by soil management (Cardoso et al., 2013; Lal, 2016).

In general, the variance explained by the mixed effect models was not similar, but varied between SOC and its labile fractions HWEC and MBC. It became clear that SOC and the labile fractions HWEC and MBC are not fully correlated but quantitatively quite distinct SOM pools with different ~~annual~~ dynamics (Wander, 2004; Tokarski et al., 2020). Not last, the faster turnover of the labile fractions is one of the reasons for the lower explained variability by the different models. HWEC is a measure of bioavailable and degradable organic carbon (Weigel et al., 1998). Although it is closely correlated to SOC (R^2 =0.75) it is best estimated by distinct parameter combinations compared to SOC, which is explained by the substantially higher variability of HWEC (Table 3 and 4). Changes in HWEC are mostly assigned to inputs of organic fertilizer substrates (Weigel et al., 1998) and the soil management (Ghani et al., 2003). For MBC especially soil management and factors such as C-input, climate, soil texture and soil pH are relevant (Wardle, 1992). Accordingly, the effect of land use but also of soil texture was most relevant for MBC accumulation. Similar to findings of Ludwig et al. (2015), MBC increased with the content of silt and clay but declined with sand, which is explained amongst other by the contribution of MBC to aggregate formation, the habitable surface and accessibility of SOC (Totsche et al., 2018). Additionally, management practices such as tillage and the application of organic fertilizer directly influence MBC (Liang et al., 1997). ~~Decreasing~~Lower explained variance of HWEC and MBC compared to SOC were based on a smaller relevance of the mineral phase parameters for their accumulation. ~~Further~~Labile fractions such as HWEC and MBC, containing larger proportions of bioavailable and easily degradable ~~compartments~~organic compounds, ~~leading to~~ are subject to~~a~~ faster turnover (Landgraf et al., 2006; Lorenz et al., 2021) ~~and a lower ability to interact with the mineral phase~~.

5 Conclusions

The reliable estimation of SOC and of its labile fractions HWEC and MBC is a task of growing importance in order to manage soil properties and functioning. That task will most often focus on local soilscapes with minor variation range in soil properties. This study showed that local models are superior to total~~global~~ models. Mixed ~~parameter~~ effect models combined with random effects yielded best estimates and highest explained variance for SOC and even its labile and quite dynamic fractions HWEC and MBC. For this purpose, the application of multivariate approaches to estimate SOC, HWEC and MBC clearly resulted in a higher explained variance compared to~~outperforms~~ models based on bivariate linear regressions~~correlations~~. Even a reduced dataset, representing parameters of the soil mineral phase is suited to estimate contents of SOC as well as HWEC and MBC. ~~Application of models from total datasets to local lead to a smaller explained variance while RMSE increased.~~ The inclusion of overall factors such as parent material, soil texture class and land use as random effects further improves the models. ~~t~~Total ~~Global~~ or even global models, developed from large-scale studies across countries or continents, often reach best estimates; however, they are subordinate for the above-mentioned small-scale areas and low sample numbers. Application of total models to local datasets leads to a smaller explained variance and higher RMSE. ~~For further research we suggest to identify possible clusters and to prove if these clusters were well explained by the overall total dataset. If otherwise we suggest to search of most relevant parameters to achieve a site adapted estimation to improve the overall understanding to SOC and its labile fractions on different landscapes.~~ From a practical perspective, the selected set of soil mineral phase parameters can be easily determined by using well-established methods and the parameters are rather stable over a longer-term. Thus, using such parameters for the ~~sufficient~~ estimation of SOC, HWEC and MBC is expedient. The presented research will be further enlarged by studying larger datasets containing more clusters in order to better identify local drivers of SOC and of its labile fractions.~~s~~ Our research shows that local models, considering site-specific parameter combinations, are superior to total models, although they are based on much smaller datasets. If such local datasets and models are available, they should be preferred. For further research we suggest to assess even larger datasets, in order to find out whether local subclusters can be identified and to examine if these clusters are best explained by total or local models. Furthermore, research is needed to determine most relevant parameters for a site adapted estimation of SOC and its labile fractions on different landscapes.

6 Code/Data availability

The raw data is available upon request to the authors.

7. Author contribution

MO, TU, MV, STB conceived, and designed the study. MO, MS, SS performed the sampling and analysis. MO wrote the first draft. All authors (MO, MS, SS; UT, MV, STB) contributed to generating and ~~and~~ reviewing the subsequent versions of the manuscript.

8. Competing interests

The authors declare that there is no conflict of interest.

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Authors response to review submitted on 06 Dec 2021 for soil-2021-81

Dear authors,

Thanks a lot for considering the feedback I gave on the initial version of your manuscript. You have incorporated most of my comments adequately, but I would like you to clarify a couple of things in the manuscript:

The authors are thankful for your additional advice to improve the quality of our manuscript. We clarified the suggested points.

- With respect to the title: how about '[...] mineral phase characteristics', instead of 'mineral phase parameters'?

It is a good option, we decided to change it according to your suggestion.

- The Discussion section is still one uninterupted text. The readibility would be increased considerably by splitting this into subsections.

Agreed, subsections were added to the discussion

- With respect to my comment to line 41, about POC: would be good to include this argumentation in the manuscript, so it's clear to the reader why POC was not studied

Thank you for this valuable hint, we added the explanation to these lines.

- With respect to my comment to line 108-109, about the abbreviations: I leave this up to you, but I think the readibility of the text will be increased substantially by using more intuitive names for your study sites

We decided to keep the abbreviations even if they are perhaps not fully intuitive. The full terms would increase the length of sentences too much. Shorter abbreviations are difficult because letters always appear in several terms.

- With respect to my comment to line 134, about CFE: As CFE is generally performed on fresh soil, to make sure the microbial community is as little disturbed as possible at the time of analysis, I would like to ask the authors to justify performing the analysis on frozen soil (either through citing articles showing that this has little effect on tbe measured MBC, or by providing the data that's not shown). In addition, I would like to ask the authors to mention in the manuscript that CFE was performed on samples that were frozen prior to analyses, this is important methodological information that is currently not mentioned.

According to Stenberg et al. (1998) freezing of soil samples at -20°C does not affect the microflora, so it is a widely accepted method for sample preservation in soil microbiology.

Stenberg, B., Johansson, M., Pell, M., Sjödahl-Svensson, K., Stenström, J., Torstensson, L., 1998. Microbial biomass and activities in soil as affected by frozen and cold storage. Soil Biology and Biochemistry 30, 393-402.

- With respect to my comment to line 205-206: Table 1 describes much more than 10 parameters, so this is not clear.

We added the information that only 10 from 23 parameters were selected, further we added information to Table 1 indicating which parameters were chosen.

- With respect to the previous formulation of models of 'sufficient extent': Would be good to clarify in the Material and Methods section what you consider a sufficiently good model

Classification of explained variance regarding their quality is for examples given by Cohen (1988) or Achen (1990). Cohen for example termed explained variance (R^2) above 0.26 as ‘high’. (For our study, however, an explained variance not much larger than 0.26 is not really high. To stay away from such discussion we focused on a relative assessment of models. If a model had a higher explained variance and a lower RMSE, it was termed as ‘superior’ to models with lower explained variance. Following the reviewer’s advice, we removed insufficient terms of model quality and added additional information to material and methods: ‘Both R^2 and RMSE were used for a comparative assessment of different models rather than for an absolute valuation.’.

Cohen, J. (1988). *Statistical power analysis for the behavioral sciences (2nd ed.)*. Hillsdale, N.J.: L. Erlbaum Associates.
Achen, C. H. (1990). What Does “Explained Variance” Explain?: Reply. *Political Analysis*, *2*(1), 173–184. doi:10.1093/pan/2.1.173

- With respect to my comment to line 243: This has not been changed at this location in the manuscript, please do so

We rephrased the sentence using a more neutral term.

- With respect to my comment to line 309-310: As you discuss the results of your model in the previous sentences, starting this sentence with 'accordingly' refers to those sentences. Would be good to rephrase this, and make it clear that this statement refers to the article you cite at the end, e.g.: 'For example, Kaiser and Guggenberger showed that ...'

We adapted this sentence to avoid any confusion.

- With respect to my comment to line 342: Please clarify this in the manuscript as well

We added some information to explain what ‘multidimensional’ means

- With respect to my comment to line 381-382: I would like to ask the authors to change this wording. You cannot assume that a property you didn't investigate contributes to concentration of SOC fraction, and 'explains' the gap in explained variance. However, you can hypothesize this.

Agreed, we changed it accordingly.