



Soil organic matter and labile fractions depend on specific local parameter combinations

Malte Ortner¹, Michael Seidel², Sebastian Semella², Thomas Udelhoven³, Michael Vohland², Sören Thiele Bruhn¹

5 ¹Soil Science Department, University of Trier, Trier, 54296, Germany

6 ²Geoinformatics and Remote Sensing, Institute for Geography, Leipzig University, Leipzig, 04103, Germany

7 ³Department of Remote Sensing & Geoinformatics, University of Trier, Trier, 54296, Germany

8 Correspondence: Malte Ortner (ortner@uni-trier.de), Sören Thiele-Bruhn (thiele@uni-trier.de)

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Abstract. Soil organic matter (SOM) is an indispensable component of terrestrial ecosystems. Soil organic carbon (SOC) dynamics 11 are influenced by a number of well-known abiotic factors such as clay content, soil pH or pedogenic oxides. These parameters 12 13 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 14 parent material, soil texture class and land use. To this end, topsoils were sampled from arable and grassland sites in southwestern 15 Germany at four regions with different soil parent material. Principal component analysis (PCA) revealed a distinct clustering of 16 data according to parent material and soil texture that varied largely between the local sampling regions, while land use explained 17 PCA results only to a small extent. The obtained global and the different local clusters of the dataset were further analyzed for the 18 relationships between SOC and mineral phase parameters in order to assess specific parameter combinations explaining SOC and 19 20 its labile fractions. 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 global dataset, we found significant correlations 21 between SOC and its labile fractions hot water-extractable C (HWEC) and microbial biomass C (MBC), respectively and the 22 23 predictors, yet correlation coefficients were partially low. 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 24 models-predicted SOC values revealed acceptable to very good regression coefficients ($R^2 = 0.41-0.91$). Thereby, the predictors and 25 predictor combinations clearly differed between models obtained for the whole data set and the different cluster groups. At a local 26 27 scale site specific combinations of parameters explained the variability of organic matter notably better, while the application of global models to local clusters resulted in less sufficient performance. Independent from that, the overall explained variance 28 generally decreased in the order SOC > HWEC > MBC, showing that labile fractions depend less on soil properties than on organic 29 30 matter input and turnover in soil.





1 Introduction 32

33 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 34 ongoing research to define models and parameter sets that best describe and predict soil organic carbon (SOC) contents of soils. 35 Further it is required to identify the driver for SOC storage at different scales and sites to adapt the management of soils. Overall, 36 the relevance of parameters for quantification of SOC is often described by bivariate relationships (Hassink et al., 1993; Barré et 37 38 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 39 accumulation of SOC is increasing (Hobley et al., 2015; Heinze et al., 2018). 40 In addition to total SOC, its labile subfractions such as hot water extractable carbon (HWEC) or microbial biomass carbon (MBC) 41 42 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 43 44 and Zeitz, 2012). The MBC is a quantitative measure of the microbial community that plays an indispensable role for the turnover 45 of SOC. Therefore, MBC is expedient to explain SOC dynamics (Liang et al., 2017). In contrast, much less research and attempts for quantitative modeling of these labile fractions compared to SOC have been done in the past (Liddle et al., 2020). 46 47 It is well known that factors such as climate, topography, vegetation, parent material and time are major factors influencing contents 48 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 49 (Wiesmeier et al., 2014; Gray et al., 2015). Consequently, vegetation and anthropogenic influence by land use and land use changes 50 are essential factors to model SOC accumulation and dynamics (Poeplau and Don, 2013; Dignac et al., 2017). The relevance of the 51 parent material for SOC sequestration and stocks was discussed for sites and small landscapes of a few km² (Barré et al., 2017; 52 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 53 54 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 55 56 at larger scales or at landscapes with a high variability concerning these factors. In contrast, for smaller, local study areas or rather 57 uniform areas with a low factor variability an inclusion of these factors as variables is less 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, 58 59 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 60 mostly known as indicators for stabilization of SOC such as content of fine silt, clay and pedogenic oxides or microbial parameters 61 such as microbial biomass and amino sugars (Angst et al., 2018; Quesada et al., 2020). There are indications that for the explanation 62 of SOC variability on a local to regional scale soil parameters instead of factors are especially suitable. Models based on soil 63 parameters also allow to identify possible drivers of SOC stabilization while using the above mentioned general factors would not 64 65 deliver a satisfying result (Wiesmeier et al., 2019; Adhikari et al., 2020). 66 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-67

mineral associations (Arrouays et al., 2006; Lützow et al., 2007). On one hand coarse particle size fractions such as sand, coarse silt 68 (cSilt) and medium silt (mSilt) contribute less to interactions between SOC and the mineral phase while on the other hand fine silt 69

(fSilt) and clay dominate such interactions (Ludwig et al., 2003). In addition, the mineral composition of the fine fraction, i.e. types 70

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of clay minerals and pedogenic oxides, is relevant for the interactions of SOC with the mineral phase (Kleber et al., 2015; Porras et 72

al., 2017). Especially iron and aluminum oxides interact with SOC leading to sequestration (Mikutta et al., 2006). Stabilization of 73 SOC is further enhanced by multivalent cations such asCa²⁺ and Mg²⁺ 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 74





properties the effective cation exchange capacity (ECEC) provides an overall measure to model cation impact on SOC storage 75 76 (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 77 saturation effect in soils with a high rock fragment content in consequence of a disproportionately high input of organic matter in 78 79 the fine soil fraction (Bornemann et al., 2011). 80 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 81 predicted by a variety of soil mineral phase parameters instead of a single predictor. Thereby combinations of parameters or factors 82 83 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 correlation models that are often unsuited at the level of local and regional 84 soilscapes (Jian-Bing et al., 2006). The latter especially applies for studies that are limited to a single specific location or only 85 contain a limited number of categorical variables or estimated soil parameters (Liddle et al., 2020). On the other hand, predictions 86 87 based on global models are often less site-specific and thus can possibly lead to an insufficient quantification of SOC at certain sites. 88 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 89 90 as well as its labile fractions by using local and global models. Differences regarding the relevance of a predictor in local vs. global models have to be identified to boost model performance and to fit adequate datasets using the best set of parameters for the 91 prediction of SOC at the investigated location. This overall aim was investigated in this study using a dataset from four local 92 93 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 94 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 global dataset they represent a broad range of soil properties typical for soils in temperate 95 regions. Therefore, the dataset enables to verify whether the global dataset is able to cover the local variability of SOC and its labile 96 97 fractions. Objectives of this study were, (i) based on identified differences in soil properties to determine best fitting factors and 98 parameter combinations that explain the variability in SOC and its labile fractions HWEC and MBC. (ii) It was aimed to determine 99 the relevance of local models in comparison to global models to achieve a sufficient quantification for local landscapes with distinct 100 properties. To this end, linear regression, principal component analysis (PCA) and mixed effect models were used in order to find 101 out whether global models or local models are better fitting. (iii) It was assessed if local datasets show a distinct combination of 102 significantly contributing predictor parameters compared to other local datasets and the entire dataset.

103 2 Material and Methods

104 2.1 Study area

105 The study was conducted in the greater area of Trier in southwestern Germany (Fig. 1). Bulk samples from topsoil horizons, i.e. 0-

106 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

107 (150) and grassland (49). Similar numbers of samples were taken from four regional areas with different parent materials. Parent

108 materials were Devonian clay schist (DCS), Luxemburg sandstone (LBS), sandy dolomitic limestone (DLS) from the Muschelkalk,

109 and Permian siltstone and fine sandstone (PSS) from the Rotliegend (Wagner et al., 2011).





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



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117 2.2 Analysis of soil properties

Samples were sieved < 2 mm and the stone content (> 2 mm) was determined gravimetrically. For further analysis, samples were 118 119 divided and stored at -20°C or air-dried, respectively. Soil pH was measured in 0.01 M CaCl₂ solution using a pH/Con 340i glass 120 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 121 122 this end, 2 g air-dry soil were extracted with a mixture of 1 g sodium dithionite, 40 ml sodium citrate and 10 ml NaHCO₃. Oxalate 123 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 NH₄⁺-oxalate (pH 3) and filtered afterwards. Extraction for the determination of the effective cation exchange 124 capacity (ECEC) was conducted using 1 M NH₄Cl. Elemental analyses for pedogenic oxides and ECEC (Na, K, Fe, Mn, Al, Ca, 125 126 Mg) were done using atomic absorption spectrometry (Varian AA240 FS Fast Sequential Atomic Absorption Spectrometer; Darmstadt, Germany). 127 For estimation of total carbon (TC) and nitrogen soil was dried at 105°C, grinded and measured by an Elemental Analyzer EA3000 128

129 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 EA3000 Series, HEKAtech 130 131 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 132 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 MgSO4 was added and samples 133 134 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 CaCl₂. Extracts of HWEC, HWEN, microbial biomass carbon (MBC) and nitrogen (MBN) were 135 analyzed with a TOC-VCPN analyzer (Shimadzu, Duisburg, Germany). For MBC and MBN correction factors kEC = 0.45 and kEN 136 137 = 0.4 respectively, were used (Joergensen, 1996; Joergensen and Mueller, 1996). Soil respiration was measured according to 138 Heinemeyer et al. (1989). Therefore, 25 g dry equivalent of sieved field moist soil were weighted in a tube that was flushed with 200 mL min⁻¹ of CO₂-free, humid air for 24 hours. Evolved CO₂ was determined after the soil passage using an infrared gas analyzer 139 140 (ADC 225 MK3, The Analytical Development, Hoddesdon, England).

141 2.3 Data analysis

Principal component analysis (PCA) was carried out to identify clusters within the dataset. For that purpose, 24 parameters 142 describing the mineral phase as well as SOM were included (Table 1). To conduct the PCA applied variables were log transformed, 143 144 centered and scaled to achieve standardized and comparable variables. Ellipses were defined by 95 % of the confidence interval 145 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). Linear regressions were performed to identify significant impact of mineral phase parameters on SOC, HWEC and MBC 146 147 for the entire dataset as well as for the identified clusters. Mixed effect models were determined for the entire dataset and for 148 identified clusters. To this end, selected soil properties of the mineral phase (Fe_{d-0} [g/kg], Fe₀ [g/kg], Al₀ [g/kg], sand [%], cSilt plus 149 mSilt [%], fSilt plus clay [%], (Ca + Mg)ECEC [mmolc/kg], stones [%] and pH) were used as fixed effect while, 'parent material', 150 '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 151 152 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, clavey and loamy soils). The additional implementation of the soil texture groups was done to consider the 153 154 potential different intercepts of the specific groups. Land use as random effect comprised the two management practices arable and 155 grassland. Maximum likelihood was applied as estimation procedure for the mixed effect models. At the beginning, all selected soil 156 properties were included in each model. Stepwise removal of parameters was conducted until all properties included in the models 157 significantly contributed to SOC, HWEC or MBC, respectively. Additional, the relevance of variables was visualized by the mean values of the clusters multiplied with their coefficient received from the mixed effect models. To avoid collinear behavior of the 158 159 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. 160 Furthermore, ECEC was excluded from mixed effect models to avoid overfitting due to collinearity with (Ca+Mg)ECEC. Residuals 161 162 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. To examine performance of mixed effect models, predicted 163 values were tested against measured values of SOC, HWEC and MBC, respectively using linear regressions. Data are shown as 164 mean (\pm SE) if not indicated otherwise. Statistical significance was indicated with *p < 0.05, **p < 0.01 and ***p < 0.001. Statistical significance was indicated with *p < 0.05, **p < 0.01 and ***p < 0.001. Statistical significance was indicated with *p < 0.05, **p < 0.01 and ***p < 0.001. Statistical significance was indicated with *p < 0.05, **p < 0.01 and ***p < 0.001. Statistical significance was indicated with *p < 0.05, **p < 0.01 and ***p < 0.001. Statistical significance was indicated with *p < 0.05, **p < 0.01 and ***p < 0.001. Statistical significance was indicated with *p < 0.05, **p < 0.01 and ***p < 0.001. 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Fable 1. Soil proper \sqrt{a} alues are means ± 3	ties in agricul SD.	ltural topsoils	for the comp	lete dataset ar	nd defined gro	up levels acc	ording to paren	t material, land	l use and soil t	exture class.
	Dataset	DCS	LBS	DLS	PSS	Sandy soils	Loamy soils	Silty soils	Arable	Grassland
	(n=199)	(n= 50)	(n=50)	(n=50)	(n=49)	(n=54)	(n=98)	(n=42)	(n=150)	(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 [%]	$0.20\pm0\ 10$	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]	753 ± 322	1071 ± 353	661 ± 163	732 ± 214	545 ± 252	570 ± 199	813 ± 319	782 ± 276	669 ± 231	1010 ± 410
HWEN [µg/g]	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]	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]	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	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
[µg CO ₂ -C _g d-m- h]										
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
Hq	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]	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
$Ca + Mg_{ECEC}$	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
[mmolc/kg]										
Fe _o [g/kg]	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]	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]	1.26 ± 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





169 3 Results

170 The dataset covers soils and topsoil properties with broad ranges of 24 parameters and parameter ratios, respectively, of SOM, 171 soil mineral phase and microbial biomass (Table 1). For example, soil pH ranged from very strongly acidic (pH 3.8) to slightly 172 alkaline (pH 7.4); soil texture varied from sandy to clayey texture. Thereby, parent materials essentially influenced 173 characteristics of the mineral phase related parameters such as texture, e.g. soils developed from sandy parent material such as 174 LBS had a sandy texture with sand content of up to 91.9 %. Soils developed from DCS and DLS parent material had elevated 175 contents of fine silt plus clay (33.4-53.3% and 16.7-44.8, respectively). Additionally, high contents of pedogenic oxides were 176 found in soils from DCS while ECEC and especially the contents of the polyvalent cations (Ca+Mg)ECEC were high in soils 177 developed from DLS (Table 1). Higher contents of SOC, HWEC and MBC were found for all parent material substrates in 178 grassland soils compared to arable soils (Table 1 and SI Table A). For the entire dataset, SOC ranged from 0.38 to 5.32 %, while 179 ranges from 237 to 1889 µg/g and 52.4 to 810 µg/g were determined for HWEC and MBC, respectively. SOC was strongly 180 correlated with HWEC ($R^2 = 0.75$) while the correlation with MBC was substantially lower ($R^2 = 0.40$). The dissimilar 181 correlations of SOC with the two labile fractions indicate differences between HWEC and MBC, which was further confirmed 182 by the mediocre correlation between HWEC and MBC ($R^2 = 0.55$). 183 To identify possible local clusters due to different sampling sites, parent material or land use systems within the dataset, PCA 184 was conducted including all 24 soil parameters and parameter ratios (Fig. 2). Principal component (PC) 1 to 3 explained 65 % 185 of the variance and had eigenvalues > 1 (Table 2). Parameters related to the soil mineral phase loaded on all three PCs. 186 Additionally, highest loadings on PC 1 were found for parameters describing the composition of SOM. For PC 2 high loadings 187 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 188 189 that were strongly related to the parent materials according to the different sampling sites (Fig. 2 A). In addition, samples clustered somewhat different when assigned to different soil texture classes (Fig. 2 B). Land use, however, was insufficient to 190 191 explain separation into different local clusters (Fig. S1). Instead, it could be used as a global cluster covering soils with separated 192 effects due to land use management. Compared to the entire dataset, the identified clusters based on parent material and soil 193 texture showed distinct properties of the SOM and the mineral phase (Table 1). In contrast to the local clusters, the global cluster 194 according to land use classes showed mostly properties quite similar to the entire dataset. Overall, identified clusters strongly 195 depended on the composition of SOM as well as on specific properties of the soil mineral phase, e.g. texture or soil pH related 196 properties. With a smaller relevance, parameters regarding the characteristics of soil microorganisms separated the dataset into 197 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

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	201	Table 2. Loadings	of the variables	on the first three	principal co	omponents
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	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

203





205 In order to test whether single parameters are suitable predictors of SOC, HWEC and MBC ten independent parameters 206 describing the properties of the soil mineral phase were selected from the dataset (Table 1). Regressions were calculated based on the total dataset (n = 199), for further global clusters (e.g. arable or grassland soils) and the local clusters that were identified 207 208 in PCA, i.e. subgroups based on the four parent rock materials and major texture classes (Table 3). Using the complete dataset, 209 highly significant regressions of SOC, HWEC and MBC to most soil mineral phase parameters were found, yet predominantly 210 at a low level of explained variance (Table 3). Compared to the complete dataset substantially different soil parameters explained 211 SOC, HWEC and MBC especially for smaller clusters such as soils from the parent materials DCS or LBS. Yet, clusters 212 comprising large sample numbers, where soil parameters cover broad ranges such as the clusters of loamy, arable or grassland 213 soils, showed significantly contributing parameters that largely matched with those found for the complete dataset. All clusters 214 differed in their pattern of significant parameters. However, for the complete dataset as well as for the clusters the explained 215 variance decreased from SOC to the labile fractions HWEC and MBC (Fig. 3 and Table 3). Only some properties such as sand. 216 ECEC or (Ca+Mg)_{ECEC} showed for MBC a higher explained variance compared to SOC and HWEC (Table 3). For the entire 217 dataset the content of SOC was best explained by Al_o and Fe_o as predictor parameter ($R^2 = 0.63$ and 0.56, respectively) while 218 soil texture related properties such as sand or fSilt plus clay explained SOC on a lower level (Table 3). Other determined mineral 219 phase parameters such as cSilt plus mSilt or ECEC explained variance to a negligible extent (Table 3). With lower values for 220 R², HWEC was explained by similar soil mineral phase parameters, as it was the case for SOC. With R² of 0.39 and a variance 221 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 222 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 223 variance of MBC compared to HWEC (R² = 0.27 and 0.16, respectively). Nevertheless, none of the applied parameters could 224 explain in all cases the complete variance of SOC, HWEC or MBC to a sufficient extent. Explained variance of SOC and its 225 labile fractions varied strongly between the parent material clusters. In general, the variance in these clusters was explained to a 226 substantially lower extent compared to the whole dataset (Table 3). In most cases, parameters of soil texture and pedogenic 227 oxides correlated significantly with SOC, HWEC and MBC. Additional to these parameters, (Ca+Mg)ECEC was useful to predict 228 SOC and MBC for some parent material clusters (Table 3). Highest values of R² were reached for the regression between SOC 229 and Al_o and Fe_o (0.47, 0.42) in the cluster DCS and fSilt plus clay (0.37) in the cluster PSS. R² was even lower in the clusters 230 LBS and DLS with maximum values of 0.21 and 0.20 respectively. Further, the cluster of loamy soils was also best described 231 by parameters representing pedogenic oxides and texture. Much lower R² were found for the sandy and silty soil clusters with 232 Al_0 and texture parameters (sandy) and additionally Fe_0 (silty) as best descriptors. While for SOC, HWEC and MBC mostly the 233 same descriptors were found (yet on different level of R²), they were partially different for MBC of the clusters silty and loamy 234 soils.





soils	Hq		0.02	0.06^{***}	0.04^{**}		0.02	0.03*	0.21^{***}	0.00	0.05	0.00		0.02	0.04	0.01	0.10^{*}	0.00	0.06	0.03	0.02	0.06	0.02	0.08^{*}	0.10^{*}		0.04	0.11^{*}	0.01	0.01	0.04	0.06	0.10^{**}	0.15^{***}	0.00
respectively, for a	(Ca+Mg) _{ECEC}		0.05**	0.02*	0.28^{***}		0.05**	0.04*	0.53^{***}	0.04	0.00	0.11^{*}		0.00	0.00	0.00	0.11^{*}	0.04	0.17^{**}	0.20^{**}	0.04	0.19^{**}	0.27^{***}	0.09*	0.17^{**}		0.02	0.04	0.05	0.03	0.02	0.19^{**}	0.02	0.00	0.15^{***}
MBC [µg kg ⁻¹] 1	ECEC Immole ka ⁻¹ 1		0 07***	0.03*	0.29^{***}		0.09***	0.08^{***}	0.61^{***}	0.04	0.00	0.11^{*}		0.00	0.00	0.00	0.10^{*}	0.05	0.20^{**}	0.20^{**}	0.04	0.19^{**}	0.30^{***}	0.10^{*}	0.16^{**}		0.02	0.03	0.07	0.03	0.01	0.17^{**}	0.04^{*}	0.00	0.14^{***}
, HWEC and	Stones	[~]	0 24***	0.11^{***}	0.06^{***}		0.29^{***}	0.17^{***}	0.12^{***}	0.44^{***}	0.30^{***}	0.15^{**}		0.00	0.03	0.06	0.00	0.00	0.00	0.20^{**}	0.06	0.08*	0.04	0.12^{*}	0.02		0.01	0.03	0.00	0.00	0.04	0.05	0.36^{***}	0.13^{***}	0.00
ce of SOC [%]	fSilt + clay	٢٥/٦	0 46***	0.27^{***}	0.43^{***}		0.46^{***}	0.28^{***}	0.51^{***}	0.59^{***}	0.47^{***}	0.67^{***}		0.03	0.00	0.01	0.08^{*}	0.01	0.21^{***}	0.08^{*}	0.00	0.11^{*}	0.37^{***}	0.20^{**}	0.35^{***}		0.07	0.08*	0.00	0.27^{***}	0.08	0.07	0.56^{***}	0.24^{***}	0.13^{***}
aining the variand and use	cSilt + mSilt	All samples	0.04**	0.04^{**}	0.29^{**}	Land use	0.05^{**}	0.06^{**}	0.52^{***}	0.02	0.02	0.13^{**}	Parent materia	0.04	0.01	0.03	0.11^{*}	0.01	0.19^{**}	0.00	0.00	0.00	0.23^{***}	0.29^{***}	0.37^{***}	Texture	0.19^{***}	0.06	0.12^{*}	0.22^{***}	0.08	0.00	0.01	0.01	0.02
ameters expl il class and l	Sand [%]	[~]	0 23***	0.16^{***}	0.45^{***}		0.23^{***}	0.18^{***}	0.64^{***}	0.25^{***}	0.21^{***}	0.41^{***}		0.00	0.00	0.00	0.11^{*}	0.01	0.21^{***}	0.02	0.00	0.05	0.36^{***}	0.30^{***}	0.44^{***}		0.18^{**}	0.08*	0.08*	0.01	0.00	0.16^{**}	0.41^{***}	0.20^{***}	0.12^{***}
it R ² for para	Al _o Γα ŀα ⁻¹ 1	1 S 1 S 1	0.58***	0.38^{***}	0.10^{***}		0.61^{***}	0.37^{***}	0.06^{**}	0.73^{***}	0.59^{***}	0.24^{***}		0.47^{***}	0.17^{**}	0.06	0.18^{**}	0.06	0.00	0.00	0.00	0.03	0.28^{***}	0.21^{***}	0.28^{***}		0.40^{***}	0.29^{***}	0.04	0.33^{***}	0.12^{*}	0.00	0.70^{***}	0.36^{***}	0.04*
n coefficien t material. n	Fed-Feo	[2 w 3]	0.16***	0.05^{**}	0.07^{***}		0.25^{***}	0.11^{***}	0.15^{***}	0.08*	0.03	0.07		0.25^{***}	0.24^{***}	0.18^{**}	0.11^{*}	0.03	0.04	0.03	0.05	0.00	0.00	0.03	0.00		0.01	0.06	0.08*	0.02	0.00	0.06	0.16^{***}	0.02	0.00
ar regressio	Feo [a ka ⁻¹]	[2 w 2]	0.56***	0.39^{***}	0.29^{***}		0.51^{***}	0.37^{***}	0.25^{***}	0.73^{***}	0.67^{***}	0.54^{***}		0.42^{***}	0.17^{**}	0.14^{**}	0.01	0.03	0.16^{**}	0.03	0.07	0.02	0.35^{***}	0.20^{**}	0.15^{**}		0.00	0.00	0.13^{**}	0.25^{***}	0.20^{**}	0.01	0.63***	0.36^{***}	0.08^{**}
able 3. Line			SOC	HWEC	MBC		SOC	HWEC	MBC	SOC	HWEC	MBC		SOC	HWEC	MBC	SOC	HWEC	MBC	SOC	HWEC	MBC	SOC	HWEC	MBC		SOC	HWEC	MBC	SOC	HWEC	MBC	SOC	HWEC	MBC
Ta			Dataset	n = 199			Arable	n = 150		Grassland	n = 49			DCS	n = 50		LBS	n = 50		DLS	n = 50		PSS	n = 49			Sandy	n = 54		Silty	n = 42		Loamy	n = 89	

Fig. 3. Predicted vs. measured content of SOC [A], HWEC [B] and MBC [C] for the global (complete) dataset. Parent materials are Devonian clay schist (DCS), sandy







SOIL Discussions





Comprising soils from all identified clusters, the set of descriptor parameters of the land use clusters were comparable to those 237 238 of the global dataset. Yet, the variance of SOC and its labile fractions were explained to a much higher extent for the global 239 dataset and the clusters of arable soils and especially grassland soils compared to the clusters based on parent material and 240 texture. Both land use types include an equal weight of samples from each parent material and act therefore as global cluster. 241 While SOC was explained by complex interactions of several different parameters for the distinct fractions, less variables 242

- showed a significant contribution to explain the variability of HWEC and MBC.
- 243 Since bivariate linear models insufficiently explained SOC, HWEC and MBC, respectively, mixed effect models were 244 developed. In these models, mineral phase parameters were applied as fixed effects, and land use, parent material and texture 245 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. 246
- 247 In general, mixed effect models explained variance in the order SOC > HWEC > MBC (Fig. 3 and Table 4). Measured and
- 248 predicted data using the mixed effect models showed a close relationship along the 1:1 prediction line while scatter increased at
- 249 higher contents of HWEC and especially of MBC, showing that estimates for grassland soils were inferior. Anyhow, correlations
- 250 between measured data and predictions of the mixed effect models ($R^2 = 0.29$ -0.91) were mostly higher than for bivariate linear
- 251 regressions ($R^2 = 0.00 - 0.73$). Independent from the applied random effect, precision of prediction results increased with sample
- 252 number and data range of parameters, respectively. Consequently, best model performance was achieved for the complete dataset
- 253 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
- 254 sandy soils revealed the poorest estimates of SOC (Table 4). In general, applying random effects such as parent material, land
- 255 use or texture for mixed effect models led to distinct results for the prediction of SOC, HWEC or MBC (Table 4). For clusters
- 256 according to land use variance was explained to a high extent (mean R² 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, 257
- 258 HWEC or MBC. Models using land use as random effect were partly distinct, though, indicating the different influence of land
- 259 use on SOC and its labile fractions (Table 4).





261	Table 4. R ² of the models for prediction of SOC, HWEC, and MBC based on the results of mixed effect models.
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	Pa	rent mater	ial+]	Land use ⁺			Texture ⁺		Mean model prediction for cluster
Sample subgroups	SOC	HWEC	MBC	SOC	HWEC	MBC	SOC	HWEC	MBC	R ²
Dataset	0.80*	0.63*	0.38*	0.77*	0.66*	0.67*	0.77*	0.61*	0.40*	0.61
					I	Land use				
Arable	0.80*	0.59*	0.70*				0.73*	0.53*	0.70*	0.68
Grassland	0.91*	0.75*	0.75*				0.89*	0.75*	0.75*	0.80
					Pare	nt mater	ial			
DCS	-	-	-	0.81*	0.78*	0.79*	0.73*	0.60*	0.56*	0.71
LBS	-	-	-	0.41*	0.34*	0.48*	0.41*	0.29*	0.30*	0.37
DLS	-	-	-	0.50*	0.35*	0.32*	0.50*	0.35*	0.25*	0.38
PSS	-	-	-	0.60*	0.55*	0.71*	0.63*	0.55*	0.61*	0.61
					7	Texture				
Sandy soils	0.79*	0.61*	0.33*	0.54*	0.50*	0.54*	-	-	-	0.55
Silty soils	0.72*	0.75*	0.48*	0.72*	0.64*	0.48*	-	-	-	0.63
Loamy soils	0.84*	0.59*	0.40*	0.81*	0.64*	0.60*	-	-	-	0.65
					Mean me	odel prec	liction			
R ²	0.81	0.65	0.51	0.65	0.56	0.57	0.65	0.53	0.51	

263 264

+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





Fig. 4. Coefficients of the mixed effect models to predict SOC, multiplied with the mean values of the specific cluster indicating 266 267 the impact of the applied variables. Differentiation into clusters and used random factors. Variables are scaled from 0 to 1.











Fig. 5. Comparison of the coefficient impact for mixed effect models to predict SOC, HWEC and MBC for the entire dataset by using



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273 The different mixed effects models particularly comprised variables (Fig. 4, Fig. 5) that also proved significant in linear 274 regressions (Table 3). Mineral phase parameters contributed with different significance to the models for SOC, HWEC and 275 MBC. The SOC and HWEC were primarily explained by pedogenic oxides followed by soil texture related parameters. Not last, 276 soil acidity indicated by pH and (Ca+Mg)ECEC was also relevant. MBC, compared to SOC or HWEC, was better explained by 277 parameters linked to soil texture. Contribution of the variables, on SOC and its labile fraction was visualized using the mean 278 values multiplied with their coefficients (Fig. 4, Fig 5). Distinct significant parameter combinations explaining SOC, HWEC 279 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, 280 within the soil texture related clusters pedogenic oxides, (Ca+Mg)ECEC, pH and texture parameters were relevant to estimate 281 SOC, HWEC and MBC. Regarding the random effects, applied mixed effect models using parent material as random effect 282 explained variability of SOC best. For MBC and HWEC, however, best model fits were mostly obtained with land use as random 283 effect. Only estimates of HWEC for the texture clusters were better when parent material was used as random effect.

The R² 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 the global model for SOC estimation to a smaller local cluster data set clearly revealed an inferior performance of the global compared to the local model (Fig. 6). The better performance of specific local models and parameter combinations was also found for other local clusters (Table 5 and SI Table 3)

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290
291 Table 5. R² for implementation of the global dataset to local clusters to estimate SOC.

			SOC			
	Par	ent material	Ι	Land use		Texture
Sample subgroups	Model	Global model to local cluster	Model	Global model to local cluster	Model	Global model to local cluster
Dataset	0.80		0.77		0.77	
DCS	-		0.81	0.68	0.73	0.65
LBS	-		0.41	0.23	0.41	0.24
DLS	-		0.50	0.30	0.50	0.35
PSS	-		0.60	0.57	0.63	0.57
Sandy soils	0.79	0.68	0.54	0.38	-	
Silty soils	0.72	0.65	0.72	0.60	-	
Loamy soils	0.84	0.83	0.81	0.79	-	
Arable	0.80	0.80			0.73	0.73
Grassland	0.91	0.87			0.89	0.87

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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].







298 4 Discussion

299 Our study showed that interactions of SOC with the mineral phase are highly relevant for the content of SOC as well as of its 300 labile fractions HWEC and MBC in soils. High correlations of SOC to fSilt plus clay (Table 3) agree with reports on the 301 relevance of organo-mineral associations for the stabilization of SOC and related to this the accumulation of the labile fraction 302 HWEC and MBC (Lützow et al., 2006). Furthermore, sandy soils contained the lowest content of SOC while loamy and silty 303 soils had an equally higher content of SOC (Table 1). This is typically expected and confirms numerous previous reports, e.g. 304 Ludwig et al. (2003) and Vos et al. (2018). In contrast, a slightly positive effect of sand on SOC was found for the in total very 305 sandy soils in the parent material cluster of LBS. This, however, is most likely a consequence of agricultural practice, with high 306 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 307 and HWEC/N as well as by a lower oxygen content of SOM compared to soils of the other parent material clusters (factor of 308 0.6; Table 1). Besides parameters directly related to soil texture, pedogenic Al- and Fe-oxides were found to be strong predictors 309 of SOC in soils. Accordingly, Al- and Fe-oxides were shown to have a relevant influence on the sequestration and stabilization 310 of SOC (Kaiser and Guggenberger, 2000; Lützow et al., 2006) as well as to have a high affinity to retain components of the 311 labile SOC fractions (Kaiser and Zech, 1998; Kaiser et al., 2002). Although soil acidity strongly affects soil processes such as 312 microbial activity and turnover that are relevant for SOC accumulation (Kemmitt et al., 2006), no clear correlation between pH 313 and SOC or its labile fractions was found by linear regression. Yet, soil parameters that are strongly related to soil acidity, i.e. 314 ECEC as well as the content of exchangeable polyvalent cations such as Ca^{2+} and Mg^{2+} , were suitable predictors for SOC and 315 its labile fractions in this and previous studies (O'Brien et al., 2015; Rasmussen et al., 2018). This is causally explained by the 316 stabilization of SOC in organo-mineral associations and the contribution of multivalent cation bridges (Ca²⁺ and Mg²⁺) to it 317 (Kaiser et al., 2012). The minor ability of ECEC and (Ca+Mg)ECEC and the higher ability of pedogenic oxides to explain variance 318 of SOC and its labile fractions in this study (Table 3), corresponds to findings of Rasmussen et al. (2018). They found a 319 prevalence of pedogenic oxides in humid areas with moderately acidic soils, while exchangeable Ca and clay prevealed in soils 320 of dry climates with circumneutral to alkaline pH. Such a prevalence of parameters to predict SOC, HWEC or MBC 321 demonstrates that it is preferred to use specific parameter sets when it is aimed to focus on local areas. The bivariate models 322 revealed that the stone content had only a small impact on SOC, HWEC and MBC. Hence, a funnel effect of the stone content, 323 by funneling more SOC into the remaining fine textured soil (Bornemann et al., 2011) was irrelevant. The combinations of 324 factors and soil properties affecting SOC and SOC fractions, respectively, were dissimilar between the different local areas 325 investigated in this study. The PCA revealed that differences according to parent material and soil texture were most relevant to 326 separate the dataset into various local clusters based on different factors (Fig. 2 A and B; Table 2). At the same time, this 327 illustrates the importance of the mineral composition (parent material) and grain size (soil texture) for the accumulation of SOC 328 as well as its labile fractions HWEC and MBC. In contrast, land use was not useful for a separation into clusters. This was 329 unexpected because typically topsoils under grassland have higher SOC contents compared to arable soils (Poeplau et al., 2020), 330 which was largely confirmed for the samples investigated in this study (Table 1). This went along with differences in the 331 composition of SOM (Table 1 and Table SI). However, data ranges of SOC, HWEC and MBC contents were largely overlapping 332 and similarities even increased in PCA when further soil properties were included. Consequently, a broad scatter of the land use 333 clusters was obtained by PCA, suggesting to treat the land use clusters as global datasets as well. 334 Several studies with large datasets covering national or continental scales, e.g. soil inventories, pointed out the relevance of 335 combinations of multiple factors and parameters instead of using single predictors to estimate SOC or its labile fractions (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 global model that was developed for the global (complete) 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.

- 342 Understanding SOC as continuum (Lehmann and Kleber, 2015) implies that accumulation of SOC is a multidimensional process 343 with various interacting factors and soil properties, respectively. The substantially lower ability of bivariate models to estimate 344 SOC compared to multiple parameter models confirmed this assumption. Accordingly, it was superior to use multiparameter 345 mixed effect models to estimate SOC and the two labile fractions. Especially parameter combinations within the land use clusters 346 gained a high-explained variance (Table 3, Table 4). A comparison with studies on regional or national scale (Vos et al., 2018; 347 Mayer et al., 2019) suggests that the importance of factors such as land use, soil texture or parent material varies with the 348 observed scale. Wiesmeier et al. (2019) reported that soil texture, land use and land management are relevant to explain SOC at 349 all scales. On regional or larger scale, also environmental factors such as climate, geology, soil use, topography are relevant for 350 SOC. Yet, at a local or smaller scale factors such as climate become less important, while parameters representing small-scale 351 soil physico-chemical properties gain importance for explaining the variability of SOC. Thereby, different factor and parameter 352 combinations were identified for the different local clusters by mixed effect modeling. The prevalence of a parameter for
- 353 quantification of SOC can differ dependent on environmental factors (Rasmussen et al., 2018).
- 354 Consequently, the quality of the multiparameter models was further improved by the implementation of local specific random 355 effects such as parent material or land use. Dependent on the random factors parent material, soil texture class and land use 356 different parameter combinations explained SOC, HWEC or MBC (Fig. 4 and Fig. 5). For the global (complete) dataset, nearly 357 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 358 359 related to soil acidity as significantly important to estimate SOC, HWEC and MBC. This highlights the importance of soil acidity 360 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 361 parameters were required that also clearly differed from the parameter combinations used in the models for SOC (Fig. 4 and 362 363 Fig. 5). Such differences concerning significantly contributing parameters were also found by other studies for specific clusters 364 or local sampling sites (Heinze et al., 2018; Quesada et al., 2020). This emphasizes that local models are required and superior 365 when it is the aim to estimate SOC and SOC fractions on a local scale. The global models used for the global dataset in this study reached the best predictions for SOC, HWEC and MBC. Yet, this was largely biased by the large samples size; applying 366 the same global models to local samples sets produced clearly poorer estimates compared to the more specific local models (Fig. 367 368 6; Table 4 and Table 5). Consequently, aggregation of smaller datasets, e.g. from a local scale, to a larger dataset enables to 369 predict SOC and its labile fractions to a satisfying extent. In opposite a global dataset applied to the local area with defined 370 properties is partially practicable, resulting in a variance explained on a lower level. Dependend on the properties of the soil 371 mineral phase, each specific cluster was controlled by other properties, which best explain the accumulation of SOC and its 372 labile fractions. This implies the importance for analysis of local clusters to avoid a subordination by models of global datasets. Comparing the results of mixed effect models using the different random effects (parent material, soil texture, land use), the 373 374 models using parent material yielded best results for the estimation of SOC. For HWEC and MBC best predictions at a sufficient 375 quality level were obtained by models using land use as random effect (Table 4). The parent material predefines the boundaries 376 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).

379 In general, the variance explained by the mixed effect models was not similar, but varied between SOC and its labile fractions 380 HWEC and MBC. It became clear that SOC and the labile fractions HWEC and MBC are not fully correlated but quantitatively 381 quite distinct SOM pools with different annual dynamics (Wander, 2004; Tokarski et al., 2020). Not last, the faster turnover of 382 the labile fractions is one of the reasons for the lower explained variability by the different models. HWEC is a measure of 383 bioavailable and degradable organic carbon (Weigel et al., 1998). Although it is closely correlated to SOC (R² =0.75) it is best 384 estimated by distinct parameter combinations compared to SOC, which is explained by the substantially higher variability of 385 HWEC (Table 3 and 4). Changes in HWEC are mostly assigned to inputs of organic fertilizer substrates (Weigel et al., 1998) 386 and the soil management (Ghani et al., 2003). For MBC especially soil management and factors such as C-input, climate, soil 387 texture and soil pH are relevant (Wardle, 1992). Accordingly, the effect of land use but also of soil texture was most relevant 388 for MBC accumulation. Similar to findings of Ludwig et al. (2015), MBC increased with the content of silt and clay but declined 389 with sand, which is explained amongst other by the contribution of MBC to aggregate formation, the habitable surface and 390 accessibility of SOC (Totsche et al., 2018). Additionally, management practices such as tillage and the application of organic 391 fertilizer directly influence MBC (Liang et al., 1997).

392 5 Conclusions

393 The reliable estimation of SOC and of its labile fractions HWEC and MBC is a task of growing importance in order to manage 394 soil properties and functioning. That task will most often focus on local soilscapes with minor variation range in soil properties. 395 This study showed that local models are superior to global models. Mixed parameter models combined with random effects 396 yielded best estimates and highest explained variance for SOC and even its labile and quite dynamic fractions HWEC and MBC. 397 For this purpose, the application of multivariate approaches to estimate SOC, HWEC and MBC clearly outperforms models 398 based on bivariate correlations. Even a reduced dataset, representing parameters of the soil mineral phase is suited to estimate 399 contents of SOC as well as HWEC and MBC. The inclusion of overall factors such as parent material, soil texture class and land 400 use as random effects further improves the models. Global models, developed from large-scale studies across countries or 401 continents, often reach best estimates; however, they are subordinate for the above-mentioned small-scale areas and low sample 402 numbers. From a practical perspective, the selected set of soil mineral phase parameters can be easily determined by using well-403 established methods and the parameters are rather stable over a longer-term. Thus, using such parameters for the sufficient 404 estimation of SOC, HWEC and MBC is expedient. The presented research will be further enlarged by studying larger datasets 405 containing more clusters in order to better identify local drivers of SOC and of its labile fractions.

406 6 Code/Data availability

407 The raw data is available upon request to the authors.

408 **7. Author contribution**

409 MO, TU, MV, STB conceived, and designed the study. MO, MS, SS performed the sampling and analysis. MO wrote the first

410 draft. All authors (MO, MS, SS; UT, MV,STB) contributed to generating and and reviewing the subsequent versions of the

411 manuscript.





412 8. Competing interests

413 The authors declare that there is no conflict of interest.

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