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Interactive comment on "Hot regions of labile and stable soil organic carbon in Germany – Spatial variability and driving factors" *by* Cora Vos et al.

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Dear Lauric Cécillon and colleagues,

Thank you very much for your comment on our discussion paper. We appreciate that you discussed the paper draft thoroughly and found some points that need more clarification to be understandable. Please find our answers to your comments below.

We have a concern regarding the use of the cross-validated regression model based on near-infrared spectroscopy to predict the size of SOC labile and stable pools in "new" samples of the German Agricultural Soil Inventory. We regret the use a regression model that has not been published yet, impeding us from a clear understanding of the actual predictive performance of the model on "new" topsoil samples. Here, the

details provided by the authors regarding the predictive performance of the multivariate regression model (see Material & methods section 2.4 at lines 189–194 and Supplementary Figure S1) do not demonstrate its ability to accurately predict the absolute content (g/kg) and proportion (%) of SOC in the POM and in the MOM fractions of the 2755 "new" samples.

Answer: The paper describing the regression model (Jaconi et al.) has been submitted to the European Journal of Soil Science. We also regret that it has not been published yet. In this paper, the model is described in detail, testing the algorithm on different datasets. In the paper the model is also validated using an independent validation dataset (consisting of one third of the total samples), which has not been part of the model calibration (two thirds of total samples). We see that it would be helpful to provide the validation results with the paper discussed here, as they are not published yet with the other paper. In the revised version we will append a table with the supplement materials (see Figure 1)

SpeciïňĄcally, the authors have only assessed the predictive performance of their model using a leave-one-out cross-validation. Leave-one-out cross-validation is not the optimal method to validate a partial least-squares (PLS) regression model when 145 samples with reference measurements are available. It may be recommended for smaller datasets when a proper validation procedure (see below) cannot be done. An acceptable procedure for validating this PLS regression model would be adding an independent validation step to the current validation scheme: i/ ïňĄrst run a leave-one-out or k-fold cross-validation on a subset of ca. 110 samples with reference measurements, that would provide a Q2 (= coefïňĄcient of determination of the model in cross-validation, not a R2), and a ïňĄrst assessment of the mean error of prediction of the PLS regression model in cross-validation (RMSECV). ii/ use this cross-validated PLS model to predict the values of the absolute content (g/kg) and proportion (%) of SOC in the POM and in the MOM fractions of the ca. 35 independent samples with reference measurements not used for cross-validation (and independent from the ca.

110 samples used for cross-validation). The coefïňĄcient of determination (actual co-efïňĄcient of determination of the model in validation,R2)and mean error of prediction of the PLS regression model in validation (RMSEP) would provide acceptable criteria for the reliable (independent) assessment of the actual predictive performance of the model for prediction on “new” topsoil samples. iii/ if the R2 and RMSEP (or RPD) of the PLS regression model obtained on the 35 independent validation samples were judged acceptable, then the model may be used to predict the values of the absolute content (g/kg) and proportion (%) of SOC in the POM and in the MOM fractions of the 2755 remaining topsoils of the German Agricultural Soil Inventory.

Answer: We agree that, if possible, the best method is always to have an independent validation dataset. We think, however, that this is not advisable in our case, as the calibration dataset was for the whole area of Germany, containing very different soils. In this case 145 samples are not a large calibration dataset. This calibration dataset was selected out of all 2900 available soil samples using the Kennard Stone algorithm, so that it contains the maximum possible spectral variability. There were also additional selection criteria for these sites, as explained in ll.125-131. This is why we do not want to split the reference dataset into calibration and validation dataset, as with every split of this dataset a large part of the variation present in German soils would be lost for the calibration.

We therefore argue that the PLS regression model based on near-infrared spectroscopy presented by the authors cannot be used in its current form to predict labile and stable SOC fractions on “new” topsoil samples of the German Agricultural Soil Inventory. At this stage (i.e. unreliable assessment of the predictive performance of the PLS regression model), the authors can only use the reference data (n = 145) of the absolute content (g/kg) and proportion (%) of SOC in the POM and in the MOM fractions to investigate the potential drivers of the distribution of SOC kinetic pools on this limited dataset. This would already be a signiïňĄcant piece of work.

Answer: As we conducted an independent validation, which showed that the predicted

values are in good accordance with the measured ones, we are sure that the model is robust enough and can be used to predict the 2755 “new” samples. Therefore, we argue that the drivers can be assessed not only using the reference data, but also the predicted ones.

Furthermore, Vos and colleagues used the particulate organic matter (POM) fraction to represent the labile SOC kinetic pool. However, the POM fraction could contain substantial (and variable) amounts of pyrogenic carbon with residence time in soils higher than the mean residence time of total SOC. This limitation of the SOC density fractionation scheme should be mentioned and discussed in the text, as it is not possible to guaranty that the POM fraction truly represents the actual labile SOC pool for all investigated samples.

Answer: We agree that this is a limitation of density fractionation, which we will address in the revised version of our paper. Pyrogenic carbon does, however, play a minor role in German soils. There is also a large section on the so-called “black sands” in Germany (ll.300-356), where we discuss explicitly why the POM fraction is not always a labile fraction.

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Table S3: Indicators of model performance for soil C fractions particulate organic carbon (POM) and mineral associated organic carbon (MOM) with calibration and independent validation dataset (mean values of 100 iterations with random selection). Table a) is for values in g C kg soil^{-1} and table b) is for the proportion (relative values).

a)

	Calibration dataset						Validation dataset					
	Q^2	**RMSECV,** g C kg soil^{-1}	**ρc_c^***	**Bias,** g C kg soil^{-1}	**RPD**	**RPIQ**	**R^2**	**RMSEP,** g C kg soil^{-1}	**ρc_v**	**Bias,** g C kg soil^{-1}	**RPD**	**RPIQ**
POM	0.83	4.92	0.91	0.34	2.5	1.8	0.82	5.38	0.89	0.44	2.5	2.0
MOM	0.87	4.92	0.93	-0.34	2.9	2.9	0.85	5.38	0.91	-0.44	2.7	2.6

ρc^* - Lin's concordance correlation coefficient

b)

	Calibration dataset						Validation dataset					
	Q^2	**RMSECV,** %	**ρc_c^***	**Bias,** %	**RPD**	**RPIQ**	**R^2**	**RMSEP,** %	**ρc_v**	**Bias,** %	**RPD**	**RPIQ**
POM	0.78	13.15	0.88	1.07	2.09	2.56	0.73	15.04	0.84	1.6	1.9	2.4
MOM	0.78	13.15	0.88	-1.07	2.00	2.48	0.72	15.04	0.83	-1.6	2.0	2.3

ρc^* - Lin's concordance correlation coefficient

Fig. 1. Table S3