# Response to the reviewers' comments

on 'EstSoil-EH v1.0 An eco-hydrological modelling parameters dataset derived from the Soil Map of Estonia', posted to the Interactive discussion.

RC1: 'Referee comment', Anonymous Referee #1, 26 Nov 2019

RC2: 'Referee Comment', Anonymous Referee #2, 21 Dec 2019

We thank the reviewers for their valuable comments. We will address the concerns raised by the reviewers point by point below. The response to the Referees are structured in the suggested sequence: (1) comments from Referees RC1/RC2, (2) author's response A, (3) author's changes in manuscript.

# Anonymous Referee #1

Received and published: 26 November 2019

(1) RC1: The manuscript of Kmoch et al. describes a methodology for deriving high resolution 3D soil property data of Estonia, which is published with the manuscript. The data basis for the methodology is the National Soil Map of Estonia and the soil properties are derived with a special focus on the parameters necessary for running the SWAT model. These parameters include the saturated hydraulic conductivity, field capacity, wilting point and the USLE K erodibility factor. Such large-scale soil data is highly valuable for soil hydrological and water quality modeling on a scale relevant for decision makers (e.g., national scale). Organizing, homogenization and distribution of soil properties on such a large scale is very challenging and I acknowledge the work the authors did here. However, there are some points that prevent the manuscript from being published at the current state.

(2) A: We appreciate the initial assessment and thank the reviewer for the value comments. We will address the concerns raised by the reviewer point by point below.

# (1) RC1: General comments

1. Structure: The manuscript is very technical and includes too many details. The main step is the transformation of a text based soil classification (Soil Map of Estonia) to soil texture, which is then (together with SOC, bulk density and topographic information) used for deriving the soil hydraulic properties. All the details (especially the grammar definition parts) makes it difficult to follow these main steps. The explanation of all codes for transforming the letter codes to texture could e.g. be a part of the dataset itself as a documentation.

(2) A: We agree, that we have included a lot of very technical information. We believe, that for the soil community in Estonia, and for countries which have similar national datasets like the original soil map of Estonia, these technical descriptions are very interesting and a topic for deeper discussion and evaluation as well. With that said, it is important to acknowledge and emphasize, that the source dataset – the original soil map of Estonia- as described in the article, is not based on modelled but on fully observed data (e.g. texture, soil profile depth, rockiness, presence of organic layer etc). Systematic mapping of Estonian soils to produce soil map in scale 1:5 000 and 1:10 000 was started in 1954 (Reintam, L., Rooma, I., Kull, A. & Kõlli, R. 2005. Soil information and its application in Estonia. In: European Soil Bureau. Research report. 9, 121-132), with most intensive field studies in period 1965-1969. Generally field mapping was carried out in scale 1:10 000 but in hilly or undulating areas with higher soil diversity in scale 1:5000. In 1982-1988 older mapping data was

updated and new areas were included with full-area soil quality (primarily fertility, rockiness, water regime, texture, erodability) assessment. In 1988-1990 soil field studies were performed in non-arable land and new mapping of ameliorated land. Forest soils were mapped in period 1976-1989. During large-scale field mapping of soils the texture was determined *in situ* based on organoleptic methods and for reference profiles laboratory analyses were performed. This enabled calibration between texture defined by organoleptic method by each researcher participating in field survey and texture determined in laboratory (Estonian Land Board, Explanation to the soil map,

https://geoportaal.maaamet.ee/docs/muld/mullakaardi\_seletuskiri.pdf?t=20091211092214). As a result of large-scale soil mapping, 119 soil varieties in Estonian national classification system have been distinguished and more than 500 combinations of textural status have been described. About 10,000 profiles (1 profile per 330ha) have been sampled and analysed for characteriation of mineral soils (Reintam, L., Rooma, I., Kull, A. & Kõlli, R. 2005. Soil information and its application in Estonia. In: European Soil Bureau. Research report. 9, 121-132; Reintam, Loit; Kull, Ain; Palang, Hannes; Rooma, Igna (2003). Large-Scale Soil Maps and a Supplementary Database for Land Use Planning in Estonia. Journal of Plant Nutrition and Soil Science-Zeitschrift Fur Pflanzenernahrung Und Bodenkunde, 166 (2), 225–231.).

Thus, the texture codes and soil types assigned to the ca. 750000 mapped soil units (polygons) are based on many decades of in-situ land surveying practices and describe quite literally the physical state of the soil based on in-situ assessment. Now, in the article and new dataset, the quality of the extraction and derivation process of the initial texture values is obviously a very critical step for the whole dataset. In many cases, scientists in Estonia have used their own "scripts" to get some numerical data out that they need for their study areas, however, no standardised approach as presented in our paper is currently available.

(3) We added this clarification to the article in section 2.1, However, we came to the decision that reducing the section 2.2.2 of preprocessing the texture codes, where the bulk of the already condensed technical description of the grammar is contained, would not improve overall readability in contrast to one of the original intentions of this dataset – to demonstrate the creation of a numerical dataset from an existing observed dataset.

(1) RC1: 2. Texture: The step of transforming a text coded soil classification into a numerical texture value is a very crucial point of the methodology. All the focus on the "grammar definition" hides the main step of the transformation, which is done with Table 2. However, it is nowhere cited or mentioned how this table was derived. Is it based on the literature or on own data? This table is the main factor influencing your final results, hence it should be carefully described how you come up with this values. Furthermore, this rises the general point of the missing validation of your final soil texture product (that then influences the hydraulic properties). You only validate your grammar-generated codes and do an "expert check". However, the texture itself is not validated with measured data (as far as I understand). You mention on page 9 line 3-9 that you validated it against SoilGrids250m, but it is important to show this validation. An expert check alone is not enough, since other user of your data cannot assess the uncertainty. You need a reliable texture database for validating your results and hence Table 2 (and Table 3). For your SOC prediction you show such a validation and you correctly mention the relevance of validation of your other data on page 15 line 27-29.

(2) A: We acknowledge the case presented here by the reviewer. As there are several arguments outlined by the reviewer we respond line by line:

L11-3: We partially agree with the reviewer that the transformation step from the extracted Estonian texture codes to the assignment of numerical values for the fine texture fractions was not well explained, however assigning the numerical values of the sand, silt and clay fractions per texture class is based on Estonian soil experts' knowledge. The emphasis on the grammar was intended to make clear that we had to put more work in to actually retrieve these codes in the first place. We added a description to make it more explicit.

Ll4-6: Lines 5-9 on page 8 are intended to describe that Estonian soil experts (co-authors Arno Kanal & Alar Astover, from the two main natural sciences universities in Estonia which are actively doing research and teaching in soil sciences) technically can assign these fractions to the historically recorded Estonian texture codes. And here again, the emphasis is on the fact, that the original soil map of Estonia is representing observed data. The recorded texture codes represent the in-situ assessment of the national soil mapping and surveying efforts. Explaining the Estonian texture code system would include a lot of technicalities and Estonian language terms, which was not desired. However, we acknowledge that this was not as clearly stated as it could have been. We improved the clarity on the creation of the table.

Ll7-15: "the texture itself is not validated with measured data (as far as I understand)" - We believe, the concern raised here again touches the understanding that the original soil map of Estonia is indeed observed data. But that is why we have to be more clear on how well we extracted the existing texture information from the original soil map. Therefore, we found it important to validate the textual extraction and not so much the decision for the assignment of fraction values for each code. Thus, we described it as our best efforts. In addition, there are detailed studies on reference soil profiles in Estonia, Latvia and Lithuania that relate original soil texture, so called Katchinsky texture system (Kachinsky NA. 1965. Fizika potchy [Soil physics], Vol. 1. Moscow: Moscow University Press[in Russian].) to USDA soil system (Calhoun, T.E., Ellermäe, O., Kõlli, R., Lemetti, I., Penu, P. & Smith, C.W., 1998. Benchmark Soils of Estonia Researched thru Baltic - American Collaboration. Problems of Estonian Soil Classification. Transactions of Estonian Agricultural University, 198, 76-114) and erosion modelling case studies where based on laboratory analyses transfer functions from Katchinsky to USDA texture classes were developed (Laas, A. & Kull, A. 2003, Application of GIS for soil erosion and nutrient loss modelling in a small river catchment. In: E. Beriatos, C.A. Brebbia, H. Coccossis, A.G. Kungolos (Eds.). Sustainable Planning and Development (525-534).. Southampton, Boston: Wessex Institute of Techonology Press.). Relationship between Katchinsky and Atterberg systems are provided by R. Kask (Kask, R. 2001. On the English Equivalents of the Estonian Terms for the Textural Classes of Estonian Soils. Journal of Agricultural Science, Vol. 14, 93-96. http://agrt.emu.ee/pdf/proceedings/toim 2001 14 kaskr.pdf) But we acknowledge the reviewers desire for numerical statistical hard data which could reveal how well and accurately the soil surveying has captured soil texture in these descriptive codes through the times. But we think, this would be beyond the scope of the current dataset because it would require inclusion of additional independent georeferenced datasets with USDA soil texture classes defined based on laboratory analysis of particle size distribution.

We added additional explanations and background to section 2.2.4.

(1) RC1: 3. Data quality: A data paper should be supportive for the dataset and help the users to evaluate the data and its quality (e.g. uncertainties). This is missing at the moment and instead of focusing on the grammar methodology you should rather present your final derived hydraulic data with e.g. appropriate diagrams.

(2) A: We agree, the data quality is not consistently reported. The texture data and soil types are observed data of many years of national surveying activities. The original observations were classified into the Estonian texture code system based on Katchinsky (1965) soil particle size standards at the time of observation (not by us). We "just" translate" the texture codes back into numbers. Therefore, we don't see a possibility to explicitly display uncertainties related to that process, as we take these as observed data and thus we can make only short reference to another study what shows that achieving 5% accuracy in organoleptic determination of clay content for lower value classes while possible error increased in case of heavy texture classes (Kokk, R. 1987.Soil texture of Estonian soils, its determination and classification. Estonian soils in figures VI. In Estonian: Eesti muldade lõimis, selle määramine ja klassifitseerimine. Eesti mullastik arvudes VI). However, we will compare the sand, silt, clay and coarse fragments fractions with other soil datasets and report on standard deviations and R2. The uncertainties for the SOC predictions are reported. The uncertainties of BD are directly related to the SOC uncertainty. AWC is directly derived from Toth et al. 2017 EU-HydroSoilGrids and we will

report the cumulative uncertainty based on our aggregation. K is predicted by ROSETTA based on our derived numerical texture values. We will report the uncertainty from these predictions. We also added Table 5: Comparison of descriptive statistics (mean, standard deviation, minimum, 25-, 50-, and 75 percentile, and maximum value) for EstSoil-Eh and SoilGrids, based on zonal aggregation of SoilGrids into the EstSoil layer polygons (SOL\*: EstSoil-EH, SGR\*\_ SoilGrids-corresponding variable) for the first out of maximum four layers in EstSoil-EH (full table in data deposit supplement: "estsoil\_vs\_soilgrids\_stats.csv")

(1) RC1: This includes the uncertainties derived from the texture + SOC classification and also the uncertainty introduced by the pedotransfer functions you used (here ROSETTA). This is also relevant for me as a referee. At the moment for me it is really difficult to evaluate your data in a feasible time. You also mention the problems to derive USDA texture from the old soviet-era based texture system, which ignores the silt fraction and has a different definition for the gravel-sand boundary (page 7 line 29-31). This of course includes a lot of uncertainty, but I understand the benefits of transforming the texture to the often used USDA

classification (e.g. usability of pedotransfer functions). I suggest to also include the soviet texture into your data. This can help to evaluate the error introduced by the two different systems and potentially allows to use the data with another "texture transfer function" (different from Table 2).

(2) A: There is no error to be assessed from the translation from one system into the USDA system. The numerical values for sand, silt and clay fractions were assigned to the Estonian texture system codes, then the values were also used to select the appropriate USDA classes based on the texture triangle. .). Relationship between Katchinsky and Atterberg systems are provided by R. Kask (Kask, R. 2001. On the English Equivalents of the Estonian Terms for the Textural Classes of Estonian Soils. Journal of Agricultural Science, Vol. 14, 93-96.

http://agrt.emu.ee/pdf/proceedings/toim\_2001\_14\_kaskr.pdf). It is not possible retrospectively to redefine minor differences in boundaries between different classes between texture systems, but we consider natural variation of texture within the soil mapping unit in scale 1:10 000 more significant than that of different texture systems. Texture transfer rules (Table 2 in manuscript) to get from Estonian texture classes to USDA particle size distributions were composed by authors according to Estonian guideline "Field Soil Survey – Muldade väliuurimine" (Astover et al. 2013) where matches of Estonian/Soviet and USDA/FAO classes for field survey is provided. In our opinion it is appropriate approach for data conversion in used mapping scale. We agree that it might increase uncertainty for point data but should be not major problem in case polygon data.

4) Dataset check: By checking randomly sampled polygons in the final GIS product (.shp) I recognized some problems with the soil layers. E.g. FID 96775 has two layers with SOC and bulk density values are shown in layer 1 and 2. However, texture values are indicated in layer 1 and 3, whereas layer 2 is empty. Similar problem was found in FID 178514 with only one layer but texture values in layer 1 and 2. Please check your data again.

(2) A: Thank you for pointing these errors out. We believe they were introduced when making assumptions about layers that have no depth reported, but are above or below a layer that has a depth reported. We are uploading an updated dataset.

(1) RC1: 5. SWAT focus: The manuscript focuses too strongly on SWAT. Although the dataset was created for using it with the SWAT model, this is not important in the data paper. Of course you can mention that the presented data is enough for many modeling purposes (e.g. SWAT), but at the moment the focus on SWAT makes the manuscript difficult to understand. E.g. on page 7 line 6-15, just mention that you have defined different layers.

(2) A: We acknowledge the reviewer's suggestion, we generalised to the need for eco-hydrological modelling, and reduced the focus on SWAT throughout the manuscript.

(1) RC1: 6. Highlight the need for your dataset: You mention similar global or regional datasets (page 2 line 4-28). However you miss to highlight the need of your dataset. What is different from the others or "better" in your dataset? Why it needs a new dataset? For calculating the available water capacity you use the dataset of Tóth et al. (2017) which is not mentioned in this section. Why is this dataset not usable for parameterizing models in Estonia?

(2) A: Other datasets are available for use in Estonia-based modelling contexts, that is correct. However, vector-based EU soil datasets are very coarse and excessively generalise large parts of the diverse Estonian landscape. High-detail datasets such as Soilgrids are themselves based predicted on a grid 1km/250m, and not based on observed data. The presented dataset is of very high spatial detail based on the original Estonian national soil map, which was created from directly surveying all of Estonia. Thus, our presented dataset much more spatially related to the landform/landuse observed there. Furthermore, the textures and SOC/BD values are directly derived from reliable observed data samples from Estonia, with a reproducible workflow, whereas this is not true for many other reported soil dataset that covers the area of Estonia. Furthermore, the method created to translate original hard copy soil map (with traditional textual codes) to digitally readable GIS-based map can be used by several other countries (e.g. Latvia, Lithuania, Ukraine etc) and this enables spatially more explicit modelling of ecosystems.

We added the explanation as highlights to the manuscript in the introduction.

(1) RC1: In summary the manuscript should rather focus on the quality of the data than on the methodology of the grammar definition. That does not mean that the grammar definition should not be part of the data or manuscript, but it should be less prioritized. If the authors are able to provide quality and uncertainty measures of the data, I suggest major revisions. Otherwise, although I think such a large scale soil hydraulic dataset is very valuable and I acknowledge the amount of work, the manuscript should be rejected since the quality cannot be guaranteed.

(2) A: We thank the reviewer for the valuable comments. However, we want to turn the interest of the reader also to one of our original motivations, which was to provide methodological approach of getting from legacy qualitative soil map to quantitative functional maps.

(1) RC1: Specific comments:

(1) RC1: Page 2 line 12-15, 27-28: Please explain the datasets at least a little if you mention them (e.g. what is SOTER or WISE?)(2) A: added to the manuscript

(1) RC1: Page 3 line 6-8: If you cannot proof it, please delete this sentence.

(2) A: deleted.

(1) RC1: Page 3 line 23-page 4 line 7: Out of context. Please give some introduction and change the structure.

(2) A: added to the manuscript

(1) RC1: Page 9 line 3: What is the second source? SoilGrids250m is just one.

(2) A: The two sources were the manually decoded dataset from the paragraph before and the second was SoilGrids250m. We rephrased.

(1) RC1: Page 11 line 9-10: Please provide a reference for this calculation (SOC = SOM / 1.724). Where does the 1.724 come from?

(2) A: Coversion factor 1.72 is widely used universal value (Soil Analysis: An Interpretation Manual. Eds. K. I. Peverill, L. A. Sparrow, D. J. Reuter. CSIRO Publishing, 2001; Soil Carbon Dynamics: An Integrated Methodology. Eds. W. L. Kutsch, M. Bahn, A. Heinemeyer. Cambride. 2012), however we acknowledge that the real value varies slightly between soils.

(1) RC1: Page 12 line

24: Add reference for the permeability classes. Figure 1 in the lower blue box: "wilting point" not "witing point"

(2) A: we updated the figure and added the reference

(1) RC1: Data file "texture\_error\_lookup.xls": In row 13 (index 11) the (1) RC1: erroneous item is "=50/LS2". Is this correct? Because it is displayed as a "#DIV/0!" in Excel.

(2) A: it is not erroneous. The cell code is "=50/ls", which is an invalid texture code. Excel interprets the "="

(1) RC1: Data structure:

I suggest to reorganize the structure of your data in the repository to make it more structured:

- the main derived map (.shp or other format)

- metadata (e.g. EstSoil-EH\_v1.0\_attribute\_fields)

- folder with figures

- folder that contains all other information used to derive this map (e.g. SOC rf

Model; original estionian soilmap, texture errors, rosetta outputs etc.)

- README

Anonymous Referee #2

Received and published: 21 December 2019 Summary

(1) RC2: In the manuscript by Kmoch et al. a new countrywide soil dataset for Estonia at 1:10000 scale is presented. Those soil properties are provided which are the most frequently required soil input variables for eco-hydrological modelling, focusing on providing soil data for the SWAT model. The data originates from the Soil Map of Estonia vector dataset (1:10000), which includes information on soil types according to Estonian soil classification, soil quality, number and depth of soil layers, information on course fragments and Estonian texture classes. Numerical soil properties are derived or through

using characteristic values of certain soil groups or computing them from available information, or if data is not available for calculation, data of external dataset is used.

# General comments

The scale of the presented soil dataset is outstanding. Detailed information about coarse fragments is unique. Descriptive or categorical type information originating from soil survey is very valuable even if uncertainty is generated when those are converted into quantitative data. The manuscript presents method to derive input information from soil survey data for those models, which require quantitative information about soil properties. This kind of data transformation has several difficulties which authors had to face. Significant amount of work has been put into the construction of the presented dataset, which has to be acknowledged. The work deserves to be published after major revision. Please find hereinafter suggestions for consideration.

(2) A: We appreciate the initial assessment and thank the reviewer for the value comments. We will address the concerns raised by the reviewer point by point below.

(1) RC2: Terminology used in international literature should be adapted in the manuscript. It is not clear what authors mean by "complex text codes" in the abstract.

(2) A: The Estonian texture information field in the original soilmap's attribute table is comprising not only of one actual texture class, but joined with classifiers for the rock content, peat soils and distinct compositional layers and their depth.

Visual examples of the meaning "complex text code" of the soil map are shown by Reintam, L., Rooma, I., Kull, A. & Kõlli, R. 2005. Soil information and its application in Estonia. In: European Soil Bureau. Research report. 9, 121-132 and Reintam, Loit; Kull, Ain; Palang, Hannes; Rooma, Igna (2003). Large-Scale Soil Maps and a Supplementary Database for Land Use Planning in Estonia. Journal of Plant Nutrition and Soil Science-Zeitschrift Fur Pflanzenernahrung Und Bodenkunde, 166 (2), 225–231.) and as an example of texture code of Skeletic Leptosol is shown "ls\_110-20/pk;r\_4ls\_1" which indicates presence of sandy silt loam, layer depth, solid limestone bedrock, rock content 50-7%.

We have included more information in the manuscript regarding the texture attribute field in the abstract, and sections 2.2.2 and 2.2.4.

(1) RC2: Please provide more precise information about the meaning of "soil profiles (e.g., layers, depths)" "layer information", which is mentioned in the abstract and introduction. Under materials and methods section authors mention that potential fertility was mapped, in the abstract and introduction soil quality is mentioned. It has to be clarified which soil property with which method was mapped, and reference or detailed description on how it was derived is needed.

(2) A: The field surveys for each polygon were made by sampling the soil to a default depth of one metre and the describing the visual and organoleptically defined texture of the soil from the surface to the depth of one metre. This is considered the observed soil profile. The assessed information was then noted on the field data sheet.

We added more information to the section 2.1.

(1) RC2: A table including metadata would be very informative in the manuscript, in which variable name, file name, description of variable,

units of measure, reference, etc. could be included, e.g. meta file of SoilGrids. The "EstSoil-EH\_v1.0\_attribute\_fields.txt" file could be a starting point for that.

(2) A: We thank the reviewer for the suggestion and added an overview table for the derived variables Table 6.

(1) RC2: The authors could put into context the novelty of providing data at
1:10000 scale – which scale is outstanding. Information on other national
soil datasets – which are considered detailed or high-resolution e.g.
https://dl.sciencesocieties.org/publications/sssaj/pdfs/82/1/186, etc. – could be referenced, and the
progress presented by EstSoil-EH v1.0 could be highlighted.

(2) A: We added the reference to the introduction in order to highlight how the EstSoil-EH v1.0 dataset preparation relates.

(1) RC2: Regarding the mapped soil properties, the following specific comments could be considered for the manuscript:

1. Soil type: Is it not clear why new soil types were added to the original dataset, how soil type was extended, e.g. was original soil type recoded based on soil profile information included in the dataset? How were Estonian soil types translated into WRB reference groups? Is there a reference document for it? Based on which soil classification system did you add new soil types and how? Please write down how many soil types were included initially and how many soil types were added. It is not clear how you got 7067 soil types in the attribute table if 120 soil types exist in Estonia. Maybe you meant something different.

(2) A: The Estonian national soil data set describes a base set of soil types, unfortunately in different literature 120-130. The difference is mainly caused because some researchers add to soil types also non-soil surface types (e.g. soilless bedrock; in total 7 types) and/or distinguish some subtypes of main soil types (e.g. Krf – recultivated open pit mining soil). It describes the most generalized level of Estonian soil classification for mapping that can be extended from these main 120-130 classes, incl. level of erosion, slope position, similar to FAO secondary identifiers, but instead of keeping them separate they just extended the main class, as the inherent "grammar" is well known in Estonia. This increased the overall number of explicit soil classes to more than 7000. We "just" extracted the main soil classes again.

(1) RC2: P4 L28: why "Overall soil type group" is differentiated from "Soil type" which is in L20?

(2) A: Original soil type is main category in Estonian soil classification and soil type group includes several soil types with main similar features. We clarified with more information in sections 2.1 and 2.2.1.

(1) RC2: 2. Texture classes: Clarification is needed on how USDA soil textural classes and then sand, silt and clay content were derived. Based on present manuscript Estonian soil textural classes were available from the official 1:10000 scale National Soil Map of Estonia. Estonian soil texture class names were translated using USDA terminology. Based on the Estonian texture class names average sand, silt and clay content were added to each soil layers. Please consider to add USDA texture class names based on the average sand, silt and clay content which characterize the Estonian texture classes. Please provide reference for the definition of the Estonian texture classes.

(2) A: The process followed a different order: The Estonian texture classes (Katchinsky, 1965 system), based on their known composition (based on how they were encoded at the time of survey)

have numerical values for sand, silt, clay fractions assigned. Then, based on these numbers the USDA texture names were assigned. The single important reference is table 2 that designates the sand silt and clay fractions for each known Estonian texture types

(1) RC2: 3. Coarse fragments content: It is not clear how - "skeleton indicator number" was derived from the shape and size of the stones and - "inferred rock content (% of volume)" was derived from "skeleton indicator number".

(2) A: We acknowledge that this was not well explained. Similar to the Estonian texture classes there exist Estonian stoniness classes, that describe a certain type of coarse fragments within the soil profile. An additional number in connection with this rock type identifier indicates the amount/volume of these rocks in 1kg of soil. We used this to characterise the coarse fragments. We clarified this in section 2.2.4

(1) RC2: 4. Soil organic carbon content: It has to be described why measured SOC data was averaged by soil units in the training dataset for deriving SOC prediction. Was not it possible to use soil profile data to derive the prediction? Predictors used in the random forest method could be listed under materials and methods section. Performance of SOC prediction could be included in a table. Variable importance could be shown in a figure.

(2) A: As several of the Estonian soil units (which contain the predictor soil profile information) would have contained a significant amount of sampling points for SOC (basically a few experimental trenches on agricultural fields) all the predictor variables (including the soil type, texture and topographical variables) aggregated for these units would be identical, this would have created a very strong bias in the training of the model. Therefore, SOC data points that lie within the same soil unit were averaged.

(1) RC2: 5. Bulk density: It is mentioned that BD is calculated based on texture and SOM, but texture is not included in Equation 4. It has to be considered that moist bulk density is required for SWAT.

(2) A: Depending on the formula indeed we are not using texture at all. Our real SOC/SOM field measurements and thus the modelled values are for dry bulk density. Removing the focus on SWAT as suggested by Reviewer1 would mitigate the conflict to provide moist bulk density. We state that this is dry BD, based on the dried SOM measurements.

(1) RC2: 6. Potential fertility: It is listed under materials and methods, but not included under the results. Reference or description for the computation would be needed.

(2) A: It was a historical data field in the original soil map. We did not use this field as the reliability and its original calculation is questionable. We remove notion of this field.

(1) RC2: 7. Organic horizon thickness: Similarly to potential fertility, it is mentioned under materials and methods, but not discussed in results section. Do you mean thickness of A horizon or thickness of soil horizon with accumulation of humified organic matter? Please add reference.

(2) A: See above, that is correct. For now we are not considering this field.

(1) RC2: 8. Please clearly state for which soil properties the performance could not be analysed because of lacking measured data.

(2) A: Yes, we have to be more precise/consistent about this. We added the reporting of data quality to manuscript.

(1) RC2: Some parts of the manuscript could be simplified by decreasing mainly technical descriptions, e.g.: P6 L3-P7 L3.

(2) A: We partially agree with RC2. However, we deem these technical details are already greatly reduced.

(1) RC2: More descriptive plots and tables could be provided for the readers about the derived dataset.

(2) A: Reviewer 1 also suggested plots regarding uncertainties and data quality. We will add these to the manuscript. We also added Table 5: Comparison of descriptive statistics (mean, standard deviation, minimum, 25-, 50-, and 75 percentile, and maximum value) for EstSoil-Eh and SoilGrids, based on zonal aggregation of SoilGrids into the EstSoil layer polygons (SOL\*: EstSoil-EH, SGR\*\_ SoilGrids-corresponding variable) for the first out of maximum four layers in EstSoil-EH (full table in data deposit supplement: "estsoil\_vs\_soilgrids\_stats.csv")

(1) RC2: Language revision of the manuscript would improve its readability.

(2) A: The manuscript had already been edited by English native professional scientific editor.

# EstSoil-EH v1.0: An eco-hydrological modelling parameters dataset derived from the Soil Map of Estonia

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Abstract. The Soil Map of Estonia is a vector dataset that maps more than 750 000 soil units throughout Estonia at a scale of 1:10 000. It is the most detailed and information-rich dataset for soils in Estonia, a Baltic country with an area of approximately 45 000 km<sup>2</sup>. For each soil unit, it describes the soil type, quality, texture, and layer information with a series of complex composite text codes, that comprises not only of the actual texture class, but also of the classifiers for the rock content, peat soils, its distinct compositional layers and their depths.- However, to use it as an input for numerical modelling using process-

15 soils, its distinct compositional layers and their depths.- However, to use it as an input for numerical modelling using processbased physical models, these text codes must be translated into numbers. Various generalisations and aggregations for agricultural soils for less-detailed versions of the map have been made at a scale of 1:100 000 and 1:200 000.

In this study, we create an extended eco-hydrological dataset for Estonia, the EstSoil-EH v1.0 (Kmoch et al., 2019a; doi:10.5281/ZENODO. 34732893473290), containing derived numerical values for the following data in all of the mapped

20 soil units in the 1:10 000 soil map: soil profiles (e.g., layers, depths), texture (clay, silt, sand components), coarse fragments and rock content, and physical variables related to water and carbon (bulk density, hydraulic conductivity, organic carbon content). Ultimately, our objective was to develop a reproducible method for deriving numerical values to support modelling and prediction of eco-hydrological processes in Estonia using the popular Soil and Water Assessment Tool.

The developed methodology and dataset will be an important resource for the Baltic region. Countries like Lithuania and Latvia have similar historical soil records from the Soviet era that could be turned into value-added datasets such as the one we developed for Estonia.

## 1 Introduction

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Eco-hydrological numerical models like Tthe Soil and Water Assessment Tool (SWAT; https://swat.tamu.edu/) or the Regional Hydro-Ecologic Simulation System (RHESSys) hasve been developed and applied during the past 30 years to evaluate the effects of alternative management decisions on water resources and non-point-source pollution in river basins through the simulation of physical processes (Arnold et al., 1998; Douglas-Mankin et al., 2010). SWAT is widely used

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internationally and is increasingly applied in Northern European and Baltic watersheds to better assess the hydrological state of the environment based on modelling of the most relevant physical processes (Piniewski et al., 2018; Tamm et al., 2016, 2018). However, a main input factor for <u>SWAT-many of these models</u> is detailed soil data, which does not exist for many countries on national scale or which exists with insufficiently fine spatial resolution. In addition, it is complicated to derive the values of the model parameters.

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At the global level, two main soil databases are available. The first was made available by the United Nations Food and Agricultural Organisation (FAO) through its Soils Portal: the Harmonized World Soil Database (HWSD) v1.2 (Fischer et al., 2008; http://www.fao.org/soils-portal/soil-survey/soil-maps-and-databases/harmonized-world-soil-database-v12/en/). The dataset resulted from a collaboration between FAO and Austria's International Institute for Applied Systems Analysis (http://www.iiasa.ac.at/), ISRIC–World Soil Information (https://www.isric.org/), the Institute of Soil Science of the Chinese Academy of Sciences (http://english.issas.cas.cn/), and the Joint Research Centre of the European Commission (https://ec.europa.eu/info/departments/joint-research-centre\_en). HWSD is a 30-arc-second raster database with more than 15000 different soil mapping units. It combines existing regional and national updates of soil information from around the world, including key soil and terrain properties of the Soil and Terrain database <u>SOTER</u> (SOTER, https://www.isric.org/explore/soter), ESD (https://esis.sc.egov.usda.gov/Welcome/pgReportLocation.aspx?type=ESD), the Soil Map of China (https://esdac.jrc.ec.europa.eu/content/soil-map-china), and homogenized sets of soil property estimates in

- the World Inventory of Soil Emission Potentials WISE (WISE, https://www.isric.org/explore/wise-databases). It also contains information from the 1:5 000 000-scale FAO-UNESCO Soil Map of the World (FAO, 1990; http://www.fao.org/soils-portal/soil-survey/soil-maps-and-databases/faounesco-soil-map-of-the-world/en/).
- 20 The other global-level soil dataset is SoilGrids250m, which provides global gridded soil information based on machine learning (Hengl et al., 2017) and is made accessible via an interactive Web interface (https://soilgrids.org/) with sophisticated standards-based data access via the OGC Web Coverage Services (https://www.opengeospatial.org/standards/wcs). SoilGrids250m provides values for sand, silt, clay, and rock fractions, and organic carbon and carbon stocks at several depths, which can be used as inputs for SWAT. At a regional level, the European
- 25 Soil Database v2.0 (Panagos et al., 2012; https://esdac.jrc.ec.europa.eu/content/european-soil-database-v20-vector-andattribute-data) is the only harmonized soil database for Europe, and also covers Estonia. It contains the soil geographical database SGDBE (vector data), which includes a number of essential soil attributes, and an associated database (PTRDB), with attribute values that have been derived through pedotransfer rules. The European database also includes the Soil Profile Analytical Database, which contains measured and predicted soil profiles for Europe as well as soil organic carbon (SOC)
- 30 projections for Europe that include 26 European countries at a resolution of 1 km. Wösten et al. (1999) developed a database of HYdraulic PRoperties of European Soils (HYPRES).

Existing national-scale soil datasets that have been developed to be used by SWAT currently only exist for the United States. Cordeiro et al. (2018) developed an official soil dataset for SWAT for Canada. Apart from these efforts, no consistent

methodology has been used to develop soil datasets at national, continental, or global scales so that the data is optimised for use in SWAT (Batjes, 1997; Dobos et al., 2005).

In Estonia, systematic large-scale soil mapping was launched in 1949, with agronomy students assisting (Estonian Landboard, 2017; "mullakaardi\_seletuskiri.pdf" ). Starting in 1954, a special survey was carried out under the supervision of 5 the Ministry of Agriculture. Aerial photographs were used as the basis for this activity. By 1992, Estonia's soil cover had been mapped by the Soil Survey Department of the former Institute of Estonian Agroprojects at a scale of 1:10 000. In addition to inspecting arable land, forests, and other land types between 1989 and 1991, the remaining former Soviet military areas were also mapped. Between 1997 and 2001, the soil map was digitized and attribute data was inserted into the database, resulting in the official National Soil Map of Estonia as a vector dataset that mapped 750 000 soil units at a scale of 1:10 000 (Estonian

- 10 Landboard, 2017; https://geoportaal.maaamet.ee/est/Andmed-ja-kaardid/Mullastiku-kaart-p33.html). It is the mosta very detailed and information-rich dataset for soils in Estonia-and, to the best of our knowledge, is also the most detailed national-scale digital soil database in the world. For each soil unit, it describes the soil type, quality, texture, and layer information using a series of complex text codes. However, to use it as an input for process-based models such as SWAT, these text codes must be translated into numbers. Processing a <u>class-based</u> soil dataset into <u>a the format readable by SWATrequired numerical</u>
- 15 variables is a time-consuming process because not all data required by SWAT are readily available (Bossa et al., 2012; Rahman et al., 2012). Various datasets have been created that generalise values for agricultural soils in Estonia to produce less detailed versions at scales of 1:100 000 and 1:200 000 (Kölli et al., 2009; Tamm et al., 2018). However, no large-scale high-resolution soil database is currently compatible available with SWAT numerical data for a range of typical eco-hydrological parameters.
- The objective of the present study was to develop a reproducible method for deriving numerical values as inputs for 20 modelling and for predicting hydrological processes with SWAT in Estonia. By developing this method, we aimed to develop a fully numeric soil database for Estonia. In this study, we derive numerical values for the key characteristics for the whole Soil Map of Estonia at a 1:10 000 scale for soil profiles (e.g., layers, depths), textures (clay, silt, and sand contents), coarse fragment and rock content, and physical variables related to water and carbon (bulk density, hydraulic conductivity, SOC) for all of the mapped soil units. The format is also suitable for use with the ArcSWAT graphical user interface 25 (https://swat.tamu.edu/software/arcswat/) for the SWAT model. We conclude with a discussion of the short-comings and uncertainties of the developed dataset.

There is no national scale dataset of measurements or predictions of SOC or BD for Estonia. However, Prévost (2004) described predictions of soil properties from the SOC content, and found that SOC was closely related to soil bulk density (BD) and porosity. Suuster et al. (2011) emphasized the importance of BD as an indicator of soil quality, site productivity, and soil compaction and proposed a PTF for the organic horizon in arable soils.

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Van Looy et al. (2017) reviewed existing PTFs and documented the new generation of PTFs that have been developed by different disciplines of Earth system science. They emphasized that PTF development must go hand in hand with suitable extrapolation and upscaling techniques to ensure that the PTFs correctly represent the spatial heterogeneity of the soils. Abdelbaki (2018) evaluated the predictive accuracy of 48 published PTFs for predicting BD using State Soil Geographic (STATSGO) and Soil Survey Geographic (SSURGO) soil databases from the United States. They also proposed and validated a new PTF for predicting BD using SOC inputs,

However, reliable estimates for SOC have been difficult to obtain due to a lack of global data on the SOC content of each soil type (Eswaran et al., 1993). Very few SOC datasets are available for countries or regions. For example, the Northern
Circumpolar Soil Carbon Database (Tarnocai et al., 2009; https://bolin.su.se/data/ncscd/) was developed to describe the SOC pools in soils of the northern circumpolar permafrost region. SOC stocks were also predicted under future climate and land cover change scenarios using a geostatistical model for predicting current and future SOC in Europe (Yigini and Panagos, 2016). Kõlli et al. (2009) published estimates of the SOC stocks for forests, arable lands, and grasslands and for all of Estonia. Nevertheless, -Tthey constrained their finding by noting that their estimates were calculated based on the mean SOC stock for
each soil type and the corresponding area in which the soil type was distributed. Putku (2016) used the large-scale Soil Map of Estonia at the polygon level for SOC stock modelling for mineral soils in arable land of Tartu county. <u>Ramcharan et al.</u> (2018) assimilate more than 200 datasets with SSURGO in order to predict\_various soil properties, SOC and BD, at 100-m

spatial resolution for the conterminous United States using statistical machine learning. Also, SOC and soil-hydraulic predictions for Estonia need to consider that Estonia is located relatively far north and hosts large areas of peatlands.

- 15 In summary, other datasets are available for use in Estonia-based modelling contexts. However, vector-based European or even global soil datasets are very coarse and excessively generalise large parts of the diverse Estonian landscape. High-detail datasets such as Soilgrids250m are predicted data on a grid 1km/250m, based on much less data points for Estonia. In this study, we derived numerical values for the following data in all of the mapped soil units in the 1:10 000 soil map: soil profiles (e.g., layers, depths), texture (clay, silt, sand components, and coarse fragments), rock content, and physical variables
- 20 related to water and carbon (organic carbon content, bulk density, hydraulic conductivity, available water capacity and erodibility factor). We present the development of a reproducible method for deriving numerical values from a Soil Map of Estonia to support modelling and prediction of eco-hydrological processes with the popular Soil and Water Assessment Tool and we create an extended ready-to-use dataset containing the additional parameters.

#### 2 Materials and Methods

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## 25 2.1 Pre-processing and screening of the initial soil database

The source dataset – the original Soil Map of Estonia - as described in the article, is not based on modelled but on fully observed data (e.g. texture, soil profile depth, rockiness, presence of organic layer etc). Systematic mapping of Estonian soils to produce soil map in scale 1:5 000 and 1:10 000 was started in 1954 (Reintam et al., 2005), with most intensive field studies in period 1965-1969. Generally field mapping was carried out in scale 1:10 000 but in hilly or undulating areas with higher soil diversity in scale 1:5000. In 1982-1988 older mapping data was updated and new areas were included with full-area soil quality (primarily fertility, rockiness, water regime, texture, erodability) assessment. In 1988-1990 soil field studies were performed in non-arable land and new mapping of ameliorated land. Forest soils were mapped in period 1976-1989.

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During large-scale field mapping of soils, the texture was determined in situ based on organoleptic methods and for reference profiles laboratory analyses were performed. This enabled calibration between texture defined by organoleptic method by each researcher participating in field survey and texture determined in laboratory (Estonian Land Board, Explanation to the soil map, https://geoportaal.maaamet.ee/docs/muld/mullakaardi\_seletuskiri.pdf?t=20091211092214). As a result of large-scale

5 soil mapping, 119 soil varieties in Estonian national classification system have been distinguished and more than 500 combinations of textural status have been described. About 10,000 profiles (1 profile per 330ha) have been sampled and analysed for characterisation of mineral soils (Reintam et al., 2003, 2005).

Thus, the texture codes and soil types assigned to the ca. 750000 mapped soil units (polygons) are based on many decades of in-situ land surveying practices.

- 10 The <u>original Soil Map of Estonia is available</u> vector layer for geographical information system software that can be downloaded from the Republic of Estonia Land Board Web site (https://www.maaamet.ee/en) in several formats under a permissive open data license. A copy with the original shapefile dataset, the related required documentation and checksums has been archived for reference (Estonian Landboard, 2017; https://datadoi.ut.ee/handle/33/103). The soil map contains the following <u>used</u> attribute fields:
- 15 Soil type: a designation of the soil name
  - Texture: texture classes defined by for fine and coarse fragments, and to which depth the same texture and coarse fragments is are observed (layer)
  - Potential fertility: estimated, prospective fertility that can be achieved after land improvement, this includes the
    potential fertility for wetlands or peatlands if they were drained
- - Rockiness: the type: i.e. material (e.g. limestone or sandstone rock), shape (e.g. flat, round, blocky) and % of the soil volume occupied by rocks (stones with a diameter  $\geq 20$  cm, in m<sup>3</sup>/ha, in the upper 30 cm of the soil, expressed with a degree of hardness)
  - -Overall soil type group: categories numbered from 0 to 22
- 25 Most-These attributes are encoded as "string" values, which include both letters and numbers. Exceptions are fertility and the generalised soil type group, which are stored as integer values. The important fields soil type and texture, are not just stored as standardised class values, but are instead a coded description based on abbreviations that are then combined with numbers for example depths and indictors for level of erosion, and are grouped together for different depths within the same attribute e field. These description-based attribute values make it difficult to derive the foundational numerical values for sand, silt, clay
- 30 and coarse fragments from the codes and to make them more consistent and usable in calculations and statistical analyses. In addition, our data screening revealed that the attribute values sometimes contradict the official legend for the Soil Map of Estonia. For example, the soil type reference sheet provided with the soil map lists ca. 120 different soil types in Estonia (Estonian Landboard, 2017; "muldade\_tabel.pdf") and the soil legend document describes 9 main texture classes and 12 soil skeleton types, i.e., coarse fragments and rock morphology (Estonian Landboard, 2017; "mullalegend.pdf"). However, the

database's attribute table contains 7067 unique variations for soil types, which resulted from the use of many specific local derivatives and transcription errors. Similarly, the texture column actually contains 87240 unique values instead of 9, 21 (9+12) or 108 (9x12). Considering the possible permutations of these soil types and textures, it would be prohibitively difficult to develop any kind of reasonable standardisation for the soil parameters before cleaning and unifying the dataset. Therefore, we performed extensive database standardisation on the original Soil Map of Estonia as the working basis and derive all further

variables based from the standardised dataset sequentially. Figure 1 illustrates the four major working packages to derived the desired eco-hydrological parameters. The subsequent sections are structured accordingly.

## 2.2 Analysis of soil type and texture codes and extraction of basic physical and textural values

## 2.2.1 Standardising soil types

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We used the main soil types from the soil type reference sheet that accompanies the Soil Map of Estonia to standardise the soil type fields in the spatial dataset and added several widely-used soil types that were not in the original reference list. We developed a short algorithm in Python to find the best match from the soil type reference list (Kmoch et al., 2019b; "01\_soilmap\_soiltypes\_textures\_layers.ipynb"). The algorithm progressively shortens the name from the right and compares the results with the "Soil type" field in the database. If no match is found, it then tries to find the name in a list of known exceptions. We created a lookup table (Kmoch et al., 2019a; "soil\_types\_error\_rules\_lookup.xlsx") that captures more than 300 entries that provide a soil type substitute code from the extended 135 soil types from the soil reference list to these not automatically identifiable soil types. The soil types and the Estonian soil names were then related to the FAO World Reference Base (WRB) soil codes (FAO, 2015) after the data have been corrected and standardised for each map unit in the extended soil dataset. An exemplary except is demonstrated in <u>Table 1Table 1</u>. The finalised table of the standardised 135 <u>main-most</u> used main soil types is provided as supplemental spreadsheet (Kmoch et al., 2019a; "soil types\_legend.csv").

#### 2.2.2 Pre-processing texture codes

The Soil Map of Estonia's "texture" field encodes the texture and general soil layer structure for each mapped soil unit in a structured, rule-based format (based on old Soviet-era paper maps). To derive meaningful numerical values for texture and other soil variables from the soil map, we developed a computer program that encodes these rules into a computer-readable grammar. In addition, we provided a lookup table for wrongly encoded texture codes and historical data-entry errors. The program provides a complete internal data structure that represents the analysed grammatical representation, which can be

evaluated and used to generate numerical values for a variety of variables.

The main implementation of this program is based on the Python library "Arpeggio" (Dejanović et al., 2016; https://pypi.org/project/Arpeggio/), which is a recursive-descent parser based on parsing expression grammars (also known as 30 the Packrat parser; http://bford.info/packrat/). This let us express rules and symbols (i.e., the grammar) in such a way that our software could parse arbitrary text and find the various definitions of the texture in the same way as the rules are described in the map legend handout.

Listing 1 provides an example of a parsing grammar. At the start of the program, the basic elements are defined, starting with the 9 main fine-textured soil types: "*plsl, pl, tsl, tls, dk, sl, ls, s, l*". The parser honours the order of their definition. Without these ordered rules, the parser will never find the more complex expression "*plsl*", because it would stop as soon as it encounters the "*pl*" part of the name. We also defined the skeleton types, i.e. coarse fragments types, and peat land soils.

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The function "def fine\_textured(): return Optional(kPlus), fine-textured\_list, Optional(amplifiers), Optional(depth\_range)" demonstrates the flexibility of how a parsing expression grammar parser can be configured. The function can find even optional (0 or 1) elements such as prefixes or suffixes within an arbitrary text stream.

- Subsequently, several separators and special indicators must be defined that can precede or be appended in combinations to the abovementioned soil type elements. These were often formatted as subscripts or using special characters. This proved to be a major source of data-entry errors, encoding mistakes, and ambiguities, which had to be handled via additional error-checking code, e.g., lookup tables which are provided in the supplemental materials (Kmoch et al., 2019b; "soil\_lib/LoimisLookups.py").
- 15 The mapped soil units also encode variations in the soil profile within a given soil unit. Thus, we must differentiate between a vertical separator for the observed soil layers, and a horizontal separator. However, we only considered the vertical component (soil horizons). In addition, these discrete vertical layers are only based the description in the original texture code. To capture and fully evaluate the possible texture codes, it was necessary to capture the meaning of any additional (rare) horizontal separators.
- 20 Because there are various data-entry errors and other ambiguities in the actual codes in the soil map dataset, we manually analysed all codes that could not be successfully evaluated by the grammar. Manual inspection was particularly required for codes that did not conform to the general rules described in the original soil legend handout. A full list of non-logical expressions, data-entry errors, and other grammar expressions that could not be easily or usefully standardised is provided as a supplemental Excel spreadsheet (Kmoch et al., 2019a; "texture\_error\_lookup.xlsx").
- 25 The parser for the defined grammar builds a data structure that can be evaluated for physical numerical parameters such as layers, depth, and the sand, silt, clay, and rock contents. This data structure is a Python dictionary object, i.e. a lookup table with nested key-value pairs that hold the parameters and the found values. In the example in Listing 2Listing 2, it becomes apparent that there is a "/" vertical layer separator (at the bottom, the "code" parameter shows the original texture code for this soil unit), and that depths and fine fractions are accessible separately from the data structure. If a skeleton coarse fraction were 30 defined in the texture code, then additional to the fine earth information, an additional "constituent" (the skeletoncoarse fraction
- type) would be part of the respective layer (i.e. the "soilparts" object). The complete parser Python module is provided as supplemental material (Kmoch et al., 2019b; "soil\_lib/LoimisGrammarV2.py").

## 2.2.3 Deriving depths and layers

In Subsection 2.2.2, we processed the textual code descriptions to compile the exact Estonian texture types in a standardised and readily available data structure. A base assumption is that most soils in Estonia were sampled to a depth of 1 m, as this is the case for a default soil profile. If larger or smaller depth information was encoded in the original soil texture code, then this would be used for the overall depth of that soil sample. The corresponding parameter required by SWAT is "NLAYERS", which represents the number of soil layers. For each of the layers, we can also read the analysed depth from the soil surface to the bottom of each layer. The SWAT-We defined parameters are named SOL\_Z# (layer 1-4) for each layer. Knowing We defined NLAYERS (the number described of layers in the profile) and depth per layer (SOL\_Z#), and we can derived the maximum soil depth (SOL\_ZMX), which represents the maximum depth of the soil profile (mm). We eliminated

- 10 additional soil parts from the dataset if their resulting layer thickness would be zero. An additional pragmatic decision was made to exclude cumulative vertical soil parts if their depth could not be reliably inferred. For example, "*sand/loamy sand*" indicates two layers, separated by "/". The base assumption is that the profiles have been sampled to the depth of one metre when no additional depth information is available. Therefore, for the given example, no depth information is available for the second layer ("*loamy sand*"). In these cases, we decide to drop the second layer and assign the full depth of 1m for the first
- 15 layer "sand". Another example is shown in Listing 2Listing 2, where the first layer depth is indicated as a range of 70-110 cm. In this case to derive a single number, the average will be taken resulting in 90 cm for the first layer. The remaining 10 cm filling up to 1m can be assigned to second layer. The Soil Map of Estonia holds depths in centimetres, whereas SWAT requires depths in millimetres. It was therefore also necessary toand for widely used conventions we convert the depths from cm to mm in this step.
- 20 In addition to the evaluation of layer and depth values we assign the extracted Estonian fine earth type and the related USDA texture class per layer in the variable EST\_TXT# (layer 1-4, Estonian texture class) and LX\_TYPE# (layer 1-4, USDA texture class). This step was conducted as part of the script in the supplemental materials (Kmoch et al., 2019b; "01\_soilmap\_soiltypes\_textures\_layers.ipynb").

#### 2.2.4 Deriving sand, silt, and clay fractions and rock content

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The foundational numerical values for fine earth and coarse fragments fractions of soil are now derived from the extracted processed and translated texture classes. There are detailed studies on reference soil profiles in Estonia, Latvia and Lithuania that relate original soil texture, so called Katchinsky texture system (Kachinsky, 1965) to USDA soil system (Calhoun et al., 1998) and erosion modelling case studies where based on laboratory analyses transfer functions from Katchinsky to USDA texture classes were developed (Laas and Kull, 2003). The relationship between the Katchinsky and Atterberg systems were provided by R. Kask (Kask, 2001).

The USDA soil taxonomy and World Reference Base soil classification systems use 12 textural classes, which are defined based on the sand, silt, and clay fractions (Ditzler et al., 2017). However, the USDA system defines fine particles as

having a diameter  $\le 2$  mm, whereas the Soviet-era maps use a diameter of  $\le 1$  mm. The Soviet soil classification also mostly ignores the silt fractions, and focuses on the clay fraction ( $\emptyset \le 0.001$  mm).

SWAT requires We defined the variables data for the extracted numerical texture input parameters for each layer as follows:

- SOL\_CLAY# (layer 1-4): clay content (% soil weight)

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- SOL\_SILT# (layer 1-4): silt content (% soil weight)
- SOL\_SAND# (layer 1-4): sand content (% soil weight)
- SOL\_ROCK# (layer 1-4): rock-coarse\_fragments content (% total weightvolumetric)

Based on the available analysis data and its structure, we derived meaningful numerical texture values using a lookup table that represents our best efforts to account for the size difference between the USDA and Soviet systems and lack of silt data in the Soviet system. The original observations were classified into the Estonian texture code system based on Katchinsky (1965) soil particle size standards at the time of observation (not by us). We translated the texture codes back into numbers. Regarding uncertainties related to that process - as we take these as observed data - achieving 5% accuracy in organoleptic determination of clay content for lower value classes while possible error increased in case of heavy texture classes. There are

- 15 many finely scaled texture classes in the Estonian system. We assigned USDA texture classes <u>based on the now defined</u> <u>numerical values for and the defined the sand</u>, silt and clay fractions. <u>Table 2Table 2</u> shows examples of the rules. For each texture code, the table provides the combination of sand, silt, and clay contents. <u>These texture transfer rules to select USDA</u> particle size distributions from the Estonian texture classes were composed by the authors according to Estonian guideline "Field Soil Survey – Muldade väliuurimine" (http://pk.emu.ee/yldinfo/uudis/2013/02/20/muldade-valiuurimine)
- 20 where matches of Estonian/Soviet and USDA/FAO classes for field survey is provided. It is not possible to retrospectively redefine minor differences in boundaries between different classes between texture systems, but we consider natural variation of texture within the soil mapping unit in scale 1:10 000 more significant than that of different texture systems. -In additional we introduced two more classes beyond the well-known USDA textures classes, i.e. "PEAT" and "GRAVELS". The former states that this soil unit is a peatland, where the peat layer thickness is at least 30 cm. For hydrological modelling reasons we
- 25 decided to still assign sand, silt and clay fractions to these units in order to provide a continuous hydrological soil surface. To soil units with the class "PEAT" a high clay content was assigned in order to represent the low vertical conductivity at the bottom theses peat bogs. However, for applications that critically evaluate clay content for soil units, the additional "PEAT" texture class (in the LX\_TYPE1-4 variable) can be used to apply additional rules to mask these soil units accordingly. The latter class "GRAVELS" is intended to demark soil units or discrete layers therein, where only a coarse fragment type but no
- 30 fine textures have been coded in the original texture codes. In these cases, depending on the type of the coarse fragment the layer can consist of gravels, large rocks or massive rock.

The rock content parameter in SWAT does not directly match the soil skeleton descriptions in the Soil Map of Estonia. Similar to the Estonian texture classes there exist Estonian stoniness classes, that describe a certain type of coarse fragments within the soil profile. An additional number in connection with this rock type identifier indicates the amount/volume of the se

rocks in 1kg of soil. We used this indicator number to designate numerical values for the coarse fragments. The soil map reference guide describes stone shapes and sizes, and ranges of these values, using a subscript indicator number that is often (but not always) appended to the skeleton code. We derived an overall percentage volume of rock based on that indicator number. Table 3Table 3 shows how we derived the rock content from the coarse fragments indicator that we obtained from the soil map encoding. This step was also conducted as part of the script in the supplemental materials (Kmoch et al., 2019b; "01\_soilmap\_soiltypes\_textures\_layers.ipynb"). This first and fundamental step concluded with a set of variables for each mapped soil unit that include now separate standardised Estonian and English/USDA texture classes per soil layer, number and depths of layers of the mapped soil unit and numerical values for fine earth and coarse fragments fractions per layer. The supplemental complete workflow is coded in the materials (Kmoch al.. 2019b: et 10 "01\_soilmap\_soiltypes\_textures\_layers.ipynb").

### 2.2.5 Evaluation and validation of extracted texture values

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We used two other sources of cross-validation to confirm the accuracy of the derived values.For validationFirst, we used a manually "decoded" part of the Estonian Soil Map for Tartu county. Tartu County covers about 10% of Estonia and offers a representative subset of the data, as it includes many different soil types, peat bogs, forest, and arable land. It contains 83 364 records. Several members of our research group cleaned and standardised the data on soil types, textures, and depth ranges over the course of several months and collated the results in a spreadsheet. We then compared the software's results with the manual classification results. Each soil unit in question was interpreted by at least two experts, and when their classifications differed, they discussed the difference until they achieved consensus about the correct classification.

- We used two other sources of cross-validation to confirm the accuracy of the derived valuesSecond, we used the ± 20 SoilGrids250m.—FirstFor that, we loaded and averaged the <u>the</u> raster layers <u>for the provided seven depths</u> from the SoilGrids250m data for the sand, silt, and clay<u>coarse fragments</u>, <u>bulk density and soil organic carbon</u>-contents <u>and saturated</u> <u>hydraulic conductivity from EU-HydroSoilGrids</u> for the top-into the layers of the EstSoil-EH datasetlayers.-Next, we rasterized the discrete polygons from the Soil Map of Estonia, including the newly generated extended values, for the same attributes provided by SoilGrids250m to the same raster resolution</u>. For each parameter, we <del>subtracted calculated descriptive statistics</del>
- 25 and plotted value distribution and an overview of the spatial pattern of the EstSoil-Eh parameters against the SoilGrids250m/EU-HydroSoilGrids values from our value to assess the magnitude of the deviation\_differences (Table 5 and Figure 9). We observed strong similarity in the general patterns. However, the variances ranged from 30-10 to 5030%. One main cause for this high variation is the scale difference between thedefinition of discrete polygon-values for the Estonian texture classes in our data and the more continuous distribution of raster values in the SoilGrids250m dataset.

## 30 2.3 Adding topographic variables as predictor variables

For the subsequent step of SOC prediction via the Random Forest machine-learning model, we calculated mean, median and standard deviation of several topographic and environmental variables as additional predictor variables. Topographic variables slope, Topographic Wetness Index (TWI), Terrain Ruggedness Index (TRI), and LS-factor were all calculated by using SAGA-GIS software based on a digital elevation model (Conrad et al., 2015). The LiDAR-based Digital Elevation Model with resolution 1 m was obtained from Estonian Land Board.

## 2.3.1 Topographic Wetness Index (TWI)

The TWI is a topo-hydrological factor proposed by Beven and Kirkby (Beven and Kirkby, 1979) and is often used to quantify topographic control on hydrological processes (Michielsen et al., 2016; Uuemaa et al., 2018) which also are relevant in the soil evolution. TWI controls the spatial pattern of saturated areas which directly affect hydrological processes at the watershed scale. Manual mapping of soil moisture patterns is often labor-intensive, costly, and not feasible at large scales. TWI provides an alternative for understanding the spatial pattern of wetness of the soil (Mokarram et al., 2015). It is a function

10 of both the slope and the upstream contributing area:

$$TWI = \ln \left(\frac{a}{\tan b}\right) \tag{1}$$

where a is the specific upslope area draining through a certain point per unit contour length  $(m^2 m^{-1})$ , and b is the slope gradient (in degrees).

## 2.3.2 Terrain Ruggedness Index (TRI)

TRI reflects the soil erosion processes and surface storage capacity which again is relevant from soil evolution perspective. The TRI expresses the amount of elevation difference between neighboring cells, where the differences between the focal cell and eight neighboring cells are calculated:

$$TRI = Y[\sum (x_{ij} - x_{00})^2]^{1/2}$$
(2)

where  $x_{ij}$  is the elevation of each neighbor cell to cell (0,0). Flat areas have a value of zero, while mountain areas with steep ridges have positive values.

## 2.3.3 LS-factor

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The potential erosion in catchments can be evaluated using LS factor as used by the Universal Soil Loss Equation (USLE). The LS factor is length-slope factor that accounts for the effects of topography on erosion and is based on slope and specific catchment area (as substitute for slope length). In SAGA-GIS the calculation is based on (Moore et al., 1991):

$$LS = (n+1) {\binom{A_s}{22.13}}^n {\binom{\sin\beta}{0.0896}}^m$$
(3)

where n=0.4 and m=1.3.

## 2.3.4 Drainage area per mapped soil unit

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In addition, we calculated the area per mapped soil unit in m<sup>2</sup> (area\_drain) and in percent of area, which is under drainage (drain\_pct). The drainage regimen considered both underground tile drainage and ditch based drainage systems. The drainage information used for this was compiled based on the Estonian Topographic Data Set (ETAK) and the official register of drainage systems (https://portaal.agri.ee/avalik/#/maaparandus/msr/systeemi-otsing) managed by the Agricultural Board of

Ministry of Rural Affairs of Estonia. All the variables were calculated using the GIS software packages QGIS and SAGA.

#### 2.4 Predicting Soil Organic Carbon (SOC) and Bulk Density (BD)

The main information described in the Soil Map of Estonia is the soil type and the soil texture. However, soil hydraulic properties and SOC data are needed for many different applications in soil hydrology, and especially for SWAT. Pedotransfer functions (PTFs) have proven to be useful to indirectly estimate these parameters from more easily obtainable soil data (Van Looy et al., 2017). Therefore, several soil parameters like soil organic carbon, bulk density and saturated hydraulic conductivity must be derived via PTFs and other data assimilation methods. To apply PTFs and other data-assimilation methods, third-party datasets can be used as secondary sources. In the previous steps we have prepared a wide set of input variables, including the numerical fractions for the textural properties, standardised classes for soil type and soil textures, and additional topographic variables, which we can apply as predictor variables to model the value distribution for SOC and BD. The SWAT modelWe develop defines these two extended soil physical input parameters as follows:

- SOL\_CBN# (layer 1-4): organic carbon content in % soil weight
- SOL\_BD# (layer 1-4): moist dry bulk density in Mg/m<sup>3</sup> or g/cm<sup>3</sup>

In order to map the spatial distribution of SOC in Estonia a machine learning model random forest (RF) was used to predict SOC based on parameters derived from the soil map. RF was preferred to more advanced ML algorithms (e.g., neural networks) because it has shown to be relatively resilient towards data noise and not require preliminary hyperparameter tuning (Breiman, 2001; Caruana and Niculescu-Mizil, 2006). In addition, feature importances can be extracted from the model to determine the most influential predictor variables.

- For training, we used measurements of soil organic matter (SOM) or soil organic carbon (SOC) from forest areas (samples sizes: n=100), 4 datasets of samples from Estonian open and overgrown alvars and grasslands (n: 94, 137, 146, 69), peatlands (n=175) and from arable soils transects (n=8964) resulting in 3373 distinct point locations (Kriiska et al., 2019; Noreika et al., 2019; Suuster et al., 2011). Where necessary, the SOM values were translated into SOC via: *SOC* = *SOM* / 1.724. Many samples from peatlands and arable fields were often sampled within the same mapped soil unit. For these soil units (polygons) the respective soil measurement data was averaged and joined to the respective soil units to reduce the bias
- 30 of the prediction. After joining the sample size reduced to the 397 distinct training samples for machine learning (Figure 2).

This data was then randomly split into training (60%) and test (40%) sets. An RF regression model was fitted to the training set using the *RandomForestRegressor* function from the Scikit-learn Python library. The model was evaluated by predicting SOC based on the predictor variables of the test set. Finally, the model was applied to soil map polygons without available SOC measurements to predict SOC content in Estonian soils.

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Subsequently, we calculated soil bulk density based on texture values and predicted soil organic carbon for each layer in each mapped soil unit polygon, with following PTF (Adams, 1973; Kauer et al., 2019):

 $BD = 1 / (0.03476 \times SOM + 0.6098)$  (4)

where:  $SOM = SOC \times 1.724$ 

The conversion factor 1.72 is a widely used universal value (). However, we acknowledge that the real value varies slightly

10 <u>between soils.</u> The workflow of SOC and BD calculation is coded in Python and provided in the supplemental materials (Kmoch et al., 2019b; "03\_SOC\_RF\_preps.ipynb").

## 2.5 Assimilation of additional hydrological variables

In order for this dataset to be more useful in eco-hydrological modelling we develop and add two additional hydrological variables. Saturated hydraulic conductivity (*K*<sub>sat</sub>) relates soil texture to a hydraulic gradient and is quantitative measure of water movement through a saturated soil. In addition to the ability of transmitting water along a hydraulic gradient we also add available water capacity (AWC) as a variable. AWC describes the soil's ability to hold water and quantifies how much of that water is available for plants to grow. For SWAT these We develop two variables are defined as follows:

- SOL\_K(layer 1-4): saturated hydraulic conductivity (mm/hr)
- SOL\_AWC(layer 1-4): available water capacity of the soil layer (mm H2O/mm soil)
- 20 We calculated K<sub>sat</sub> using the improved Rosetta3 software, which implements a pedotransfer model with improved estimates of hydraulic parameter distributions (Zhang and Schaap, 2017). It is based on an artificial neural network (ANN) for the estimation of water retention parameters, saturated hydraulic conductivity, and their uncertainties. For each standardised texture class, we used the numerical fine earth fractions for sand, silt and clay as inputs for the Rostta3 software and calculated K<sub>sat</sub> for each layer in each mapped soil unit polygon. We provide a copy of the Rosetta program in the supplemental materials (Kmoch et al., 2019b; "Rosetta-3.0").

In order to calculate available water capacity, we summarized the field capacity (FC, at -330 cm matric potential -0.03 MPa) and wilting point (WP, at -15,848 cm matric potential -1.5 MPa) variables of the 7 soil depths of the EU-SoilHydroGrids 250m resolution raster datasets (Tóth et al., 2017) for each mapped soil unit for the provided depths of 0, 5, 15, 30, 60, 100, and 200 cm. The available water capacity is then calculated for each of the 7 depths by a raster calculation:

30 AWC = FC - WP (Dipak and Abhijit, 2005). The resulting 7 AWC raster layers are then averaged into the respective depth ranges for each of the discrete layers of the Estonian mapped soil units. The Python code of the process for the extraction of FC and WP from the EU-SoilHydroGrids is provided with the supplemental materials (Kmoch et al., 2019b; "05\_hydrogrids\_extents\_and\_awc\_extract.ipynb").

## 2.6 Calculating the USLE K erodibility factor

To account for erosion, we used the universal soil loss equation (USLE) soil erodibility (K) factor (USLE\_K) based on the exact values for clay, silt, sand, and rock contents, modified by accounting for the mean SOC content. SWAT requires USLE\_K for the top layer of the soil. To calculate USLE\_K values for Estonia, we used the previously derived texture classes and SOC content. It was also necessary to provide a soil structural class (s) related to the texture, which is defined in the

European Soil Database as majority of particles of matter that fit through a sieve of the given size:

- s = 1 means very fine granular (1 to 2 mm) G (good)
- s = 2 means fine granular (2 to 5 mm) N (normal)
- s = 3 means medium or coarse granular (5 to 10 mm) P (poor)
- 10 s = 4 means blocky, platy or massive (> 10 mm) H (humic or peaty top soil)

As in previous sections, we used the Estonian texture code to derive the value using a simple decision tree based on the texture types (1 or 2), amount of rocky material (2 to 3), and the presence of peat soils (4).

Next, we defined soil permeability classes (*p*, see Table 4<u>Table 4</u>, as suggested by the SWAT 2012 IO documentation p.309, https://swat.tamu.edu/media/69296/swat-io-documentation-2012.pdf) and the related saturated hydraulic conductivity

15 ranges to derive a permeability class for each soil unit, which became an input for the final USLE\_K equation. These classes function similarly to the SWAT hydrologic groups and were derived for major soil textural classes, where *p* ranges from 1 (very rapid) to 6 (very slow).

We defined the *p* value for the USLE\_K using based on the already predicted hydraulic conductivity  $K_{sat}$ . We then calculated the required term for an intermediate factor (*M*) that accounts for the balance among the silt, sand, and clay contents:

(5)

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## $M = (m_{ m silt} + m_{ m sand}) \times (100 - m_{ m clay})$

where m represents the % fraction of weight for the silt, sand, and clay contents (respectively). K is then calculated from M using the following equation:

 $K = \{(2.1 \times 10^{-4} \, M^{1.14}) \times (12 - om) + 3.25(s - 2) + 2.5(p - 3)\} / 100 \tag{6}$ 

where *om* represents organic matter, which we fill in from the predicted SOC (SOC×1.724). The joint process of loading
 calculated *K*<sub>sat</sub> values from the Rosetta3 output, averaging and assimilating the AWC values based onn the FC and WP datasets
 from the EU-SoilHydroGrids and consequently, calculating USLE\_K is described and provided in the supplemental materials
 (Kmoch et al., 2019b; "02\_soilmap\_update\_Ksat\_AWC\_USLE-K.ipynb").

## **3** Results

In this study, we developed a Python module that is capable of analysing, extracting, and standardising the soil type 30 and soil texture data from the official Soil Map of Estonia into a reusable, reproducible soil dataset that uses World Reference Base and FAO soil classes and texture descriptions. Figure 4Figure 4 shows a map of the classified topsoil texture classes derived from the original Estonian texture codes. In addition, it shows the peat soils that cover up to 20% of Estonia, and are an important soil type in such northern countries.

To make such soil information usable in an eco-hydrological modelling context, we derived numerical values for each of the soil units. These values include the number of discretized soil layers (NLAYERS) - a maximum of 4 separate vertical distinct soil layers where described in the original texture codes –the depth of each layer (SOL\_Z1-4), and the maximum depth of the sampled profile for each mapped soil unit (SOL\_ZMX). Based on the layer information and the extract texture classes we could define the percent fractions per volume of sand (SOL\_SAND1-4), silt (SOL\_SILT1-4), clay (SOL\_CLAY1-4), and coarse fragments (SOL\_ROCK1-4) per layer. Figure 5 shows the percent fractions for sand, silt, clay and coarse fragments for the top layer. Table 6 contains the full list of variable and parameters per mapped soil unit contained in the EstSoil-EH dataset.

## 10 3.1 Validation of soil type and texture classes extraction and standardisation

For the main soil types, we achieved 97.7% agreement between the software's result and the manual classification. The manual verification of the validation revealed several re-labelling issues from the error lookup table. A visual assessment by two soil sciences senior research staff asserted that the level of similarity of the soil types that were selected by the automated process were closely related. However, the mismatches (1943 records, equivalent to 2.3% of the total records) indicated that

- 15 the soil experts tended to interpret "errors" based on personal knowledge that may not be reproducible in a strictly automated fashion. For example, some landforms (e.g. eroded material filling low slopes or collapsed cliffs) were originally classified as exceptions to the general classification rule based on the local knowledge of the landscape. When standardising these expert interpretations with the same more general soil type, we reduced the number of mismatched soil type identifiers to 0. Furthermore, it should be emphasised that humans tend to make mistakes when performing repetitive procedures. Therefore,
- 20 we consider the high accuracy (97.7%) to be a very good result.

For the validation of textures, we used several steps. First, given the high agreement between the software-generated codes and the human-generated codes, we accepted the software's texture codes for use in our subsequent evaluations. Next, we compared the extracted main texture for each layer with the manually coded value:

- 77 870 of 83 364 records (93.4%) showed identical parsing of the full texture code
- 71 635 of the records (85.9%) showed identical interpretation of the first layer's texture type (10 312 records were differently coded, and 1417 produced "no value" errors, in which either the source or validation dataset contained no value, preventing a comparison with the other dataset's value)
  - 65 000 of the records (78.0%) showed identical interpretation of the second layer's texture (with 2325 differently coded textures, and 16 038 "no value" errors, of which 15 461 occurred in the automated processed new dataset, and only 577 occurred in the validation dataset)
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82 507 of the records (99.0%) showed identical interpretation of the third layer's texture (with most errors caused by a non-existent third layer, 334 differently coded, and 523 with a "no value" error)

Our manual assessment of the mismatches indicated the same problem that occurred with the soil types. The expert assessments aimed to keep as much information as possible available in their decoded classification, and this did not always agree with the automated processing rules. Furthermore, the complexity of the Estonian texture rules and the reliance on human judgement creates high uncertainty in some cases, even for human interpretation. In addition, to derive the grammar rules, we added a

5 few simplifying elements, such as omitting some rarely used additional information in the soil texture descriptions. For example, the Estonian rules allow specification of several soil parts, but as a horizontal distribution within the same mapped soil unit rather than as vertical layers. This is understandably complex, making it difficult to classify this variable soil as a single soil unit. Consequently, it is inevitable that some of these descriptions will not agree with the software's classification.

## 3.2 SOC prediction and validation of Random Forest model

- 10 We also calculated several extended soil properties, i.e. SOC content and BD. The RF regression model was implemented with the RandomForestRegressor function from the Scikit-learn Python library. The model was evaluated by predicting SOC based on the predictor variables of the test set for the 60:40 split. Figure 3Figure 3 illustrates the cross-validation scatterplots of observed vs. predicted SOC values for the test/validation sample splits. Following characteristics are reported for the chosen RF model:
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- coefficient of determination (R<sup>2</sup>) score: 0.69
- score of the training dataset with out-of-bag estimate (oob score): 0.58
- Pearsons r correlation coefficient, training: 0.90, validation: 0.83

RF feature importances, top 6:

- Clay content (SOL\_CLAY1): 0.65
- Terrain Roughness Index, standard deviation (tri\_stdev): 0.04
- Sand content (SOL\_SAND1): 0.03
- LS-factor, median (ls\_median): 0.028
- Area under drainage in percent (drain\_prct): 0.027
- Coarse fragments rock content (SOL\_ROCK1): 0.024

25 Figure 6Figure 6 shows the predicted values of SOC and BD for the top layer. On visual inspection the spatial distribution for the SOC content matches comparatively well with known agricultural areas, where low carbon content prevails, as well as with the peat land areas, which have a very high carbon content.

## 3.3 Extended variables results

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Based on the variables derived in previous steps, we could also calculate soil hydraulic parameters, such saturated 30 hydraulic conductivity ( $K_{sat}$ ) and available water capacity (AWC). Figure 7 shows the spatial distribution of  $K_{sat}$ and AWC for the first layer. The predicted  $K_{sat}$  values for peat areas and wetlands also corresponds with ranges reported in the literature for the sand-silt-clay ratios provided (Gafni et al., 2011). The USLE *K* erodibility factor for each soil unit was also calculated (Figure 8Figure 8). We compiled all parameters into a dataset that can now be easily used with SWAT or other ecohydrological and land-use-change models. As we are not changing the general geometry or underlying spatial data model of the original soil map, all parameters are only added to the existing mapped soil units and thus, all original soil polygons remain discernible. The dataset (Kmoch et al., 2019a; doi:10.5281/ZENODO.3473290) and the software codes (Kmoch et al., 2019b; https://zenodo.org/record/3473210) have been deposited online.

## 4 Discussion and Future Work

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The Soil Map of Estonian is a valuable resource for hydrological, ecological and agricultural studies. It is widely used in Estonia. But before our analysis, a large amount of the dataset's information was not readily usable beyond the field or farmscale because of the need to manually interpret the specialised soil types and the complexity of the rules that describe the texture or other characteristics of the soil units. The presented dataset is of very high spatial detail based on the original Estonian national soil map, which was created from directly surveying all of Estonia. Thus, our presented dataset much more spatially related to the landform/landuse observed there. Furthermore, the textures and SOC/BD values are directly derived

- from reliable observed data samples from Estonia, with a reproducible workflow, whereas this is not true for many other
  reported soil datasets that cover the area of Estonia. Furthermore, the method created to translate original hard copy soil map (with traditional textual codes) to a digitally readable numerical GIS-based map can be used by several other countries (e.g., Latvia, Lithuania, Ukraine etc) which enables spatially more explicit modelling of ecosystems. We used a multi-step approach to derive a generalised and standardised numerical dataset that will have many potential applications for users of Estonian soil information, including support of economic, agricultural, or environmental management and input for decision-making and to support more reproducible scientific research based on Estonian soil information. Until the present analysis, numerical and
- process-based eco-hydrological modelling with tools and models like SWAT or the Regional Hydro-Ecologic Simulation System (RHESSys) were greatly hampered by the need to manually derive useful values from the Soil Map of Estonia to support the modelling.
- One challenge in terms of validation is that the datasets we used for validation are informed to some extent by previous reports about Estonian soil characteristics that are not necessarily more accurate than the results of our classification. Although we accounted for this problem by providing additional comparisons, the scale mismatch between continuous raster datasets and polygon-based data inevitably introduced errors and trade-offs into the comparison. One solution to these problems would be to perform supplemental field sampling to ground-truth the source data and confirm the accuracy of our model's classification based on the field data.
- 30 A direct interpretation on the derived discrete layer information as soil horizons needs should not be generalized but checked on per case basis. From the point of end-user, the first layer is not a default 30 cm deep top soil layer. All physical, chemical and hydraulic properties are based on the analysis of the original texture code per mapped soil units and the resulting

discrete layers per unit. This is an important usage constraint, for example in sense of biological activity, as 30 cm soil layer is most active, but for each soil unit it needs to be checked which layers extend into which actual depths. Also the *SOC* content and *BD* are not modelled in a vertical continuum but per discrete values per unit and layer. However, fertile soils, like Luvisols contain a lot of *SOC* also in deeper layers. But such additional expert knowledge is not encoded in original Soilmap of Estonia,

- 5 nor in the processing algorithms that derived the extended parameters for this newly generated dataset. However, such additional knowledge, as well as more appropriate models for peatland areas, could be included as additional rules in a subsequent improvement of this dataset. The original purpose of this dataset was to derive values for hydrological modelling purposes and at the same time to stay as close to the original data as possible. From that perspective peat soil units are currently modelled with assumptions to have a similar behaviour to clay hydrologically. Therefore, the spatial distribution of clay
- 10 percentage in particular, but also the concurrent physical fractions of sand and silt do not make scientific sense for these areas where peat is prevalent. In order to make the dataset as useful as possible and to identify peatland areas, we introduced the additional class "PEAT" into the USDA classification. While sand, silt, clay and rock content are directly derived values from the original texture codes, *SOC* and *K<sub>sat</sub>* are modelled via statistical machine-learning algorithms, which include additional uncertainty. This should be considered when evaluating *BD* and USLE *K*, which are calculated using *SOC* as an input variable.
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The only variable which we did not model based in dependence of already modelled parameters is AWC. Here we summarised the EU-SoilHydroGrids 250m (Tóth et al., 2017) raster datasets for FC and WP as inputs an external data integration. This is not ideal and can be considered a trade-off between introducing too much uncertainty and an external unrelated data source.

In the future, we foresee step-wise improvement of our software by developing better PTFs to estimate parameters 20 and to better integrate the presence of peat soils and other specific landscapes and environments in Estonia. Furthermore, statistical machine-learning or neural network and deep learning methods could be tested in order to improve soil classifications and express more complex relationships between soil types and textures. Currently, one specificity of the newly created EstSoil-EH dataset is its discrete nature, as we are only adding derived numerical variables to the existing mapped soil units (polygons). We do not predict a continuous surface in this study, thus, comparisons with continuous surface parameters 25 predicitons such as in SoilGrids (Hengl et al., 2017) or EU-SoilHydroGrids (Tóth et al., 2017), are not directly possible. However, the workflow could potentially be extended also for creating continuous surface. With appropriate modification (e.g., to use the soil characteristic codes more consistently for a different country), our methodology could also be applied in

(e.g., to use the soil characteristic codes more consistently for a different country), our methodology could also be applied other countries such as Lithuania or Latvia that share similar historical land- and soil surveying practices.

## Code and data availability.

30 The described "EstSoil-EH v1.0" dataset including all supplemental tables and figures is deposited on Zenodo, doi:10.5281/ZENODO. <u>3473289</u>3473290 (Kmoch et al., 2019a). Supplemental software and codes that were used, e.g. the texture-code parsing scripts, the machine learning model and the parameter calculation Jupyter notebooks are maintained on

GitHub (https://github.com/LandscapeGeoinformatics/EstSoil-EH\_sw\_supplement/releases) and were also deposited on Zenodo, doi:10.5281/ZENODO.3473210 (Kmoch et al., 2019b). The original National Soil Map of Estonia (https://geoportaal.maaamet.ee/est/Andmed-ja-kaardid/Mullastiku-kaart-p33.html ) was archived for reference on the DataCite- and OpenAire-enabled repository of the University of Tartu, DataDOI, doi:10.15155/re-72 (Estonian Landboard, 2017).

## Author contributions.

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A. Kmoch designed the experiments and code. A. Kmoch, E. Uuemaa, A. Astover, A. Kanal validated soil types and texture values. E. Uuemaa completed terrain analysis and statistics. A. Kull, A. Helm, M. Pärtel, I. Ostonen cleaned and organized the input SOC datasets. H. Virro developed the SOC RF machine-learning code and experiment. A. Kmoch and E. Uuemaa drafted the manuscript and created the figures, and all authors contributed to the paper writing.

## Competing interests.

The authors declare that they have no conflict of interest.

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Figure 1: Flowchart for executed processing steps grouped into the four major work packages



Figure 2: Distinct soil unit polygons including all sampling locations for the ML training sample.



5 Figure 3: Random Forest model cross-validation scatterplot of observed vs. predicted SOC values for the test/validation sample splits: a) training subsample and b) validation subsample



Figure 4: USDA topsoil textures derived from the original Estonian texture codes by the software developed in the present study, including additional classes "PEAT" and "GRAVELS".



Figure 5: Physical soil properties: assigned soil texture fractions of a) sand, b) silt, c) clay, and d) coarse fragments in the first soil layer based on texture classes.



Figure 6: Extended physical soil parameters: a) predicted soil organic carbon (SOC) and b) bulk density (BD) of the first layer.



Figure 7: Soil hydraulic parameters: a) saturated hydraulic conductivity (K\_sat) and b) available water capacity (AWC) in the first layer.



Figure 8: Calculated USLE K erodibility factor based on the numerical parameters derived from the Soil Map of Estonia dataset.



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supplemen	tal spreadsheet ("soil_types_legend.csv")		
Estonian soil code	Estonian name	Scientific English	WRB_code
Ag	Gleistunud lammimuld	Endogleyic Fluvisols	FL-gln
AG	Lammi gloimuld	Clavic Eluvisols	EL al

Table 11: Examples of the final list of standardised soil types and the added English WRB classes, full list as

soil code			
Ag	Gleistunud lammimuld	Endogleyic Fluvisols	FL-gln
AG	Lammi-gleimuld	Gleyic Fluvisols	FL-gl
AG1	Lammi-turvastunud muld	Histic Fluvisols	FL-hi
AM'	Väga õhuke lammi-madalsoomuld	Rheic Sapric Histosols (fluvic)	HS-sa.rh-fv
AM"	Õhuke lammi-madalsoomuld	Rheic Sapric Histosols (fluvic)	HS-sa.rh-fv
Dg	Gleistunud deluviaalmuld	Endogleyic Umbrisols (deluvic,	UM-gln-
		novic)	del.nv
E2I	Keskmiselt erodeeritud kahkjas leetunud ja leetunud	Dystric Regosols	RG-dy
	muld		
E2k	Keskmiselt erodeeritud rähkmuld	Epicalcaric Regosols	RG-cap
E2o	Keskmiselt erodeeritud leostunud ja leetjas muld	Eutric Brunic Regosols	RG-br.eu
E3I	Tugevasti erodeeritud kahkjas leetunu ja leetunud muld	Dystric Regosols	RG-dy
E3k	Tugevasti erodeeritud rähkmuld	Epicalcaric Regosols	RG-cap
E3o	Tugevasti erodeeritud leostunud ja leetjas muld	Eutric Brunic Regosols	RG-br.eu

5 Table 22: Example of the basic rules for deriving numerical values for texture (sand, silt, and clay contents) from the Estonian texture codes and assigned new English and USDA texture classes. These rules were selected by the authors. The full table is provided as a supplemental Excel spreadsheet ("texture\_rules\_lookup.xlsx")

Estonian				Proporti	on (%) of t	otal weight
texture	Estonian name	English name	USDA texture code	Sand	Silt	Clav
code						
1	Liiv	sand	S	90	5	5
$l_1$	sõre liiv	coarse sand	S	95	5	0
12	sidus liiv	fine sand	S	90	3	7
sl	saviliiv	loamy sand	LS	82	9	9
$sl_1$	saviliiv	loamy sand	LS	82	9	9
ls	liivsavi	loam	L	55	30	15
$ls_1$	kerge liivsavi	sandy loam	SL	65	20	15
$ls_2$	keskmine liivsavi	loam	L	55	30	15
s	Savi	clay	С	25	30	45

Table <u>33</u>: The relationship between the coarse fragments (rock content and shape) indicator from the soil map encoding and the rock content as a % of the total volume. We used the average of each defined range as the singular value required by the SWAT model

	Sca	le of c	onversi	ion for	rock co	ontent
"Skeleton" indicator number	1	2	3	4	5	6
Inferred rock content (% of volume)	6	15	25	40	60	85

5

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## Table 44: Permeability classes used in the USLE\_K equation as suggested by the SWAT documentation.

Texture	Saturated hydraulic
	conductivity (mm $h^{-1}$ )
Sand	> 61.0
Loamy sand, sandy loam	20.3-61.0
Loam, silty loam	5.1-20.3
Sandy clay loam, clay loam	2.0-5.1
Silty clay loam, sand clay	1.0-2.0
Silty clay, clay	< 1.0
	Texture Sand Loamy sand, sandy loam Loam, silty loam Sandy clay loam, clay loam Silty clay loam, sand clay Silty clay, clay

Table 5: Comparison of descriptive statistics (mean, standard deviation, minimum, 25-, 50-, and 75 percentile, and maximum value)for EstSoil-Eh and SoilGrids, based on zonal aggregation of SoilGrids into the EstSoil laver polygons (SOL\*: EstSoil-EH, SGR\* SoilGrids-corresponding variable) for the first out of maximum four lavers in EstSoil-EH (full table in data deposit supplement: "estsoil vs\_soilgrids\_stats.csv")

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variable	mean	std	min	<u>25 %</u>	<u>50 %</u>	<u>75 %</u>	max
SOL_Z1	787.67	<u>304.97</u>	20.00	<u>500.00</u>	1000.00	1000.00	<u>30750.00</u>
SOL_SAND1	<u>68.70</u>	24.16	0.00	55.00	82.00	<u>90.00</u>	100.00
SGR_SAND1	55.12	<u>6.42</u>	0.00	<u>50.55</u>	54.40	<u>59.00</u>	80.08
SOL_SILT1	14.15	<u>9.83</u>	0.00	5.00	<u>9.00</u>	20.00	<u>50.00</u>
SGR_SILT1	30.12	<u>4.77</u>	0.00	27.17	30.88	<u>33.58</u>	46.17
SOL_CLAY1	17.15	<u>18.99</u>	0.00	5.00	<u>9.00</u>	15.00	70.00
SGR_CLAY1	14.74	3.17	0.00	12.58	14.65	16.75	35.67
SOL_ROCK1	5.46	15.71	0.00	0.00	0.00	<u>6.00</u>	85.00
SGR_ROCK1	8.42	1.60	0.00	7.36	<u>8.28</u>	<u>9.27</u>	38.17
SOL_SOC1	<u>9.37</u>	7.18	<u>1.20</u>	5.05	<u>6.69</u>	<u>9.38</u>	<u>29.98</u>
SGR_SOC1	<u>9.66</u>	4.56	<u>1.18</u>	<u>6.20</u>	<u>8.64</u>	12.16	47.62
SOL_BD1	<u>0.94</u>	0.23	0.00	0.85	<u>0.99</u>	<u>1.10</u>	<u>1.47</u>
SGR_BD1	1.33	0.07	0.80	1.29	<u>1.34</u>	1.38	<u>1.51</u>
SOL_K_SAT1	<u>55.27</u>	<u>66.43</u>	0.00	<u>9.20</u>	<u>37.54</u>	133.21	<u>645.68</u>

SGR_K_SAT1	773.84	193.29	24.38	588.33	701.33	870.83	1884.17
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## Table 6: Description of variables and parameters available in the EstSoil-EH dataset

<u>name of variable per</u>		
mapped soil unit	<u>data type</u>	description
upd_siffer	<u>string</u>	Estonian soil type
WRB_code	<u>string</u>	FAO WRB soil type (1st and 2nd level)
<u>wrb_main</u>	<u>string</u>	FAO WRB main soil type (1st level)
Loimis1	<u>string</u>	Estonian texture description
loimis_rec	<u>string</u>	reconstructed error-free interpretation of
		Estonian texture description
<u>nlayers</u>	<u>number</u>	number of recognized layers/horizons
<u>SOL_ZMX</u>	float64	depth in mm: max depth of the sample
		analysed soil profile in the mapped soil unit
<u>SOL_Z1-4</u>	<u>float64</u>	depth in mm: the bottom of the layer
EST_TXT1-4	<u>string</u>	Estonian texture class
LXTYPE1-4	<u>string</u>	USDA texture class
EST_CRS1-4	<u>string</u>	Estonian coarse fragment type
SOL_SAND1-4	<u>int64</u>	% mass of Sand in fine earth fraction
SOL_SILT1-4	<u>int64</u>	% mass of Silt in fine earth fraction
SOL_CLAY1-4	<u>int64</u>	% mass of Clay in fine earth fraction
SOL_ROCK1-4	<u>int64</u>	<u>% volumetric in kg soil</u>
SOL_SOC1-4	float64	<u>% soil weight</u>
SOL_BD1-4	float64	<u>g/cm<sup>3</sup></u>
<u>SOL_K1-4</u>	float64	<u>mm/hr</u>
SOL_AWC1-4	float64	mm H2O/mm soil
<u>USLE_K</u>	float64	<u>K factor</u>
<u>HYDGRP</u>	<u>object</u>	SWAT hydrological group, A-D
<u>slp_mean</u>	float64	mean slope, calculated from DEM
<u>slp_median</u>	float64	median of slope
<u>slp_stdev</u>	float64	standard deviation
<u>twi mean</u>	float64	mean terrain wetness index, calculated from DEM
twi_median	float64	median of terrain wetness index
<u>twi_stdev</u>	float64	standard deviation
<u>ls mean</u>	float64	Is-factor, calculated from DEM
<u>ls_median</u>	float64	median ls-factor
<u>ls_stdev</u>	float64	standard deviation
<u>tri_mean</u>	float64	terrain roughness index, calculated from DEM
<u>tri median</u>	float64	median of terrain roughness index
tri stdev	float64	standard deviation

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<u>area_drain</u>	<u>float64</u>	<u>area per unit under a (e.g. tile-)drainage</u>
		<u>regimen</u>
drain_pct	float64	percent of the area of the soil unit under
		<u>drainage</u>
<u>Huumus</u>	string	textual description of A or O horizon, if
		<u>available</u>
ao hor thick	float64	thickness in mm of A (or O) horizon
<u>ao hor type</u>	string	type of A (or O) horizon
geometry	geometry	EPSG:3301 Estonian National Grid

# at the first the basic elements are defined, starting with the actual soil texture fine-textured soils ("peenes") types
def l(): return 'l'  # liiv, en: sand
def pl(): return 'pl' # pl - peenliiv, en: fine sand (täiendina peenliivakas)
def plsl(): return 'plsl' # plsl - peenliivakas saviliiv, en: fine clayey sand
# other " finely textured" types
def fine textured list(): return [plsl, pl, tsl, tls, dk, sl, ls, s, l]
def fine_textured(): return Optional(kPlus), fine_textured_list, Optional(amplifiers), Optional(depth_range)
# turfs, aka, peat bogs and similar are specially handled types
def t(): return 't' # t - turvas, en: peat
def th(): return 'th' # th 15 or th 15-20 humus thickness
def turfs(): return Optional(kPlus), [th, t], Optional(amplifiers), Optional(depth_range)
# soil skeleton ("koores") types, for stone content and shape in the soil part
def kr(): return 'kr' # kr - kruus, en: gravel
def r(): return 'r'  # r - rähk, en: grit, rubble
# and other " skeleton " types
def skeleton list(): return [kr, kb, pk, ck, lu, v 0, k 0, r 0, r, v, k, p, d]
def skeleton(): return Optional(kPlus), skeleton_list, Optional(amplifiers), Optional(depth_range)
# several separators and special indicators can precede or be appended in combinations with the above soil elements
def deoth number(): return RegExMatch(r'\d+') # at least two digits for deoth numbers (well might as well be one)
def depth_range(): return Optional(kPlus), depth_number, ZeroOrMore('-', depth_number)
def vertiSep(): return '/'
def horiSep(): return ';'
# and eventually get composed into aggregated lists of components per encoded profile
def constituent(): return ZeroOrMore(skeleton), ZeroOrMore([fine textured, turfs, Optional(alternateComma)])
def paraSeq(): return OneOrMore(constituent)
def soilParts(): return paraSeq, ZeroOrMore(vertiSep, paraSeq)
def texture grammar(): return OneOrMore(soilParts, sep=horiSep), EOF

Listing 1: Examples of grammar definitions. The grammar is built upon the defined basic combinations of text and symbols that are found in the database, and comprises the rules for processing those encodings. The full grammar is presented in the supplemental materials (Kmoch et al., 2019b; "soil\_lib/LoimisGrammarV2.py" Python module)



Listing 2: The data structure that results from a computed grammatical evaluation. At the bottom, the original texture code for this soil unit is shown.