Response to Editor and Reviewers

Editor Decision:

Reconsider after major revisions (further review by editor and referees) (08 Feb 2018) by Roberto Greco
Comments to the Author:
Dear Authors,
both the two Referees suggest that the manuscript would benefit of a more sound evaluation of the quality of the predictions of Ksat based on the IE and the novel soil particle size classes you propose.
In fact, even if you claim that you are not looking for a PTF nor to a tool for predicting Ksat, and rather your aim is to "find out whether a relationship can be found among the newly used parameters and (...) Ksat", focusing on "the strength of such relationship", (this is what you write in one of your answers), I think that the comparisons suggested by both the Referees, and the rigorous validation required by the second, point exactly in the direction of evaluating the strength of the found relationship, and its potential use to predict Ksat.
Indeed, the relationship you establish between your proposed measure of heterogeneity of PSD and Ksat is purely statistical. No discussion is attempted about the physical reasons why a choice of size classes should perform better than another, and you evaluate your results merely on the basis of data correlations. So, I definitely agree with both Referees that such a statistical analysis should be improved.
I look forward to receiving the revised manuscript for furher evaluation.
Best regards
Roberto Greco

Response to Editor:

Dear Editor:

We have redone the Ksat, and log(Ksat), linear regressions, against all possible IE values. But this time, in order to get a more sound evaluation of the quality of these regressions, we have employed the bootstrap method (see references Shaap and Leij, 2000; Efron and Tibshirani, 1993; T. Hastie et al. 2003 included in the new version of the manuscript). This technique allows for inference on any of the parameters obtained in the regression, in particular the R2 and RMSE statistics. This is described in Page 3, Line 25 onwards of the revised document.

This way one can statistically validate the strength of the linear relationships and the statistical analysis is improved.

Also, all the comments on first’s reviewer supplement PDF have been introduced in the text. Besides the misspellings and grammar suggestions, which can be found in the coloured differences document, particularly important changes are:

- we have eliminated the 0.4% of soils that whose Ksat was estimated using falling head method from the database, which were all silty clays. Thus the total number of soils and all regressions were discarded and re-done (Page 2, section 2.1, Line 26 onwards)

- We have manually classified all soils that were “unclassified” in the previous version. Soils were initially classified into their textural classes using R package “soiltexture” (see https://cran.r-project.org/web/packages/soiltexture/index.html or http://soiltexture.r-forge.r-project.org/). This software classified some soils as belonging to more than one textural class. We checked all these soils and correctly classified them into only one textural class. Thus, the number of soils in some textural classes changed. See Page 2, Section 2.1 and Page 3 Section 3.1. Also Page 17 Table 1.
- The bootstrap results varied slightly in some textural classes. Therefore the two superclasses used in this study changed. Now sandy clay belongs to SC2. Furthermore, we have left out of either superclass the textural classes with N<50, as the choice of the superclasses was based on information on Table 3 (Page 19). All these changes can be tracked in Page 5, Section 3.3, Line 32 onwards.
- Finally, as all the calculations had to be re-done with the bootstrapping technique, the whole results section has undergone changes: numbers have slightly changed in most cases, and also have tables. No significant changes, in the sense of physical interpretation of these regressions, which was ultimately the purpose of the paper, were found. These changes can be found in all tables and in Section 3, Page 4 of the revised paper.

Finally, please note that tables do not appear in the coloured-differences pdf, as they have been fully changed. Now tables contain mean and standard deviation values for the bootstrap repetitions. Numbers change slightly due to the randomness included in the method.

Response to reviewers:

Both reviewers were answered through “Copernicu’s online manuscipt tracker”.
Here we copy/paste the claims of the reviewers and we answer the comments in detail.

Reviewer #1:

R. A. Armindo
Received and published: 13 January 2018
The manuscript "Saturated Hydraulic Conductivity and Textural Heterogeneity of Soils" brings an interesting approach in predicting Ksat values based on IE and textural hetereogenity behaviour. A grand USDA data set was used to test this approach. However, I think that a comparison of the obtained Ksat results against other results published on literature (which have used other methods) would be very nice. It could be a simple table showing R^2 and RMSE results with a text discussion for Ksat under the same textural classes ranging different methods and authors or other idea of authors. Thus, readers could have an idea of how is the performance of this method in front of other known methods. Title of this manuscript could be more specific about used method. I would write someting like: "Prediction of Saturated Hydraulic Conductivity based on Textural Heterogeneity and Information Entropy of Soils". Some comments and details are presented in attached in other to help authors.

Please also note the supplement to this comment:
https://www.hydrol-earth-syst-sci-discuss.net/hess-2017-706/hess-2017-706-RC1-supplement.pdf

Response to reviewer #1:

Received and published: 17 January 2018

Dear referee:
we are grateful for the insightful review and the useful comments.
We did not try to develop pedotransfer functions in this work. We set the objective as the "exploration of relationships between Ksat values and entropy metric of soil texture heterogeneity using different size limits of coarse intermediate and fine fractions."

See Page 2, Last paragraph of Introduction. Line 14.

In other words, we tried to develop and inspect a physics-inspired possibility of relationships between the Ksat and the proposed heterogeneity parameter in the attribute spaces determined by various soil texture representations. For that reason, we did not do the common steps of PTF development, i.e. split of data into development and testing datasets, cross-validation, comparison with other PTF results, etc. We did not intend to do Ksat predictions.
There undoubtedly are interesting PTF-related research questions regarding the use of IE in PTF development. It is quite possible that if the IE will be used as a PTF input, additional inputs, e.g. organic matter content, will be needed and useful. It is also possible that the performance of PTF with IE as input may be database-dependent in comparison with existing PTFs. Computing IE from different textural triplets may affect its efficiency as a PTF input. Using various textural triplets may stimulate the re-use of existing databases in PTF development sine these databases include more detailed representation of sand fraction in comparison with the representation that is commonly used in PTF and does not differentiate between different sand fractions. Overall, your suggestion of possible use IE as a effective input to pedotransfer functions is most interesting. We took the liberty to include your suggestion in the Discussion section as the possible avenue for the future research.

See Section 3.6 Final Comments, Page 8, Line 15

We are very thankful for the detailed comments on the supplement. The manuscript was modified by taking into account all of them.

Reviewer #2:

Received and published: 19 January 2018

Manuscript hess-2017-706 investigates whether entropy measures for the soil texture are better predictors for the saturated hydraulic conductivity (Ks) than the traditional three class texture information (sand/silt/clay). An (to my knowledge) innovative variant of calculating information entropies (IE) from the 7 USDA standard texture classes is introduced. Furthermore regressions between the IE and Ks are established. Most of them are breathtakingly good (avg. R2 = 0.734), considering that Ks is notoriously difficult to predict (with typical R2 of around 0.2 in cases where realistic validation approaches are undertaken). It is difficult to understand why the use of a 7 texture class derived entropy measure should outperform prior pedotransfer functions (PTF) by such a large margin. From the methods section of this article, I am missing a description of a proper validation approach. I therefore suspect that the authors are presenting training errors which are known to be overly optimistic. Also the authors choice to perform their regressions on binned data has probably helped to imprve the goodness of fit. I therefore advise against publishing the paper in its present form as it would have considerable potential to mislead the reader.

It is difficult to understand why the authors miss the chance of presenting their regression equations and trying to use them to predict Ks in a cross-validation approach. Without the regression equations and proper cross-validations, I am seeing little value in publishing this manuscript. I therefore request the authors to introduce both of it in their article. If they could show that the regressions based on their IE's predict Ks with an R2 of clearly more than 0.2 in a source-wise cross-validation, they would demonstrate the usefulness of their entropy measures for real. With "source-wise" cross-validation I mean the following: a) train regression relationships using all data from 44 of your 45 data sources and b) then try to predict the Ks of the samples from the 45th data source. You will obtain an idea of how well you could predict the Ks for newly sampled soil. Preferably do the cross-validation sample wise (not binned), so that the range of prediction error for individual samples becomes obvious. I recommend major revisions.

Minor comments

The Ks is known to be log-normal distributed (you could even check it for your data). It is therefore advisable to only predict logarithmized Ks values. If the Ks in your database would rather be normal distributed, only use the plain Ks values instead of the log Ks.

The explanation and terminology used for the different texture class triplets is difficult to follow. It needs to be better explained. Moreover, how about denoting the triplets using the grain diameters for the boundaries between coarse, medium and fine texture. E.g. the classic texture classification (now '5-1-1') would be referred to as 50/2 (for the equivalent grain diameters at the sand/silt and silt/clay boundaries in micron). Or '3-2-2' would become 250/50. I would find such a naming convention much more intuitive.

I do not think that the manuscript is ready for more detailed comments, yet.

Answer to reviewer #2:

Received and published: 26 January 2018

Please note that our work is not aimed constructing pedotransfer function for Ksat using the heterogeneity parameters obtained from the texture fractions. We do not intend to predict Ksat. Therefore we do not intend to compare our regressions to previously obtained pedotransfer functions. We do not need a validation exercise. Sure a development of a PTF can be undertaken in further work, and, at that time, the cross-validation you propose should be done. Even more, further soil information, such as organic matter, can be included in the PTF. Our work is a natural continuation of the published work "On soil textural classifications and soil texture-based estimations" on Solid Earth (https://doi.org/10.5194/se-2017-84), where the relationship among the new heterogeneity parameters (IE) and soil bulk density is investigated. In that work, as in this one, a physical interpretation of this relationship is intended, not a PTF development. Our regressions are not intended to be used as predicting tools, but to find out whether a relationship can be found among the newly used parameters and an important soil hydraulic property as Ksat. The focus of the work is the strength of such relationship. We agree however that R2 should not be the only indicator of the relationship strength, and it is possible to research residual distributions within the textural triangles. About the nomenclature change you propose: this nomenclature was previously used and published in the Solid Earth paper. We believe that altering it now might bring confusion.

Additional joint response to reviewers #1 and #2:

Received and published: 1 February 2018

Besides to the previous responses, we want to say that we have included, in the discussion section of the article, an explanation saying that development of PTFs has not been the objective of this work, but can be undertaken in future, and that may be a promising avenue for expanding the research of the current paper.

See Section 3.6 Final Comments, Page 8, Line 15

Saturated Hydraulic Conductivity and Textural Heterogeneity of Soils

Carlos García-Gutiérrez[1], Yakov Pachepsky[2], and Miguel Ángel Martín[1]

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Abstract. Saturated hydraulic conductivity (K_{sat}) is an important soil parameter that highly depends on soil's particle size distribution (PSD). The nature of this dependency is explored in this work in two ways, (1) by using the Information Entropy as a heterogeneity parameter of the PSD and (2) using descriptions of PSD in forms of textural triplets, different than the usual description in terms of the triplet of sand, silt and clay contents. The power of this parameter, as a descriptor of K_{sat} and ~~$\log K_{sat}$~~$\ln K_{sat}$, was tested on a database ~~of >19K soils. We found~~ larger than 19,000 soils. Bootstrap analysis yielded coefficients of determination of up to 0.977 for ~~$\log K_{sat}$~~ $\ln K_{sat}$ using a triplet that combines very coarse, coarse, medium and fine sand as coarse particles, very fine sand and silt as intermediate particles, and ~~silt and~~ clay as fines. The power of the correlation ~~is~~ was analysed for different textural classes and different triplets ~~. Overall, the use of textural triplets different than traditional, combined with IE, may provide a useful tool for predicting K_{sat} values.~~ using a bootstrap approach.

This heterogeneity parameter can lead to new descriptions of soil PSD, other than usual clay, silt and sand, that can describe better different soil physical properties, that are texture dependant.

1 Introduction

Saturated hydraulic conductivity (K_{sat}) is the measure of soil's ability to conduct water under saturation conditions (Klute and Dirksen, 1986). It is an essential parameter of soil hydrology. Soil K_{sat} affects many aspects of soil functioning and soil ecological services, like infiltration, runoff, groundwater recharge ~~,~~ and nutrients transport. Knowing values of soil K_{sat} appears to be essential in designing management actions and practices, such as irrigation scheduling, drainage, flood protection, and erosion control.

The dependence of K_{sat} on soil texture has been well documented (Hillel, 1980). Different parameterizations of particle size distributions (PSDs) were suggested to relate K_{sat} and soil texture. It was proposed to use d10, d20, and d50 particle diameters (Chapuis, 2004; Odong, 2007) or slope and intercept of the particle size distribution curve ~~(Alyamani and Sen, 1993)~~(Arya and Paris, 1980; Also various functions were fitted to PSDs, and the fitting parameters were related to K_{sat}. For example, Chapuis et al. (2015) proposed to use two lognormal distributions to fit the detailed particle size distribution and to use the lognormal distribution parameters to predict the K_{sat}.

A common way to parameterize the PSD for K_{sat} estimation purposes is using the textural triplet that provides the percentage of coarse particles (sand), intermediate particles (silt), and fine particles (clay). K_{sat} values are estimated using the contents of one or two triplet fractions or just the textural class (Rawls et al., 1998). Representing PSD by textural triplets is the common way to estimate a large number of soil parameters (Pachepsky and Rawls, 2004). The coarse, intermediate, and fine fractions need not to be sand, silt and clay. Martín et al. (2017) showed that different definitions of the triplet, e.g. coarse sand, sand, and medium sand as coarse, fine sand, very fine sand as intermediate, and silt and clay as fine triplet fractions, provide much better inputs for bulk density estimation compared with the standard textural triplet.

The heterogeneity of particle size distributions appears to be an important factor affecting hydraulic parameters of soils, including the saturated hydraulic conductivity. Values of K_{sat} depend on both distribution of sizes of soil particles, i.e. soil texture, and the spatial arrangement of these particles, i.e. soil structure. Soil structure can be to some extent controlled by soil texture, since packing of particles is affected by the particle size distributions ~~(e.g Gupta and Larson, 1979; Assouline and Rouault, 1997; Jorda~~
It was recently proposed to use the information entropy as the parameter of the PSD heterogeneity for predicting soil water retention (Martín et al., 2005) and soil bulk density (Martín et al., 2017). Previously, information entropy was used, together with other predictor ~~vaiables~~ variables to estimate K_{sat}, using multivariate analysis (Boadu, 2000).

The objective of this work was to test the hypothesis that combining two recent developments -the description of the PSD by different textural triplets, that may focus on different soil properties, and the information entropy as a PSD heterogeneity parameter that depends on the triplet used for its description- may ~~improve estimation~~ yield a better description of K_{sat} and may be seen as a step forward to study the effect of heterogeneity widely recognized in the majority of works that studied the particle size - hydraulic conductivity relationships. We ~~used~~ explored the possible relationships between K_{sat} values and an entropy metric of soil texture heterogeneity using different size limits of coarse intermediate and fine fractions, using the large USKSAT database on laboratory measured K_{sat} ~~.~~ containing more than ~~19000~~ 19.000 samples.

2 Materials and Methods

2.1 Database description and textural triplet selection

For this study we used USKSAT database ~~. Detailed~~ in which detailed information can be found in ~~(Pachepsky and Park, 2015)~~Pachepsky an
This database consists on soils from different locations of the USA and contains soils from 45 different sources. We selected only those sources which (a) had data on both K_{sat} and on the seven textural fractions, and (b) presented measurements of K_{sat} made in laboratory ~~; K_{sat} was deteremined using~~ with the constant head method~~in 99.6% of cases and falling head metod in 0.4% of cases~~. From those, we subset those soils whose sum of mass in the seven textural fractions, i.e. (1) very coarse sand, (2) coarse sand, (3) medium sand, (4) fine sand, (5) very fine sand, (6) silt and (7) clay ~~differed from 100% not more than by 2~~ranged from 98 to 102%. The final number of soils considered was ~~19193.~~ 19.121. By USDA textural classes the total number of soils are: ~~12068 sands, 1779~~ 12.068 sands, 1.780 loamy sands, ~~2123~~ 2.123 sandy loams, ~~106 loams, 178~~ 104 loams, 135 silt loams, 36 silts, ~~1982~~ 2004 sandy clay loams, ~~80~~ 78 clay loams, ~~48~~ 41 silt clay loams, ~~334~~ 345 sandy clays, ~~7 silty clays , 414 clays and 38 soils that were classified into more than one class~~0 silty clays and 407 clays.

We used all possible triplets formed from seven textural fractions. Triplets consisted of coarse, intermediate, and fine fractions. The symbols for triplet showed how the fractions were grouped. For example the “coarse” fraction for the triplet ‘3-2-2’ included very coarse sand, coarse sand and medium sand, the “intermediate” fraction included fine sand and very fine sand , and “fine” included silt and clay; triplet ‘5-1-1’ was the standard one where “coarse” included all five sand fractions, “intermediate” included silt, and “fine” included clay. The amount of possible triplets with 7 textural fractions was 15.

2.1.1 Heterogeneity metric calculation

The Entropy based parametrization of textures introduced in ~~(Martín et al., 2001)~~ Martín et al. (2001) has as central concept in the Information Entropy (Shannon, 1948). Assuming the texture interval divided into k textural size ranges and that the respective textural fraction contents are $p_1, p_2, \ldots, p_k$, $1 \leq i \leq k$, with $\sum_{i=1}^{k} p_i = 1$, the Shannon Information Entropy (IE) (Shannon, 1948) is defined by

$$IE = -\sum_{i=1}^{k} p_i \log_2 p_i \tag{1}$$

where ~~$p_i \log p_i = 0$~~ $p_i \log_2 p_i = 0$ if $p_i = 0$. The IE is a widely accepted measure of the heterogeneity of distributions (Khinchin, 1957). In case of three fractions, the minimum value of IE is zero when only one fraction ~~os~~ is present, and the maximum value is 1.57 when three fractions are present in equal amounts ~~.~~ (see Fig. 1~~.)~~).

For each soil in this study, we grouped the 7 available textural fractions in the 15 possible triplet combinations and calculated the respective triplet’s IE using formula (1). Fig 2 shows heatmaps of IE calculated for all the soils available in this study but using two different triplets as input. It is clear that, by changing the triplet, the calculated IE values vary differently along the same textural triangle. IE is a measure of heterogeneity, but the triplet used is the substrate for this measure~~. We will notate this combination together~~: (IE,*triplet*), i.e., (IE,‘5-1-1’).

We followed the binning method of Martín et al. (2017) to research the relationship between K_{sat} and soil heterogeneity. Specifically, the range of values of IE was divided into ten bins, the average value of K_{sat} was plotted against the average IE for the bin, i.e. the bin midpoint.

Linear regressions ‘bin midpoint vs. average bin K_{sat}’ and ‘bin midpoint IE value vs. average bin ~~$\log K_{sat}$~~ $\ln K_{sat}$’ were computed. ~~These regressions were obtained for each of 15 triplets and for those of USDA textural classes that were represented by more than 50 samples, i. e. sands, loamy sands, sandy loams, loams, silt loams, sandy clay loams, clay loams, sandy clays,~~ The goodness-of-fit of these regressions was tested using the coefficient of determination R^2 and the Root-mean-square error, RMSE

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n} (\hat{y}_t - y_y)^2}{n}}$$

where $\hat{y}_t$ are the predicted and y_t are the measured values of K_{sat}, and ~~clays~~ n is the number of soils.

In order to make some inference on these parameters we employed the bootstrap method, which has been used in a very similar context by Schaap and Leij (2000). The bootstraph method is a tool for assessing statistical accuracy. It assumes that one can obtain multiple samples from a single data set, by randomly drawing data with replacement from the original sample. Thus, one can perform the same statistical analysis multiple times in different data sets, obtaining slightly diferent regression models, thus resulting in an uncertainty in each of the parameters of the model. All of the samples used have the same size as the original sample they were drawn from, so the are generated by random sampling with replacement. We used 1.000 bootstrap data sets, resulting in 1.000 linear regression models. In particular we obtained not just one R^2 and one $RMSE$ value for each IE vs. triplet regression, but one thousand of them, that were summarized into a mean and a standard deviation values. More information on this method can be found in (Efron and Tibshirani, 1993; T. Hastie, 2003).

~~The regression relationships were characterized by~~ We took 1.000 samples with size equal the total amount of soils, with repetition, and calculated, for each sample, the coefficient of determination, R^2 ~~,~~ and the Root-mean-square error

~~$RMSE = \sqrt{\frac{\sum_{i=1}^{n} (\hat{y}_t - y_y)^2}{n}}$~~

~~where $\hat{y}_t$ are the predicted and y_t are the real valuesof K_{sat}, and n is the number of soils~~, RMSE. Finally, the mean and standard deviation from these two values, for the 1.000 samples were calculated.

These regressions were obtained for each of 15 triplets and for those of USDA textural classes that were represented in the selected database by more than 50 samples, i.e. all of them except silty clay loams and silts.

3 Results and Discussion

3.1 The Dataset Overview

Fig. 3 presents the ~~19193~~ 19.121 soils used in this study in the USDA textural triangle and in the modified '3-2-2' triangle. The density of points reflects the dominance of coarse textural soils in the database. When the triplet is changed, the distribution of points across the triangle changes. By setting the textural fractions to be the '3-2-2' triplet, the distribution of points/soils in the new textural triangle spreads. While there is still a high concentration of soils in the stripe of bigger than 85% of the ~~Coarsefraction~~Coarse fraction, where Coarse 3 includes very Coarse Sand, Coarse sand a Medium Sand, now those soils spread fully from 10 to 100% of the Intermediate-2 fraction, where Intermediate-2 contains Fine and Very Fine Sand. On the USDA textural triangle, most of the soils are clustered in the subtriangle limited by the lines "more than 70% sand" and "less than 20% silt". This new textural triangle allows for a finer look into the sand fraction, revealing the distribution of soils within the USDA sandy textural classes. This finer look might prove itself useful to study physical properties of these soils that are mainly related to the type and amount of sand in them.

Table **??** shows the K_{sat} statistics for the soils in the study. A total of ~~19420~~ 19.420 soils were used in this study, from which ~~39 (0.2%) could not be classified as they belonged to more than one textural class~~299 (1.53%) had to be rejected due to missing values. The textural class sand comprises the ~~62.3~~63.1% of all the soils, followed by sandy loam (~~11.12~~11.1%) and sandy clay loam (~~10.77~~10.48%). ~~Six~~ Five textural classes were poorly represented with percentages less than 1% of the total soils. The K_{sat} values varied between 0.0005 and 841 cm/h being 22.57 the mean value.

3.2 Regression in binned data: IE as a predictor of K_{sat} ~~/ $\log K_{sat}$)~~and $\ln K_{sat}$

Linear regressions for K_{sat} and ~~$\log K_{sat}$~~ $\ln K_{sat}$ were done to find out the predictive power of the proposed parameter, (IE,triplet), with the 15 possible different triplets that could be archived by grouping the available textural data. Table **??** shows the computed R^2 and $RMSE$ values for the linear regressions using 10 interval bins.

The best triplet for the K_{sat} regression was '2-3-2', i.e. 'very coarse sand + ~~sand + medium~~ coarse sand' as coarse, 'medium sand + fine sand + very fine sand' as intermediate and 'silt + clay' ~~sa fime~~ as fine factions, with the highest mean R^2 value (~~R^2~~mean = 0.885, std = 0.020) and this triplet also had the lowest RMSE value (RMSE=~~3.609~~3.649 cm/h). Figure 4 shows a heatmap representation of the K_{sat} values of the soils of the study on the textural triangle compared to a heatmap representation of the IE values of the same soils computed using the ’2-3-2’ triplet. The sandy soils had high K_{sat} values, and the IE values on that part of the triangle were low. The triangle presents high K_{sat} values in a stripe between 0 and 20% sand. This stripe has also low (IE,'2-3-2') values, so there is a reasonable visual relationship between these two values. It is also worth noting that the '4-1-2' triplet, i.e. 'very coarse + coarse + medium + fine sands' as coarse fraction, 'very fine sand' as intermediate and 'silt + clay' as fines had a very similar mean R^2 value (0.880) but a lower standard deviation (0.007).

For the ~~$\log K_{sat}$~~ $\ln K_{sat}$ regression, the best triplet in terms of highest mean R^2 value was '4-2-1', with a ~~R^2 value~~ mean of 0.977 and a standard deviation of 0.002, but the lowest mean RMSE value (~~RMSE~~mean=~~0.194~~0.207, std = 0.030) was attained with the '1-2-4' triplet. Figure 5 shows the same comparison as figure 4, but using the ~~$\log K_{sat}$~~ $\ln K_{sat}$ heatmap and the IE computed with the '4-2-1' triplet. There is a higher visual similarity between these two images, with high ~~$\log K_{sat}$~~ $\ln K_{sat}$ value zones, near the lower corners (sandy and silty soils) that correspond to low (IE,'4-2-1') values. The ~~$\log K_{sat}$~~ $\ln K_{sat}$ values tend to decrease towards the centre of the triangle. On the other hand, the (IE,'4-2-1') values tend to increase around this point.

The standard triplet ('5-1-1') yielded, for the K_{sat} regression, a mean R^2 value of ~~0.776 and~~ 0.775 with standard deviation equal to 0.010 and a mean RMSE value of ~~7.528~~7.555 with standard deviation of 0.190; for the ~~$\log K_{sat}$~~ $\ln K_{sat}$ regression, the R^2 value with this triplet ~~was~~ had a mean of 0.960 and ~~the RMSE value was 0.340~~a standard deviation of 0.005; the RMSE mean value was 0.339 with a standard deviation of 0.021. Regressions against ~~$\log K_{sat}$~~ $\ln K_{sat}$ were in average better: the average of the R^2 ~~value~~ mean values of the regressions with all possible triplets for ~~$\log K_{sat}$ was 0.734~~$\ln K_{sat}$ was 0.727, whilst the average R^2 value for the K_{sat} regression was ~~0.673~~0.667.

3.3 Predictive power of IE among the USDA textural classes

In this section we show how IE works differently among textural classes: using different triplets we can find that the textural classes are predicted differently; what works for some, for others is counterproductive.

Table **??** shows the best triplet, chosen in terms of highest mean R^2 value of all the possible regressions, for each textural class that had $N > 50$~~, and the~~. In the table are shown the mean and standard deviation for R^2 ~~value~~, of the 1.000 bootstrap samples for both, K_{sat} and ~~$\log K_{sat}$~~$\ln K_{sat}$, linear regressions. The best R^2 values were obtained for the regression of the sand textural class against the (IE,'5-1-1'), i.e., the IE computed with the standard '5-1-1' clay-silt-sand USDA triplet (means equal to R^2=~~0.907~~ 0.905 for the K_{sat} regression and R^2=~~0.989 for the $\log K_{sat}$~~0.987 for the $\ln K_{sat}$). A possible explanation for this triplet being the best among all the other possible triplets, is that sandy soils are the ones that contain percentages of the sand fraction higher than 70%, so their distribution is highly heterogeneous. Minor fractions are now silt and clay, and the information about this two fractions could be very important for the hydraulic properties of the soil, thus the (IE,'5-1-1') triplet yielded the best regression result. One might think that, having such a high concentration of sand particles, is now silt and clay the fractions that made the difference in the packing properties, thus in the saturated hydraulic conductivity values. The high value of R^2 indicates that the relation is very strong in this case.

~~The~~ Almost all sandy textural classes had the highest regression coefficients~~(R^2>0.655 for all classes), in constrast to the non-sandy classes (R^2<0.56). This motivated the classification of all the soils in the study in~~. Table **??** suggested grouping the textural classes into two superclasses: ~~sandy (SC~~SC1~~) and not-sandy class (NSC). SC comprised the textural classes sandyclay~~, comprising the textures sandy, sandy clay loam, sandy loam ~~, loamy sandand sand.~~ and loamy sand; and SC2, with sandy clay, clay, clay loam, loam and silty loam. Soils in ~~NSC~~SC1 ~~comprised the other seven textural classes~~are mostly sandy soils, with the exception of the sandy clay textural class which is within the SC2 soils which are mostly clayley and loamy soils. The first superclass, SC1, had K_{sat} mean R^2 values above 0.608 and for the second superclass, the biggest mean R^2 value was of 0.416. Even more, the lowest mean R^2 value for the $\log K_{sat}$ regressions in the SC1 superclass was 0.742 and the highest one for the SC2 class was 0.604. Total number of soils in ~~SC~~SC1 was ~~18286 (95.27~~17975 (94.06% of total soils in the database). ~~NSC~~SC2 contained ~~869 soils (4.53~~1069 soils (5.59% of total). Tables ~~**??** and **??**~~ **??** and **??** show the R^2 and RMSE values for all regressions (K_{sat} and ~~$\log K_{sat}$~~$\ln K_{sat}$) for the soils in ~~SC~~SC1 and ~~NSC~~SC2.

For the ~~SC~~SC1 we observed that the best regression (R^2=~~0.888~~0.885) against K_{sat} was reached with (IE,'2-2-3'), and being (IE,'2-3-2') a close runner-up (R^2=~~0.880~~0.868) and a lower RMSE value. Both these triplets make a distinction among the sand fractions, putting very coarse and coarse sand in the coarse fraction in the first case, and adding medium sand in the second case. Also, the fines fraction contains either very fine sand or not. Comparing this to the sandy textural class results, where the best triplet was '5-1-1', we observed that now more information from the sandy fraction was required to infer hydraulic properties. The area that the ~~SC~~SC1 soils cover in the textural triangle and the hydraulic property variation of these soils can be related with a heterogeneity metric associated to triplets that distinguish well among the predominant fraction in that area of the triangle, i.e., sand.

For the ~~NSC~~SC2, best triplet in both regressions (K_{sat} and ~~$\log K_{sat}$~~$\ln K_{sat}$) was '~~4-1-2~~1-1-5', with R^2=~~0.232~~ 0.202 for K_{sat} and R^2=~~0.769 for $\log K_{sat}$~~0.623 for $\ln K_{sat}$. Regression results were worse than for ~~SC~~SC1, but this might be just provoked by the nature of ~~NSC~~SC2 itself: these are soils with less sand, thus higher content in clays and aggregating particles. The packing -and consequently the K_{sat}- of these soils is not just mainly affected by the PSD, but also by aggregation, which cannot be accounted for in the IE value, regardless of the triplet used.

Furthermore, the best triplet, '~~4-1-2~~1-1-5', also pointed in this direction: the fines fraction contains medium sand, fine sand, very fine sand, silt and sand particles, while the intermediate fraction contains only the ~~very fine~~ coarse sand, leaving the coarse fraction with ~~most of the~~ the very coarse sand, thus giving more importance to the possibly aggregating particles than a triplet like, '~~1-3-3~~1-4-2' which had R^2 values equal to ~~0.051~~ 0.014 (K_{sat}) and ~~0.019 (log K_{sat}~~0.033 (ln K_{sat}).

3.4 Triplets and Scaling Break

In the regressions made with all the soils, it was noteworthy the behaviour of the (IE,'3-1-3'). The average mean value R^2 for all the K_{sat} regressions was ~~0.673~~0.667, but the R^2 using (IE,'3-1-3') gave a R^2 equal to ~~0.0002~~0.005, far below the next lowest one, which was (IE,'3-2-2') with a mean R^2 value of ~~0.433~~0.428. The same happened in the ~~log K_{sat}~~ ln K_{sat} regressions, where the average value of all triplets was ~~0.734~~0.727, but (IE,'3-1-3') gave a exceptionally low R^2 value of ~~0.111~~0.087, being the next lowest (IE,'2-2-3') with a mean R^2 value of ~~0.229~~0.235.

The '3-2-3' triplet groups fine sand with silt and clay, and coarse and very coarse sand with medium sand. Kravchenko and Zhang (1998); Wu et al. (1993); Tyler and Wheatcraft (1992) reported the break in scaling where the powerlaw scaling of soil texture occurred in the size range of fine sand The Particle size distribution scales in a different way in two different regions of the size intervals, and that the change of scaling is produced around the fine sands. The triplet '3-1-3' separates these two regions, maybe bringing forth this scaling break effect. Fig 6. shows how the relationship between K_{sat} (and ~~log K_{sat}~~ln K_{sat}) and (IE,'3-1-3') could be nonlinear, maybe due to the absence of global selfsimilarity showed in the scaling break.

On the other hand, it is also noteworthy that regressions against (IE,'3-1-3') were actually quite good (R^2=~~0.855~~ 0.837 for K_{sat} and R^2=~~0.955 for log K_{sat}~~0.939 for ln K_{sat}) in the ~~SC~~SC1, while in the ~~NSC~~SC2 they were moderate (R^2=~~0.204~~ 0.047 for K_{sat}, and R^2=~~0.267 log K_{sat}~~0.045 ln K_{sat}). Furthermore, even though (IE,'3-1-3') presented the lowest R^2 values for all soils, this triplet yielded the best R^2 results for ~~some soils belonging to silty loam ($N = 178$) and~~ soils belonging sandy clay loam (~~$N = 1982$) textures~~$N = 2.004$) texture, for K_{sat} regressions. Nevertheless, for other textures, the '3-1-3' triplet had, generally, a very low value.

When all the soils are considered together, then (IE,'3-1-3') might fail, due to the scaling break, but when we restrict the study to a certain part of the textural triangle, that effect might diminish to a point where this triplet is even useful to predict some textural derived properties, or maybe the scaling break effect is also restricted to some textural classes and should be further investigated.

As results show, IE is not powerful K_{sat} predictor by itself, but combined with an input triplet. By changing the triplet, we may focus on certain physical aspects of the soils, but it is also important to keep in mind that this might not work statistically for random groupings of soils that belong to different textures.

3.5 IE variation as a spatial function in the textural triangle

Heatmaps were used to visually correlate the IE values calculated with the K_{sat} (or ~~log K_{sat}~~ln K_{sat}) values of the soils in the study. Also, a less visual, but more ~~quantifyable~~ quantifiable approach, to find out how much of K_{sat} could be explained through IE variation was to find out what ranges of IE are available for soils in different textural classes and compare them to the range of K_{sat} values of soils inside those same textural classes. Also, in order to compare the new tool (IE triplet), we compared these ranges to the ranges computed for (IE,'5-1-1') , i.e. to the values of the IE computed with the usual description of soil texture. We want to find out if, by changing the triplet, we obtain a wider range of variation in IE for a given range of K_{sat}. This way we compare if the new descriptions of texture, in form of different triplets, might be suitable for explaining soil physical properties, in particular K_{sat}.

For each textural class, we ~~calculated~~ did a sensitivity analisis by calculating the ratio of the range of K_{sat} values inside the textural class versus the range of K_{sat} values of all the soils in the study. The same was done for IE for each triplet. Table **??** shows, for each textural class, the ratio of the percentage of (IE,'5-1-1') against the percentage of K_{sat} range. The same ratio was also calculated using IE for the triplet that gave the best R^2 value in the linear regression against K_{sat}. These values can be thought of as how much range of (IE,*triplet*) can be used to explain a certain variation of K_{sat} inside each textural class, i.e. as how much parametrizing power is available by the IE. In all the textural classes, except clay, where the regressions were done, the parametrizing power of the alternative triplet was higher than the one by using the usual clay-silt-sand triplet. For the clay textural class, the relative difference was of 2.2%. For the sand textural class, the triplet which gave the best R^2 regression was '5-1-1' thus the results are the same; the average value of the parametrizing power for the usual triplet was 2.46, while when we change the triplet we obtained ~~4.80~~5.10. This shows how, by considering different triplets, combined with IE, a better description/parametrization of K_{sat} can be reached.

3.6 Final Comments

Textural heterogeneity is a crucial factor affecting soil K_{sat}, but it acts along many other ecological factors, as animal activity, root exudates, soil aggregation, etc. In this work we showed that a proper representation of textural heterogeneity, by IE, allows one to (1) demonstrate its effect on K_{sat} by binning samples based on the textural heterogeneity and (2) to statistically parametrize this effect for some textures.

This work has limitations, in particular, the limited available texture data of only seven fractions in the database. The boundaries between coarse, intermediate, and fine fractions can be moved with data from continuous measurements of texture in the fine sand-silt-clay range of particle sized. This may bring the improvements in mean bin K_{sat} estimates for non-sandy soils that could not be achieved in this work.

Although globally the IE computed from different triplets show a potential to reflect the effect of soil texture on the K_{sat} values, the different relationship between the IE and the K_{sat} depending on the triplet used might have different possible explanations. While the IE/K_{sat} relationship is found satisfactory in some textural classes, results seem to indicate that the IE parameter cannot reflect with the same efficiency the K_{sat} values in other classes predominating fine particles, in which other processes as aggregation or weathering can not been elucidated by the single textural data input.

Overall, the heterogeneity parameter, IE, combined with the different triplet information, appears to be a strong candidate as an input for the development of new pedotransfer functions (PTFs) to predict K_{sat} and probably other soil physical parameters which are strongly dependant on soil particle size distribution. While PTFs are a useful tool to predict difficult-to-measure soil properties, they exhibit highly non-linear relationships which are difficult to interpret. While the objective of this paper was the exploration of the physical relation of the new tools and the saturated hydraulic conductivity, the future development of PTFs is promising avenue for expanding this research.

4 Conclusions

The PSD coarse, intermediate,and fine fractions in soil textural triplets can be redefined from standard ‘sand-silt-clay’ to other fraction size ranges. The textural heterogeneity parameters obtained for some of the new triplets correlate with soil saturated hydraulic conductivity averaged by ranges of the heterogeneity parameters. This approach allows one to quantify the effect of the textural heterogeneity of saturated hydraulic conductivity of soils. Given that size boundaries of sand, silt, and clay fractions have not originally been established for the purposes of prediction of soil hydraulic conductivity, it may be beneficial to look for other size based subdivisions of particle size distributions which, when used along with other soil properties such as bulk density and organic matter content, may provide better predictions of the saturated hydraulic conductivity.

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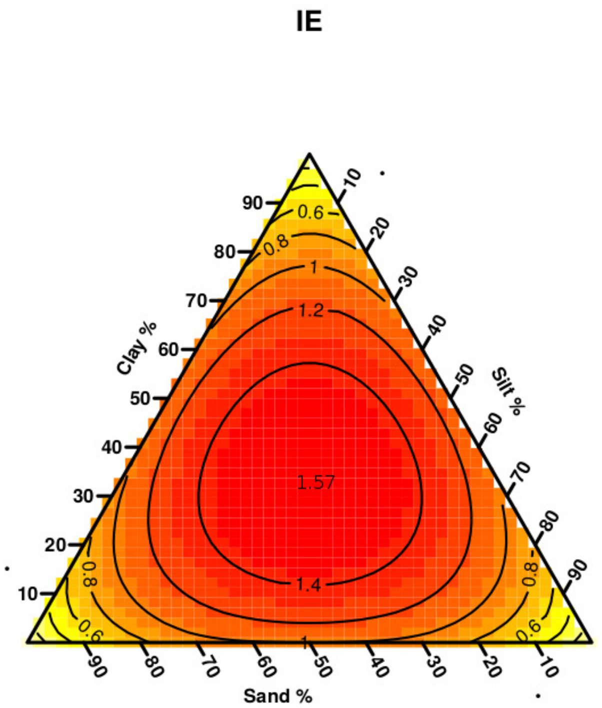
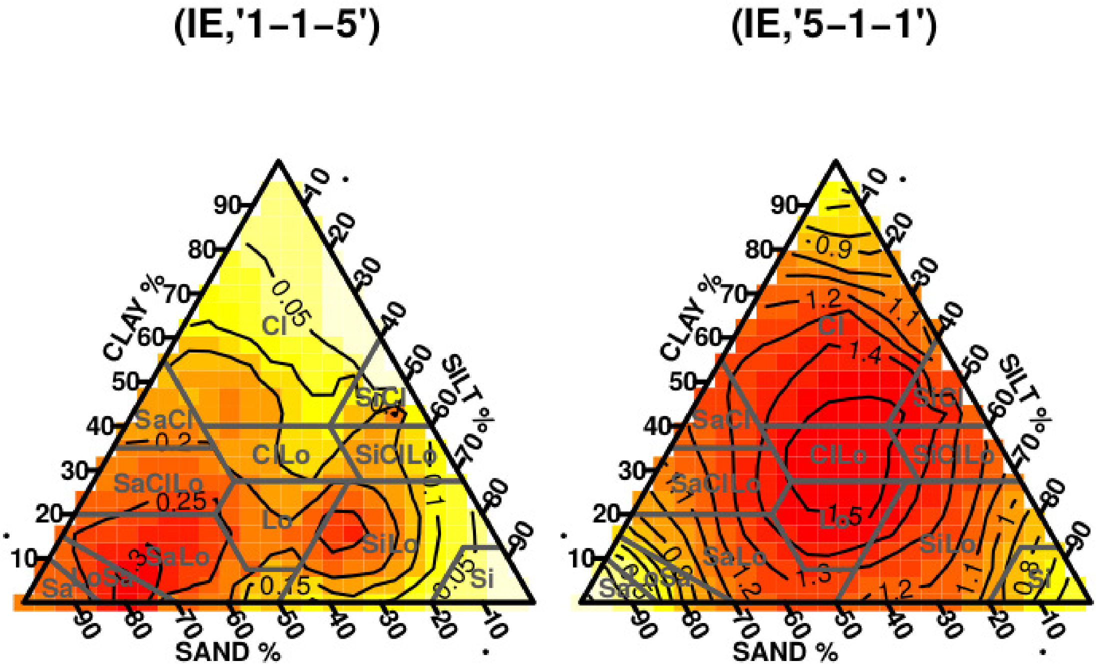


Figure 1. IE numerical approximation heatmap: IE is computed for a sample of 5051 evenly distributed soils in the USDA textural triangle using the clay, silt and sand fractions as input triplet. This distribution of IE is repeated for any textural triangle, when the fractions used for its calculations are the ones at the axes of the triangle. The lowest values for the IE are near the vertex of the triangle, i.e. where one fraction dominates above the others. Biggest values are located towards the centre of the triangle, where the distribution fractions are more balanced.



(IE,'1–1–5')

(IE,'5–1–1')

Figure 2. Heatmaps for IE calculated for the soils of the study but using different triplets. The usual clay, silt and sand triplet ('5-1-1') was used at the left and the grouping seven textural fractions into '1-1-5' was used as input for the right.

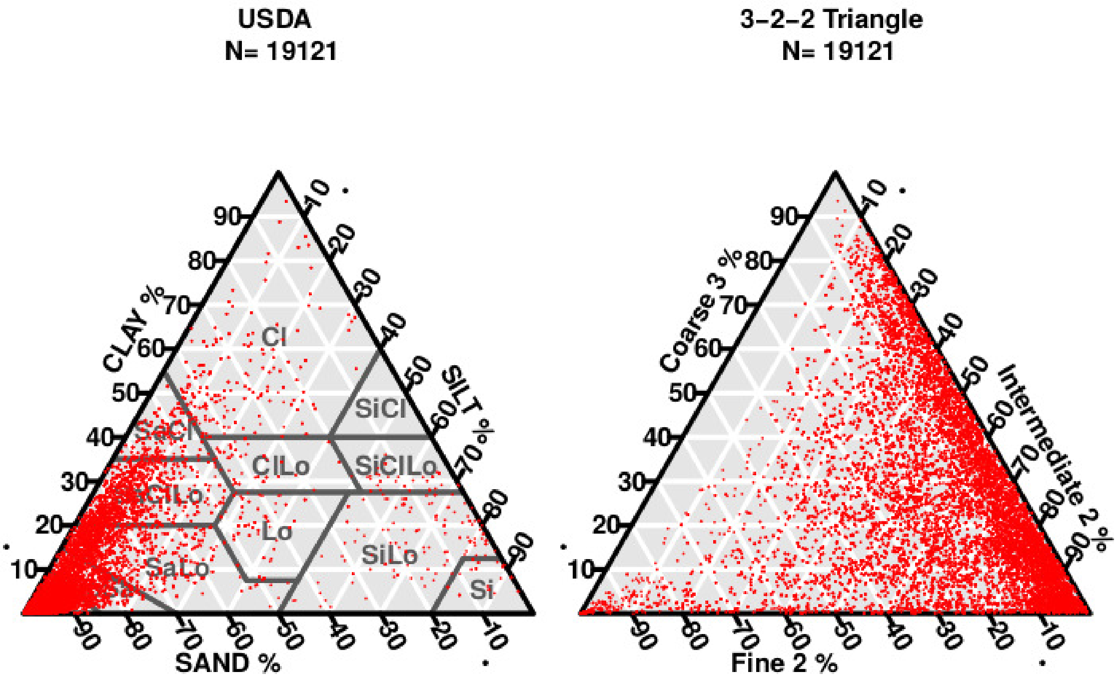


Figure 3. Representation in the USDA textural triangle of the 19193 soils used in this study. (a) standard sand-silt-clay, i.e. '5-1-1' triplet. (b) the '3-2-2' triplet.

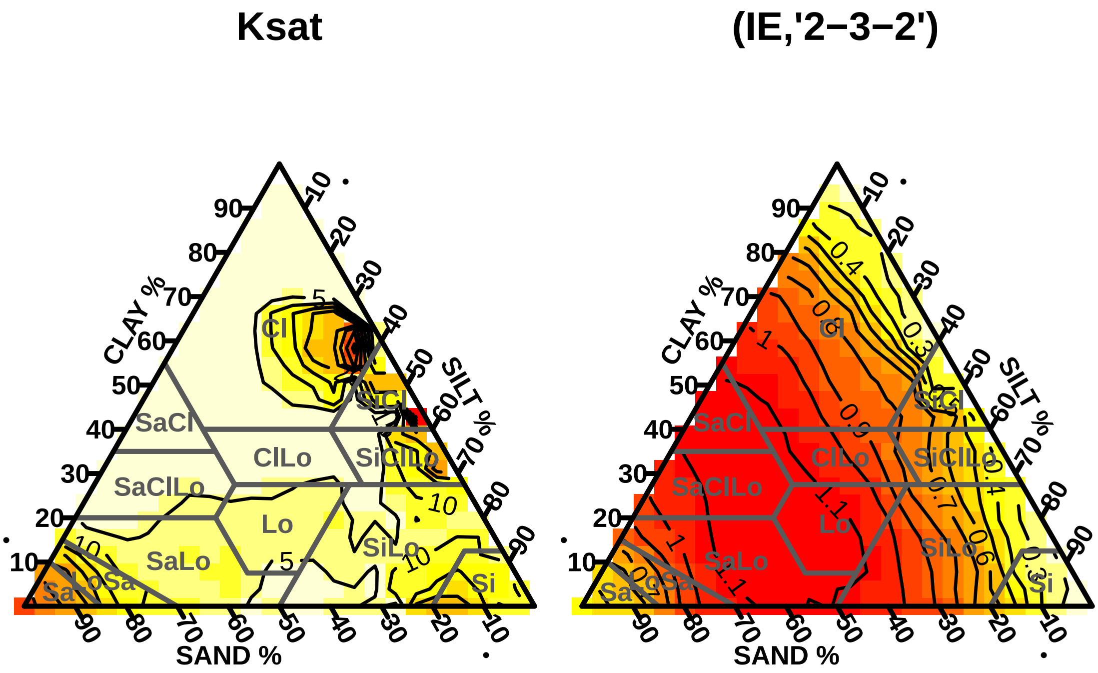
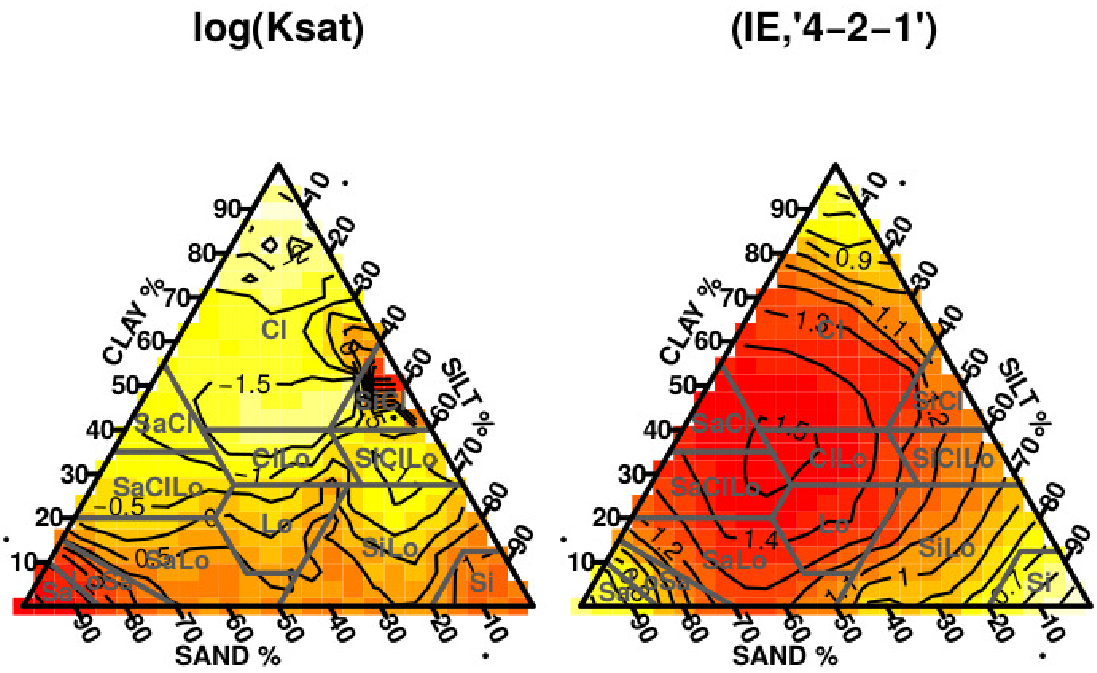


Figure 4. Heatmaps for the K_{sat} and the (IE,'2-3-2'), represented in the USDA textural triangle.



log(Ksat)

(IE,'4–2–1')

Figure 5. Heatmaps for ~~$\log K_{sat}$~~ $\ln K_{sat}$ and $(IE,$‘4-2-1’$)$ represented in the USDA textural triangle.

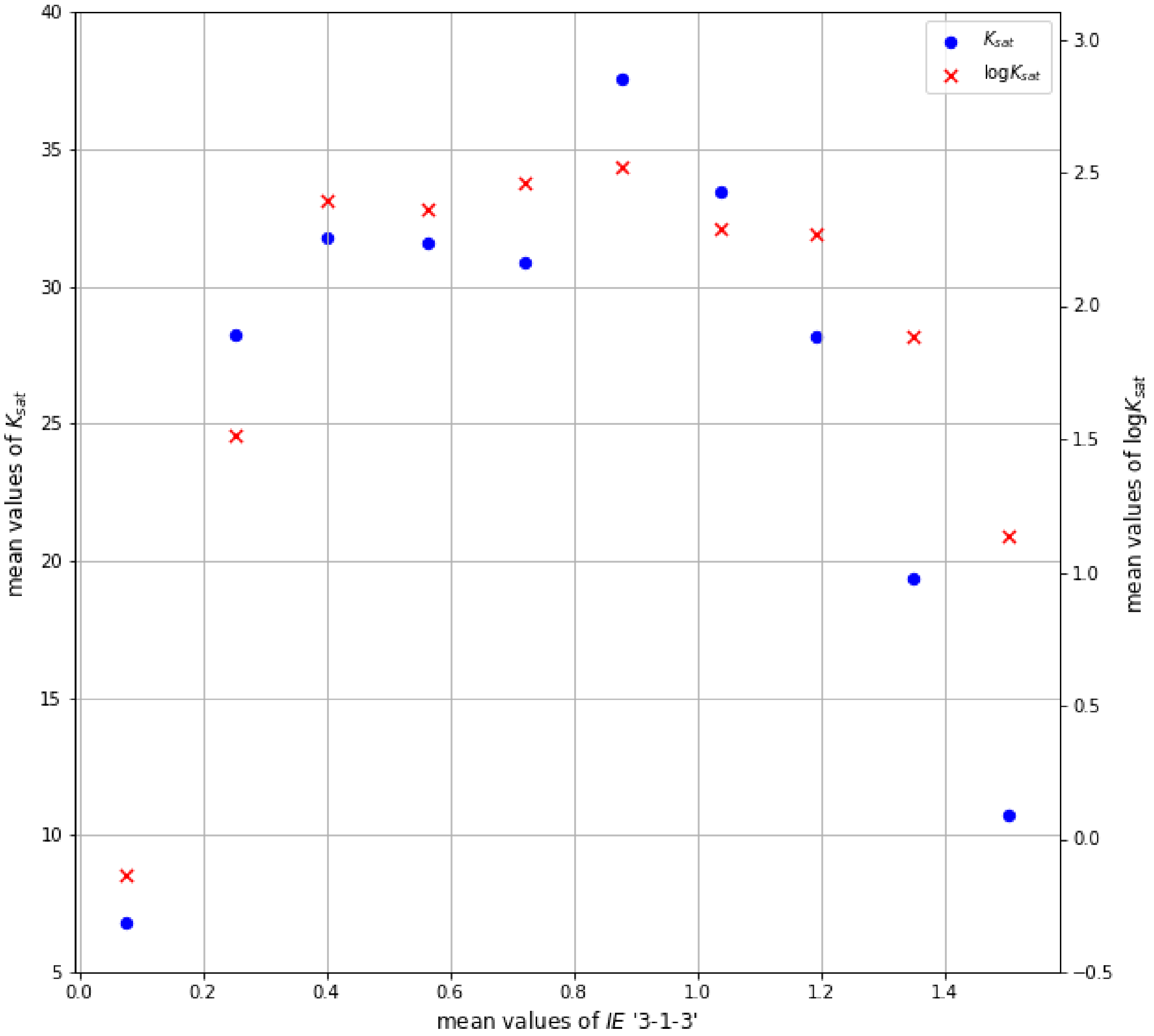


Figure 6. K_{sat} (~~top~~cm/h) (circles) and ~~$\log K_{sat}$~~ $\ln K_{sat}$ (~~bottom~~crosses) values against IE calculated with the '3-1-3' triplet in 10 interval binnings.~~The lines are the regression lines.~~