SoilKsatDB: global soil saturated hydraulic conductivity measurements for geoscience applications

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Abstract. Saturated soil hydraulic conductivity (Ksat) is a key parameter in many hydrological and climatic modeling applieations. Ksat values are primarily determined from soil textural properties and may vary over several orders of magnitude. Despite availability of Ksat datasets in the literature, significant efforts are required to import and combine the data before it can be used for specific applications. In this work, a total of 13,267 Ksat measurements from 1,910 sites were assembled from published literature and other sources, standardized (units made identical), and quality-checked in order to provide a global database of soil saturated hydraulic conductivity (SoilKsatDB). The SoilKsatDB covers most regions across the globe, with the highest number of Ksat measurements from North America, followed by Europe, Asia, South America, Africa, and Australia. In addition to Ksat, other soil variables such as soil texture (11,591 measurements), bulk density (11,269 measurements), soil organic carbon (9,787 measurements), field capacity (7,389) and wilting point (7,418) are also included in the dataset. To show an application of SoilKsatDB, we fit Ksat pedotransfer functions (PTFs) for temperate regions and laboratory-based soil properties (sand and clay content, bulk density). Accurate models can be fitted using a Random Forest machine learning algorithm (best concordance correlation coefficient (CCC) = 0.70 and CCC = 0.73 for temperate and laboratory based measurements, respectively). However, when these temperate and laboratory based Ksat PTFs are applied to soil samples from tropical climates and field measurements, respectively, the model performance is significantly lower (CCC = 0.52 for tropical and CCC = 0.10 for field samples). These results indicate that there are significant differences between Ksat data collected in temperate and tropical regions and measured in lab or the field. The SoilKsatDB dataset is available at 'version 0.3' https://doi.org/10.5281/zenodo.3752721 (Gupta et al., 2020) and the code used to extract the data from the literature, for the quality control and applied random forest machine learning approach is publicly available under an open data license.

1 Introduction

Soil saturated hydraulic conductivity (Ksat) describes the rate of water movement through water saturated soils and is defined as the ratio between water flux and hydraulic gradient (Amoozegar and Warrick, 1986). It is a key variable in a number of hydrological, geomorphological, and climatological applications, such as rainfall partitioning into infiltration and runoff

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(Vereecken et al., 2010), optimal irrigation design (Hu et al., 2015), as well as the prediction of natural hazards including catastrophic floods and landslides (Batjes, 1996; Gliński et al., 2000; Zhang et al., 2018). Accurate measurements of Ksat in the laboratory and field are laborious and time consuming and most samples are taken from agricultural soils (Romano and Palladino, 2002).

5 Efforts to produce reliable and spatially refined datasets of hydraulic properties date back to the 1970's with the proliferation of distributed hydrologic and climatic modeling. Some of these early notable works also provided basic databases (some of which are used in this study) for Australia (McKenzie et al., 2008; Forrest et al., 1985), Belgium (Vereecken et al., 2017; Cornelis et al., 2001), Brazil (Tomasella et al., 2000, 2003; Ottoni et al., 2018), France (Bruand et al., 2004), Germany (Horn et al., 1991; Krahmer et al., 1995), Hungary (Nemes, 2002), the Netherlands (Wösten et al., 2001), Poland (Glinski et al., 1991), and USA (Rawls et al., 1982). Nemes (2011) discussed the available datasets on Ksat and other hydro-physical properties in detail. Collaborative efforts have resulted in the compilation of multiple databases, including the Unsaturated Soil Hydraulic Database (UNSODA) (Nemes et al., 2001), the Grenoble Catalogue of Soils (GRIZZLY) (Haverkamp et al., 1998), and the Mualem cataloge (Mualem, 1976) —these, however, focused on soil types and not on the spatial context of Ksat mapping. In an effort to provide spatial context, Jarvis et al. (2013), Rahmati et al. (2018) and Schindler and Müller (2017) published global databases for soil hydraulic and soil physical properties. Likewise, the European soil data center also started projects such as SPADE (Hiederer et al., 2006) and HYPRES (Wösten et al., 2000), for generating spatially referenced databases for several countries. Since HYPRES represents only western European countries, Weynants et al. (2013) gathered data from 18 countries and developed the European Hydropedological Data Inventory (EU-HYDI) database—this dataset is, however, not publicly available and was not included in this compilation. The datasets mentioned above cover almost all climatic zones except tropical regions, where Ksat values can be significantly different due to the strong local weathering processes and different clay mineralogy (Hodnett and Tomasella, 2002). Recently, Ottoni et al. (2018) published a dataset named HYBRAS (Hydrophysical Database for Brazilian Soils) improving the coverage of South American tropical regions. In addition, Rahmati et al. (2018) recently published the Soil Water Infiltration Global database (SWIG) eollecting information on Ksat for the whole globe. In SWIG database, some Ksat values were extracted from literature and other Ksat values were deduced from infiltration time series. In contrast to lab measurements that determine Ksat as ratio of flux density to gradient, infiltration-based methods determine Ksat by fitting infiltration dynamics to-parametric models (using three-parameter infiltration equation of Philip (Kutílek and Krejca, 1987) or simplified form of Haverkamp et al. (1994)).

The ever increasing demand for highly resolved description of surface processes require commensurate advances in Ksat representation for modern Earth System Model (ESM) applications. Several existing Ksat datasets miss either coordinates or these have been recorded with unknown accuracy thus limiting their applications for spatial modeling. For example, the SWIG dataset misses information on soil depth and assigns a single coordinate for entire watersheds. Similarly, the UNSODA dataset does not provide coordinates and soil texture information for all samples. For a few locations, HYBRAS uses a different coordinate system. Taken together, these limitations highlight that, to prepare spatially referenced global Ksat datasets for large scale applications, a serious effort to compile, standardize and quality check all literature (available publicly) is often required.

The objective of the work here is to provide a new global standardized Ksat database (SoilKsatDB) that can be used for geoscience applications. To do so, a total of 13,267 Ksat measurements have been collected, standardized, and cross-checked to produce a harmonized compilation which is analysis-ready (i.e., it can directly be used for model fitting and spatial analysis). We compiled data from existing datasets and, to improve the spatial coverage in regions with sparse data, we further conducted a literature search to include Ksat measurements in geographic areas that were not yet eovered in other existing databases. In the manuscript, we first describe the data compilation process and then describe methodological steps used to spatially reference, filter, and standardize the existing datasets. As an illustrative application of the dataset, we derive PTFs for different regions and measurement methods and discuss their transferability to other regions/measurement methodologies. We fully document all importing, standardization and binding steps using the R environment for statistical computing (R Core Team, 2013), so that we can collect feedback from other researchers and increase the speed of further updates and improvements. The newly created data set (SoilKsatDB) can be accessed via 'version 0.3' https://doi.org/10.5281/zenodo.3752721 and directly used to test various Machine Learning algorithms (Casalicchio et al., 2017).

2 Methods and materials

2.1 Data sources

To locate and obtain all compatible datasets for compilation, a literature search was conducted using different search engines, including Science Direct (https://www.sciencedirect.com/), Google Scholar (https://scholar.google.com/) and Scopus (https://www.scopus.com). We searched soil hydraulic conductivity datasets using keywords such as "saturated hydraulic conductivity database", "Ksat", and similar. The collected datasets are listed in Table 1 together with number of Ksat observations for each study, and can be classified into three main categories, namely: i) Existing datasets (in form of tables) published and archived with a DOI in a peer-review publication; ii) legacy datasets in paper/document format (e.g., legacy reports, PhD theses, and scientific studies), iii) on-line materials.

Existing datasets include published datasets such as HYBRAS (Ottoni et al., 2018), UNSODA (Nemes et al., 2001), SWIG (Rahmati et al., 2018), and the soil hydraulic properties over the Tibetan Plateau (Zhao et al., 2018), from which we extracted the required information as described in Table 2a. The major challenge with making the existing datasets compatible for binding (standardization, removing redundancy), was to obtain the locations for a particular sample as well as the corresponding measurement depths. For instance, the UNSODA database empletely lacks geographical locations. To fill the gaps and make the data suitable also for spatial analysis, we used Google Earth to find the coordinates based on the given location (generally an address or a location name). We separated the UNSODA data based on laboratory and field measurements and we computed sand, silt and clay contents based on the particle diameters between 0-2 µm (clay), 2-50 µm (silt), and >50 µm (sand) from the available particle-size data, assuming a log-normal distribution as described in Nemes et al. (2001). We further note that, in some datasets, the coordinates were missing or reported in diverse coordinate systems. For example, in the HYBRAS database, the locations needed to be converted from UTM to a decimal degrees. In the SWIG database, the information related to location (coordinates for each point), soil depth and measurement method (laboratory or field) was completely missing, so we

went through each publication referenced in Rahmati et al. (2018) (except the unpublished literature) and added coordinates and applied the necessary conversions.

In the case of legacy datasets (paper or document format, data from journals, theses, and legacy reports with and without peer-reviewed publications), we invested a significant effort to digitize tabular data, clean it and make it analysis-ready. After the digitization process, all data values were cross-checked one more time with the original PDFs to avoid any artifacts or error in the final database.

Two datasets were also collected directly from project websites that might be peer reviewed such as the NASA project based on hydraulic and thermal conductivity (retrieved from https://daac.ornl.gov/FIFE/guides/Soil_Hydraulic_Conductivity_Data. html and described in Kanemasu (1994)) and the Florida database from Grunwald (2020).

There are many biomes and climatic regions, such as desert dunes, peatlands and frozen soils, where very few data of Ksat were publicly available. Because it is essential for global modeling to provide some values or range to reduce the uncertainty in the spatial maps, we have also intensively searched for these areas and, in addition to the major datasets (SWIG, UNSODA HYBRAS), we have also found several minor studies (that contain less than 5 Ksat measurements) to cover these regions. We thus digitized Ksat values from these studies (shown either in bar charts or line plots), georeferenced the maps where necessary, and then converted the data into tabular form. All these datasets are also listed in Table 1. In some cases, we also contacted colleagues that worked in these regions to ask for data support.

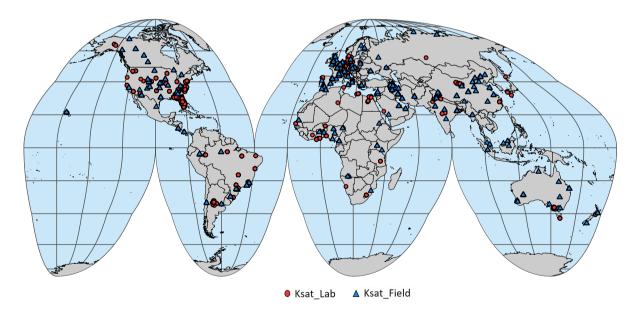


Figure 1. Spatial distribution of Ksat points (red and blue for laboratory and field measurements, respectively) in the SoilKsatDB. A total of 1,910 spatial locations are on this map.

Table 1. List of reference articles and digitized Ksat datasets, and number of points (N) per data set used to generate the new SoilKsatDB product.

Reference	N	Reference	N	Reference	\overline{N}
Rycroft et al. (1975)	1	Abagandura et al. (2017)	3	Jabro (1992)	18
Waddington and Roulet (1997)	1	Habel (2013)	3	Greenwood and Buttle (2014)	18
Takahashi (1997)	1	Nyman et al. (2011)	3	Wang et al. (2008)	19
Katimon and Hassan (1997)	1	Bhattacharyya et al. (2006)	4	Deshmukh et al. (2014)	19
El-Shafei et al. (1994)	1	Lopes et al. (2020)	4	Price et al. (2010)	20
Lopez et al. (2015)	1	Yasin and Yulnafatmawita (2018)	4	Bonsu and Masopeh (1996)	24
Kramarenko et al. (2019)	1	Daniel et al. (2017)	6	Bambra (2016)	24
Zakaria (1992)	1	Anapalli et al. (2005)	7	Verburg et al. (2001)	26
Ramli (1999)	1	Arend (1941)	7	Southard and Buol (1988)	27
Singh et al. (2011)	1	Helbig et al. (2013)	7	Chang (2010)	30
Campbell et al. (1977)	1	Gwenzi et al. (2011)	7	Yao et al. (2013)	33
Chief et al. (2008)	1	Päivänen et al. (1973)	9	Becker et al. (2018)	34
Conedera et al. (2003)	1	Mahapatra and Jha (2019)	9	Baird et al. (2017)	50
Ebel et al. (2012)	1	Amer et al. (2009)	9	Keisling (1974)	56
Ferreira et al. (2005)	1	Radcliffe et al. (1990)	10	Rahimy (2011)	56
Imeson et al. (1992)	1	Vogeler et al. (2019)	10	Hao et al. (2019)	57
Johansen et al. (2001)	1	Singh et al. (2006)	10	Kanemasu (1994)	60
Lamara and Derriche (2008)	1	Kelly et al. (2014)	10	Tete-Mensah (1993)	60
Parks and Cundy (1989)	1	Elnaggar (2017)	11	Zhao et al. (2018)	65
Ravi et al. (2017)	1	Ganiyu et al. (2018)	12	Hinton (2016)	77
Smettem and Ross (1992)	1	Cisneros et al. (1999)	12	Vieira and Fernandes (2004)	86
Helbig et al. (2013)	2	Niemeyer et al. (2014)	12	Houghton (2011)	88
Boike et al. (1998)	2	Sharratt (1990)	14	Tian et al. (2017)	91
Andrade (1971)	2	Habecker et al. (1990)	14	Li et al. (2017)	118
Beyer et al. (2015)	2	Nielsen et al. (1973)	14	Forrest et al. (1985)	118
Blake et al. (2010)	2	Robbins (1977)	15	Richard and Lüscher (1983/87)	121
Bonell and Williams (1986)	2	Sonneveld et al. (2005)	15	Sanzeni et al. (2013)	127
Kutiel et al. (1995)	2	Quinton et al. (2008)	16	Vereecken et al. (2017)	145
Martin and Moody (2001)	2	Simmons (2014)	16	Coelho (1974)	176
Mott et al. (1979)	2	Ouattara (1977)	17	Kool et al. (1986)	240
Rab (1996)	2	Hardie et al. (2011)	17	Nemes et al. (2001)	283
Soracco et al. (2010)	2	Baird (1997)	17	Ottoni et al. (2018)	326
Varela et al. (2015)	2	Kirby et al. (2001)	17	Rahmati et al. (2018)	3637
Sayok et al. (2007)	3	Yoon (2009)	17	Grunwald (2020)	6532

2.2 Georeferencing Ksat values

Georeferencing of Ksat measurements is important for using data for local, regional or global spatial modeling. Once georeferenced, points can be directly used in hydrological and land surface models. Although many studies provided information on the geographical location of the measurements, the studies conducted in the 70's and 80's only provided the name of the locations and approximate distance from the exact location. Therefore, we extracted the latitude and longitude of the location using Google maps for some datasets (which did not provide the spatial locations). We digitized provided maps or sketches with locations of the points. We first georeferenced these maps using ESRI ArcGIS software (v10.3) and then digitized the coordinates from georeferenced images. Some of the documents we digitized (e.g. Nemes et al. (2001)) provided the names specific locations, and hence we used Google Earth to obtain the coordinates. We estimate that the spatial location accuracy of these points is roughly between 0 to 5 km. Similarly, spatial maps in jpg format (e.g. Becker et al. (2018)) were geo-referenced with 100–500 m location accuracy. In contrast, few studies (e.g. Yoon (2009)) provided the extract location of the sampling with assumed location accuracy of 10–20 m.

2.3 Standardization and quality assignment

The database was cleaned to remove unrealistic low values. For example, In the SWIG database, Ksat values computed using infiltration time series were less than 10^{-14} m/day, which seems unreasonable, so they were not included in the database. All datasets were cross-checked to avoid redundancy. For example, UNSODA data consist of Vereecken et al. (2017) and Richard and Lüscher (1983/87) datasets and SWIG database used Zhao et al. (2018). Hence we removed these datasets from UNSODA and SWIG database and used the original sources. Moreover, in the SWIG database, soil depth information was not available, so we assumed that infiltration experiments were conducted close to the surface and assigned a depth of 0–20 cm.

To describe position accuracy of each dataset, we assigned each Ksat value to one of seven 'accuracy classes' ranging from highest (0 - 100 m) to lowest accuracy (more than 10000 m or non available information (NA)). For example, Forrest et al. (1985), Zhao et al. (2018) and Ottoni et al. (2018) provided detailed site coordinates, thus we assigned a location accuracy of 0-100 m (i.e., highly accurate) (see Table 3 for more details). After data extraction from literature, geo-referencing and standardization, all information was collected in tabulated form in the new data base SoilKsatDB 'version 0.3' (https://doi.org/10.5281/zenodo.3752721). The database consists of 22 columns (various sample properties) and 13,268 rows (a header and 13,267 samples). An excerpt of the database with some key properties is shown in Table 2b.

2.4 Statistical modeling of Ksat

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To show a possible application of the database, we computed various pedotransfer functions (PTFs). The PTF models were fitted using a random forest (RF) machine learning algorithm (Breiman, 2001) in the R environment for statistical computing (R Core Team, 2013). We tested fitting the RF model for log-transformed (log_{10}) Ksat values as function of primary soil properties. For 15% of samples with information on bulk density and soil texture, the value of organic content (OC) was not

Table 2a. Description and units of some key variables listed in the database. The complete list can be found in the link to the data base '*version 0.3*' (https://doi.org/10.5281/zenodo.3752721) in the readme-file. We used the same codes adopted in the National Cooperative Soil Survey (NCSS) Soil Characterization Database (National Cooperative Soil Survey, 2016).



Headers	Description	Dimension
site_key	Data set identifier	_
longitude_decimal_degrees	Ranges up to +180 degrees down to -180 degrees	Decimal degree
latitude_decimal_degrees	Ranges up to +90 degrees down to -90 degrees	Decimal degree
location_accuracy_min	Minimum value of location accuracy	m
location_accuracy_max	Maximum value of location accuracy	m
hzn_top	Top of soil sample	cm
hzn_bot	Bottom of soil sample	cm
hzn_desgn	Designation of soil horizon	_
db	Bulk density	${\rm g~cm^{-3}}$
w3cld	Soil water content at 33 kPa (field capacity)	vol %
w1512	Soil water content at 1500 kPa (wilting point)	vol %
tex_psda	Soil texture classes based on USDA	_
clay_tot_psa	Mass of soil particles, < 0.002 mm	%
silt_tot_psa	Mass of soil particles, > 0.002 and < 0.05 mm	%
sand_tot_psa	Mass of soil particle, > 0.05 and < 2 mm	%
oc_v	Soil organic carbon content	%
ph_h2o_v	Soil acidity	_
Ksat_lab	Soil saturated hydraulic conductivity from lab	${\rm cm~day}^{-1}$
Ksat_field	Soil saturated hydraulic conductivity from field	${\rm cm~day^{-1}}$
source_db	Sources of the datasets	_
location_id	Combination of latitude and logitude	_
hzn_depth	Mean depth of soil horizon	_

reported. Therefore, we expressed the PTF for Ksat as a function of bulk density, clay and sand content only. We derived two PTFs for Ksat:

1. *PTFs for temperate regions*: the map of Ksat locations were overlaid on the Köppen-Geiger climate zone map (Rubel and Kottek, 2010; Hamel et al., 2017) and then divided based on climatic regions (temperate, tropical, boreal, and arid) to account for differences in climate and related weathering processes (Hodnett and Tomasella, 2002). A total of 8,296 temperate climate based Ksat values that contain information on sand, clay, and bulk density were used to develop PTF. The data set was randomly divided into a training (6,637 samples, 80%) and testing dataset (1,659 samples, 20%).

Table 2b. Example of Ksat database structure with key variables (from left to right: reference, longitudinal and latitudinal coordinates (decimal degree), top and bottom of soil sample (cm), bulk density (g cm⁻³), soil textural class, clay, silt and sand content (%) and saturated hydraulic conductivity measured in lab or field (cm day⁻¹)). NA is 'no value'. Column names are explained in Table 2a.

aita kar	longitude_	latitude_	hzn_	hzn_	db	tex_	clay_	silt_	sand_	ksat_	ksat_
site_key	decimal_	decimal_	top	bot	ab	psda	tot_	tot_	tot_	lab	field
	degrees	degrees					psa	psa	psa		
Saseendran_2005	-103.15	40.15	15	30	1.33	Loam	23.4	44.3	32.3	232.08	NA
Saseendran_2005	-103.15	40.15	30	60	1.32	Loam	22.3	40.7	37.0	232.08	NA
Saseendran_2005	-103.15	40.15	60	90	1.36	Loam	17.6	36.7	45.7	337.92	NA
Saseendran_2005	-103.15	40.15	90	120	1.40	Loam	12.0	42.3	45.7	284.88	NA
Saseendran_2005	-103.15	40.15	120	150	1.42	Loam	10.0	41.7	48.3	259.20	NA
Saseendran_2005	-103.15	40.15	150	180	1.42	Loam	10.0	41.7	48.3	259.20	NA
Becker_2018	-110.13	31.73	0	15	NA	Sandy loam	NA	NA	NA	NA	26.40
Becker_2018	-110.09	31.72	0	15	NA	Sandy loam	NA	NA	NA	NA	27.84
Becker_2018	-110.09	31.69	0	15	NA	Sandy loam	NA	NA	NA	NA	21.60
Becker_2018	-110.05	31.74	0	15	NA	Loam	NA	NA	NA	NA	23.76
Becker_2018	-110.04	31.72	0	15	NA	Sandy loam	NA	NA	NA	NA	39.12
Becker_2018	-110.04	31.69	0	15	NA	Sand	NA	NA	NA	NA	102.96

Table 3. Number of samples (N) assigned to each elass of spatial accuracy. A minimum and maximum accuracy is defined for each class. NA are samples without information on spatial accuracy.

Minimum location error	Maximum location error	N
0 m	100 m	9937
100 m	250 m	1422
250 m	500 m	959
500 m	1000 m	516
1000 m	5000 m	163
5000 m	10000 m	128
10000 m	NA	142
Total		13,267

2. *PTFs from laboratory-based Ksat values*: In a second application, the dataset (total 13,267) was divided into laboratory and field based Ksat values. The laboratory dataset (8,498 soil samples) was used for training (6,798) and testing (1,700) following the same method as used for the temperate climate PTF (i.e., 80% for training and 20% for testing).

Table 4. Instruments and methods used to estimate Ksat. A key reference with further details is given for all methods. In some cases, 'ponding' or 'permeameter' methods were listed in original studies without specification (18 samples in total).

Lab Ksat methods	N	Field Ksat methods	N
Constant head method (Klute and Dirksen, 1986)	8014	Mini-infiltrometer (Leeds-Harrison et al., 1994)	739
Falling head method (Klute, 1965)	766	Tension infiltrometer (Reynolds et al., 2000)	705
Triaxial cell (ASTM D 5084) (Purdy and Suryasasmita, 2006)	99	Double ring infiltrometer (Bodhinayake et al., 2004)	625
Cylinder method or soil core method (Reynolds et al., 2000)	27	Disc infiltrometer (Soracco et al., 2010)	584
Hydraulic head (Robbins, 1977)	15	Single ring (Bagarello and Sgroi, 2004)	467
Pressure plate (Sharratt, 1990)	14	Guelph Permeameter (Reynolds and Elrick, 1985)	156
Oedometer test (UNI CEN ISO/TS 17892-5) (Terzaghi, 2004)	9	BEST method (Bagarello and Sgroi, 2004)	147
Oedometer test (ASTM D2435-96) (Sutejo et al., 2019)	12	Aardvark permeameter (Hinton, 2016)	142
		Guelf Infiltrometer (Gupta et al., 1993)	87
		Piezometer slug test (Baird et al., 2017)	72
		Tensiometers (Nielsen et al., 1973)	70
		Rainfall simulator (Gupta et al., 1993)	55
		Hood infiltrometer (Schlüter et al., 2020)	40
		Micro-infiltrometer (Sepehrnia et al., 2016)	35
		Mini Disc infiltrometer (Naik et al., 2019)	32
		Disc permeameter (Mohanty et al., 1994)	27
		Constant head permeameter (Amoozegar, 1989)	22
		Steady infiltration (Scotter et al., 1982)	16
		Permeameter	10
		Ponding	8
		Philip–Dunne permeameter (Muñoz-Carpena et al., 2002)	6
		Augur method (Mohsenipour and Shahid, 2016)	5
Unknown	206	Unknown	83
Total	9162		4133

Table 5. Mean values of soil hydro-physical properties for each soil textural class. The number of samples (N) is given in parenthesis under each soil variable for each soil texture classes. N values marked with * correspond to undefined soil texture classes. N values marked with * correspond to undefined soil texture classes. N values marked with * correspond to undefined soil texture classes. N values marked with * correspond to undefined soil texture classes. N values marked with * correspond to undefined soil texture classes. N values marked with * correspond to undefined soil texture classes. N values marked with * correspond to undefined soil texture classes. N values marked with * correspond to undefined soil texture classes. N values marked with * correspond to undefined soil texture classes. N values marked with * correspond to undefined soil texture classes. N values marked with * correspond to undefined soil texture classes. N values marked with * correspond to undefined soil texture classes. N values marked with * correspond to undefined soil texture classes. N values marked with * correspond to undefined soil texture classes. N values marked with * correspond to undefined soil texture classes. N values marked with * correspond to undefined soil texture classes. N values marked with * correspond to undefined soil texture classes. N values marked with * correspond to undefined soil texture classes. N values marked with * correspond to undefined soil texture classes. N values marked with * correspond to undefined soil texture classes. N values marked with * correspond to undefined soil texture classes. N values marked with * correspond to undefined soil texture classes. N values marked with * correspond to undefined soil texture classes. N values marked with * correspond to undefined soil texture classes. N values marked with * correspond to undefined soil texture classes. N values marked with * correspond to undefined soil texture classes. N va

Texture Classes	Clay	Silt	Sand	BD	OC	FC	WP	$Ksat_l$	$Ksat_f$
	(N)	(N)							
Clay	56.3	23.6	20.0	1.27	2.00	43.2	30.0	8.22	110.07
	(830)	(830)	(830)	(639)	(448)	(447)	(449)	(499)	(331)
Silty Clay	45.2	45.1	9.6	1.18	3.83	49.9	30.2	3.63	196.65
	(181)	(181)	(181)	(175)	(116)	(46)	(46)	(85)	(96)
Sandy Clay	39.3	8.1	52.5	1.52	0.23	34.7	23.4	14.16	
	(176)	(176)	(176)	(172)	(140)	(158)	(158)	(172)	(4)
Clay Loam	31.4	38.6	29.9	1.27	2.49	37.2	22.1	13.34	60.56
	(544)	(544)	(544)	(382)	(360)	(76)	(76)	(127)	(417)
Silty Clay loam	33.1	57.1	9.7	1.24	2.67	46.2	23.9	1.57	48.45
	(335)	(335)	(335)	(283)	(227)	(57)	(56)	(113)	(222)
Sandy Clay Loam	26.3	12.1	61.6	1.53	1.26	28.7	17.1	19.43	14.23
	(1148)	(1148)	(1148)	(966)	(950)	(805)	(759)	(876)	(272)
Silt	7.7	84.6	7.6	1.16	1.65	51.4	7.5	13.27	
	(25)	(25)	(25)	(19)	(11)	(12)	(11)	(25)	
Silt Loam	15.2	66.8	17.9	1.34	3.65	35.2	15.6	5.87	44.63
	(810)	(810)	(810)	(618)	(498)	(148)	(138)	(447)	(364)
Loam	19.0	39.1	41.7	1.29	2.16	32.07	14.2	45.62	34.21
	(692)	(692)	(692)	(600)	(561)	(101)	(104)	(226)	(466)
Sandy Loam	13.5	16.8	69.7	1.49	1.33	24.2	11.0	39.71	74.57
	(1601)	(1601)	(1601)	(1492)	(1337)	(806)	(792)	(1078)	(523)
Loamy Sand	7.3	8.5	84.0	1.55	1.13	17.3	6.5	95.37	132.33
	(736)	(736)	(736)	(711)	(674)	(582)	(586)	(637)	(99)
Sand	2.2	3.1	94.6	1.51	0.62	8.2	2.5	488.46	209.55
	(4513)	(4513)	(4513)	(4437)	(4179)	(4063)	(4062)	(4409)	(106)
Total	11,591	11,591	11,591	10,494	9,501	7,301	7,236	8,694	2,900
	(17*)		(38*)	(775*)	(286*)	(88*)	(182*)	(468*)	(1,233*)

The 'ranger' package version 0.12.1 (Wright and Ziegler, 2015) was implemented to process the large dataset. The PTFs developed for temperate regions and for laboratory data were then applied to test their applicability in tropical climate (1,111).

samples) and for field measurements (1,998 samples), respectively. The code for generating and testing the PTFs is provided in the supplementary file.

2.5 Evaluation of Ksat PTFs

The relative importance of the covariates to determine the PTF was assessed by the increase in node purity. It is calculated using the Gini criterion from all the splits (in our case 3 splits) in the forest based on a particular variable (Rodrigues and de la Riva, 2014). Furthermore, the accuracy of the predictions was evaluated using bias, root mean square error (RMSE, in log-transformed Ksat measurement) and concordance correlation coefficient (CCC) (Lawrence and Lin, 1989).

Bias and RMSE are defined as:

$$bias = \sum_{i=1}^{n} \frac{(y_i - \hat{y}_i)}{n} \tag{1}$$

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

where y and \hat{y} are observed and predicted Ksat values, respectively, and n is the total number of cross-validation points.

In addition, Concordance Correlation Coefficient (CCC) (as measure of the agreement between observed and predicted Ksat values) of cross validation (Lawrence and Lin, 1989) is defined as:

$$CCC = \frac{2 \cdot \rho \cdot \sigma_{\hat{y}} \cdot \sigma_{y}}{\sigma_{\hat{y}}^{2} + \sigma_{y}^{2} + (\mu_{\hat{y}} - \mu_{y})^{2}} \tag{3}$$

where $\mu_{\hat{y}}$ and μ_y are predicted and observed means, $\sigma_{\hat{y}}$ and σ_y are are predicted and observed variances and ρ is the Pearson correlation coefficient between predicted and observed values. CCC is equal to 1 for a perfect model.

3 Results

3.1 Data coverage of SoilKsatDB

Based on the literature search and data compilation, we have assembled a total of 13,267 values of Ksat from 1,910 sites (one site is equal to one location 'id') across the globe. Figure 1 shows the global distribution of the sites used in this study. Most data originate from North America, followed by Europe, Asia, South America, Africa, and Australia. With respect to climatic regions, 10,093 Ksat values belong to the temperate region and 1,443, 1,113, 582, and 36 to tropical, arid, boreal, and polar regions, respectively. The points are often spatially clustered with the biggest cluster of points (1,103 site stions with 6,532 Ksat values) in Florida (Grunwald, 2020). Ksat data include 4,133 values from field measurement and 9,162 values from

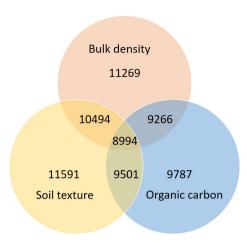


Figure 2. Venn diagram illustrating the number of samples containing information on bulk density, soil texture, and organic carbon. Out of 13,267 samples, 11,269, 11,591 and 9,787 samples have values of bulk density, soil texture and organic carbon, respectively. Furthermore, 10,494, 9,266 and 9,501 samples have information of bulk density and soil texture, bulk density and organic carbon and soil texture and organic carbon, respectively. 8,994 samples have information of all three soil properties. Note that the size of the intersecting areas does not represent the correct fractions (otherwise the intersection with 8,994 would be much bigger).

laboratory measurements. In particular, different types of infiltrometers (e.g., Mini-infiltrometer, Tension infiltrometer, double ring infiltrometer) and permeaters (e.g., Guelf permeameter, Aardwark permeameter) were used for-Ksat field measurements, whereas constant or falling head methods were predominantly, used in laboratory analyses, as shown in Table .4.

Out of the 13,267 Ksat measurements, 11,591, 11,269, 9,787, 7,389 and 7,418 points had information on soil texture, bulk density, organic carbon, field capacity and wilting point, respectively, while 8,994 samples had information for all soil basic properties (bulk density, soil texture and organic carbon) (Figure 2). The methods used to compute these soil properties (as much as we could extract from the literature and existing databases) were listed in the supplementary CSV file sol_ksat.pnts_metadata.csv available at 'version 0.3' https://doi.org/10.5281/zenodo.3752721. Note that in addition to 11,591 soil texture values, 75 samples have soil texture information with total (sand+silt+clay) less than 98% or greater than 102%. We did not use these values in the PTF development. Moreover, the database contains total of 13,295 Ksat values because few studies have reported both field and lab measurements for the same sampling point.

3.2 Statistical properties of SoilKsatDB

The distribution of soil samples based on soil texture classes is shown on the USDA soil texture triangle in Figure 3a. The database covers all textural classes, with a high clustering in sandy soils due to the numerous samples from Florida (Grunwald, 2020). The violin distribution plot in Figure 3c shows the range of Ksat values for the different databases. Most of the datasets report Ksat values between $\approx 10^{-2}$ and $10^{2.5}$ cm/day, with a wider range of Ksat values observed in measurements from theses and reports (including studies with extreme values from sandy desert soils and low conductive clay soils) and from the SWIG

database (databases 9 and 6 in Figure 3c, respectively). Likewise, Figure 3d shows the violin distribution of Ksat based on soil texture classes. Sand and loamy sand soils showed the highest arithmetic mean (i.e., 2.6 and 1.99, respectively), while the lowest mean values were found for silt and silty loam (i.e., 1.12 and 1.15, respectively). The significance between each soil texture class was also tested using a t-test (Kim, 2015) and results are presented in the supplementary file. Table ST1 shows that the Ksat values under sand and loamy sand soil texture class are significantly different from all other soil texture classes, however, silt, silty clay, and silty clay loam elass are not significantly different from clay, sandy clay, and sandy clay loam Ksat values.

Average values of Ksat and other hydro-physical properties are shown in Table 5. Higher average organic carbon and bulk density values were observed in clayey and loamy soils compared to sandy soils. Ksat values obtained from field measurements were on average higher (depending on the type of instrument used) than those obtained from laboratory Ksat values Particularly, for the clay texture class much lower Ksat values were observed for laboratory (mean Ksat ≈ 8 cm/day) compared to field (mean Ksat ≈ 110 cm/day) measurements (Table 5). Figure 3b further illustrates the higher range of Ksat values obtained for finer texture soils (clay and loam) compared to coarser soils (sand).

3.3 Ksat PTFs derivation

As a test application of SoilKsatDB, two PTFs were derived for Ksat (i.e., for temperate regions and based on laboratory measurements) using basic soil properties as covariates. Such basic soil properties are plotted against Ksat in Figure 4, showing that Ksat decreases with increasing clay content and bulk density, and increases with sand content. The observed correlation between these soil properties and Ksat motivates their use as key variables for the estimation of PTFs. In this application, PTFs for Ksat were built on bulk density and sand and clay content. Organic carbon (OC) was not used to build the PTFs because (i) this information was missing for 15% of samples, and (ii) the correlation between OC and Ksat was poor (i.e. 0.005).

Figure S1 shows the list of relative importance of the covariates the PTFs models obtained for temperate regions and laboratory-based measurements. Clay content was found to be the most important variable followed by sand and bulk density for temperate climate PTF. On the other hand, sand content was found to be the most important variable followed by clay and bulk density for the laboratory-based Ksat PTF. CCC, bias, and RMSE were respectively equal to 0.70, -0.002, and 0.69, for the temperate region based PTF, and to 0.73, 0.0004, and 0.65 for laboratory-based PTF.

PTF models derived for temperate and laboratory-based Ksat values overestimate Ksat for tropical and field-based Ksat values, respectively (see Figure 6b and Figure 5b). CCC, bias, and RMSE values were respectively equal to 0.52, 0.2, and 0.90 for tropical Ksat values, and to 0.10, 0.21, and 1.2 for field measured Ksat values.

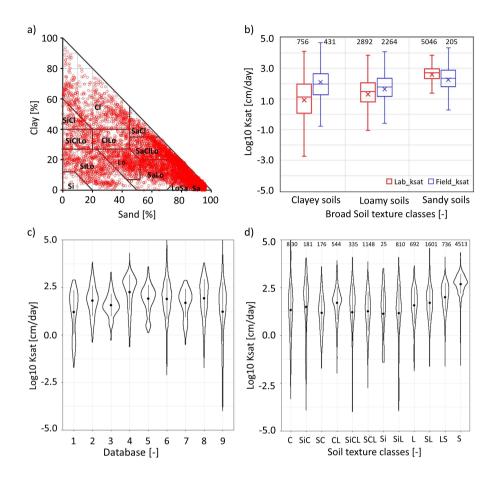


Figure 3. Characterization of collected Ksat values. (a) Distribution of soil samples on the USDA soil texture triangle. The data points cover all soil textural classes and only few samples belong to the silt textural class. b) Distribution of Ksat values using broad soil texture classes (sandy soils: sand, loamy sand; loamy soils: sandy loam, loam, silt loam, silt, clay loam, sandy clay loam; clayey soils: sandy clay, silty clay, clay) based on laboratory and field methods. The number of samples provided on the top of the figure. The increase in Ksat values in clayey and loamy soils under field methods is likely due to the effect of soil structure. A t-test showed that all broad soil texture classes are significantly different from each other except clayey soils field Ksat values and sandy soils field Ksat values (see Table ST2). The violin plot (c) represents the range of Ksat values spanned by each data source. The dot represents the mean value, and the line represents the standard deviation for each data set. The numbers 1–9 refer to different sources and databases: 1 = Australia (Forrest et al., 1985), 2 = Belgium (Vereecken et al., 2017), 3 = China (Tian et al., 2017; Li et al., 2017), 4 = Florida (Grunwald, 2020), 5 = HYBRAS (Ottoni et al., 2018), 6 = SWIG (Rahmati et al., 2018), 7 = Tibetan Plateau (Zhao et al., 2018), 8 = UNSODA (Nemes et al., 2001), 9 = all other databases in Table 1. d) Distribution of Ksat based on soil textural classes with the number of samples shown on the top of the figure. The significance was also tested for each class using a t-test (Kim, 2015) and results are presented in the supplementary file.

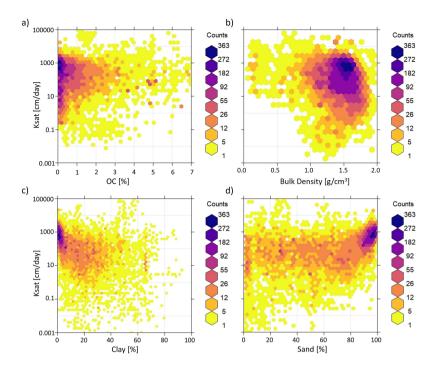


Figure 4. Partial correlation between Ksat and a) organic carbon (%), b) bulk density (g/cm³), c) clay (%) and d) sand content (%). Ksat decreases with increasing clay content and bulk density, and increases with sand content. The color of each hexagonal cell shows the number of the <u>counts</u> in each cell.

4 Discussion

4.1 Laboratory vs field estimated Ksat: effect of soil structure

The Ksat values were, on average, higher for samples measured using field methods compared to laboratory methods for most soil texture classes (Table 5 and Figures 3b and 5). The difference in laboratory and field based Ksat values and higher range of Ksat values in fine textured soil is probably related to the effect of biologically-induced soil structure that might be neglected in laboratory measurements. The omission of soil structures in many laboratory samples limits the possibility to properly reproduce field observations that are likely to be more affected by the presence of biopores (Fatichi et al., 2020). In other words, variability in the Ksat values depends on the consideration (and existence) of soil structural pores by the measurement methods. Soil structural pores change the pore size distribution and subsequently affect Ksat values (Tuller and Or, 2002). Such an effect is more likely to be neglected more in laboratory measurements compared to field studies. Presence or absence of large structural pores also depends on the scale of measurements (that is usually larger in the field). Mohanty et al. (1994), for example, compared three field methods and one laboratory method and found that the sample size affects the measurement of Ksat due to the presence and absence of open-ended pores. Similarly, Ghanbarian et al. (2017) showed that the sample dimensions (e.g., internal diameter and height) also impact Ksat. The authors further developed a sample dimension-dependent

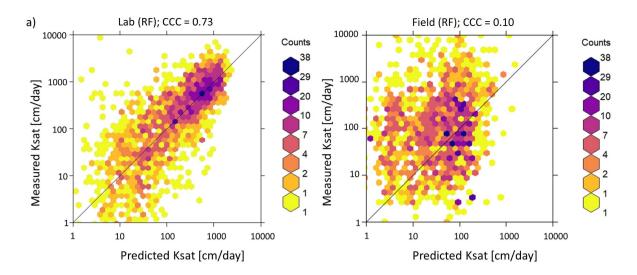


Figure 5. The correlation between observed and predicted Ksat values obtained from (a, b) random forest (RF) models. The RF-based Pedotransfer function (PTF) model was fitted using data for laboratory measurements of Ksat and tested on both laboratory (a) and field (b) measurements. Results showed reasonable agreement (CCC = 0.73) using RF algorithms for laboratory measurements, but low CCC (0.10) for field measurements. PTFs developed based on laboratory measurements do not provide accurate estimates of Ksat measured in the field.

PTF and showed a better performance compared to other available PTFs in the literature. Likewise, Braud et al. (2017) used three field methods for Ksat measurements and found significant variation between these methods of measurements. Davis et al. (1996) presents the necessity to choose the most appropriate scale of measurement for a particular soil when undertaking conductivity measurements. The authors tested small cores (73 mm wide and 63 mm high) and large cores (22 mm wide and 300 mm high) using the constant head method in the laboratory and found the difference of 1 to 3 orders of magnitude.

4.2 Temperate vs tropical soils: effect of clay mineralogy

Results showed that PTFs obtained for temperate soils performed poorly for tropical soils (Figure 6), with Ksat being underestimated by the temperate-based PTFs. This result is in agreement with Tomasella et al. (2000) who derived PTFs using data from tropical Brazilian soils, which did not properly capture observations in temperate soils. We argue that the significant differences in the models validated for tropical and temperate soils are due to the differences in the soil-forming processes defining the clay type and mineralogy. In fact, Oxisols (highly weathered clay minerals in tropical regions) are turned into inactive (non-swelling) clay minerals as a result of high rainfall and temperatures. On the other hand, in the temperate regions, active (smectite) and moderately active clay minerals (illite) are the dominant clay minerals. These swelling clay minerals retain the water within internal structures with very low hydraulic conductivity. Therefore, such a difference in clay mineralogy is likely responsible for the underestimation of Ksat in tropical soils from PTFs obtained in temperate ones. In addition, soil

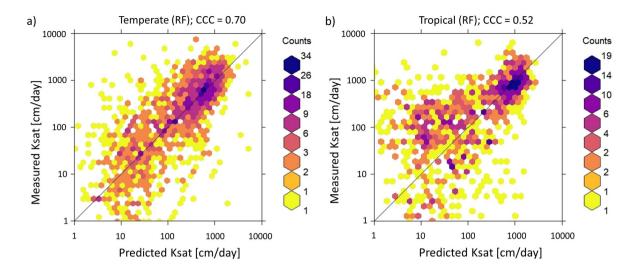


Figure 6. Correlation between observed and predicted Ksat values obtained from random forest (RF) model. The RF-based Pedotransfer function (PTF) model was obtained by fitting 6,637 training points obtained in a temperate-climate and tested on (a) temperate (1,659 samples) and (b) tropical testing points (1,111 samples). CCC is the concordance correlation coefficient. PTFs showed good performance (CCC = 0.70) for the temperate soil samples (including both laboratory and field measurements), but lower CCC values were obtained for tropical soil samples (0.52 for RF). PTFs determined for temperate regions cannot be easily transferred to tropical regions due to different soil forming processes.

structure formation processes may be different in tropical and temperate regions and intensify the differences between Ksat values measured in the two different climatic regions.

4.3 Limitations of SoilKsatDB

We have put an effort to combine laboratory and field data from most global regions. However, we acknowledge that there are still gaps in some regions such as Russia and higher northern latitudes in general, which may produce uncertainties in Ksat estimations in such regions. The SoilKsatDB could also be of limited use for fine-resolution applications because many data points were characterized by limited spatial accuracy and missing soil depth information. Specifically, the spatial accuracy of many points is between tens of meters to several kilometers (see the methodology sections regarding the extraction of the spatial locations using Google Earth). Many of the records in the SoilKsatDB come from legacy scientific reports and the original authors can not be traced and contacted, hence we advise to use this data with caution. In addition, in the SWIG database, the soil depth and measurement method information were not provided, and often one location was used to represent an entire watershed. We tried to revisit each publication and extract the most accurate coordinates of assumed sampling locations. In addition, we assumed that most of the samples were obtained from field measurements as authors used different infiltrometers to compute Ksat, so there might be few points in our SoilKsatDB that belong to laboratory measurements and that we have incorrectly assigned to field measurements.



For each measurement, a location accuracy (0-100 m = highly accurate, >10000 m = least accurate) was assigned based on the sampling location accuracy. The location accuracy can be used as a weight or probability argument in Machine Learning for Ksat mapping. We acknowledge that this was a rather subjective decision and a more objective way to assign weights would be to use the actual spatial positioning errors. Because these were not available for most of the datasets, we have opted for the definition of a location accuracy estimated from the available documentation.

4.4 Further developments

The advancement in remote sensing technology opens the doors to link the hydraulic properties with global environmental features. Using satellite-based maps of environmental properties, local information on vegetation, climate, and topography for specific areas, which are often ignored by basic PTFs, can be incorporated. For example, Sharma et al. (2006) developed PTFs using environmental variables such as topography and vegetation and concluded that these attributes, at finer spatial scales, were useful to capture the observed variations within the soil mapping units. Likewise, Szabó et al. (2019) used the random forest machine learning algorithm for mapping soil hydraulic properties and incorporated local environmental variable information.

5 Data availability

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5 All collected data and related soil characteristics are provided online for reference and are available at 'version 0.3' https://doi.org/10.5281/zenodo.3752721 (Gupta et al., 2020).

6 Summary and conclusions

We prepared a comprehensive global compilation of measured Ksat training point data (N=13,267) by importing, quality controlling, and standardizing tabular data from existing soil profile databases and legacy reports. The produced SoilKsatDB covers a broad range of soil types and climatic regions and hence is useful for global soil modeling. A higher variation in Ksat values was observed in fine-textured soil compared to coarse-textured soils, indicating the effect of soil structure on Ksat. Moreover, Ksat values obtained from field measurements were generally higher than those from laboratory measurements, likely due to impact of soil structural pores at larger scale in field measurements.

The new database was applied to develop pedotransfer functions (PTFs) for Ksat using measurements in temperate climates and laboratory based soil samples using RF algorithms. PTFs developed for a certain climatic region (temperate) or measurement method (laboratory) could not be satisfactorily applied to estimate Ksat for other regions (tropical) or measurement method (field) due to the role of different soil forming processes (inactive clay minerals in tropical soils and impact of biopores in field measurements).

There are still some gaps in the geographical representation of sampling points, especially in Russia and the higher northern latitudes, that could induce uncertainty in global modeling. Therefore, the data set can be further improved by covering the missing areas and achieve better accuracy in the hydrological applications.

The SoilKsatDB was developed in R software and is available via '*version 0.3*' https://doi.org/10.5281/zenodo.3752721. We have made code and data publicly available to enable further developments and improvements as a collective effort.

Acknowledgements. The SoilKsatDB is a compilation of numerous existing datasets from which the most significant are: SWIG dataset (Rahmati et al., 2018), UNSODA (Leij et al., 1996; Nemes et al., 2001), and HYBRAS (Ottoni et al., 2018). The study was supported by ETH Zurich (Grant ETH-18 18-1). OpenGeoHub maintains an global repository of Earth System Science datasets at www.openlandmap.org. We thank Zhongwang Wei for helping in collecting the datasets and for insightful discussions. We acknowledge Samuel Bickel (ETH Zurich) for the help with High Performance Computing. We would also like to thank two anonymous reviewers and Dr. Attila Nemes for their constructive feedback to improve the manuscript.

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