**Predicting field-saturated hydraulic conductivity of urban soils using texture and structure**

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**Acronyms:** Kfs – Field-saturated hydraulic conductivity, ANN – Artificial Neural Network, RF – Random Forest model, PTF – Pedotransfer Function

# Abstract

Pedotransfer functions (PTFs), which predict soil hydraulic parameters based on other measured properties, provide limited accuracy when estimating field-saturated hydraulic conductivity. PTF models are often constructed using laboratory-determined saturated hydraulic conductivity measurements, which typically vary from field-derived values. Current PTFs also do not account for soil structure, even though this factor can influence permeability. This study therefore had two objectives: 1) develop PTFs that accurately predict field-saturated hydraulic conductivity (Kfs) using a dataset collected in twelve U.S. cities, and 2) validate the predictive capability of these models by comparing them to measured Kfs values reported in three other urban studies. The developed PTFs included as possible inputs %sand, %silt, %clay, and soil structure type. The data were analyzed using both artificial neural networks (ANN) and Random Forest models that excluded (RF1) and included (RF2) soil structure. The developed PTFs accurately predicted Kfs in the training dataset, with adjR2 = 0.28 (ANN), 0.77 (RF1), and 0.77 (RF2), but model performance decreased substantially in the test dataset, with adjR2 = 0.27 (ANN), 0.25 (RF1), and 0.36 (RF2). However, the models still had much less error than the widely used ROSETTA model. The evaluation dataset similarly showed that the developed PTF provided much greater accuracy than ROSETTA, and that adding soil structure information improved model accuracy (adjR2 improved from 0.25 to 0.36). This study provides improved PTFs for predicting Kfs in urban soils, while demonstrating the importance of considering soil structure in such predictions.

# 1. Introduction

Field-saturated hydraulic conductivity (Kfs) influences many soil hydrological processes, including infiltration, drainage, and other subsurface water redistribution processes (Jackson et al., 2016; Libohova et al., 2018; Stewart and Abou Najm, 2018). Kfs often represents the single most important parameter to constrain when performing hydrological modeling (Ameli et al., 2015; Trinh et al., 2018), yet can be time-consuming and difficult to measure in the field. For this reason, pedotransfer functions (PTFs), which predict properties such as hydraulic conductivity from easier to measure properties such as soil texture, have become widely used. As an example, the ROSETTA PTF, which possesses a hierarchical structure with flexibility in input data, has enjoyed widespread usage due in part to its inclusion with the soil hydrological model HYDRUS (Schaap, 1999; Schaap et al., 2001; Šimůnek et al., 2008).

Most current PTFs utilize a similar set of basic parameters: either texture or %sand, %silt, and %clay (%SSC), bulk density, and water contents at various matric potentials such as -33 and -1,500 kPa. Some may also include additional information on such characteristics as type of soil horizon, organic matter content, topography, vegetation, and land management and use (Moeys et al., 2012; Sharma et al., 2006; Wösten et al., 1999). These models then develop statistical relationships between those variables and more difficult to determine parameters like saturated hydraulic conductivity (Ksat) and water retention model coefficients. More than twenty different PTFs have been developed over the years, using anywhere from six to more than 5,000 soil samples (Guber and Pachepsky, 2010). These models have incorporated a variety of techniques to estimate parameter values, from using physical relationships (Arya et al., 1999a; Arya et al., 1999b; Arya and Paris, 1981; Gimenez et al., 1997; Rawls et al., 1993) to statistical regression models (Lin et al., 1999; Wösten et al., 1999) to artificial neural networks (Parasuraman et al., 2006; Schaap, 1999; Schaap et al., 1998). These different PTFs can also be integrated together into multi-model ensemble predictive tools (Guber et al., 2006). While these various PTF approaches tend to perform well when predicting water retention characteristics, the variability between model and measurement becomes much wider when applied to Ksat values (Pachepsky and Rawls, 2003; Rawls et al., 1998). These errors may become further compounded when the PTFs are used to estimate field-saturated Kfs values.

Current PTFs often poorly predict Kfs for several reasons, including the lack of field-relevant training data and the exclusion of soil morphological information such as structure. As an example of the former, PTF models are typically trained using values collected from disturbed cores (Clapp and Hornberger, 1978; Rawls et al., 1998), which often do not reflect field-saturated hydraulic conductivity values measured in the field (Reynolds et al., 2000; Stewart et al., 2016). This discrepancy can arise because soil cores are typically saturated when analyzed, as compared to the field-saturated conditions where air still exists in trapped pockets. Soil cores can also allow water to short-circuit the soil matrix, thus exaggerating hydraulic conductivity values, though this effect may diminish as cores become longer (Anderson and Bouma, 1973). These potential inconsistencies point to the need for PTFs based on field-relevant Kfs values.

Soil structure, which describes the specific arrangement of primary soil particles into secondary units, is not incorporated into most current PTFs and thus represents a second potential reason that existing functions can prove inadequate for estimating Kfs. Structure often results in larger, better connected, and more easily drained pores, which can enhance the flow of water and gases through soils (Horn and Smucker, 2005). Lin et al. (1999) developed a set of PTFs that included soil morphological data including soil ped grade and type and macropore quantity and type, and found that those descriptors improved predictions of Kfs. Wagner et al. (2001) also found that soil structure influences predictions of Kfs, though those authors argued against including morphological data since their particular focus was on predicting unsaturated hydraulic conductivity values. The role of structure may be particularly important in urban environments, where structure may be altered or destroyed via compaction, regrading, fill materials, etc. (Batey, 2009; Herrmann et al., 2018; Shuster et al., 2015).

Soil structure can be difficult to quantitatively describe (Eck et al., 2016) or incorporate into large-scale models (Van Looy et al., 2017); however, the National Cooperative Soil Survey provides qualitative descriptions of soil structure within soil series descriptions (NCSS, 2019). These descriptions include type, grade, and class. Type describes the arrangement and geometry of soil peds, and includes categories such as granular, blocky, and platy. Grade describes the prominence of the structural features, while class conveys the size of the peds. Taken together, this information can convey information about the size and connectivity of flowpaths in the soil, and have successful been incorporated into PTFs for soil water retention (Pachepsky and Rawls, 2003). We posit here that incorporating soil structural information, specifically soil structure type, into PTF models will improve predictions of Kfs.

Based on the shortcomings of current PTF models for estimating hydraulic conductivity in urban soils, this study had two main objectives: 1) develop a set of pedotransfer functions that accurately predicts field-saturated hydraulic conductivity, Kfs, using a novel dataset collected in twelve U.S. cities, and 2) validate the predictive capability of this model by comparing it to measured Kfs values reported in four other studies on urban systems.

# 2. Methods

**2.1 Urban soil field-saturated hydraulic conductivity (Kfs) data**

Field-saturated hydraulic conductivity (Kfs) values were collected from 286 urban soil profiles located in 12 cities (Atlanta, GA; Camden, NJ; Cincinnati, OH; Cleveland, OH; Detroit, MI; New Orleans, LA; Omaha, NE; Phoenix, AZ; Portland, ME; Tacoma, WA; Majuro, RMI; and San Juan, PR). Sites were selected as part of the U.S. Environmental Protection Agency (EPA) Urban Soil Assessment [see (Herrmann, Schifman, & Shuster, 2018; Herrmann, Shuster, & Garmestani, 2017; W. D. Shuster, Dadio, Drohan, Losco, & Shaffer, 2014; William D. Shuster, Dadio, Burkman, Earl, & Hall, 2015)] for details; together, the sites represent 10 of the 12 major soil orders in the USDA soil taxonomy (Soil Survey Staff, 2014). The urban datasets are available for download through a repository maintained by the US Government (https://catalog.data.gov/harvest/about/epa-sciencehub).

Soil profiles were assessed for physical, hydrologic, and chemical characteristics. Soil texture was measured using…, The soil cores covered all 12 United States Department of Agriculture (USDA) soil textures, though the sandy clay, silt and silt loam textures had fewer samples than the other soil textures (Figure 1).

Surface infiltration rates were measured using a mini-disk tension infiltrometer (METER Group, Pullman, WA, USA) with pressure head h = -2 cm. Kfs values were then estimated using the solution of (Zhang, 1997). Kfs values in the dataset ranged from 0.02 to 50 cm h-1, with a mean of 2.0 cm h-1. The entire dataset was divided into two subsets, with 85% of the samples (n=243) used to train the Artificial Neural Network (ANN) and Random Forest (RF) models, and the remaining 15% (n=43) used to test the performance of the models.

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**Figure 1.** Textural distribution of 286 samples (blue dots in left panel) and 20 samples from historical papers (red dots in left panel) used in this study according to the United States Department of Agriculture (USDA) soil texture system; and the histogram of soil hydraulic conductivity (cm h-1, right panel).

We also collected published Kfs data from urban soils studies to verify the performance of the ANN and RF models developed in this study. We conducted a literature search through ISI Web of Science and the China National Knowledge Infrastructure (CNKI), using the keywords “urban soil hydraulic conductivity” or “urban soil infiltration”. Papers from peer reviewed journals, theses, and dissertations were included. From a total of more than 50 papers, we used the following criteria to identify appropriate sources: (1) the data came from the urban soils; (2) experiments were conducted in the field; (3) the study reported Kfs or steady-state one-dimensional infiltration rates, which we assumed was equal to Kfs (Philip, 1969); (4) %SSC were reported; and (5) the study location or field conditions were described with sufficient information to infer soil structure. Within these constraints, 20 Kfs data were extracted from three papers (Table 1). Kfs values collected from the historical papers ranged from 0.4 to 18.8 cm h-1, with a mean of 5.67 cm h-1.

**Table 1.** Summary of data from three studies used to validate pedotransfer function (PTF) models. Texture = soil texture; Sa = %sand, Si = %silt, Cl = %clay; BD = bulk density in g cm-3; Type = structure type; Kfs = field-saturated hydraulic conductivity in cm h-1; ANN = Artificial Neural Network prediction for Kfs in cm h-1; RF1 = Random Forest without soil structure prediction for Kfs in cm h-1; RF2 = Random Forest with soil structure prediction for Kfs in cm h-1; ROSE = ROSETTA model prediction for Kfs in cm h-1. NA indicates where data was not available. For structure type, SG = single grain; P = platy; SBK = sub-angular blocky; G = granular.

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| **Texture** | **Sa** | **Si** | **Cl** | **BD** | **Type** | **Kfs** | **ANN** | **RF1** | **RF2** | **ROSE** | **Citation** | **Infiltration test type** |
| Sand | 89.3 | 10.6 | 0.1 | 1.48 | SG | 18.7 | 7.75 | 9.63 | 7.36 | 340 | Gregory et al. (2006) | Double ring |
| Sand | 96.2 | 1.8 | 2 | 1.52 | SG | 16.0 | 7.75 | 9.63 | 7.36 | 872 | Gregory et al. (2006) | Double ring |
| Sand | 96.2 | 1.8 | 2 | 1.47 | SG | 18.8 | 7.25 | 9.63 | 7.36 | 872 | Gregory et al. (2006) | Double ring |
| Loam | 28 | 47 | 25 | NA | P | 0.40 | 0.38 | 0.41 | 0.29 | 13.2 | Hamilton & Waddington (1999) | Double ring |
| Silt loam | 18 | 59 | 23 | NA | P | 1.20 | 0.39 | 0.51 | 0.35 | 13.2 | Hamilton & Waddington (1999) | Double ring |
| Silt loam | 22 | 55 | 23 | NA | SBK | 1.40 | 0.99 | 1.17 | 1.61 | 13.6 | Hamilton & Waddington (1999) | Double ring |
| Sandy loam | 62 | 27 | 11 | NA | SBK | 1.40 | 0.40 | 1.19 | 0.83 | 35.0 | Hamilton & Waddington (1999) | Double ring |
| Silt loam | 23 | 58 | 19 | NA | SBK | 1.60 | 0.53 | 0.70 | 0.84 | 16.3 | Hamilton & Waddington (1999) | Double ring |
| Loam | 44 | 37 | 19 | NA | SBK | 1.80 | 0.37 | 0.49 | 0.37 | 10.1 | Hamilton & Waddington (1999) | Double ring |
| Silt loam | 14 | 63 | 23 | NA | SBK | 2.20 | 0.38 | 0.91 | 0.68 | 13.0 | Hamilton & Waddington (1999) | Double ring |
| Clay loam | 24 | 47 | 29 | NA | SBK | 2.30 | 0.40 | 0.43 | 0.31 | 12.4 | Hamilton & Waddington (1999) | Double ring |
| Silt loam | 27 | 51 | 22 | NA | SBK | 2.70 | 0.50 | 0.35 | 0.53 | 14.6 | Hamilton & Waddington (1999) | Double ring |
| Loam | 42 | 33 | 25 | NA | SBK | 2.90 | 0.42 | 0.44 | 0.47 | 7.21 | Hamilton & Waddington (1999) | Double ring |
| Loam | 32 | 43 | 25 | NA | G | 4.90 | 0.41 | 0.60 | 0.35 | 12.6 | Hamilton & Waddington (1999) | Double ring |
| Clay loam | 32 | 39 | 29 | NA | G | 5.10 | 0.38 | 0.48 | 0.36 | 9.68 | Hamilton & Waddington (1999) | Double ring |
| Silt loam | 18 | 60 | 22 | NA | G | 8.50 | 0.39 | 0.53 | 0.40 | 13.7 | Hamilton & Waddington (1999) | Double ring |
| Silt loam | 22 | 57 | 21 | NA | G | 9.80 | 0.40 | 0.59 | 0.34 | 14.6 | Hamilton & Waddington (1999) | Double ring |
| Clay loam | 30 | 41 | 29 | NA | G | 10.0 | 6.90 | 9.63 | 7.36 | 11.3 | Hamilton & Waddington (1999) | Double ring |
| Sand | 94 | 3 | 3 | NA | SG | 3.00 | 0.35 | 2.00 | 1.56 | 629 | Pitt et al. (1999) | Double ring |
| Clay | 15 | 15 | 70 | NA | SBK | 0.70 | 0.34 | 0.41 | 0.30 | 16.3 | Pitt et al. (1999) | Double ring |

The following procedure was used to estimate structure type: if the exact site location was reported, the soil structure description was taken from the soil series description; if the site location was ambiguous, the dominant soil series around the location were analyzed for most common structural descriptions, with the most frequently reported structure type assumed for the study site. In cases where this procedure gave ambiguous results, structure type was estimated based on qualitative descriptions provided in the original texts: sandy soils were assumed to have single-grained structure; well-aerated and intact A horizons were assumed to have granular structure; compacted fine-textured soils were assumed to have platy structure.

**2.2 Kfs modeling**

Artificial Neural Network (ANN) modeling was used in this study to predict urban soil Kfs according to soil texture information (sand, silt, and clay percentage). ANN technology has been widely used in the soil physical pretransfer functions (Parasuraman, Elshorbagy, & Si, 2006; Schaap & Leij., 1998). Typically, an ANN model has input, hidden, bias, and output layers; each layer is connected to the next layer of neurons (Figure 2). The input layer compiles entered data, and the hidden layer(s) process the inputs using activation functions. The bias neuron lies in between two layers, it allows the fitting curve moves to fit the prediction with the data better. In this study, the input layers included %Sand, %Silt and %Clay, and the output layer predicted Kfs (Figure 2). We varied the number of hidden layers from 1 to 3, with each layer possessing 2 to 6 neurons. As model performance was not sensitive to the number of neurons or hidden layers, we set the ANN model with 2 hidden layers, with 5 neurons for the first hidden layer and 3 for the second hidden layer (Figure 2). We conducted the ANN modeling using the “neuralnet” package in the R software (Version 3.4.3, R Core Team, 2014).

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**Figure 2.** Schematic diagram shows results of Artificial Neural Network (ANN) model. I1, I2, and I3 represent input variables: %Sand, %Silt, and %clay percentage, respectively. H1-H5 are the neurons in the first hidden layer, and H6-H8 are the neurons in the second hidden layer. O represents output layer. B1-B3 indicates bias terms added in each step.

We also developed two Random Forest (RF) models in this study. RF is a type of regression tree algorithm, which allows multiple parameters to be input (note that both numeric and categorical parameters can be used as input). Before creating the RF models, we needed to determine the number of trees and the number of variables in each tree. Usually, the required number of trees can be determined according to the mean square error (MSE) vs. number of trees plot. We set the number of trees to 100, and set the number of variables in each tree to 2, as the number of variables per tree should be smaller or equal to the total number of input variables. Our analysis found that the modeled mean square error (MSE) decreased with as number of trees increased over the range 0 to 70, but was constant when the number of trees was > 70 (Figure 3a). We thus concluded that setting the number of trees to 100 is reasonable when developing the RF models. The importance of individual input variables was also tested by quantifying the increase in model MSE as each variable was removed. This analysis determined that %Sand was the most important variable, following by %Clay, %Silt, and soil structure (Figure 3b). Similar conclusions can be obtained by examining the node purity, in which the importance of each variable was indicated as the increase in model node purity once that variable was removed (Figure 3c). RF modeling was conducted under “randomForest” package in R.

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**Figure 3.** Change of (MSE) values as number of trees increase in the Random Forest model (panel a). The trends show that MSE decreased as number of trees increased between 0 and 70, and MSE values did not change when number of trees > 70. (b) Variables importance indicated as increase of MSE if a specific variable was removed, most important variable has large effect on MSE value. The results show that percentage of silt content is the most important variable, following by sand percentage and clay percentage. (c) Variables importance indicated as increase of model’s node purity if a specific variable was removed, similar as showed from the MSE results, silt percentage is also the most important variable, following by sand percentage and clay percentage.

**2.3 Model evaluation**

Kfs values predicted by the models were compared to measured Kfs values for the test (*n* = 43) and evaluation data (*n* = 20). As an addition comparison, the ROSETTA model (Schaap et al., 2001) was also used to estimate Kfs based on reported %SSC (Table 2). Model fits were evaluated using five measures: 1) Pearson correlation [*R*; Equation (1)], 2) adjusted *R*2 [*adjR*2; Equation (2)], 3) mean error [*E*; Equation (3)]; 4) index of agreement [*d*, Equation (4)], and 5) root mean square error [RMSE; Equation (5)].

 (1)

where *n* is the number of observations, and *x* represents measured and *y* represents predicted values for Kfs. *R* ranges from -1 to +1, with higher values indicate better correlation between the regressor and the response.

 (2)

where *k* is the number of independent regressors. *adjR*2 ranges from 0 to 1, with values closer to 1 indicating better model performance.

 (3).

Mean error (*E*) close to zero indicates good simulation results, E > 0 indicates that the predicted values were overestimated relative to measured data, and E < 0 indicates that predicted values underestimate the observed data.

 (4)

where  represents the average of all measured Kfs values. Index of agreement (*d*) ≥ 0.9 shows excellent agreement between measured and predicted values, 0.80 ≤ *d* < 0.90 shows good agreement between measured and predicted values, 0.70 ≤ *d* < 0.80 shows moderate agreement between measured and predicted values, and *d* < 0.70 shows poor agreement between measured and predicted values.

 (5).

Smaller RMSE values indicate better model performance.

We also fit simple linear regression (SLR) models between the predicted and measured Kfs values; the slope and intercept of the SLRs were used to evaluate the ability of each model to provide predictions of the appropriate magnitude compared to observations.

Finally, analysis of variation with Tukey’s Honestly Significant Difference (ANOVA with Tukey’s HSD) were used to assess if the Kfs predicted by ROSETTA, ANN, RF1, and RF2 model are significantly differ from measured Kfs. All data analysis were carried out using R software (Version 3.4.3, R Core Team, 2014).

# 3. Results

**3.1 Training and testing data**

The Artificial Neural Network (ANN) model results indicated that the model can explain approximately 30% of Kfs variability (*adjR*2 = 0.28 for the training and 0.27 for the test dataset; Figure 4a and b). For the training dataset, the linear regression between predicted Kfs and field measured Kfs followed the 1:1 line, indicating that the ANN model provided proper estimates for Kfs magnitude (Figure 4a). However, for the testing dataset, the simple linear regression had a positive intercept (intercept = 1.11) and a slope smaller than 1 (slope = 0.33), indicating that the ANN model tended to overestimate Kfs at small values and underestimate Kfs at large values (Figure 4b and Table 2). The results from the other four model evaluation statistics showed that ANN model had relatively low values for absolute mean error value (*E* = -0.07) and RMSE (2.23 cm h-1), and a relatively high value for index of agreement (d = 0.71; Table 2). The *R* value was 0.51, which was equal to or lower than the results for the other four models.

The Random Forest (RF) modeling was used to explore the hierarchical importance of textural components (sand, silt, clay %) and structure on urban soil field-saturated hydraulic conductivity. The RF models provided good Kfs predictions under the training dataset (*adjR*2 = 0.77 for both RF1 and RF2, RSME = 1.19 cm h-1 for RF1 and 1.15 cm h-1 for RF2; Figure 4b and c). However, the RF1 model performance decreased under testing dataset compared to the training data (*R* = 0.51, *adjR*2 = 0.25; Figure 4e). Adding soil structure information into the Random Forest model (RF2) improved the model performance in the test data (*adjR*2 = 0.36, *d* = 0.77, and RMSE = 2.36 cm h-1; Figure 4f and Table 2). Linear regressions between predicted and field measured Kfs values showed that both RF models provided predictions much closer to 1:1 line for the test data comparing with the ANN model.

The ROSETTA model had similar *R* and *adjR*2 values for the testing data as the ANN, RF1, and RF2 models (Figure 4g and Table 2). However, the ROSETTA model had much higher mean error (*E* = 51.6) and RMSE (114 cm h-1) values, and much lower index of agreement values (*d* = 0.06) compared to the models developed in this study.

The multiple comparisons analysis for the test data indicated that there were no significant differences between field-measured Kfs versus Kfs predicted by the ANN and RF models (Tukey’s HSD; p = 0.99), but there were significant differences for the ROSETTA-predicted values (Tukey’s HSD; p < 0.001).

**Table 2.** Summary of model evaluation results for the ANN, RF1, RF2 and ROSETTA model using test data. Slope and Intercept come from simple linear regression model between modeled and measured Kfs; *R* = Pearson’s correlation; *adjR*2 = adjusted *R*2; *E* = mean error; *d* = index of agreement, RMSE = root mean square error; p-values represent results from Tukey’s HSD between modeled and measured Kfs.

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| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Test data (*n* = 43) | | | | | | | | | |
| Model | Slope | Intercept | *R* | *adjR*2 | *E* | *d* | RMSE  (cm h-1) | p-value |
| ANN | 0.33 | 1.11 | 0.51 | 0.27 | -0.07 | 0.71 | 2.23 | 0.99 |
| RF1 | 0.42 | 1.25 | 0.51 | 0.25 | 0.21 | 0.70 | 2.65 | 0.99 |
| RF2 | 0.49 | 1.13 | 0.61 | 0.36 | 0.21 | 0.77 | 2.36 | 0.99 |
| ROSETTA | 0.02 | 0.91 | 0.58 | 0.32 | 51.56 | 0.06 | 114.38 | <0.001 |

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**Figure 4.** Measured Kfs versus Kfs predicted by the Artificial Neural Network model (ANN; panels a and d), the random forest models without soil structure (RF1; panels b and e) and with soil structure (RF2; panels c and f), and the ROSETTA model (panel g), for the testing dataset. Note that the solid blue lines represent the 1:1 relationship and each dashed red line represents a simple linear model (SLR).

**3.2 Model verification**

When the field-measured verification dataset was used, the ANN and both RF models provided reasonable predictions for urban soils Kfs. The three models explained between 28% and 45% of the variability in Kfs, as determined using *adjR*2 (Figure 5a-c). the RF2 model and ANN models had higher *R* and *adjR*2 values than the RF1 model (Table 3). The ROSETTA model had similar *R* and *adjR*2 values as the ANN model, yet greatly overestimated Kfs. The mean Kfs predicted by the ROSETTA model (105 cm h-1) was more than 20 times larger than the mean field-measured Kfs value of 5.67 cm h-1. This discrepancy is reflected in the results for mean error (*E*), index of agreement (*d*), and RMSE, which all show that the ANN, RF1, and RF2 models had superior performance to the ROSETTA model.

The multiple comparisons test showed no significant differences between field-measured Kfs versus Kfs predicted by the ANN (Tukey’s HSD; p = 0.99) and RF models (Tukey’s HSD; p = 0.99), but did show significant differences for the ROSETTA-predicted values (Tukey’s HSD; p = 0.008).

**Table 3.** Summary of model evaluation statistics for the ANN, RF1, RF2 and ROSETTA model using the verification dataset. Slope and Intercept come from simple linear regression model between modeled and measured Kfs; *R* = Pearson’s correlation; *adjR*2 = adjusted *R*2; *E* = mean error; *d* = index of agreement RMSE = root mean square error; p-values represent results from Tukey’s HSD between modeled and measured Kfs.

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| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Verification data (*n* = 20) | | | | | | | | |
| Model | Slope | Intercept | *R* | *adjR*2 | *E* | *d* | RMSE  (cm h-1) | p-value |
| ANN | 1.55 | 3.02 | 0.69 | 0.45 | -3.96 | 0.61 | 5.96 | 0.99 |
| RF1 | 1.03 | 3.41 | 0.57 | 0.28 | -3.49 | 0.64 | 5.94 | 0.99 |
| RF2 | 1.48 | 2.91 | 0. 65 | 0.39 | -3.81 | 0.59 | 5.98 | 0.99 |
| ROSETTA | 0.01 | 3.59 | 0.69 | 0.44 | 141.34 | 0.05 | 313 | 0.008 |

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**Figure 5.** Field-measured urban soil Kfs versus Kfs predicted using the Artificial Neural Network model (ANN; panel a), the Random Forest models without soil structure (RF1; panel b) and with soil structure (RF2; panel c), and the ROSETTA model (panel d) for the verification dataset. Note that the solid blue lines are 1:1 lines, that each dashed red line represents a simple linear model (SLR), and that the x-axis for panel d differs from other panels.

# 4. Discussion

In this study we used a unique set of field-saturated hydraulic conductivity (Kfs) values measured in urban soil profiles to generate new pedotransfer functions (PTFs). We used three different models as PTFs, including an Artificial Neural Network (ANN) analysis and two Random Forest (RF) models that both excluded (RF1) and included (RF2) soil structure descriptions. As inputs, the models only used %sand, silt, and clay (along with soil structure type in the RF2 model). These inputs represent information that can be found almost everywhere in the conterminous United States (NCSS, 2019) and are commonly measured in other locations and studies. We then compared these three PTF models to the commonly used ROSETTA model (Schaap et al., 2001), which uses the same %sand, %silt, and %clay inputs.

We evaluated the four models using five summary statistics, along with the intercept and slope of simple linear regression models fit to the predicted versus measured Kfs values and a multiple comparisons statistical test (ANOVA with Tukey’s HSD). The model evaluation statistics conveyed different information. For example, the ROSETTA model had relatively high values for *adjR*2 and *R*, indicating linear association between the measured and modeled data. However, that model also had slopes much less than 1 when linear regression was applied to predicted versus measured Kfs (indicating overestimation in high permeability soils), low index of agreement values, and large RMSE values, which all indicate poor model fit. This observations support the contention that individual evaluation statistics only reflect specific aspects of model performance, and that no single statistic can quantify overall model performance (Bennett et al., 2013; Gilmour, 1996; Yang et al., 2014). The multiple comparisons test also showed that the ROSETTA model predicted significantly different values for Kfs compared to measurements, while the developed PTFs did not.

Looking closer at the performance of the PTFs developed in this study, the RF models in particular provided good estimates for measured Kfs values ≤ 3 cm h-1, whereas the ANN model had low sensitivity in that range (Table 1). As urban soils often have moderate to high levels of compaction and relatively low infiltration rates (Gregory et al., 2006; Hamilton and Waddington, 1999), this result offers confidence that the RF models can provide accurate prediction Kfs in such soils. Further, when considering all of the evaluation statistics together, the RF2 model, which includes soil structure description, provided the best predictions for Kfs values, as it ranked at or near the top of the evaluated models in all statistical categories. Soil structure thus provides additional information that can be used to infer and predict hydraulic conductivity values, even when qualitatively described (Lin et al., 1999).

The three PTF models developed in this study were all constructed using mini-disk tension infiltrometer data with the pressure source *h* = -2 cm, while the verification data tests were all conducted using double ring infiltration tests (Table 1). These two types of flow experiments thus differ in their boundary condition (positive versus negative pressure heads) and the type of pores that they potentially activate (macropores versus matrix pores). Despite the differences in experimental conditions, the PTFs provided estimates for Kfs that were mostly of the same order of magnitude as the field-measured values. There are several possible reasons for the good model performance. For one, the double-ring experiments were run until steady-state conditions were attained, meaning that any large but disconnected pores at the surface likely became filled and no longer hydraulically active at the time of measurement. The tension infiltrometers would likewise bypass such large but inert pores during measurements. Urban soils often have compacted layers and other subsurface heterogeneities that restrict water movement, so we contend that the flow conditions used in these experiments are more representative of the actual system behavior than other protocols (e.g., short-term single ring infiltration tests). At the same time, soil structural features may be more likely to exist throughout a horizon and connect to other pores, so the results shown here suggest that the infiltration tests used to build, test and verify this model likely captured some aspects of flow through these morphological features.

Altogether, the results of this study suggest that PTF performance may improve when those functions are developed using field-derived data. There is currently a large-scale effort to compile field infiltration measurements from across the globe (Rahmati et al., 2018), with emphasis on hydraulic and structural characterization of soils. As datasets such as this one continue to grow and develop, it is likely that they can help produce even more flexible and realistic pedotransfer functions.

# 5. Conclusion

In this study, we developed three pedotransfer functions (PTFs) to predict field-saturated hydraulic conductivity (Kfs) in urban soils based on %sand, silt, clay, and soil structure information. Our results show that the model with soil structure information (RF2 model) had the best overall performance in the training, testing, and verification dataset, which supports the hypothesis that including soil morphological information such as structure can improve PTF performance when estimating Kfs. Even without soil structure information, however, the developed PTFs provided superior estimates for Kfs compared to the commonly used ROSETTA function in both the testing and verification datasets. The ROSETTA model was developed using hydraulic conductivity measurements on saturated soil cores, which may explain why that model tended to over-predict hydraulic conductivity compared to observations made in the field. At the same time, the soils used to develop ROSETTA primarily originated in agricultural soils, while the measurements used to develop the PTFs in this study came from measurements conducted in twelve U.S. cities. The PTFs developed in this study did much better than ROSETTA when predicting Kfs from a set of independent studies conducted in urban soils (i.e,. the verification dataset), suggesting that pedotransfer functions may perform best when the underlying data is appropriately aligned with the system being studied.

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