Agropedology 2009, 19 (1), 47-56

Development and evaluation of pedotransfer functions for saturated hydraulic conductivity of seasonally impounded clay soils

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Abstract : Data on hydraulic properties of soils are often not available. Hence, pedotransfer functions (PTFs) are used to estimate hydraulic properties of soils. PTFs formulate a relationship between basic soil properties and property of interest (mostly any hydraulic property). Little information is available on the hydraulic properties of clay soils that are impounded by water for the entire monsoon season (known as 'Haveli') in large tracts of Madhya Pradesh. This study was conducted to calibrate and evaluate PTFs to predict saturated hydraulic conductivity (K_s) using basic soil properties. Global PTF 'Rosetta' was also evaluated for its validity in predicting K_s of the 'Haveli' soils. Available data on the 'Haveli' soils was used for the analysis. It included information on particle-size distribution, bulk density and water retention characteristics. PTFs were calibrated using regression as well as artificial neural networks. Imprecise estimates of K_s indicated that the calibrated PTFs were not reliable. However, excluding the samples with unusually low field capacity (<0.3 m^3 m^{-3}) despite clay content (> 50%) resulted in PTFs that performed with precision. Estimates of K_s obtained by implementing hierarchical rules in generic PTF 'Rosetta' were poor in precision but improved with inclusion of field capacity and permanent wilting point as predictor variables. The study indicated limitations of calibrated as well as generic PTFs in predicting saturated hydraulic conductivity.

Additional key words: *Pedotransfer functions, artificial neural network, saturated hydraulic conductivity, clay soils, Rosetta*

Introduction

Simulation of water flow through the vadose zone requires information on hydraulic properties of soils. Saturated hydraulic conductivity is one of the two soil properties (the other being water retention characteristics), which is vital to any such simulation. Soil hydraulic properties are usually measured in laboratory. The procedure is, however, complex and time-consuming. Because of the considerable spatial variability in soil hydraulic properties, field and laboratory observations often exhibit high levels of uncertainty (Kutilek and Nielsen 1994). Discrepancies are known to occur between laboratory and field measurements (Ratliff *et al.* 1983). In attempts to alleviate these problems and to estimate soil hydraulic properties from easily obtainable soil information, such as, particle-size distribution, bulk density, organic carbon content, etc, many authors (Cosby *et al.* 1984; Jain *et al.* 2004; Rawls and Brakensiek 1983; Leij *et al.* 2002; Saxton *et al.* 1986; van Genuchten 1992; Veerecken *et al.* 1990) have used pedotransfer functions (PTFs). Schaap and Leij (1998) and Wosten *et al.* (2001) have discussed the accuracy and reliability of PTFs. Schaap and Leij (1998) found that the performance of PTFs may strongly depend on the calibration and evaluation of data sets. PTFs could be developed using different techniques (Wosten *et al.* 2001) like regression (Rawls and Brakensiek 1985; Wosten *et al.* 1995) and artificial neural networks (ANNs) (Jain *et al.* 2004; Minasny *et al* 1999; Minasny and McBratney 2002; Pachepsky *et al.* 1996; Schaap *et al.* 1998). Schaap *et al.* (1998) developed an ANN-based PTF which reportedly performed better than four published PTFs in estimating water retention data and six published PTFs in estimating the saturated hydraulic conductivity. They used a dataset of 4515 samples in the USA. Later, Schaap *et al.* (2001) developed ANN-based computer code, '*Rosetta*' (public domain) which implements hierarchical PTFs for the estimation of water retention and the saturated and unsaturated hydraulic conductivity. The dataset used for calibrating *Rosetta* was derived from soils in temperate to subtropical climates of North America and Europe. These studies have shown effectiveness of ANN in prediction of hydraulic properties. However, it must be noted that the PTFs were based on large datasets.

Little is known about the predictive quality of generic PTFs when employed to predict hydraulic characteristics of problematic soils. A study by Nemes *et al.* (2003) indicated that the PTFs developed at one scale (regional, national, continental) may not be suitable at other scales. In their study, PTFs derived from a small local database, were shown to perform better than large but general database. Romano and Palladino (2002) examined the prediction of soil hydraulic properties from soil physical properties and terrain information. Their work showed that the use of PTFs was not advisable if the scale varied. Recent publications focus on comparing PTF predictions with independent data sets of hydraulic properties measured in the laboratory. Some publications indicate good agreement (Cornelius *et al.* 2001; Rawls *et al.* 2001; Wagner *et al.* 2001) or moderate agreement (Givi *et al.* 2004) whereas few discrepancies are also reported (Chen and Payne 2001; Pachepsky and Rawls 2003; Soet and Stricker 2003).

Limited information is available related to validity of generic PTFs or calibrated PTFs in estimating K_s at small or field scale for seasonally impounded soils. Low hydraulic conductivity of these soils is attributed to high clay content that impedes drainage causing impounding of water. It is, however, not known to what extent clay content affects the K_s and whether generic PTFs, to predict K_s, could be validated. Further, most of the reported PTFs were developed to predict soil water retention and PTFs to predict K_s are relatively few. This study was conducted to calibrate regression and neural PTFs at a field scale using basic soil data including particle-size distribution, bulk density, field capacity (soil water retained at 33 kPa) and permanent wilting point (soil water retained at 1500 kPa), determine the best combination of inputs for prediction and comparing the performance of the field-scale PTF with the published neural PTF '*Rosetta.*'

Materials and Methods

Study Area

The study area is located in Jabalpur district of Madhya Pradesh. The district lies between 22°49' and 24°80' N latitude and 78°21' and 80°58' E longitude. The starting point of this analysis was the database on 'Haveli' soils (Patil 2006). It contained data on basic soil properties, i.e. textural composition, dry bulk density, nine point soil water retention data and saturated hydraulic conductivity values for 41 soil profiles (175 horizons). The 'Haveli' tract derives its name from the ingenuous system of impounding water during the rainfall season and using it during the winter (*rabi*) season. It occupies nearly 5 M ha area which accounts for 50% area of Jabalpur district (Rajput *et al.* 2004). The tract receives, on an average, 1300–1500 mm rainfall mostly during rainy season. The soils of the area are mainly clayey and classified as Vertisols and associated soils (Tomar *et al.* 1996). Low infiltration rate (poor vertical drainage) of the soils combined with plain topography (poor horizontal drainage) and high amount of rainfall received in relatively short period of time make the agricultural lands inundated.

Calibration of PTFs

PTFs were calibrated using statistical regression and neural network tools. Two computer codes, namely, 'Neurointelligence' (evaluation version) developed by Alyuda Inc. and 'Neuropath' (version 1.2) developed by Minasny and McBratney (2002) of Australian Centre for Precision Agriculture were used in this study for calibrating neural PTFs. Code 'Neurointelligence' provides choice of many types of possible neural networks. According to Maier and Dandy (2000), feed-forward neural networks (FF-NNs) are the most widely adopted network architecture for the prediction and forecasting of geophysical variables. A rare use of radial-based function was seen in the literature. Hence, feed forward network was selected. Typical FF-NN consists of three layers-an input layer, hidden layer, and output layer. The number of nodes in an input layer corresponds to the number of inputs considered for the PTF. The input layer is connected to the hidden layer with weights that determine the strength of the connections. The hidden layer nodes consist of the activation function, which helps in non-linearly transforming the inputs into linearly separable form. Often sigmoidal or hyperbolic tangent transfer function that provides a graded, non-linear response is used by the researchers. Hidden layer provides the network's non-linear modeling capabilities. As a general rule, the total hidden units should be half the number of units. Thus, in the present analysis, maximum inputs being seven, 3-4 hidden units were believed to serve the purpose. However, the search for a good network invariably yielded a single layer network with two hidden units. For hidden layer activation, hyperbolic tangent function was used because of its reported ability to perform better than logistic function. For output, the logistic function performed well. The hyperbolic tangent function has restrictions in that it can only be used on network with a single output unit, for small network, and it is meant for the sum squared error function and hence is appropriate only for regression problems. The data was bisected into training and testing sets. For training, Levenberg-Marquardt (L-M) algorithm was chosen due to the fact that the data is small. Mayr and Jarvis (1999), van Genuchten *et al.* (1992) and other researchers have used the same algorithm to develop PTFs. Further, for fair comparison between regression and ANN models, it was desirable to seek minimization of sum of squares error. It is also the fastest algorithm available for multi-layer perceptrons. The data was partitioned as 68% (71 horizons) for training, 16% (16 horizons) for validating and testing each. Another ANN computer code, Neuropath, is a single layer network that uses hyperbolic tangent function and feeds forward network. For validation, neuropath makes use of bootstrap *i.e.* a copy of validation sample remains in the training set. Neuropath performance was observed to be better with 4-6 hidden units.

The neural network typically consists of *'j'* input neurons, *'k'* hidden neurons, and *'l'* output neurons. Symbolically, the ANN architecture shown in fig. 1 can be represented as *ANN (j,k,l)*.

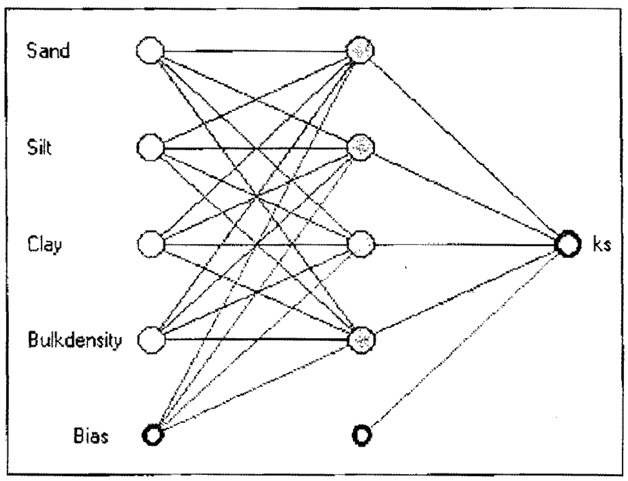

Fig.1 A typical neural network with input neurons of sand, silt, clay and bulk density relating to output neuron-saturated hydraulic conductivity.

A systematic search of different network configurations and user-adjustable parameters was performed to obtain the optimal network architecture, while minimizing the cost function. The network architecture was chosen based on the least cost function criteria (minimizing mean sum of squares of the network errors).

$$MSE = 1/n\sum_{i=1}^{n}(y_i - y_i')^2 \qquad (2)$$

where, y_i and y_i' stand for measured and estimated value and n is the number of trainings. ANN model is developed in two steps - 1) training and 2) testing. In training process, connection weights between different layers and the bias values of the neural network were optimized by minimizing the cost function.

Four levels of available information were classified for the study.

- Input level 1 Sand, silt, and clay content (SSC)
- Input level 2 Level 1 + bulk density data (SSCBD)
- Input level 3 Level 2 + field capacity (SSCBDFC)
- Input level 4 Level 3 + permanent wilting point (SSCBDFCPWP)

These four input sets were related by regression and neural network to K_s resulting in four PTFs to estimate K_s.

Performance Evaluation

The performances of the PTFs were evaluated based on (i) root mean square error (RMSE), (ii) index of agreement (d), (iii) maximum absolute error (ME) and iv) mean absolute error (MAE). RMSE, d, ME, and MAE statistics were calculated using following equations, respectively, where n represents the number of data used for modeling and E_i and M_i represent measured and computed value, respectively. The units of errors are same as that of K_s i.e. L/T.

Root Mean Square Error $$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(Ei - Mi)^2}{n}} \quad (3)$$

Index of Agreement $$d = 1 - \frac{\sum_{i=1}^{n}(Ei - Mi)^2}{\sum_{i=1}^{n}\left(\left|Ei - \overline{M}\right| + \left|Mi - \overline{M}\right|\right)^2} \quad (4)$$

Maximum Absolute Error $$ME = Max\left|Ei - Mi\right| \quad (5)$$

Mean Absolute Error $$MAE = \sum_{i=1}^{n}\frac{\left|Ei - Mi\right|}{n} \quad (6)$$

The RMSE statistic indicates the model's ability to predict away from the mean. RMSE imparts more weight to high values because it involves square of the difference between observed and predicted values. Ideally, the model should have the smallest MAE and smallest overall dispersion (RMSE). The units of error in this paper are cm d^{-1}. RMSE was applied as a primary indicator of model precision, whereas other indicators were secondary. When the measured K_s values are used for developing equation and correspondence between measured and predicted values is tested, it indicates goodness of fit or 'accuracy' of the equation. Thus, when neural networks were trained, they were first tested for their ability to represent the same data used for training dataset (accuracy) and then evaluated for 'reliability' by using independent dataset (outside the training dataset). Thus, when the measured values are different (the estimates are obtained using other properties) from the ones used for developing equation, correspondence between measured and estimated values indicates 'reliability' of the equation.

Results and Discussion

Analysis of the soil samples indicated that 103 out of 175 horizons had clay texture (USDA classification). Clay loam and sandy clay loam textures was observed in 18 and 22 horizons, respectively. These three textures constituted 82 % of the entire dataset. Rest of the 32 horizons were dispersed over other textural classes. Analysis discussed here pertains to clay texture. Statistical summary of soil properties is presented in table 1(a). Coefficient of uniformity indicates that the variation in clay content of the samples was relatively low, mean being 53.47%. Sand content varied to a greater extent and variation of similar magnitude was noted in saturated hydraulic conductivity data. In general, soils were low in organic carbon content as shown by mean per cent (0.28). Correlation matrix of soil properties (Table 1b) shows negative relationship between K_s and clay. High bulk density (mean 1.44 Mg m^{-3}) showed the strongest negative relationship with K_s followed

Table 1(a). Statistical summary of soil properties of 'Haveli' tract

Statistic	Sand (%)	Silt (%)	Clay (%)	BD (Mg m^{-3})	OC (%)	FC (m^{3}m^{-3})	PWP (m^{3}m^{-3})	K_s (cm d^{-1})
Mean	20.50	25.52	53.47	1.44	0.28	0.32	0.16	15.02
SE	0.87	0.54	0.86	0.01	0.015	0.00	0.00	0.57
SD	8.82	5.46	8.74	0.12	0.12	0.04	0.03	5.82
Variance	77.72	29.76	76.45	0.02	0.018	0.00	0.00	33.90
CV	0.43	0.21	0.16	0.09	0.428	0.13	0.19	0.39
Minimum	3.12	8.04	40.50	1.20	0.15	0.22	0.08	3.12
Maximum	36.70	39.11	71.50	1.73	0.5	0.40	0.24	25.92

BD-bulk density, FC-field capacity, PWP-permanent wilting point, K_s-saturated hydraulic conductivity, SE-standard error, SD-standard deviation, CV-coefficient of variation

Table 1(b). Correlation matrix of soil properties

	Sand	Silt	Clay	BD	FC	PWP	K_s
Sand	1						
Silt	-0.31**	1					
Clay	-0.81**	-0.3**	1				
BD	-0.3**	-0.17	0.41**	1			
FC	-0.56**	0.29*	0.39**	0.14	1		
PWP	-0.51**	0.2	0.41**	0.41**	0.64**	1	
K_s	0.32**	0.07	-0.36**	-0.6**	-0.16	-0.22	1

*significant at $p<0.05$, ** significant at $p<0.01$

Table 2. Regression PTFs to estimate saturated hydraulic conductivity

PTF	Input level
K_s =-9.50369+0.225644*Sand+0.177611*Silt+0.123012*Clay	1
K_s =.232089+0.167218*Sand+0.122096*Silt+0.128874*Clay-10.7378*BD	2
K_s =9.375558+0.158644*Sand+0.118295*Silt+0.122676*Clay-10.8216*BD -1.00354*FC	3
K_s =21.93144+0.052977*Sand+0.00767*Silt+0.012036*Clay-12.1265*BD - 6.5644*FC+13.77544*PWP	4

by PWP and FC in that order. The relationship with sand was strongly positive. The sets of calibrated regression equations (PTFs) are presented in table 2.

Accuracy (fitting to the measured/observed data) and reliability (ability to predict data) of the models were judged using the statistical indices ('statistic'). In accuracy testing, not withstanding input level, RMSE (Table 3) tended to be high though at higher input levels (3 and 4), marked improvement could be observed. It ranged from 0.88 to 1.77 for the relatively accurate PTFs (by 'Neuropath'). The range for regression and 'Neurointelligence' was 1.87 to 2.25 and 1.29 to 2.26, respectively. The highest mean absolute error and mean error were observed in predictions by regression PTFs (R). Magnitude of these errors was relatively low in A1 followed by A2. The degree of agreement values also indicated that the neural PTF predictions were closer to the measured data than the regression PTF estimates. The best agreement (0.96) was observed in A2 PTFs, when tested for accuracy. However, all these indices showed tenfold or more increase, when 'reliability' was evaluated. In general, PTFs developed by 'Neuropath'

Table 3. Evaluation indices denoting 'accuracy' and 'reliability' of the calibrated PTFs in predicting saturated hydraulic conductivity

	Input level	1		2		3		4	
Index	Method	ACCU	REL	ACCU	REL	ACCU	REL	ACCU	REL
	R	2.25	12.88	1.88	64.09	1.88	65.63	1.87	67.67
RMSE	A1	2.26	2.12	1.47	1.68	1.29	1.58	2.21	1.72
	A2	1.77	6.61	1.41	6.54	0.88	6.73	1.03	6.58
	R	1.81	12.48	1.53	61.55	1.53	63.00	1.52	64.42
MAE	A1	1.86	1.82	1.17	1.36	0.98	1.16	1.57	1.29
	A2	1.47	6.22	0.96	6.17	0.65	6.30	0.69	6.16
	R	5.23	16.71	4.45	88.17	4.39	90.39	4.32	96.53
ME	A1	5.10	3.36	3.91	3.20	5.15	3.57	7.94	3.58
	A2	4.31	9.96	6.54	10.04	3.40	10.02	4.70	10.09
	R	0.50	0.21	0.75	0.05	0.75	0.05	0.75	0.05
D	A1	0.42	0.50	0.87	0.81	0.91	0.84	0.76	0.81
	A2	0.77	0.35	0.91	0.36	0.96	0.34	0.95	0.35

R-regression, A1-Neurointelligence, A2-Neuropath, ACCU-Accuracy, REL-Reliability

fitted better than others with a tendency to underestimate at input levels 1, 3 and 4 and overestimate at level 2. However, in reliability testing, irrespective of the input levels though, PTFs developed using 'Neurointelligence' were comparatively better, the errors were large and unacceptable. Thus, no PTF could be identified for application/utility.

Estimates of K_s obtained by hierarchical input in 'Rosetta' were also evaluated with the same set of statistical indices. Again, irrespective of input used, the error component (Table 4) in estimates was large warranting rejection. A clear pattern of improvement in predictions with increase in input was discernible as RMSE and MAE decreased from 8.83 and 7.17 to 5.58 and 0.83, respectively. Mean error (ME) decreased in the input level 2, but increased for level 3 before decreasing again for level 4. Thus, even with maximum input, the predictions as indicated by mean error, were not better than predictions with minimum input.

While the modeling efforts using regression and ANN tools failed to formulate the PTF for estimating saturated hydraulic conductivity, we felt that the hydraulic behaviour of these soils differ from other clay soils because of the unique hydromorphic environment caused by continuous ponding of water over unknown years (it is said to be a 50 years old practice but there are no records to substantiate). We then screened soil samples with field capacity < 0.3 m^3/m^3 and excluded

Table 4. Evaluation indices denoting 'reliability' of the PTF 'Rosetta' in predicting saturated hydraulic conductivity

Input	1	2	3	4
RMSE	8.83	8.31	7.84	5.58
MAE	7.17	7.02	4.71	0.83
ME	17.23	16.68	26.54	17.61
d	0.30	0.62	0.76	0.83

Table 5. Evaluation indices denoting 'reliability' of the PTF 'Rosetta' in predicting saturated hydraulic conductivity of screened samples

input	1	2	3	4
RMSE	7.64	8.24	2.67	0.17
d	0.48	0.59	0.96	0.99
MAE	5.93	7.08	1.63	0.13
ME	16.99	16.56	9.51	0.42

from analysis. A total of six profiles (profile no. 5, 6, 8, 9, 12 and 31) were found to constitute 21 of the 28 horizons that had lower (< 0.3 m^3m^{-3}) field capacity. All these profiles were within 500 m distance from the river and are exposed to greater period of waterlogging every year. We feel that the aggregation that would have otherwise occurred was prohibited by the longer period of ponding and it led to change in hydraulic behaviour. Further, these soil samples had mean sand content 25.60%, silt 22.26% and clay content 51.79 %. The increase in sand and silt contents and reduction in clay content along with less bulk density could also explain less water retention. Mean K_s also increased to 15.44 as against 15.01 cm d^{-1}. With the new dataset, there was a marked improvement in RMSE (Table 5), especially for input level 3 and 4.

Graphical presentation of these results is made in figures 2 and 3, which shows an improving trend with the increasing input. With inputs of texture, bulk density, field capacity and permanent wilting point, excellent agreement was noted in measured and predicted K_s. Use of FC and especially PWP with the other soil physical properties (in the PTF models) increased precision of predicted K_s. It may be attributed to the fact that soil moisture constants in water retention curve provide more information about soil pore structure than texture and bulk density. Other indices also showed improvement and possible validity of 'Rosetta'. Soil structure in sandy soils is dominantly single grained. Substantial difference in K_s, due to soil structure is, therefore, unlikely in sandy soils. Nevertheless, soil structure in clay soil can be blocky, which in addition to soil texture, can introduce substantial difference in K_s estimates. Similarly, the PTF evaluation using screened samples indicated an improving trend with increase in input variables. The error values shown in Table 6 imply that the calibrated PTFs were reliable (RMSE, MAE, ME

Table 6. Evaluation indices denoting 'accuracy' and 'reliability' of the calibrated PTFs in predicting saturated hydraulic conductivity of screened samples

	Input level	1		2		3		4	
Index	Method	ACCU	REL	ACCU	REL	ACCU	REL	ACCU	REL
	R	2.31	3.02	1.81	2.18	1.67	2.03	1.68	0.59
RMSE	A1	2.06	2.87	1.77	1.98	1.85	1.92	0.13	0.12
	A2	2.1	2.95	1.89	2.04	1.58	1.99	0.63	0.48
	R	1.91	2.7	1.51	1.9	1.42	1.82	0.88	0.91
MAE	A1	1.75	2.38	1.35	1.64	1.29	1.54	0.32	0.25
	A2	1.86	2.35	1.42	1.71	1.34	1.68	0.44	0.58
	R	5	4.67	4.23	4.23	4.1	3.25	4.01	0.44
ME	A1	4.5	4.8	3.95	4.05	3.85	3.11	3.68	0.17
	A2	4.82	4.4	4.1	4.17	4.12	3.21	3.85	0.28
	R	0.28	0.405	0.72	0.7	0.78	0.78	0.78	0.77
d	A1	0.5	0.38	0.78	0.7	0.8	0.77	0.82	0.81
	A2	0.48	0.29	0.72	0.61	0.77	0.65	0.74	0.78

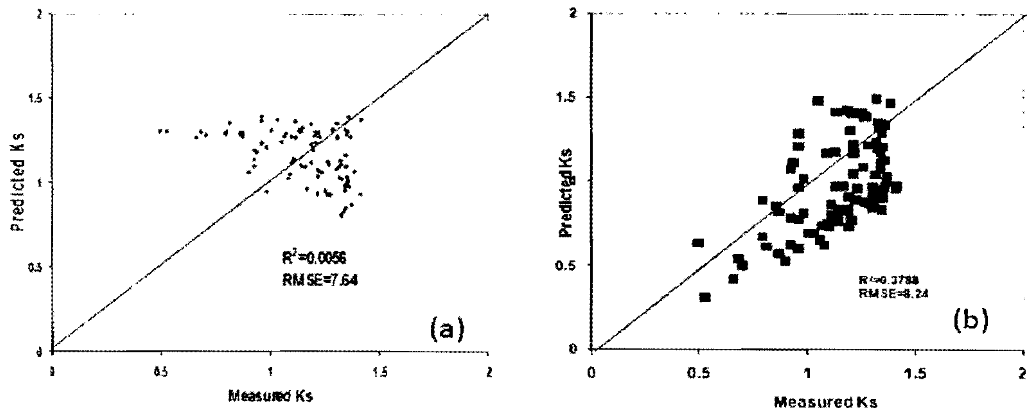

Fig. 2. Measured and predicted saturated hydraulic conductivity (cm d^{-1}) using texture (a), and texture and bulk density (b) as an input in 'Rosetta'

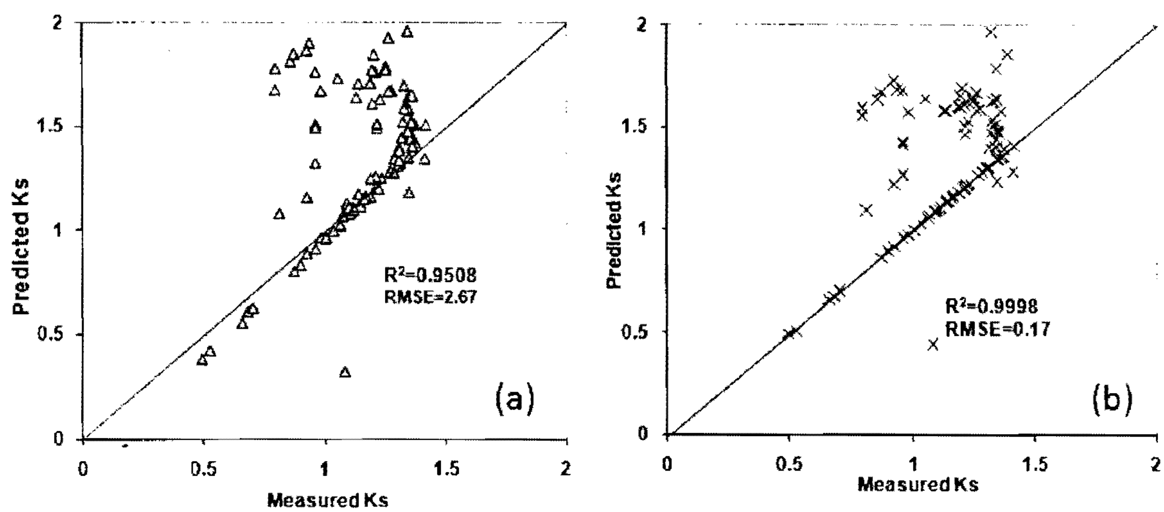

Fig. 3. Measured and predicted saturated hydraulic conductivity (cm d^{-1}) using texture, bulk density, and field capacity (a), and texture, bulk density, field capacity and permanent wilting point (b) as an input in 'Rosetta'

and d being 0.12, 0.25, 0.17 and 0.81, respectively at highest input level), when neural PTFs developed by using A1 were assessed. PTFs developed by the regression method performed poorly with lowest accuracy and reliability. The improvement with inclusion of FC and PWP as predictor variables was again conspicuous as the error (RMSE, MAE and ME) showed reducing trend with increase in input, whereas the degree of agreement increased. However, the reason for low water retention despite high clay content and inability to model K_s for the excluded data warrants further investigations. Possible variation in clay mineralogy was ruled out as it was identical for the region. It may be noted that the input requirement was greater for acceptable PTFs. Soil data on texture, bulk density and field capacity were necessary for acceptable estimates. We infer that the 'Haveli' tract should further be divided into two units based on period of impounding and more data need to be collected for further investigations.

Conclusion

Prediction of saturated hydraulic conductivity using PTFs is limited by their (PTFs') inability to mimic behaviour of impounded soils, irrespective of tools used to calibrate PTFs. Applicability of generic PTF 'Rosetta' was observed to be limited. However, improved performance of calibrated PTFs after screening the samples for field capacity (>0.3 m^3m^{-3}) imply that the proposed PTFs could be used as a primary tool of prediction and refined further by widening the database and investigating influence of soil variables that directly affect saturated hydraulic conductivity.

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Received on : June 2008, Accepted on : March 2009