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Development of pedotransfer functions for predicting soil bulk density: A case study in Indonesian small island

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Abstract: Unlike many other countries, tropical regions such as Indonesia still lack publications on pedotransfer functions (PTFs), particularly ones dedicated to the predicting of soil bulk density. Soil bulk density affects soil density, porosity, water holding capacity, drainage, and the stock and flux of nutrients in the soil. However, obtaining access to a laboratory is difficult, time-consuming, and costly. Therefore, it is necessary to utilise PTFs to estimate soil bulk density. This study aims to define soil properties related to soil bulk density, develop new PTFs using multiple linear regression (MLR), and evaluate the performance and accuracy of PTFs (new and existing). Seven existing PTFs were applied in this study. For the purposes of evaluation, Pearson's correlation (*r*), mean error (*ME*), root mean square error (*RMSE*), and modelling efficiency (*EF*) were used. The study was conducted in five soil types on Bintan Island, Indonesia. Soil depth and organic carbon (SOC) are soil properties potentially relevant for soil bulk density prediction. The *ME*, *RMSE*, and *EF* values were lower for the newly developed PTFs than for existing PTFs. In summary, we concluded that the newly developed PTFs have higher accuracy than existing PTFs derived from literature. The prediction of soil bulk density will be more accurate if PTFs are applied directly in the area that is to be studied.

Keywords: bulk density, multiple linear regression, pedotransfer function, soil property

INTRODUCTION

Soil bulk density is one of the critical physical variables for evaluating soil. It is important for identifying soil density, porosity, water holding capacity, and drainage, as well as for assessing the stock and flux of nutrients [MARTIN *et al.* 2011]. Bulk density measurement is lacking due to the difficulty involved in the collection of samples for laboratory tests, which is a time-consuming, and costly process [BERNOUX *et al.* 1998; HEUSCHER *et al.* 2005; HOLLIS *et al.* 2012; MANRIQUE, JONES 1991; MINASNY, HARTEMINK 2011; SOUZA *et al.* 2016; TOMASELLA, HODNETT 1998; TRANTER *et al.* 2007]. Pedotransfer functions (PTFs) are an empirical approach to estimating soil bulk density from soil properties. They provide an alternative method to overcome these difficulties.

Multiple linear models are often used to develop PTFs from soil properties, as they are the simplest and fastest way to do it [SOUZA *et al.* 2016]. The PTFs developed in China rely on the combination of multiple linear regression (MLR) and artificial neural network (ANN) methods [QIAO *et al.* 2019; XIANGSHENG *et al.* 2016]. The same was done in Tunisia in Northern Africa [BRAHIM *et al.* 2012]. Over the last decade, a considerable empirical equations of PTFs has been developed for predicting soil bulk density from soil properties. The PTFs were developed in tropical areas [MINASNY, HARTEMINK 2011; TRANTER *et al.* 2007], Brazilian soils [BERNOUX *et al.* 1998], Amazon region soils [TOMASELLA, HODNETT 1998], soils in the United States and several countries in Central America [MANRIQUE, JONES 1991], in European soils [HOLLIS *et al.* 2012], and on the basis of soil data from USDA-NRCS National Soil Survey [HEUSCHER *et al.* 2005].

Typically, such PTFs are not transferrable to other regions with acceptable accuracy [McBratney *et al.* 2002].

In Indonesia, there are currently no publications predicting soil bulk density with the application of PTFs. This study is aimed to (1) define soil properties that are correlated with soil bulk density, (2) develop new PTFs to predict soil bulk density, and (3) evaluate the performance and accuracy of PTFs (new and existing) on a small tropical island in Indonesia.

MATERIALS AND METHODS

STUDY AREA

The study was conducted on a small tropical island called Bintan Island, Riau Islands province (Fig. 1). It comprises pre-tertiary and quarter sedimentary formations and igneous rocks, consisting of granite and diorite [Kusnama *et al.* 1994]. The soil types were Oxisols, Entisols, Ultisols, and Inceptisols [USDA 2014]. The topography is predominantly an undulating hillock, with slopes varying from 0–3% in the flat region to more than 40% in the hilly areas. The difference in elevation between the sea level (0) and the highest peak at Bintan Mountain (345 m a.s.l.) on Bintan Island is not significant.

The streams flow in the North and South directions, forming sub-parallel patterns, while the tributaries form a semi-radial pattern. The rivers are predominantly short, shallow, and not too wide. The largest watershed is the Jago watershed covering an area of 135.8 km^2, followed by the Kawal watershed covering 93.0 km^2. The average temperature ranges from 26.1 to 26.7°C, while the average air humidity ranges from 70 to 95%. The rainy season occurs twice a year. May and December generally bring the highest annual rainfall, while the lowest rainfall is recorded in August. During the rainy season, the monthly rainfall is about 200–390 mm, and in the dry season, the monthly rainfall is about 170 mm. Assuming that a dry month is defined as a month in which precipitation falls below 80 mm, there are no proper dry months in Bintan Island, according to average monthly rain figures.

SOIL DATASET

This soil profile sampling was carried out from May to July 2018. Geo-referenced surface soil samples and field analysis tools included soil auger, soil ring cylinder, clinometer, pH stick, and distilled water. Fifteen sampling sites covering different soil-type zones were selected for the purposes of the study (Fig. 1). For each soil profile, disturbed and undisturbed soil samples were collected at three different depths (0–30 cm, 30–60 cm, and 60–90 cm). A total of 45 soil samples (disturbed and undisturbed) were collected at all sites to determine soil properties. Each disturbed soil sample consisted of approximately 1 kg of soil placed in a plastic bag. The samples were taken and air-dried at room temperature. Disturbed samples were utilised for determining the soil pH, measured with a pH meter, and soil organic carbon (SOC) [Walkley, Black 1934]. The sieve-hydrometer method was used to measure particle size distribution [Gee, Bauder 1986]. A soil ring cylinder with an inner diameter of 7.6 cm and a height of 4 cm was used for the undisturbed soil sample. The core method was applied for soil bulk density (BD) analysis [Grossman, Reinsch 2002].

PEDOTRANSFER FUNCTIONS (PTFs) FOR SOIL BULK DENSITY ESTIMATION

Seven existing PTFs for bulk density estimation were applied in this study, as presented in Table 1. The soil properties used in constructing new PTFs differ from the properties used to develop

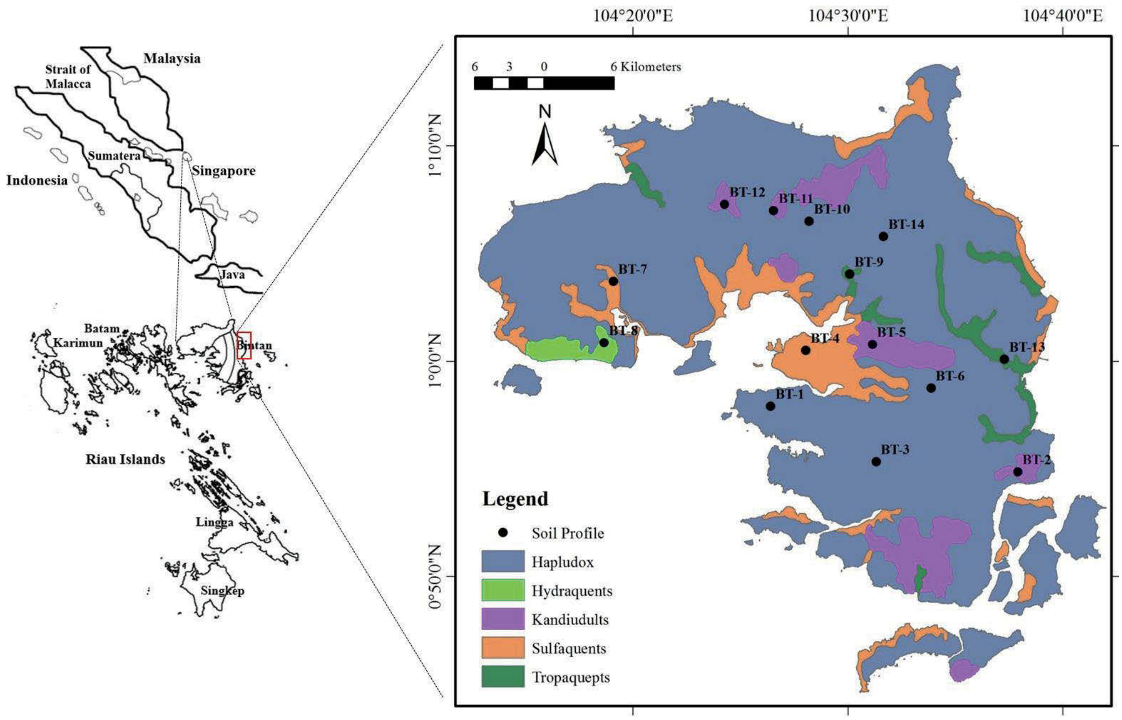

Fig. 1. Map of soil profile locations; source: own elaboration

the seven existing PTFs. In tropical areas [MINASNY, HARTEMINK 2011], PTFs were developed on the basis of organic matter, depth, and sand fraction properties; clay, sand, organic carbon, and pH were used to develop PTFs in Brazilian Amazon soils [BERNOUX *et al.* 1998]; silt, clay, and organic carbon were used in the Amazon Region soils [TOMASELLA, HODNETT 1998]; organic carbon was used in the United States and several countries in Central America [MANRIQUE, JONES 1991]; clay and soil depth were used in European soils [HOLLIS *et al.* 2012], sand and soil depth [TRANTER *et al.* 2007], while clay, organic carbon, and soil depth were used in USDA-NRCS National Soil Survey soil data [HEUSCHER *et al.* 2005].

Table 1. List of selected PTFs used for bulk density estimation

PTFs No.	Formula
1	*BD* = 100/[(OM/0.935 + 0.049 log depth) + (0.0055 sand) + (0.000065 (sand – 38.96)^2)] + [(100 – OM)/0.224)]
2	*BD* = 1.524 – (0.0046 clay) – (0.051 SOC) – (0.0045 pH) + (0.001 sand)
3	*BD* = 1.578 – (0.054 SOC) – (0.006 silt) – (0.004 clay)
4	*BD* = 1.660 – (0.318 SOC$^{1/2}$)
5	*BD* = 1.3894 – (0.0252 clay) + (0.000372 clay) [2 – (0.07897 log depth)]
6	*BD* = 1.35 + (0.0045 sand) + (44.7 – sand) 2(–6·10^{-5}) + (0.06 log depth)
7	*BD* = 1.148 – (0.144 SOC$^{1/2}$) + (1.05·10^{-5} clay^3) + (0.00181 depth)

Explanations: PTFs = pedotransfer functions; 1 = MINASNY and HARTEMINK [2011]; 2 = BERNOUX *et al.* [1998]; 3 = TOMASELLA and HODNETT [1998]; 4 = MANRIQUE and JONES [1991]; 5 = HOLLIS *et al.* [2012]; 6 = TRANTER *et al.* [2007]; 7 = HEUSCHER *et al.* [2005]; *BD* = bulk density; OM = organic matter; SOC = soil organic carbon; pH = decimal logarithm of the reciprocal of the hydrogen ion activity.
Source: own elaboration based on literature.

STATISTICAL ANALYSIS

New PTFs were developed alongside existing PTFs using multiple linear regression (MLR). The evaluations were required for both existing and new PTFs. Many statistical indices have been used to evaluate and validate PTFs [PATIL, SINGH 2016]. A graphical plotting between measured and predicted values was used to evaluate each of the PTFs. Each of the selected PTFs was evaluated with the coefficient of determination (R^2), mean errors (*ME*) (Eq. 1), root mean errors (*RMSE*) (Eq. 2), and modelling efficiency (*EF*) (Eq. 3):

$$ME = \frac{\sum_1^N (\widehat{y}_i - y_i)}{N} \tag{1}$$

$$RMSE = \sqrt{\frac{\sum_1^N (\widehat{y}_i - y_i)^2}{N}} \tag{2}$$

$$EF = \frac{\sum_1^N (y_i - \overline{y_i})^2 - \sum_1^N (\widehat{y}_i - y_i)^2}{\sum_1^N (y_i - \overline{y_i})^2} \tag{3}$$

where: y_i is the measured value, $\hat{y}_i$ is the predicted value, $\tilde{y}_i$ is the mean of the measured values, and N is the total number of observations.

A perfect match of PTFs predicted models should have the lowest *ME* [PATIL, SINGH 2016; WEYNANTS *et al.* 2009], an overall dispersion of *RMSE*, which is a favoured indicator [MCNEILL *et al.* 2018; VEREECKEN *et al.* 2010]. The *EF* value should be close to 1 [RUSTANTO *et al.* 2017].

RESULTS AND DISCUSSION

DESCRIPTIVE STATISTICS

The descriptive statistics of the soil dataset used to derive the PTFs are shown in Table 2. The average bulk density values for the five profile sampling sites were as follows: 1.32 g·cm^{-3} (Hapludox), 1.04 g·cm^{-3} (Hydraquents), 1.27 g·cm^{-3} (Kandiudults), 1.18 g·cm^{-3} (Sulfaquents), and 1.24 g·cm^{-3} (Tropaquepts).

Our findings conclude that the soil bulk density values come in the following order: Hapludox > Kandiudults > Tropaquepts > Sulfaquents > Hydraquents. The highest soil bulk density is recorded for the Hapludox soil type and the lowest is recorded for the Hydraquents soil type. Soil bulk density is influenced by the soil particle size distribution [JONES 1983], especially by sand content. Hydraquents soil type has the lowest bulk density, due to the sand fraction average. The highest soil organic carbon is found in Hydraquents, while the lowest is encountered in Hapludox soil type. A decrease in soil organic carbon will increase bulk density and reduce porosity, thus reducing soil infiltration and water and air storage capacity [WALL, HEISKANEN 2003].

The results of Pearson correlation analysis for soil properties, performed with the confidence levels of 95 and 99%, were presented in Table 3. The obtained soil organic content, depth, and clay data were found to be significantly correlated with bulk density at the 0.05 significance level (Tab. 3). Soil organic carbon and clay have a negative correlation with bulk density. On the other hand, depth has a positive correlation with it. Soil organic carbon (–0.63) showed higher Pearson correlation coefficients followed by the depth (0.45) and clay fraction (–0.33). A negative correlation between clay and soil bulk density [JONES 1983] existed, while sand and silt fraction positively correlated with soil bulk density [CHAUDHARI *et al.* 2013]. The negative correlation of clay is also observed in Entisols, Vertisols, and Aridisols soil type [SAKIN *et al.* 2011] and Cryrendoll soil, China [LI *et al.* 2007]. In soil data from the USDA-NRCS National Soil Survey, organic C content has shown 25% of bulk density variation [HEUSCHER *et al.* 2005]. The higher the soil organic carbon, the lower the soil bulk density [LEIFELD, KÖGEL-KNABNER 2005].

NEW PTFs DEVELOPED USING MLR METHODS

Existing PTFs, except for PTFs no. 5 and PTFs no. 6, included organic content (OM/OC/SOC) as predictor variables. Soil organic carbon is considered an important factor in bulk density prediction [XIANGSHENG *et al.* 2016]. The particle size class is used as a predictor variable for all existing PTFs, except for PTFs no. 4

Table 2. Summary statistics for the bulk density (*BD*) and other soil properties

Sampling sites of soil type	Variables	Min	Max	Ave	*SD*
Hapludox (5 profiles)	*BD* ($g \cdot m^{-3}$)	1.15	1.35	1.32	0.10
	sand (%)	32.00	39.00	35.00	3.61
	silt (%)	20.00	52.00	35.67	16.01
	clay (%)	9.00	46.00	29.33	18.77
	SOC (%)	0.30	0.39	0.34	0.05
	pH	5.14	5.80	5.45	0.33
Hydraquents (1 profile)	*BD* ($g \cdot m^{-3}$)	0.95	1.20	1.04	0.14
	sand (%)	47.00	82.00	68.00	19.92
	silt (%)	8.00	43.00	25.00	17.52
	clay (%)	9.00	29.00	16.00	11.27
	SOC (%)	0.50	2.01	1.08	0.82
	pH	5.13	6.45	5.58	0.76
Kandiudults (4 profiles)	*BD* ($g \cdot m^{-3}$)	1.09	1.42	1.27	0.17
	sand (%)	53.00	56.00	54.00	1.73
	silt (%)	11.00	41.00	23.67	15.53
	clay (%)	3.00	36.00	22.33	17.21
	SOC (%)	0.36	1.11	0.65	0.41
	pH	4.85	5.71	5.15	0.49
Sulfaquents (2 profiles)	*BD* ($g \cdot m^{-3}$)	1.17	1.19	1.18	0.01
	sand (%)	30.00	33.00	31.33	1.53
	silt (%)	7.00	22.00	12.67	8.14
	clay (%)	47.00	61.00	56.00	7.81
	SOC (%)	0.39	0.53	0.46	0.07
	pH	4.98	5.14	5.09	0.09
Tropaquepts (2 profiles)	*BD* ($g \cdot m^{-3}$)	1.14	1.46	1.24	0.16
	sand (%)	58.00	75.00	59.00	8.89
	silt (%)	9.00	38.00	18.67	16.74
	clay (%)	4.00	20.00	13.33	8.33
	SOC (%)	0.30	0.78	0.49	0.26
	pH	5.56	6.07	5.81	0.26

Explanation: Min = minimum; Max = maximum; Ave = average; *SD* = standard deviation; *BD* = bulk density; SOC = soil organic carbon; pH = decimal logarithm of the reciprocal of the hydrogen ion activity.
Source: own study.

[Manrique, Jones 1991]. Further, variables considered as predictors included soil thickness (depth), which was used in *BD* prediction, except for PTFs no. 2, PTFs no. 3, and PTFs no. 4. pH was included respectively at PTFs no. 2, and there may have been indirect relationships between soil pH and bulk density.

The new PTFs were developed based on the three correlated variables (Tab. 3) with three different combinations (models), using MLR methods (Tab. 4). The combination of depth and soil organic carbon (model 2) resulted in the highest R^2 (0.425) and similar *RMSE* with model 3 (depth + soil organic carbon + clay combinations). The lowest *RMSE* was obtained from model 1 (only soil organic carbon variable) with *RMSE* 0.118 but had a higher *ME* than was obtained for the other model.

Table 3. Pearson's correlation matrix for bulk density (BD) and other soil properties

Variable	Depth	Sand	Silt	Clay	SOC	pH	*BD*
Depth	1.00						
Sand	0.29	1.00					
Silt	0.13	–0.25	1.00				
Clay	–0.35	–0.67**	–0.55*	1.00			
OC	–0.50	0.01	0.07	–0.07	1.00		
pH	0.50	0.68**	0.07	–0.64*	–0.26	1.00	
BD	0.45*	0.12	0.16	–0.33*	–0.63*	0.11	1.00

Explanations: * significant correlation at 0.05 significance level; ** significant correlation at 0.01 significance level; *BD* = bulk density; SOC = soil organic carbon; pH = decimal logarithm of the reciprocal of the hydrogen ion activity.
Source: own study.

Table 4. Statistical indices for the models developed using MLR

Model	Input variables	R^2	*ME*	*RMSE*
1	SOC	0.353	0.120	0.118
2	depth + SOC	0.425	0.064	0.120
3	depth + SOC + clay	0.330	0.048	0.120

Explanations: MLR = multiple linear regression; SOC = soil organic carbon; R^2 = coefficient of determination; *ME* = mean errors; *RMSE* = root means square errors.
Source: own study.

Based on Table 4, a perfect match of new PTFs should have the R^2 value close to 1, the lowest *ME* and *RMSE*. Therefore, the combination of input variables comprises depth and soil organic carbon. Despite this, clay is not a strong predictor of bulk density due to the distribution of bulk density as a clay function. Clay is characterised by a lower R^2 value (0.05) than soil organic carbon and depth, for which the value amounts to 0.399 and 0.207, respectively. In Table 4, Model 2 was used to develop new PTFs by MLR, according to Eq. (4):

$$BD = 1.2684 + (0.0011\ \mathrm{depth}) - (0.1774\ \mathrm{SOC}) \tag{4}$$

EVALUATION OF EXISTING AND NEW PEDOTRANSFER FUNCTIONS (PTFs)

Figure 2 shows the scatterplot for the new and existing PTFs for measured and predicted soil bulk density. PTFs by Tranter *et al.* [2007] showed an extreme estimation and biases along the horizontal axis (Fig. 2g) and the best predictive power among the seven existing selected PTFs by Manrique and Jones [1991] (Fig. 2e), whereas the most accurate of these predictions was the one proposed by this study.

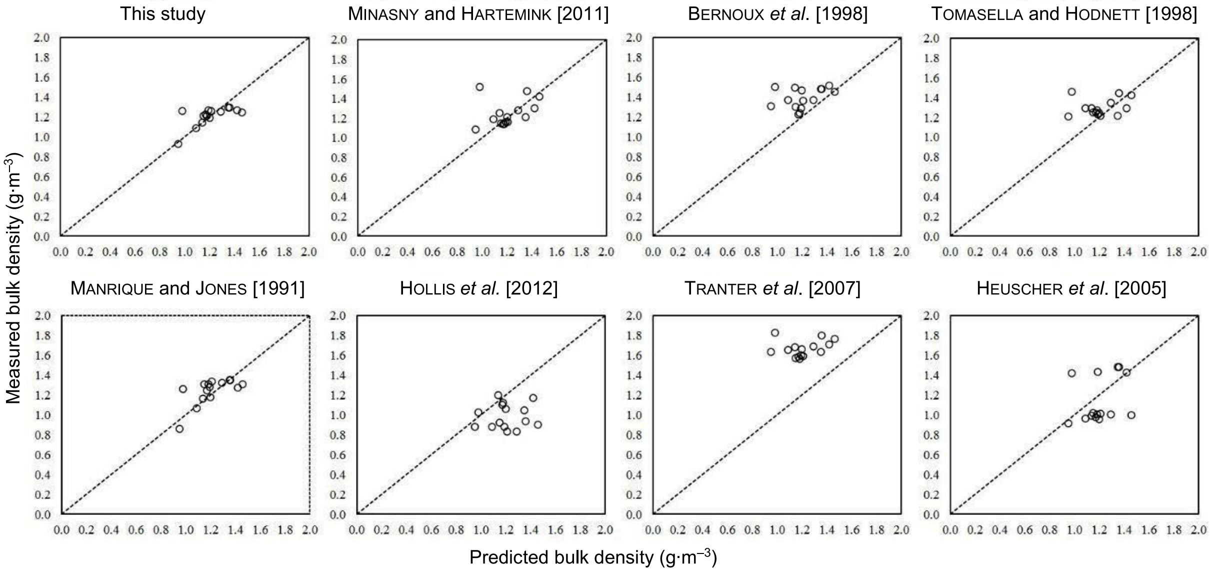

Fig. 2. Measured and predicted bulk density using new and existing pedotransfer functions (PTFs); source: own elaboration

The existing PTFs, as derived from literature, included estimated bulk density with R^2 ranging from 0.005 to 0.426, *ME* ranging from –0.223 to 0.457, *RMSE* ranging from 0.117 to 0.480, and *EF* ranging from –10.471 to 0.316 (Tab. 5). Among the existing PTFs, PTFs developed by Manrique and Jones [1991] showed the best performance, with R^2 at 0.426, *ME* at 0.032, *RMSE* at 0.117, and *EF* at 0.316, followed by Minasny and Hartemink [2011] with *ME* at 0.038, *RMSE* at 0.160, and *EF* at –0.271. PTFs with poorer performance and larger *RMSE* (0.480) were proposed by Tranter *et al.* [2007]. The performance of PTFs proposed by Hollis *et al.* [2012] and Heuscher *et al.* [2005] is underestimated, as reflected by a negative *ME* value (Tab. 5), while the other PTFs gave a positive ME value.

None of the existing PTFs performed better than the PTFs developed in this study (Fig. 2a, Tab. 5). The new PTFs obtained by us have the lowest *ME* (0.002) and *RMSE* (0.108), and higher *EF* (0.424) compared to the existing PTFs. The application of PTFs must be adjusted to the geographical domain of the soil dataset. The differences of geographical domain characteristics between the region in which the PTFs were developed and the area in which PTFs are used result in inadequate PTFs [McBratney *et al.* 2002] and allow the inclusion of soil morphological data [Tranter *et al.* 2007].

CONCLUSIONS

The average bulk density values for the five soil profile sites in Bintan island were 1.32 g·cm^{-3} (Hapludox), 1.04 g·cm^{-3} (Hydraquents), 1.27 g·cm^{-3} (Kandiudults), 1.18 g·cm^{-3} (Sulfaquents), and 1.24 g·cm^{-3} (Tropaquepts). Pearson correlation delivered the negative correlation between bulk density and soil organic carbon and clay, but a positive correlation with soil depth. Depth and soil organic contents were the most important input variables for predicting soil bulk density. Performance evaluations for the seven existing and newly developed PTFs considered in this study allow us to draw the following conclusions about using PTFs for predicting soil bulk density. PTFs derived from our

Table 5. Evaluation indices for existing and new pedotransfer functions (PTFs)

PTFs	R^2	*ME*	*RMSE*	*EF*
Minasny and Hartemink [2011]	0.111	0.038	0.160	–0.271
Bernoux *et al.* [1998]	0.129	0.183	0.231	–1.648
Tomasella and Hodnett [1998]	0.048	0.088	0.171	–0.462
Manrique and Jones [1991]	0.426	0.032	0.117	0.316
Hollis *et al.* [2012]	0.005	–0.223	0.286	–3.069
Tranter *et al.* [2007]	0.049	0.457	0.480	–10.471
Heuscher *et al.* [2005]	0.106	–0.069	0.230	–1.637
This study	0.425	0.002	0.108	0.424

Explanation: R^2 = coefficient of determination; *ME* = mean errors; *RMSE* = root means square errors; *EF* = modelling efficiency.
Source: own study.

study showed higher accuracy than PTFs derived from literature. New PTFs are characterised by a lower mean error, root means square error, and modelling efficiency value than existing PTFs. These results indicate that soil bulk density prediction will be more accurate if PTFs developed directly on the basis of the data collected in the study area are used. We developed the first set of PTFs for predicting soil bulk density on a small tropical island in Indonesia, which will be important for further soil research in Indonesia in general.

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