Development and Evaluation of Pedotransfer Functions to Estimate Soil Moisture Content at Field Capacity and Permanent Wilting Point for South African Soils

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Abstract: This study was undertaken to develop new pedotransfer functions (PTFs) for the estimation of soil moisture content at field capacity (FC, at −33 kPa) and permanent wilting point (PWP, at −1500 kPa) for South African soils based on easily measurable soil physico-chemical properties. The new PTFs were developed using stepwise multiple linear regressions with the dependent variable (either FC or PWP) against clay, silt, sand and soil organic carbon (SOC) content from a total of 3171 soil horizons as the explanatory variables. These new PTFs were evaluated and compared with five well-established PTFs using a total of 3136 soil horizons as an independent dataset. The coefficient of determination ($r^2$) values for the existing PTFs ranged from 0.65–0.72 for FC and 0.72–0.81 for PWP, whilst those developed in this study were 0.77 and 0.82 for FC and PWP, respectively. The root mean square error (RMSE) values for the well-established PTFs ranged from 0.052–0.058 kg kg$^{-1}$ for FC and 0.030–0.036 kg kg$^{-1}$ for PWP, whilst those developed in this study were 0.047 and 0.029 kg kg$^{-1}$ for FC and PWP, respectively. These findings suggest that PTFs derived locally using a large number of soil horizons acquired from different agro-climatic locations improved the estimation of soil moisture at FC and PWP. Due to the range of conditions and large soil datasets used in this study, it is concluded that these new PTFs can be applied with caution in other regions facing data scarcity but with similar soil types and climatic conditions.

Keywords: modelling; multiple linear regressions; soil hydraulic properties; soil physico-chemical properties; validation

1. Introduction

There has recently been increasing interest in the accurate modelling of water dynamics in soil-plant-atmosphere systems within the context of climate change modelling and adaptation [1]. Within this context, biophysical models such as AquaCrop [2], APSIM [3], CropSyst [4], DSSAT [5], SPAW [6] and SWAT [7] are often applied to estimate crop yields, solute movements and irrigation water requirements. These biophysical models are also used for the assessment of water balance components such as drainage, runoff and evapotranspiration to support efficient management and allocation of resources in different countries of the world [1,8–12]. These models are therefore becoming more important to solve numerous water-related challenges posed by climate change in the fields of agriculture, ecology, environment, hydrology and soil sciences [13,14].

The application of biophysical models requires knowledge of soil hydraulic properties at a high spatial resolution, specifically the soil moisture content at field capacity.
(FC, at −33 kPa) and permanent wilting point (PWP, at −1500 kPa) for each soil horizon [1,8,9,13,15–17]. Water retention at FC and PWP are the two critical soil hydraulic properties that are required for the computation of plant-available water in the soil profile [12,13,17]. However, measurements of these soil hydraulic properties are expensive, labour-intensive, time-consuming and sometimes impractical or financially unattainable, especially for regional studies [8,13,18–22]. Furthermore, laboratory apparatus such as pressure plates that are used for the determination of these soil hydraulic properties are costly and are often unavailable in many developing countries [18,23,24].

Alternatively, these soil hydraulic properties are often estimated using pedotransfer functions (PTFs) based on easily measurable soil properties that are readily available from soil surveys such as soil particle size distribution (sand, silt and clay), bulk density and soil organic carbon (SOC) content [11–13,17–19,24–28]. Generally, PTFs are developed using correlations between these readily available or easily measurable soil properties and measurements of water retention at different pressure heads. Many PTFs with different data input requirements have been developed and validated for the estimation of soil hydraulic properties [9,20,25,26,28–38]. Some of these PTFs have been incorporated into biophysical models such as Aquacrop, CropSyst, DSSAT, SPAW and SWAT amongst others as the ready-to-use PTFs to fill in missing information of soil moisture content at FC and PWP [12,13,17].

Research on the evaluation of the existing PTFs has shown that they are often only reliable and applicable for regions with similar characteristics to those of their origins [9,12,13,39–42]. The limited transferability of PTFs across different regions is attributed to the significant variations in geological, climatic and soil bio-physico-chemical properties across regions [14,18,43]. Therefore, PTFs applied outside the soils and climatic conditions from which they were derived may result in poor performance [8,13,18,20]. Inaccurate estimation of hydraulic properties may result in the poor modelling of the water dynamics and could give misleading overall results from a biosphere model, resulting in inefficient use and management of natural resources [12,13]. Therefore, the existing PTFs developed internationally still need to be calibrated and validated locally against measurements before they can be reliably used to estimate hydraulic properties in new sites that are located in different regions from their origins [12,44–46]. However, the lack of representative information on soil hydraulic properties hinders the validation of the existing PTFs and the development of local PTFs in many countries of the world [12,24,46,47]. Consequently, the existing PTFs are often applied without any calibration or validation in many regions as the result of data constraints [15,46,48]. Therefore, the reliability of the estimated soil hydraulic properties from the existing PTFs in regions outside their origins with different geological, climatic and soil bio-physico-chemical properties is questionable.

Very few PTFs have been developed specifically for use within the agro-climatic conditions of Africa [25,28,31,32], which is widely described as a major hotspot for climate change [49–52]. Thus, the need for accurate modelling of water dynamics is of utmost importance for efficient management and use of natural resources as water-related challenges posed by climate change are expected to increase in this region. Some work has been done to develop and evaluate PTFs to estimate water retention at different pressure heads for South African soils [28,53–56]. The major drawback of these earlier studies is that they used a limited number of samples (<450) collected from a limited range of soil types and under specific climatic conditions. Therefore, the applicability and reliability of these existing PTFs for the estimation of water retentivity of the soils over a wide range of agro-climatic conditions in South Africa is questionable. Furthermore, most of these existing PTFs require measurements of bulk density as an input requirement, which is often not readily available from the soil surveys or is measured with difficulty, especially in developing countries [18]. Therefore, existing PTFs that require bulk density as an input variable may be of limited use in countries such as South Africa that are facing data constraints.
For regions facing data constraints, the evaluation of the widely-used PTFs or development of local PTFs that can be reliably used to estimate soil water retention over a wide range of soil types and climate conditions without bulk density would be more beneficial for the improved estimation of water dynamics [26]. The availability of the South African national soil database of the Land Type Survey Staff [57] provided a unique opportunity to develop new PTFs that do not require bulk density data and to evaluate the performance of the existing PTFs over a wide range of soil types and climatic conditions of this country. Given the diversified nature of the southern Africa region in terms of climatological, biogeographical, pedological and lithological characteristics, this study is expected to reveal the strengths and weaknesses of the existing PTFs with the aim of improving them or developing new PTFs for better estimation of water retention in future studies. Therefore, this study aimed to improve the estimation of soil moisture content at FC and PWP from minimal soil physico-chemical properties that are usually available from surveys or easily measured in most countries of the world. The first objective was to develop new PTFs for the estimation of soil moisture content at FC and PWP for a wide range of soil types and climatic conditions in South Africa using the national soil database. These new PTFs were evaluated and compared with five well-established PTFs using an independent dataset to evaluate their applicability and reliability over a wide range of the most typical soil types and climatic conditions found in South Africa.

2. Materials and Methods

2.1. Soil Database

A total of 7219 soil horizons from 2800 profiles with measured gravimetric soil moisture content at FC (%, kg kg\(^{-1}\)), PWP (%, kg kg\(^{-1}\)), particle size distribution (%) and soil organic carbon (SOC, %) were extracted from the Agricultural Research Council of South Africa (ARC) soil database. The choice of these soil properties was based on the soil hydraulic and physico-chemical properties that are available from the South African national soil database of the Land Type Survey Staff [57]. The pressure plate apparatus was used to determine water retention at pressure heads of 33 kPa and 1500 kPa using disturbed soil samples. Five or seven original particle size classes (%) were measured with the double pipette method, i.e., coarse sand (2.0–0.5 mm), medium sand (0.25–0.5 mm), fine sand (0.10–0.25 mm), and very fine sand (0.05–0.10 mm), coarse silt (0.02–0.05), fine silt (0.002–0.02 mm) and clay (<0.002 mm) [58]. These particle size classes were then summed into three classes, i.e., sand (2.0–0.05 mm), silt (0.05–0.002 mm) and clay (<0.002 mm) [59]. The Walkley–Black method was used to determine the SOC content [60].

A data quality routine was undertaken to identify and eliminate obvious errors. For example, soil horizons with no geographical coordinates, negative values of soil moisture content at FC or PWP, soil moisture content at PWP greater than FC or total textural content of either below 95% or above 105%. A similar data quality protocol was undertaken by Van Tol et al. [61] to clean datasets for the development and validation of pedotransfer functions for the estimation of Atterberg limits in South African soils. After this process, a total of 6307 soil horizons from different soil profiles, representing a wide range of soil types, geology, parent materials and climatic conditions found in South Africa, were used for the development and evaluation of PTFs in this study (Figure 1). The choice of these sites was based on the availability of quality data of water retentivity with corresponding particle size distribution and SOC. Rainfall is one of the key factors that significantly affects vegetation distribution [62–64] and is also one of the key agents of weathering, resulting in variation in soil types [65]. Thus, variations in long-term mean annual rainfall (from the year 1960 to 2020) were used as an additional indicator of the wide range of soil types in the dataset for this study (Figure 1).
2.2. Development of New PTFs

Previous studies have reported improved performance of the PTFs that were developed using a large number of soil horizons acquired from different soil depths, soil types, geographic and climatic conditions of a specific region [17,24,26]. Therefore, in this study, a total of 6307 soil horizons were grouped regardless of their soil depth, soil type, textural class, geographic and climatic location then randomly divided per granulometric range into two groups, with one group used for the development of new PTFs and the other for validation of the PTFs. The new PTFs for estimating soil moisture at FC and PWP were developed using stepwise multiple linear regressions with the dependent variable (either soil moisture content at FC or PWP) against weight percentages of sand, silt, clay and SOC content as the explanatory variables. The highest coefficient of determination ($r^2$) was used to select the best fit of the linear regression functions. A similar approach has been widely used to develop and validate PTFs [9,17,26,29,37].

2.3. Evaluation and Comparison of PTFs

The new PTFs developed in this study were evaluated and compared with five well-established PTFs using an independent dataset (Table 1). The selection of the five existing PTFs was based on them being well established for the estimation of gravimetric soil moisture content at FC and PWP using only particle size distribution and SOC as the input requirements.

2.4. Statistical Analysis

The root mean square error (RMSE, kg kg$^{-1}$), mean bias error (MBE, kg kg$^{-1}$) and index of agreement ($d$) were used for the evaluation of PTFs and were computed following the procedure of Willmott et al. [67]:

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}(w_{e,i} - w_{o,i})^2}{n}}$$  \hspace{1cm} (1)

$$\text{MBE} = \frac{\sum_{i=1}^{n}(w_{e,i} - w_{o,i})}{n}$$  \hspace{1cm} (2)
\[ d = 1 - \left[ \frac{\sum_{i=1}^{n}(w_{e \ i} - w_{0 \ i})^2}{\sum_{i=1}^{n}(|w_{e \ i} - w_{0 \ i}| + |w_{0 \ i} - w_{o}|)^2} \right] \]  

(3)

where \( i \) is the data pair index, \( w_e \) and \( w_o \) are estimated and measured gravimetric moisture content, respectively, while \( w_o \) is the mean of \( w_o \) and \( n \) is the number of observations. A linear regression between \( w_e \) and \( w_o \) values was also computed:

\[ w_e = mw_o + c \]  

(4)

where the slope \( (m) \) was used as a measure of accuracy and \( c \) is the y-intercept \((\text{kg kg}^{-1})\). The coefficient of determination \( (r^2) \) was used to quantify the degree of the linear correlation, while the RMSE is the measure of the accuracy expressing the magnitude of the error in prediction. Based on these statistics, better performance of the PTFs is indicated by RMSE, MBE and \( c \) values approaching zero whilst \( d \), \( r^2 \) and \( m \) values approach 1 [67].

Table 1. List of well-established PTFs for estimating soil moisture content at FC and PWP evaluated in this study.

| Source                  | Abbreviation | Output                                                                 | Geographical Domain |
|-------------------------|--------------|------------------------------------------------------------------------|---------------------|
| Arruda et al. [30]      | AR           | FC = 0.29 × (Cl + Si) + 9.93 PWP = 0.27 × (Cl + Si) + 1.07            | Brazil              |
| Chakraborty et al. [33] | CH           | FC = 27.447 + (0.078 × Cl) + (0.248 × Si) − (0.241 × Sa) PWP = 20.695 + (0.021 × Cl) − (0.028 × Si) − (0.179 × Sa) | India               |
| Dijkerman [25]          | DI           | FC = 0.3697 − (0.0037 × Sa) PWP = 0.0074 + (0.0039 × Cl)              | Sierra Leone        |
| Lal [31]                | LA           | FC = 0.065 + (0.004 × Cl) PWP = 0.006 + (0.003 × Cl)                 | Nigeria             |
| Pidgeon [32]            | PI           | FC = (100 × w_{FC} − 3.77) + 95 where: \( w_{FC} = 0.0738 + (0.0016 × Si) + (0.003 × Cl) + (0.03 × SOC) \) PWP = −0.0419 + (0.0019 × Si) + (0.0039 × Cl) + (0.009 × SOC) | Uganda              |

where FC (\%, kg kg\(^{-1}\)) is the gravimetric soil moisture content at field capacity, PWP (\%, kg kg\(^{-1}\)) is the gravimetric soil moisture content at permanent wilting point, Cl (\%) is clay content, Si (\%) is silt content, Sa (\%) is sand content and SOC (\%) is soil organic carbon content.

3. Results and Discussion
3.1. Description of Soil Datasets
3.1.1. Distribution of USDA Soil Textural Classes

Newly developed PTFs still need to be tested for suitability over a wide range of soil types from different climatic conditions before they can be utilized with confidence to estimate soil moisture content at FC and PWP. The soil horizons were classified according to the textural triangle of the United States Department of Agriculture (USDA) classification scheme [59]. The results showed a uniform distribution of eleven textural classes across the development and validation datasets (Table 2). Furthermore, clay, sandy loam and sandy clay loam were the dominant textural classes across both the development and validation datasets, respectively. These findings indicate that the datasets used in this study represent a wide range of textural classes for the most typical soil types found in South Africa [58,68]. Thus, these datasets are suitable for the development and validation of PTFs for the estimation of soil moisture content at FC and PWP under a wide range of agro-climatic conditions in South Africa.
Table 2. Percentage distribution of USDA soil textural classes between development and validation datasets.

| Textural Class     | Development Dataset \(n = 3171\) | Validation Dataset \(n = 3136\) |
|--------------------|----------------------------------|-------------------------------|
| Clay               | 22.93                            | 21.01                         |
| Clay loam          | 7.03                             | 7.78                          |
| Loam               | 4.82                             | 5.10                          |
| Loam sand          | 9.93                             | 10.17                         |
| Sand               | 8.14                             | 7.81                          |
| Sandy clay         | 4.95                             | 4.78                          |
| Sandy clay loam    | 18.92                            | 20.09                         |
| Sandy loam         | 20.47                            | 20.63                         |
| Silty clay         | 0.85                             | 0.86                          |
| Silty clay loam    | 1.10                             | 0.92                          |
| Silty loam         | 0.85                             | 0.83                          |

3.1.2. Descriptive Statistics of Soil Datasets

The soil physico-chemical properties for all sampling sites illustrated a wide range of soil types attributed to the heterogeneity of South African parent material, geology and climatic conditions (Table 3). The summary statistics of all datasets showed that sand content ranged from 2–97%, and silt, clay and SOC content ranged from 1–68%, 1–83% and 0.01–11.7%, respectively. The results showed that soil moisture content at FC and PWP ranged from 0.01–0.50 kg kg\(^{-1}\) and from 0–0.31 kg kg\(^{-1}\), respectively. The development and validation datasets had similar ranges for all soil physico-chemical properties.

Table 3. Descriptive statistics for all datasets, development datasets and validation.

| Dataset       | Parameter          | \(n\) | Min  | Max  | Mean  | Std. Dev |
|---------------|--------------------|-------|------|------|-------|---------|
| All data      | Sand (%)           | 6307  | 2.00 | 97.00| 55.06 | 23.69   |
|               | Silt (%)           | 6307  | 1.00 | 68.00| 16.40 | 11.78   |
|               | Clay (%)           | 6307  | 1.00 | 83.00| 27.25 | 17.27   |
|               | SOC (%)            | 6307  | 0.01 | 11.70| 0.73  | 0.80    |
|               | FC (kg kg\(^{-1}\))| 6307  | 0.01 | 0.50 | 0.18  | 0.10    |
|               | PWP (kg kg\(^{-1}\))| 6307 | 0.00 | 0.31 | 0.11  | 0.07    |
| Development   | Sand (%)           | 3171  | 2.00 | 97.00| 54.72 | 24.06   |
| data          | Silt (%)           | 3171  | 1.00 | 64.00| 16.34 | 11.84   |
|               | Clay (%)           | 3171  | 1.00 | 83.00| 27.65 | 17.61   |
|               | SOC (%)            | 3171  | 0.01 | 9.36 | 0.75  | 0.82    |
|               | FC (kg kg\(^{-1}\))| 3171 | 0.01 | 0.50 | 0.18  | 0.10    |
|               | PWP (kg kg\(^{-1}\))| 3171 | 0.00 | 0.31 | 0.11  | 0.07    |
| Validation    | Sand (%)           | 3136  | 2.00 | 97.00| 55.39 | 23.30   |
| data          | Silt (%)           | 3136  | 1.00 | 68.00| 16.45 | 11.72   |
|               | Clay (%)           | 3136  | 1.00 | 80.00| 26.85 | 16.91   |
|               | SOC (%)            | 3136  | 0.01 | 11.70| 0.72  | 0.78    |
|               | FC (kg kg\(^{-1}\))| 3136 | 0.01 | 0.50 | 0.17  | 0.10    |
|               | PWP (kg kg\(^{-1}\))| 3136 | 0.00 | 0.30 | 0.11  | 0.07    |

where \(n\) is the number of soil samples, Min is minimum, Max is maximum, Std. dev is the standard deviation, SOC is the soil organic carbon, FC is soil moisture at field capacity, and PWP is soil moisture at permanent wilting point.

3.2. Correlation Analysis

Prior to the development of the PTFs for estimating soil moisture content at FC and PWP, it was critical to understand the relationships between FC, PWP and selected soil physico-chemical properties to inform the choice of possible explanatory variables to be included in the new PTFs. The correlation coefficients among the soil physico-chemical properties of the development dataset are presented in Table 4. The results showed that both soil moisture at FC and PWP had significant \((p < 0.01)\) and positive correlations.
with clay, silt and SOC, but were significantly and negatively correlated with sand. These findings confirm that small particles such as clay and silt have a higher water holding capacity as a result of their relatively larger surface area, as well as their large number of small pores that enhance the soil moisture absorption capacity [41,59,69]. Furthermore, the results indicate that soils with high SOC have a higher water absorption capacity as the result of the larger surface area of SOC that enhances the moisture absorption capacity of the soil [26,70]. Moreover, SOC acts as a binding agent that improves the moisture absorption capacity of the soil [70]. These findings agree with earlier studies that reported that silt, clay, and SOC are significantly and positively correlated to both FC and PWP [16,17,21,42,71,72]. The findings of this study suggest that sand, silt, clay, and SOC content can be used as the explanatory variables in the estimation of soil moisture content at both FC and PWP.

Table 4. Pearson’s correlations between measured soil physico-chemical properties.

| Parameters | Sand | Silt | Clay | SOC | FC | PWP |
|------------|------|------|------|-----|----|-----|
| Sand       | 1.00 |      |      |     |    |     |
| Silt       | -0.70 ** | 1.00 |      |     |    |     |
| Clay       | -0.87 ** | 0.27 ** | 1.00 |     |    |     |
| SOC        | -0.40 ** | 0.37 ** | 0.27 ** | 1.00 |    |     |
| FC         | -0.83 ** | 0.43 ** | 0.82 ** | 0.35 ** | 1.00 | |
| PWP        | -0.83 ** | 0.35 ** | 0.87 ** | 0.34 ** | 0.94 ** | 1.00 |

where SOC is the soil organic carbon, FC is soil moisture content at the field capacity, PWP is soil moisture content at permanent wilting point and ** is correlation significant level at 0.01.

3.3. New PTFs for Estimating Soil Moisture Content at FC and PWP

The stepwise multiple linear regressions were used to develop new PTFs for estimating soil moisture content in FC and PWP from readily available soil physico-chemical properties (Table 5). The results indicated that the new PTF for estimating soil moisture content at FC explained 73% of the total variation while the new PTF for estimating soil moisture content at PWP explained 79% of the total variation. The results further revealed that clay, SOC and silt content were the most significant \((p < 0.001)\) explanatory variables for the prediction of soil moisture content at FC and PWP, with standard errors less than 0.002 kg kg\(^{-1}\) suggesting the robustness of these new PTFs. These findings agreed with the previous studies that reported that clay, SOC and silt content were the key input variables for the reliable estimation of soil moisture content at FC and PWP [16,26,32].

Table 5. Results of the stepwise multiple linear regressions for the new PTFs.

| Parameter | Variable | SE  | \(p\)  | \(r^2\) | Output Equations |
|-----------|----------|-----|--------|-------|-----------------|
| FC (kg kg\(^{-1}\)) | Constant | 0.002 | <0.001 | 0.73 | FC = 0.014 + (0.005 × Cl) + (0.009 × SOC) + (0.002 × Si) |
|           | Clay     | 0.000 | 0.000  |      |                 |
|           | SOC      | 0.001 | <0.001 |      |                 |
|           | Silt     | 0.000 | <0.001 |      |                 |
| PWP (kg kg\(^{-1}\)) | Constant | 0.001 | 0.894  | 0.79 | PWP = (0.003 × Cl) + (0.001 × Si) + (0.007 × SOC) |
|           | Clay     | 0.000 | 0.000  |      |                 |
|           | Silt     | 0.000 | <0.001 |      |                 |
|           | SOC      | 0.001 | <0.001 |      |                 |

where \(SE\) is the standard error (kg kg\(^{-1}\)), \(p\) is the level of significance, \(r^2\) is the coefficient of determination, SOC (%) is the soil organic carbon, FC (kg kg\(^{-1}\)) is the gravimetric soil moisture content at field capacity, PWP (kg kg\(^{-1}\)) is the gravimetric soil moisture content at permanent wilting point, Cl (%) is clay content (%) and Si (%) is silt content.

3.4. Evaluation of PTFs for Estimating FC and PWP

3.4.1. Performance of the PTFs for Estimating Soil Moisture Content at FC and PWP

To evaluate the performance of new PTFs for estimating soil moisture content at FC and PWP, comparisons were performed for soil moisture content measured and estimated at FC and PWP using an independent dataset. Furthermore, five existing PTFs for estimating
soil moisture content at FC and PWP were also evaluated using an identical validation dataset. The results indicated reasonable relationships between measured and estimated soil moisture content at FC and PWP for all PTFs evaluated (Figures 2 and 3, respectively; Table 6).

Figure 2. Comparison between measured and estimated soil moisture contents at field capacity (FC) using six different pedotransfer functions (PTFs). TS is the new PTF developed in this study, DI is the PTF of Dijkerman [25], AR is the PTF of Arruda et al. [30], PI is the PTF of Pidgeon [32], LA is the PTF of Lal [31] and CH is the PTF of Chakraborty et al. [33].
Figure 3. Comparison between measured and estimated soil moisture contents at permanent wilting point (PWP) using six different pedotransfer functions (PTFs). TS is the new PTF developed in this study, DI is the PTF of Dijkerman [25], AR is the PTF of Arruda et al. [30], PI is the PTF of Pidgeon [32], LA is the PTF of Lal [31] and CH is the PTF of Chakraborty et al. [33].
Table 6. Performance of the new and well-established PTFs using the validation dataset (PTFs were ranked based on RMSE).

| Parameters | PTFs | $c$ (kg kg$^{-1}$) | $r^2$ | RMSE (kg kg$^{-1}$) | MBE (kg kg$^{-1}$) | $d$ |
|------------|------|-------------------|-------|---------------------|-------------------|-----|
| FC         | TS   | 0.853             | 0.039 | 0.77                | 0.047             | 0.002 | 0.93 |
|            | DI   | 0.700             | 0.054 | 0.72                | 0.052             | 0.003 | 0.91 |
|            | AR   | 0.575             | 0.125 | 0.73                | 0.052             | 0.003 | 0.81 |
|            | PI   | 0.632             | 0.063 | 0.72                | 0.053             | 0.003 | 0.90 |
|            | LA   | 0.576             | 0.072 | 0.71                | 0.053             | 0.003 | 0.88 |
|            | CH   | 0.729             | 0.076 | 0.65                | 0.058             | 0.003 | 0.87 |
| PWP        | TS   | 0.759             | 0.021 | 0.82                | 0.029             | 0.001 | 0.96 |
|            | PI   | 1.025             | 0.010 | 0.81                | 0.030             | 0.001 | 0.94 |
|            | LA   | 0.667             | 0.015 | 0.80                | 0.030             | 0.001 | 0.90 |
|            | DI   | 0.867             | 0.019 | 0.80                | 0.030             | 0.001 | 0.96 |
|            | CH   | 0.547             | 0.050 | 0.76                | 0.033             | 0.001 | 0.96 |
|            | AR   | 0.775             | 0.133 | 0.72                | 0.036             | 0.001 | 0.61 |

where PTFs is pedotransfer functions, $m$ the slope, $c$ the y-intercept, $r^2$ the coefficient of determination, RMSE the root mean square error, MBE the mean bias error, $d$ index of agreement, FC and PWP are the soil moisture content at field capacity and permanent wilting point, respectively, whilst TS is the new PTF developed in this study, DI is the PTF of Dijkerman [25], AR is the PTF of Arruda et al. [30], PI is the PTF of Pidgeon [32], LA is the PTF of Lal [31] and CH is the PTF of Chakraborty et al. [33].

The $r^2$ values for the well-established PTFs ranged from 0.65–0.72 for FC and 0.72–0.81 for PWP, whilst those developed in this study were 0.77 and 0.82 for FC and PWP, respectively. Amongst the existing PTFs, the PTF of Dijkerman [25] performed better (RMSE = 0.052 kg kg$^{-1}$) in the estimation of soil moisture content at FC while the PTF of Pidgeon [32] performed better (RMSE = 0.030 kg kg$^{-1}$) in the estimation of soil moisture content at PWP. In contrast, the PTF of Chakraborty et al. [33] had the worst performance in the estimation of soil moisture content at FC (RMSE = 0.058 kg kg$^{-1}$) and the PTF of Arruda et al. [30] was the worst in the estimation of soil moisture content at PWP (RMSE = 0.036 kg kg$^{-1}$).

The findings of this study agree with those of Botula et al. [13] who reported RMSE values of 0.053, 0.040, 0.075 and 0.045 kg kg$^{-1}$ for the PTFs of Arruda et al. [30], Dijkerman [25], Lal [31] and Pidgeon [32], respectively, for estimation of soil moisture content at FC for soils in the Democratic Republic of the Congo. Furthermore, their study reported RMSE values of 0.021, 0.032, 0.058 and 0.028 kg kg$^{-1}$ for the PTFs of Arruda et al. [30], Dijkerman [25], Lal [31] and Pidgeon [32], respectively, for estimation of soil moisture content at PWP [13].

The results of this study indicate better performance of the new PTFs developed with RMSE values of 0.047 and 0.029 kg kg$^{-1}$ for soil moisture content at FC and PWP, respectively. These findings suggest that PTFs derived locally using a large number of soil horizons acquired from different soil depths, soil types, geographic and climatic locations improved the estimation of soil moisture content at FC and PWP. Furthermore, this study indicates restricted applicability, reliability and transferability of the existing PTFs across different regions, thus the need for the development of new PTFs for each specific region is indisputable. The findings also confirmed that the PTFs applied outside the soils and climatic conditions from which they were derived may result in poor performance [8,13,18,20,73]. This is in agreement with previous studies that reported better performance of locally-derived PTFs over the existing PTFs that were developed for specific regions with different climatological and pedological properties [9,12,13,39–43].

The results showed that soil moisture content at PWP could be estimated with a higher degree of accuracy ($r^2 = 0.82$ and RMSE = 0.029 kg kg$^{-1}$) compared to FC ($r^2 = 0.77$ and RMSE = 0.047 kg kg$^{-1}$) using the new PTFs that were developed in this study. The relatively lower accuracy of estimated soil moisture content at PWP could be attributed to the lack of information regarding soil structure in these new PTFs that could have been probably provided by including the bulk density as one of the explanatory variables. These findings are in agreement with previous studies that reported better performance of the PTFs in the estimation of soil moisture content at PWP compared to FC [13,73,74]. The results of
this study indicate that the performance of all PTFs evaluated decreased with an increase in gravimetric soil moisture content. The relatively lower performance of the PTFs at the wetter range could be attributed to soil water retention at the wet range being primarily controlled by the soil structure, whereas, at the dry range, it is primarily controlled by soil texture [74]. Thus, since all PTFs evaluated in this study did not include bulk density (an indicator of soil structure) and used disturbed soil samples for the determination of soil moisture content at FC and PWP, these PTFs did not explicitly take the effects of soil structure on soil water retention into consideration.

3.4.2. Overall Discussion

The new PTFs developed in this study were capable of estimating soil moisture content at FC and PWP from particle size distribution and SOC with acceptable levels of confidence. These new PTFs are time-efficient and could reduce the cost and labour requirements in the estimation of soil moisture content at FC and PWP that are required by biophysical models to solve numerous challenges related to soil water in the fields of agriculture, ecology, environment and hydrology [13,14,37]. The new PTFs are expected to improve the estimation of the plant-available water, not only in South Africa where the need for efficient water use is of paramount importance under the threat of water scarcity but also in other regions facing data scarcity that have similar soil types and climatic conditions. Thus, due to the range of conditions for which these new PTFs were derived, they should be used with caution in other regions to estimate soil moisture content at FC and PWP from minimal soil physico-chemical properties that are usually available from surveys or are easily measured in most countries of the world. Moreover, this study is expected to raise awareness to the model users regarding the potential errors and implications attributed to the use of the ready-to-use PTFs within the models that were developed for specific regions with different soil types and climatic conditions.

To the best of our knowledge, this is the first study in southern Africa that has developed new PTFs and evaluated them against existing ones for the estimation of soil moisture content at FC and PWP using a large number of soil horizons (6307) acquired from different soil types, geographic and climatic conditions. Thus, for the wide applicability of the new PTFs that were developed in this study, a soil moisture retentivity (SMR) calculator that is user-friendly, quick and reliable was developed. In this calculator, a user is required to enter the percentages of clay, silt and SOC content to calculate the soil moisture content at FC and PWP instantaneously. The SMR spreadsheet is freely available on request from the authors.

4. Conclusions

The application of biophysical models requires the knowledge of soil moisture content at field capacity and permanent wilting point for each soil horizon. However, measurements of these soil hydraulic properties are time-consuming, labour-intensive, expensive and sometimes impractical or financially unattainable, especially in regional studies. Therefore, this study was undertaken to develop new pedotransfer functions for the estimation of soil moisture content at FC and PWP for a wide range of soil types and climatic conditions in South Africa. These new PTFs were evaluated and compared with five well-established PTFs using an independent dataset.

This study indicated a limited transferability of PTFs across different regions, particularly in regions with different geological, climatic and soil bio-physico-chemical properties to those of their origins. Therefore, existing PTFs still need to be tested for suitability before they can be utilized with confidence to estimate soil moisture content at FC and PWP for regions with different soil types and climatic conditions from which they were derived. Furthermore, the development of new PTFs for each region using a large number of soil horizons acquired over a wide range of soil types, geographic and climatic conditions is indisputable for the improved estimation of soil moisture content at FC and PWP.
The PTFs developed in this study reliably estimate soil moisture content at FC and PWP over a wide range of soil types and climatic conditions found in South Africa. These new PTFs are quick, reliable and could reduce the cost and labour requirements in the estimation of soil moisture content at FC and PWP required by biophysical models. Due to the large soil datasets and wide range of soil types, geographic and climatic conditions over which these PTFs were derived, they can be applied with caution in other regions facing data scarcity but with similar soil types and climatic conditions. To allow wide applicability of the new PTFs that were derived in this study, a quick, reliable and user-friendly soil moisture retentivity calculator was developed that uses clay, silt and SOC content as input requirements to compute soil moisture content at FC and PWP. For future studies, it is recommended that undisturbed soil samples are collected for the determination of soil moisture content at FC and PWP to improve the accuracy of the PTFs. It is also recommended that future studies explore the benefits of the development of PTFs for each specific agro-climatic condition of the region, unlike the current study where we developed the generic PTFs for the whole of South African soils.

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