Geoderma 401 (2021) 115346

Contents lists available at ScienceDirect

Geoderma

journal homepage: www.elsevier.com/locate/geoderma

Predicting field capacity in undisturbed stony soils

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ARTICLE INFO

Handling Editor: Cristine L.S. Morgan

Keywords:
Rock fragment water content
Field capacity
Low porosity rock fragments
Undisturbed stony soil
Pedotransfer function

ABSTRACT

An increasing number of studies around the world are showing that a long-held assumption that rock fragments (RFs) are inert with respect to water retention is incorrect. Yet very few pedotransfer functions (PtFs) account for water held by RFs or the effect RFs have on the water retention of the fine earth. The few PtFs that incorporate the water content (WC) of RFs have relied upon measurement methods that may not be representative of field conditions. This indicates a gap in research regarding the characterisation of the water holding behaviour of stony soils *in situ* using soil volumes that adequately represent the soil. We address this gap in research by developing PtFs that predict the field capacity WC of stony soils using soil water storage measurements from 52 pits excavated into stony soils on the Canterbury Plains, New Zealand. These soils comprise sediment derived from a Mesozoic hard sandstone. The soils at each site were watered to saturation, and then after two days of drainage (a proxy for field capacity), a 30 × 30 cm pit was excavated in 10 cm increments to a depth of 60 cm. Matric potential was measured *in situ* for each increment, and soil WC was calculated from samples taken back to the laboratory. Our results showed it was possible to accurately predict the field capacity WC of stony soils using only explanatory variables that could be easily measured or estimated from a minimalistic field survey. An existing PtF calibrated on NZ soils (logit PtF), which was constructed on the assumption that RFs had no effect on WC at FC other than reducing the volume of the fine earth, performed worse than our models. By modifying the logit PtF, we conclude that its poorer performance stems from its inability to account for deviations from 1) the matric potential it assumes for field capacity (−10 kPa), 2) water held by RFs, and 3) the effect of RFs on the water retention characteristics of the fine earth. Our results demonstrate that even the low porosity RFs measured in this study can significantly affect model performance, but by including two variables (depth and volumetric proportion of RFs) that are routinely measured or estimated in most soil sampling projects, it is possible to improve prediction accuracy in established models.

1. Introduction

Worldwide, there are concerns about rising nutrient concentrations in surface and groundwater systems (McDowell et al., 2020). A leading source of leached nutrients is agricultural land, which has expanded significantly with the global demand for food (McDowell et al., 2020; Wu et al., 2014). To mitigate nutrient leaching, more effective land management practices operating within an appropriate regulatory environment are necessary, making knowledge of soil water and nutrient retention properties indispensable. However, soil hydraulic properties are costly and time-consuming to measure, making it difficult or impossible to provide representative soil hydraulic properties at the farm scale, let alone regional and national scales. Therefore, models have been developed to provide estimates of soil retention properties like field capacity (FC) using more readily available field data (Vereecken et al., 1990). When applied to soil mapping units, these models (known as pedotransfer functions or PtFs) can be utilised for management and regulation purposes at the national scale when appropriate uncertainty analysis is included (Johnston et al., 2003; Lilburne et al., 2012). But PtFs for water retention properties often rely on the

Abbreviations: PtF, pedotransfer function; FC, field capacity; RF, rock fragment; SSA, specific surface area; VWC, volumetric water content.

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https://doi.org/10.1016/j.geoderma.2021.115346
Received 18 January 2021; Received in revised form 13 June 2021; Accepted 5 July 2021
Available online 15 July 2021
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assumption that rock fragments (RFs) in the soil are inert, such that all retention estimates are based solely on soil fine earth (<2 mm fraction) properties and its volumetric proportion.

Several studies have demonstrated that RFs can account for a significant proportion of the water held in a soil (Hanson and Blevins, 1979; Poesen and Lavee, 1994; Schoeman et al., 1997). For instance, Tetegan et al. (2011) found the soil available water content (WC) of a horizon containing 30% RFs could be underestimated by 5–33% depending on the lithology of the RFs. Similarly, Jones and Graham (1993) found large volumes of low porosity granite could hold more plant available water than the surrounding fine earth in soils under forest. As a result, a potentially significant error could exist for predictions of FC WC in stony soils (soils with over 30–35% RFs by volume), which represent large areas of land in many countries, including ~30% of Western Europe (Tetegan et al., 2011) and >60% of land in the Mediterranean area (Poesen, 1990). This is especially important considering PtFs that do not account for RF WC are used in national soil information systems (Lilburne et al., 2012; McNeill et al., 2018) and are used in digital soil information projects consistent with specifications of the GlobalSoilMap initiative (Román Dobarco et al., 2019a; Román Dobarco et al., 2019b). For instance, S-Map (the national soil information system of New Zealand; Lilburne et al., 2012) do not incorporate the WC of RFs in FC predictions, even though two-thirds of the irrigated land area in one of New Zealand's most important agricultural region (Canterbury) is on stony soil (Carrick et al., 2013). The few PtFs that incorporate the WC of RFs (Cousin et al., 2014; Parajuli et al., 2017; Scheinost et al., 1997; Wang et al., 2013) have relied upon measurement methods that may not be representative of field conditions: they used small sample sizes, relied upon repacked soil, or neglected to include the effect RFs may have on fine earth *in situ*. This indicates a gap in research regarding the characterisation of the water holding behaviour of stony soils *in situ* using soil volumes that adequately represent the soil.

This paper aims to develop PtFs that incorporate characteristics of the skeletal material in soils, and thus implicitly account for water held by RFs. We use variables that may reasonably be expected to affect the response variable, for example, depth (Minasny et al., 2016; Szabó et al., 2021), carbon (Moreno et al., 2014) and bulk density (Pollacco, 2008). There are also variables that have not been described in the literature as predictor variables for water retention but might reasonably be expected to have an association such as phosphate retention (as a proxy for soil weathering and structural development, Hewitt, 2010; Saunders, 1965), geomorphic surface age (as a proxy for post-depositional soil development processes acting over time, Robertson et al., 2021a), total nitrogen (as a proxy for organic matter, Cotrufo et al., 2019, and as a global soil map attribute) and irrigation treatment (due to its effect on soil carbon and soil physical attributes, Drewry et al., 2021; Mudge et al., 2021). The combined effect of all these variables is unknown and is therefore another novel aspect of this paper. The PtFs are calibrated on data derived from representative elementary volumes of stony soils *in situ* on alluvial fans in Canterbury, New Zealand. To develop better PtFs for FC in stony soils worldwide, we identify variables that have predictive value and are easy to measure. We then use them to augment the logit model of McNeill et al. (2018) to demonstrate how they may improve model performance in stony soils.

2. Materials and methods

2.1. Soil data

The soil data used to develop the FC PtFs was sourced from Robertson et al. (2021a) and Robertson et al. (2021b). Data from these studies are derived from 52 soil pits located throughout the Canterbury Plains of New Zealand. The Plains are approximately 180 km long and 70 km at their widest and consists of geomorphic surfaces of latest Pleistocene and Holocene age. The Plains have been built of coalescing aggrading Pleistocene glacial outwash fans constructed by large rivers sourced in the Southern Alps. The large rivers are now entrenched within the Pleistocene fans to form inset fans of Holocene age. Most of the soils on the Canterbury Plains are shallow stony soils (Carrick et al., 2013) comprising RFs of indurated muddy fine sandstone (greywacke) of the Rakaia terrane (Coates and Cox, 2002; Forsyth et al., 2008). On the late Pleistocene surfaces, Pallic and Brown soils dominate, while Holocene surfaces are dominated by Recent soils in the NZ Soil Classification (Hewitt, 2010). The stony soils of the Canterbury Plains include Firm Brown Soils (Dystrudepts and Dystrustepts) and Fluvial Recent Soils (Fluvents and Ustepts).

We adopt Webb and Lilburne's (2011) definition of stony soils as applied at the family level (level 4) of the NZ Soil Classification; specifically, soils with >35% rock fragments by volume within 45 cm of the soil surface. This definition is comparable to soil families of the USDA *Soil Taxonomy* system with the skeletal or fragmental particle sizes classes; or taxa having the skeletic soil qualifier for the second-level units of the WRB (IUSS Working Group WRB, 2015).

The 52 soil pits spanned 24 sites on land under pasture for at least three years and were predominately grazed by dairy cattle. At each site, a minimum of two pits were sampled. One pit was under spray irrigation for at least two years, while the other pit was in the same paddock but in soil that had never been irrigated (e.g. in the corner of a paddock outside the arc of a centre pivot irrigator). For each sampling location, the soil was first wet-up by applying >100 mm from a bespoke trickle irrigation system designed to wet a local area. The soil was allowed to drain for two days, which was used as a proxy for FC. A 30 cm by 30 cm pit was then excavated in 10 cm increments to a depth of 60 cm. The soil profile was then described according to the terminology of Milne et al. (1995) and classified to the subgroup level of the New Zealand Soil Classification according to Hewitt (2010). Each increment was equal to ~9000 cm^3, a volume that Novák and Hlaváčiková (2019) suggest is a representative elementary volume for measuring hydraulic properties in stony soils with gravels (2–75 mm RFs). The volume of each increment was determined using the pit and bead method (Hedley et al., 2012). After each increment was excavated, matric potential was measured by inserting a UMS T5 pressure transducer tensiometer horizontally into the pit wall, as described in Robertson et al. (2021a). Excavated material from each increment was then analysed following the process outlined in Robertson et al. (2021b) to determine a suite of attributes: the whole soil and fine earth bulk density; the volumetric proportion of fine earth (<2 mm) and RFs (>2mm); RF size distribution; WC of whole soil and fine earth. A subsample of <2 mm fine earth material was used for particle size analysis (Claydon, 1989), particle density (Gradwell and Birrell, 1972), specific surface area of the fine earth (Kirschbaum et al., 2020), WC of the fine earth at −1500 kPa (Gradwell and Birrell, 1972), phosphate retention (Saunders, 1965), total nitrogen (Leco, 2003) and organic carbon (Leco, 2003).

Some manipulation of raw data was required prior to statistical analyses. Because the proportion of sand (p_{sand}), silt (p_{silt}), and clay (p_{clay}) in the fine earth form a ternary simplex, a structural correlation exists (McNeill et al., 2018). As a result, conditions that may only affect clay for instance, will have an apparent statistical effect on sand and silt even though no functional relationship is present, as changes to one fraction alter the other two. For computational convenience, texture proportions were transformed to a Cartesian system as this generally reduces the apparent correlation between texture fractions by removing the structural correlation component. As per the method used by McNeill et al. (2018) and Cornell (1981), the texture proportions were transformed to a Cartesian system by generating two auxiliary variables as follows,

$$\omega_1 = 2p_{sand} - p_{silt} - p_{clay} \quad (1)$$

$$\omega_2 = p_{silt} - p_{clay} \quad (2)$$

The data set was also censored according to relative errors in data values. Many of the variables used for model development are derived from calculations on primary variables, with inherent uncertainty.

Table 1
Variables used in initial models for PtF development.

Optimal PtF	Practical PtF
Soil order	Soil order
Irrigation treatment (irrigated, dryland)	Irrigation treatment (irrigated, dryland)
Geomorphic surface age[*]	Geomorphic surface age[*]
Depth[#]	Depth[#]
Measured FC matric potential	Texture class[^]
Phosphate retention	Texture group[~]
Total nitrogen	Specific surface area
Organic carbon	Proportion of vol. that is RFs
Total porosity	Proportion of vol. that is 2–6 mm RFs
Particle density	Proportion of vol. that is 6–20 mm RFs
−1500 kPa WC	Proportion of vol. that is 20–60 mm RFs
Texture class[^]	Proportion of vol. that is >60 mm RFs
Texture group[~]	
ω_1	
ω_2	
Specific surface area	
Proportion of vol. that is RFs	
Proportion of vol. that is 2–6 mm RFs	
Proportion of vol. that is 6–20 mm RFs	
Proportion of vol. that is 20–60 mm RFs	
Proportion of vol. that is >60 mm RFs	
ρ_b[+]	
$\rho_{<2}$[-]	

[*] Pleistocene, Holocene and Pleistocene to Holocene.
[#] The depth increment at which variables were measured, such as 0-10 cm, 10-20 cm and 50-60 cm.
[^] Such as sand, silt loam and loamy clay.
[~] Namely, sandy, loamy, silty and clayey texture groups.
[+] Whole soil bulk density.
[-] Fine earth bulk density.

Those uncertainties compound and grow in relative magnitude, especially where subtractions and divisions are involved. We quantified the magnitude of errors, both absolute and relative, by applying Gaussian error propagation (refer to Supplementary file). Increments were removed if the relative error for an increment's fine earth VWC, fine earth bulk density or total porosity was >25%. As the New Zealand Soil Classification Order (top level of the NZSC, Hewitt, 2010) was used as an explanatory variable, increments from soils belonging to rare soil orders (Pallic (2 pits) and Gley (2 pits)) were excluded. The texture group of a soil was also an explanatory variable, making it necessary to remove increments from the rare clayey texture group (4 increments). The resulting dataset had 230 measured increments.

2.2. *Statistical modelling*

For modelling purposes, the dataset was randomly split 70:30 into training and validation datasets, respectively. Two multiple linear regression models to predict total FC WC (matrix plus RFs) were constructed in R version 4.0.2 (R Core Team, 2016) using different combinations of independent variables (Table 1).

These models constituted PtFs referred to as an optimal and a practical PtF (Fig. 1). The optimal PtF included all the explanatory variables measured in the experiment and was developed as a standard to compare the relative accuracy of the other models. The practical model used explanatory variables that could be easily measured or estimated from a minimalistic field survey. The explanatory set of variables for each model (PtF) was refined by selecting only significant variables according to a backwards selection process based on finding the model with the lowest Akaike information criterion value (AIC). This method of development is commonly found in modelling literature (Burnham and Anderson, 2002).

2.3. *An existing New Zealand PtF*

To quantify the value of implicitly accounting for the effects of RFs on soil water retention we sought a model that considered the fine earth only, which we could apply to our data to compare predictions against. McNeill et al. (2018) developed PtFs calibrated on NZ soil data to predict soil water retention when evaluating modelling methods for NZ's S-Map

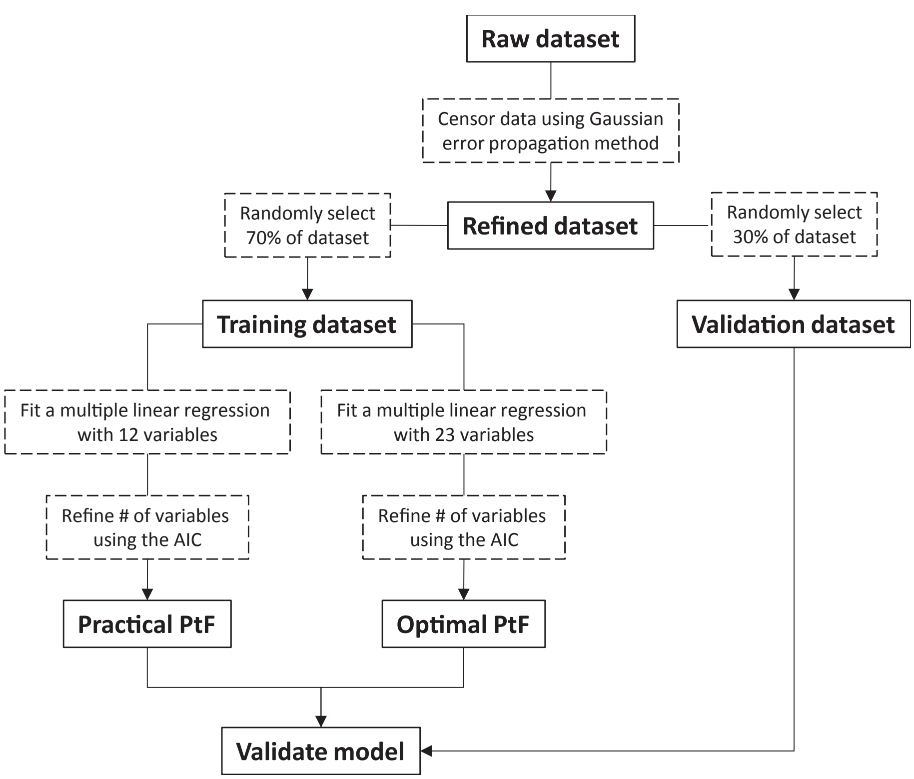

Fig. 1. Schematic methodology of practical and optimal PtF optimisation and validation.

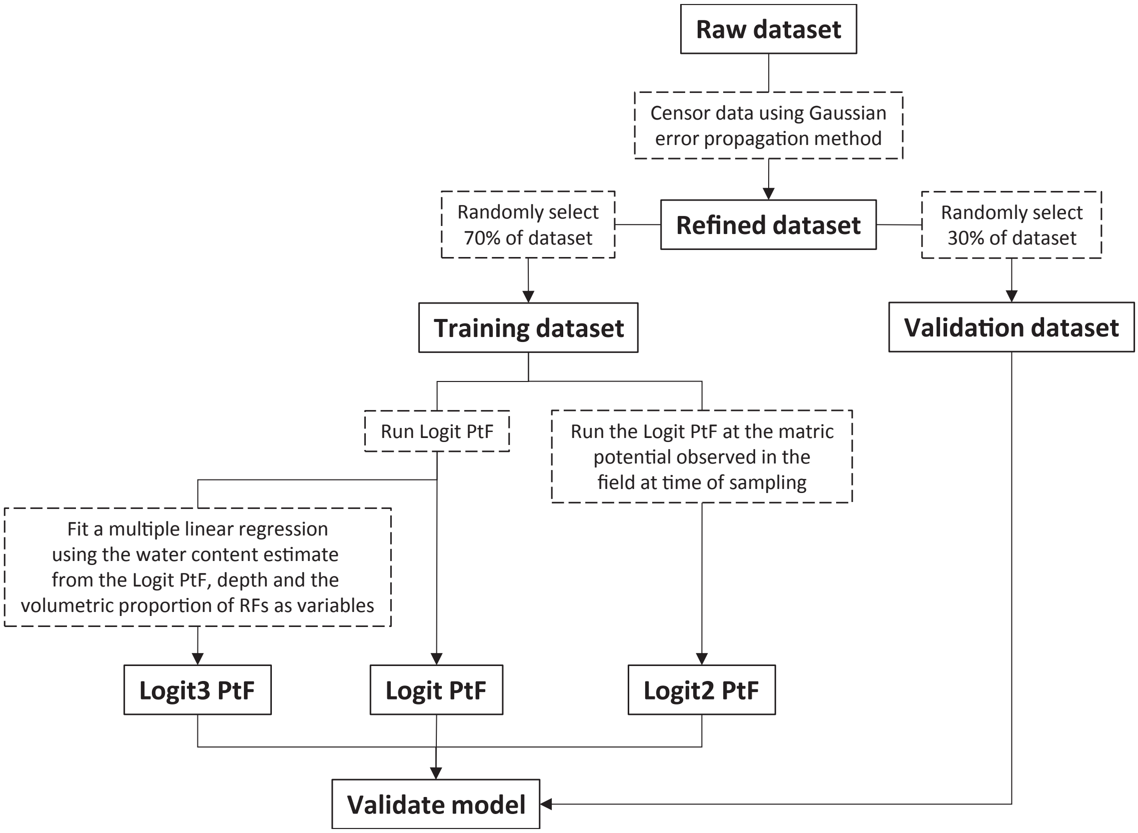

Fig. 2. Schematic methodology of the optimisation of the Logit3 PtF and the validation of the Logit, Logit2 and Logit3 models.

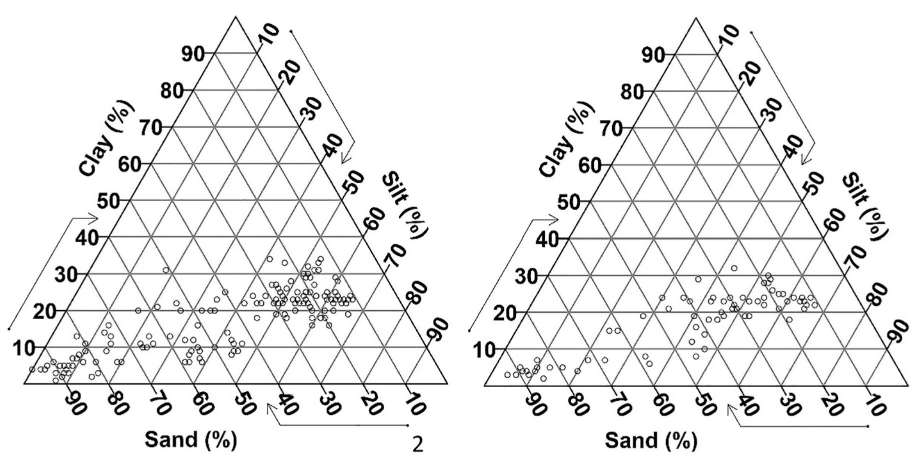

Fig. 3. Soil texture diagram displaying textures for each increment in the training dataset (left) compared to those of the validation dataset (right).

spatial soil information system. They concluded a logit-transformation model (logit PtF) had the lowest RMSE estimates and was the most stable, so we compared our results directly with output from that PtF.

The logit PtF was derived from eight explanatory variables, namely, soil order (top level of the NZSC, Hewitt, 2010), natural soil drainage, rock class of the fine earth, two auxiliary texture variables (ω_1 and ω_2), ped size, a topsoil identifier, tephra descriptor and consistence (for more information on variables see Milne et al., 1995; Webb and Lilburne, 2011). Interactions were permitted for the topsoil identifier and the two auxiliary texture variables.

Unlike the PtFs developed in this paper (the optimal and practical PtFs), the logit PtF was able to predict the water release curve of the fine earth (from 0 kPa to −1500 kPa). This was achieved by first fitting the logit transformed WC at −1500 kPa, $logit(\theta_{1500kPa})$, using a linear model,

$$logit(\theta_{1500kPa}) = f(\cdots) + \varepsilon \tag{3}$$

where $f(\cdots)$ is the linear function of the explanatory variables defined above and ε is the uncertainty, which is assumed to be Gaussian distributed. The explanatory set of variables was optimised using the AIC. The difference in WC between matric potentials (Δ) was then used as the response variable for another six PtFs:

$$\Delta_1 = \frac{logit(\theta_{100kPa}) - logit(\theta_{1500kPa})}{1 - logit(\theta_{1500kPa})} = f(\cdots) + \varepsilon \tag{4}$$

$$\Delta_2 = \frac{logit(\theta_{40kPa}) - logit(\theta_{100kPa})}{1 - logit(\theta_{100kPa})} = f(\cdots) + \varepsilon \tag{5}$$

Table 2
Descriptive statistics for training and validation databases.

		Training data set					Validation data set				
		Min	Median	Mean	SE	Max	Min	Median	Mean	SE	Max
Clay	%	1.00	20.0	17.9	0.68	34.0	2.00	21.0	17.5	1.02	32.0
Silt	%	0.00	46.0	40.5	1.52	67.0	4.00	46.0	40.6	2.20	67.0
Sand	%	11.0	29.0	41.7	2.07	96.0	11.0	34.0	41.9	3.07	93.0
Prop. RF by vol.	%	0.00	33.0	35.5	0.02	78.8	0.00	43.1	39.5	0.03	83.2
Carbon	%	0.21	1.88	2.11	0.10	5.15	0.26	1.58	1.97	0.14	4.98
-Topsoil~		1.97	3.90	3.68	0.18	5.15	1.62	3.57	3.52	0.32	4.98
-Subsoil>		0.21	1.17	1.20	0.08	3.30	0.26	1.24	1.26	0.10	2.95
ρ_b	*	1.13	1.74	1.77	0.03	2.41	1.16	1.89	1.82	0.04	2.43
FC VWC	^	0.02	0.25	0.24	0.01	0.44	0.04	0.21	0.22	0.01	0.47

* $Mg\ m^{-3}$.
^ $m^3\ m^{-3}$.
~ Average carbon (%) in 0–20 cm increments.
> Average carbon (%) in 20–60 cm increments.

Table 3
Multiple linear regression results for the optimal PtF.

Coefficients		Estimate	Std Error	t-value	$Pr(>\lvert t\rvert)$	
(Intercept)		1.15	7.29E-01	1.58	0.116	
Depth	10–20 cm	−2.12E-02	6.07E-03	−3.50	6.29E-04	***
	20–30 cm	−2.49E-02	8.25E-03	−3.02	3.01E-03	**
	30–40 cm	−2.62E-02	1.01E-02	−2.59	0.0107	*
	40–50 cm	−2.34E-02	1.11E-02	−2.11	0.0363	*
	50–60 cm	−2.13E-02	1.19E-02	−1.79	0.0750	.
Particle.density		5.61E-01	2.37E-01	2.37	0.0194	*
Total.N		3.26E-01	4.46E-02	7.30	1.84E-11	***
Total.porosity		−2.55	1.293528	−1.97	0.0504	.
Phosphate.retention		9.32E-04	1.53E-04	6.10	9.3E-09	***
Fine.earth.bulk.density		−0.958	4.86E-01	−1.97	0.0509	.
Whole.soil.bulk.density		1.44E-01	3.30E-02	4.35	2.54E-05	***
Vol.proportion.RFs		−4.74E-01	4.31E-02	−11.0	8.87E-21	***
15.bar.WC		1.23E-03	3.42E-04	3.60	4.42E-04	***
Treatment.irrigated		1.13E-02	3.33E-03	3.39	9.12E-04	***
ω_1		−3.28E-04	4.33E-05	−7.58	3.87E-12	***
Geomorphic surface	Pleistocene	−2.41E-02	5.31E-03	−4.54	1.18E-05	***
	Pleistocene to Holocene	−1.55E-02	9.34E-03	−1.66	0.0987	.
Residual standard error: 0.01918 on 143 degrees of freedom						
Multiple R-squared: 0.9783, Adjusted R-squared: 0.9757						
F-statistic: 379.4 on 17 and 143 DF, p-value: <2.2e-16						
Significance codes: '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1						

Table 4
Multiple linear regression results for the practical PtF.

Coefficients		Estimate	Std Error	t-value	$Pr(>\lvert t\rvert)$	
(Intercept)		0.320	1.37E-02	23.3	1.78E-51	***
Depth	10–20 cm	−0.0120	6.80E-03	−1.76	0.0798	.
	20–30 cm	−0.0321	7.70E-03	−4.17	5.26E-05	***
	30–40 cm	−0.0344	8.74E-03	−3.93	1.30E-04	***
	40–50 cm	−0.0451	1.03E-02	−4.37	2.34E-05	***
	50–60 cm	−0.0530	1.09E-02	−4.88	2.74E-06	***
Vol.proportion.RFs		−0.307	1.34E-02	−23.0	1.29E-50	***
Treatment.irrigated		0.0124	4.41E-03	2.82	5.44E-03	**
SSA		0.00141	2.12E-04	6.64	5.6E-10	***
Geomorphic surface	Pleistocene	−0.0132	6.10E-03	−2.16	3.24E-02	*
	Pleistocene to Holocene	−0.00688	1.29E-02	−0.533	0.595	
Texture.group	Sandy	−0.0363	7.83E-03	−4.64	7.61E-06	***
	Silty	0.0164	8.20E-03	2.00	0.0470	*
Residual standard error: 0.02672 on 148 degrees of freedom						
Multiple R-squared: 0.9564, Adjusted R-squared: 0.9529						
F-statistic: 270.8 on 12 and 148 DF, p-value: <2.2e-16						
Significance codes: '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1						

$$\Delta_3 = \frac{logit(\theta_{20kPa}) - logit(\theta_{40kPa})}{1 - logit(\theta_{40kPa})} = f(\cdots) + \varepsilon \tag{6}$$

$$\Delta_4 = \frac{logit(\theta_{10kPa}) - logit(\theta_{20kPa})}{1 - logit(\theta_{20kPa})} = f(\cdots) + \varepsilon \tag{7}$$

Table 5
Multiple linear regression results for the logit3 PtF.

Coefficients		Estimate	Std Error	t-value	Pr(>|t|)	
(Intercept)		0.193	2.04E-02	9.49	4.4E-17	***
logit.prediction		0.520	4.97E-02	10.5	1.21E-19	***
Depth	10–20 cm	−0.0179	7.14E-03	−2.51	0.0132	*
	20–30 cm	−0.0281	8.08E-03	−3.48	6.57E-04	***
	30–40 cm	−0.0292	9.47E-03	−3.08	2.45E-03	**
	40–50 cm	−0.0420	1.10E-02	−3.82	1.93E-04	***
	50–60 cm	−0.0432	1.21E-02	−3.56	4.98E-04	***
Vol.proportion.RFs		−0.244	1.44E-02	−16.9	6.17E-37	***

Residual standard error: 0.02889 on 153 degrees of freedom
Multiple R-squared: 0.9474, Adjusted R-squared: 0.945
F-statistic: 393.5 on 7 and 153 DF, p-value: <2.2e-16
Significance codes: '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

$$\Delta_5 = \frac{logit(\theta_{5kPa}) - logit(\theta_{10kPa})}{1 - logit(\theta_{10kPa})} = f(\cdots) + \varepsilon \tag{8}$$

$$\Delta_6 = \frac{logit(\theta_{0kPa}) - logit(\theta_{5kPa})}{1 - logit(\theta_{5kPa})} = f(\cdots) + \varepsilon \tag{9}$$

where $f(\cdots)$ is the same linear function as for the $logit(\theta_{1500kPa})$ and each set of explanatory variables was optimised using the AIC (Appendix A). Collectively, the 7 models span the water release curve and will collectively be referred to as the logit PtF.

In the logit PtF, the WC of a stony soil is estimated as the predicted WC of the fine earth scaled on a volumetric basis by the concentration of RFs (McNeill et al., 2018). Thus, it does not take account of the water held in RFs or the effect of RFs on the water retention of the fine earth. For example, when estimating FC WC, the logit PtF predicts the volumetric WC (VWC) of the fine earth only at a default FC matric potential of −10 kPa (θ_{10kPa}). The FC VWC of stony soils ($\theta_{FCstony}$) is then estimated by adjusting θ_{10kPa} by the volume proportion of RFs in an increment (χ), which are considered inert;

$$\theta_{FCstony} = \theta_{10kPa}(1 - \chi) \tag{10}$$

To explore the limitations and avenues for improvement of the logit PtF, we generated two variants, logit2 and logit3. Logit2 was essentially the same statistical model as the logit PtF but evaluated at the matric potential observed in the field at the time of sampling (θ_{FC}) instead of −10 kPa (Fig. 2). This model could never be used in practice because matric potential at field capacity is rarely going to be available. Logit3 was a new linear regression model, which incorporated the logit-predicted WC plus two variables that were identified as significant to FC predictions in our practical model, namely increment depth (z) and the volume proportion of RFs. The significance of the two variables was determined by a variable scaling procedure, which is explained in more detail in the Comparing models section. The model was calibrated using 70% of the measured data like the optimal and practical PtFs (Fig. 2).

2.4. Comparing models

The five models were compared by using the validation dataset. Each of the models were used to predict the whole soil FC VWC of the validation dataset and were then ranked using the mean bias, mean absolute error (MAE) and the root mean square error (RMSE) of predictions. As per McNeill et al. (2018), distributions of the three error measures above

Table 6
Model performance based on the means of error measure distributions obtained from bootstrap sampling.

	Order	Bias	RMSE	MAE
Optimal PtF	1	0.0001	0.020	0.016
Practical PtF	2	0.001	0.026	0.021
Logit3 PtF	3	0.0016	0.029	0.023
Logit2 PtF	4	0.006	0.045	0.038
Logit PtF	5	0.027	0.043	0.036

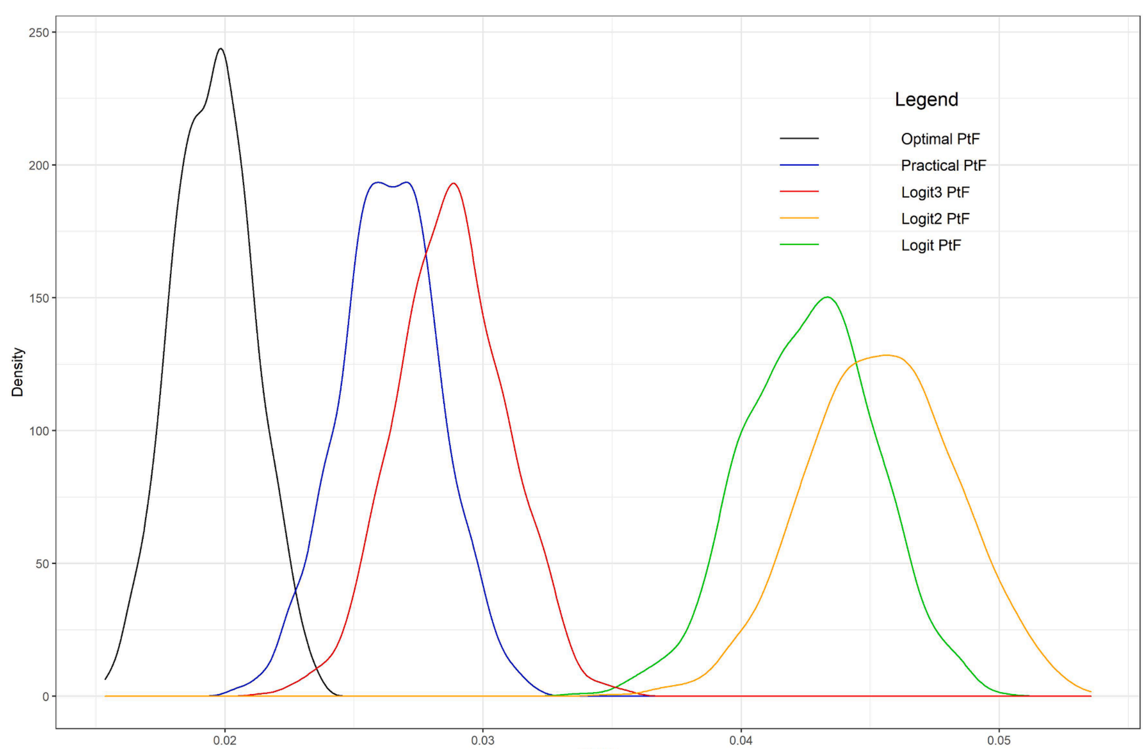

Fig. 4. Density plots of the root mean square error for the five regression models for FC WC. Ranked in order of lowest to highest bias, the PtFs follow the sequence: optimal, practical, logit3, logit2, and logit. The mean bias for all but the logit PtF were within ±0.01 m^3/m^3 of 0, showing the PtFs had no substantial positive or negative biases overall. The 0.027 bias of the logit PtF indicates a pattern of underestimation.

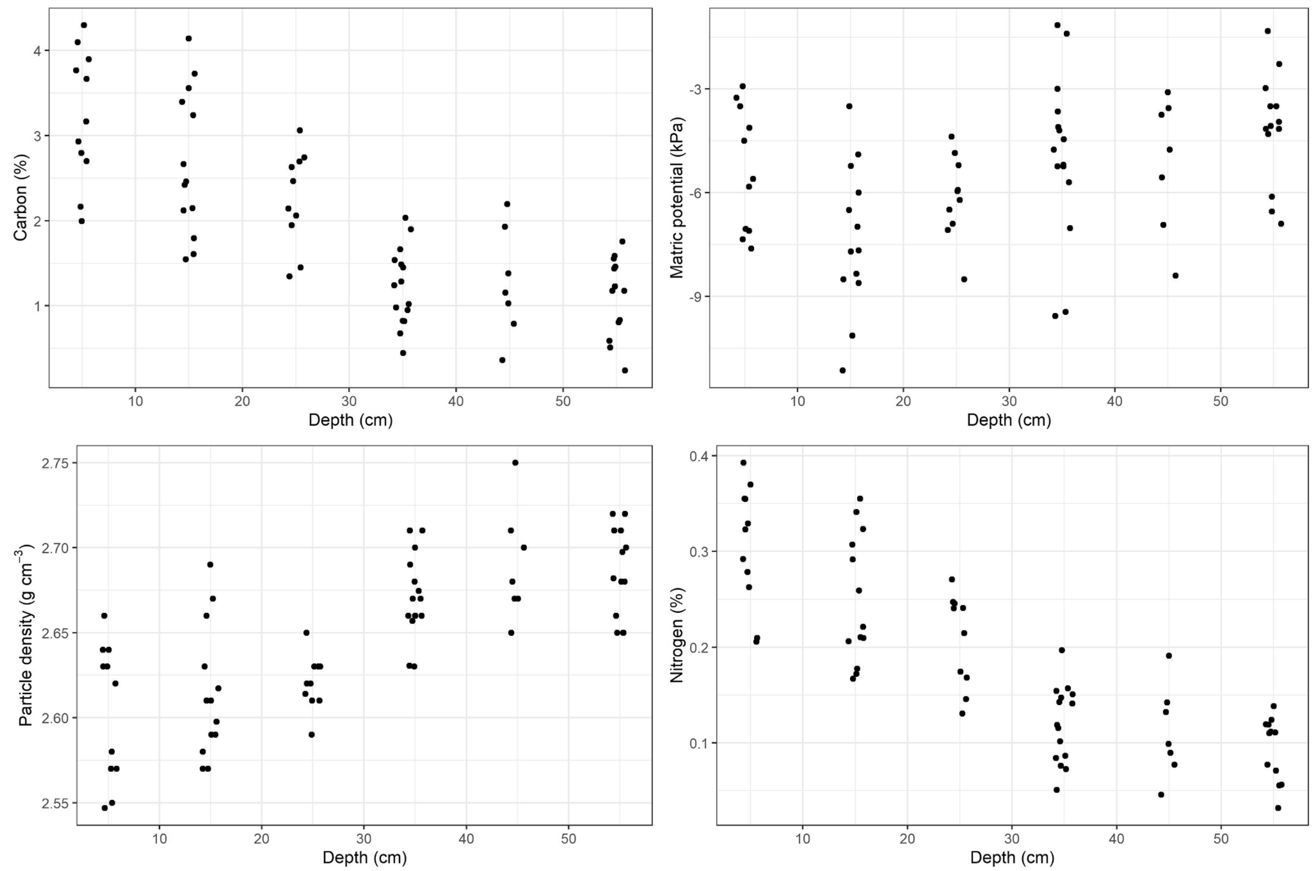

Fig. 5. Correlations between soil variables (carbon, matric potential, particle density and total nitrogen) and depth. Note, data points within each increment have had slight adjustments to their depth to aid readability.

were made by bootstrap sampling the training data. An error estimate (e.g. RMSE) was derived using the validation dataset for each bootstrap, resulting in a distribution of each error measure. This analysis was used because the distributions indicate the likely range of error as a result of all possible training data, as opposed to the more limited information derived from the more commonly used single-value estimates of error.

To understand variation in model performance and to identify the influential variables (which were incorporated in the logit3 model), the "standardised" function in R was also used to centre all the model variables and scale by the standard deviation. Following this scaling procedure, the size of the coefficients can be used as a direct measure of relative importance – large coefficients indicate strong influence, and small coefficients indicate weak influence.

3. Results and discussion

3.1. Descriptive statistics

Descriptive statistics of soil properties were similar between the training and validation datasets (Fig. 3, Table 2).

Soil textures fell within 6 of the 11 soil texture classes used by the NZSC (Milne et al., 1995). There were no samples in the clay, loamy clay, silt, sandy clay loam or silty clay textures. Textural distribution was biased toward the sand and silt-dominated textures with silt loam representing ~50% of the dataset (Table 2). Distributions of soil variables remained similar between training and validation datasets (Table 2), so the changes in variables with depth will now be described as an average of the two datasets. On average, the volume of RFs accounted for <15% of the total soil volume in the 0–10 cm increment, but >60% for the 40–50 cm and 50–60 cm increments. Whole soil bulk density increased from an average of 1.37 g cm^{-3} in the 0–10 cm increment to 2.04 g cm^{-3} in the 50–60 cm increment. As expected, the average organic carbon content decreased with depth from 3.6% in the topsoil to 1.2% in the subsoil (Table 2), while the FC VWC of the whole soil decreased from 0.35 in the 0–10 cm increment, to 0.09 in the 50–60 cm increment. Brown Soils were the dominant soil order, accounting for ~60% of the total dataset, while Recent Soils accounted for ~40%. Pits were distributed over two geomorphic surfaces: ~79% were on Late Pleistocene glacial outwash, ~17% were on Holocene alluvial deposits and ~5% were on Late Pleistocene to Holocene alluvial deposits.

3.2. Model structures and performance

The optimal PtF had an $R^2 = 0.98$ and included 12 of 23 variables once those that did not minimise the AIC were removed (Table 3).

The practical PtF, generated from 12 pre-selected, easily measured soil variables, had an R^2 of 0.95 and retained 6 of 12 variables after the AIC was applied (Table 4).

The logit and logit2 PtFs are established models that did not require model formulation and thus no regression results are presented. The logit3 PtF, generated from three variables, had an R^2 of 0.95 and retained all three variables after the AIC was applied (Table 5).

The five PtFs produced distinct distributions of RMSE (Fig. 4), bias and MAE (Table 6) when applied to the validation dataset.

3.3. Is less more? predicting FC WC with field survey variables

Despite displaying the best performance, the relative improvement of the optimal model in comparison to the practical model is only modest considering the increase in explanatory variables. We expected the optimal model would perform much better considering the practical model does not include a number of variables commonly associated with

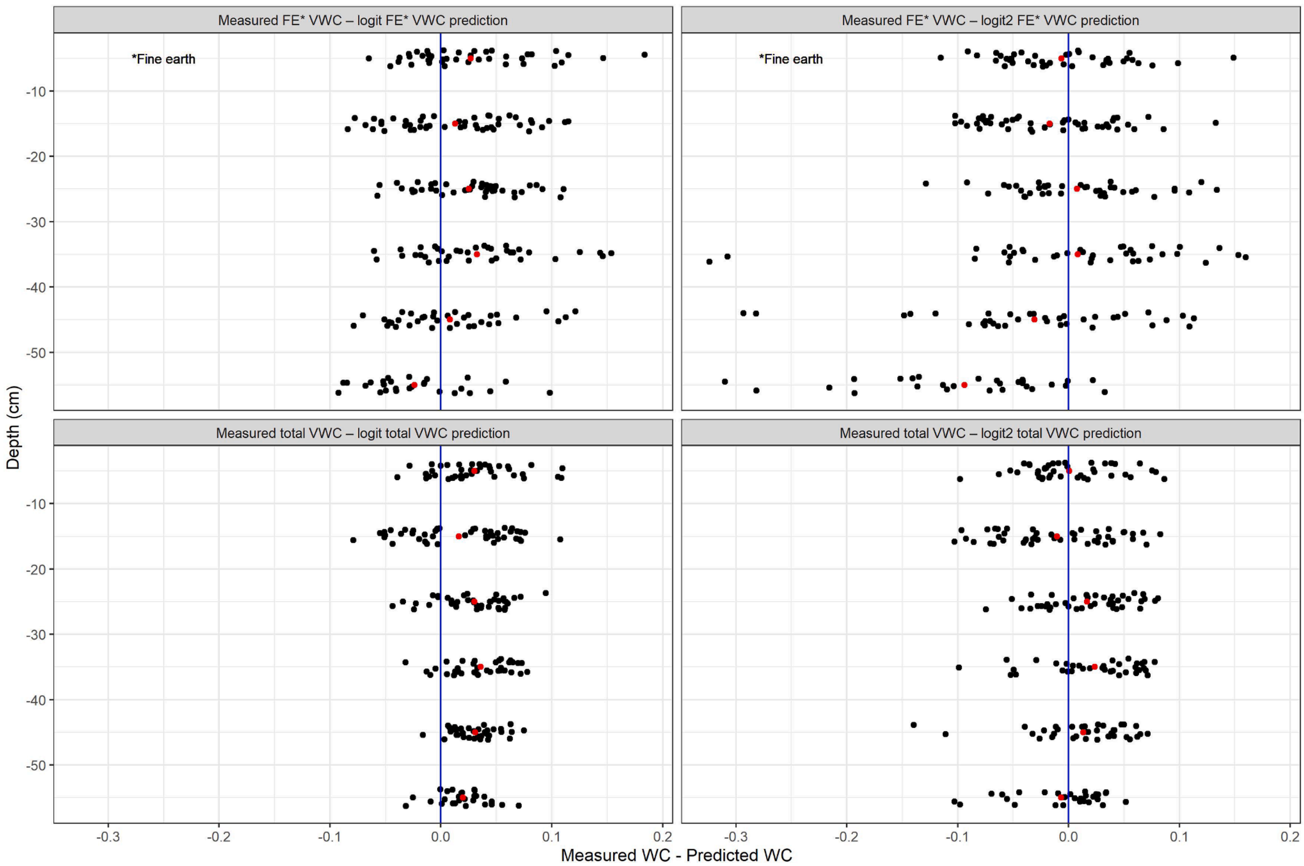

Fig. 6. Difference between logit predictions and measured values for fine earth and total VWC. Blue line depicts zero error, red dots are the average error for an increment. Note, data points within each increment have had slight adjustments to their depth to aid readability.

predicting soil VWC, such as carbon, bulk density (whole soil or fine earth) or even continuous measures of texture (i.e. proportion sand, silt or clay) (Mohamed and Ali, 2006; Ostovari et al., 2015; Pollacco, 2008; Román Dobarco et al., 2019b; Santra et al., 2018). Regardless of the absence of these 'standard' variables, the RMSE of the practical PtF (0.026 m^3/m^3) is still low when compared to the logit PtF or the performance of other PtFs in the literature, which commonly predict FC with RMSE > 0.04 m^3/m^3 (Ostovari et al., 2015; Pollacco, 2008; Román Dobarco et al., 2019b).

Using the "standardised" scaling procedure in R, it was found that the proportion of RFs, geomorphic surface and total nitrogen content were the most influential variables in the optimal PtF (Appendix B), while the practical model was mostly influenced by the proportion of RFs and depth (Appendix C). The depth variable in the practical model was correlated with a number of variables found in the optimal PtF (such as total nitrogen and particle density) as seen in Fig. 5. As such, depth may act as a proxy for several other variables, allowing the practical model to predict accurately even with a limited number of variables. These results are consistent with international literature that have also found depth to be a significant explanatory variable for many soil properties including soil carbon, texture, soil development and solute transport (Fontaine et al., 2007; Minasny et al., 2016; Vasques et al., 2010).

3.4. Do RFs affect prediction accuracy? a review of logit and logit2 performance

The average error for whole soil VWC showed logit predictions were underestimates at all depths, while the logit2 predictions were more evenly distributed around a mean error of 0 (Fig. 6A and 6B). To understand the cause of this bias, the logit and logit2 predicted fine earth WCs were compared to the measured fine earth WC. The measured fine earth WC was greater than the logit predictions in all but the 50–60 cm increment (Fig. 6C). Alternatively, logit2 predictions of fine earth WC generally exceeded measured fine earth WC at all depths except the 20–40 cm increments (Fig. 6D).

These results demonstrate that on average, logit underestimates the WC of the fine earth, while logit2 maintains a near-zero bias in the 0–40 cm increments with substantial overestimation in the 40–60 cm increments. However, as logit2 considers RFs to be inert (when they in fact hold water; Robertson et al, 2021b), bias in total WC predictions tends towards zero or underestimation. For instance, in the 50–60 cm increment, logit2 (which takes into account actual matric potential) overestimates fine earth WC by 0.09 m^3 m^{-3} on average, but total WC is overestimated by only 0.007 m^3 m^{-3}. By chance, the greater overestimation of fine earth WC by logit2 better compensates for the neglected WC of RFs in the 40–60 cm increments, resulting in logit2 having a lower average error compared to the logit PtF when predicting the whole soil WC.

3.5. How to calibrate the logit PtF to alluvial stony soils; identifying variables with predictive value

The inclusion of depth and RF proportion variables in logit3 substantially improved model performance in comparison to logit, with logit3 demonstrating a similar accuracy to the practical model (Fig. 7). Model performance may have improved because depth acts as a proxy for several variables as discussed previously (Fig. 5). Furthermore, including RF proportion as a predictor variable may capture the influence of the WC of the RFs, as well as the indirect effects RFs have on water retention of the fine earth, by way of changes to soil properties such as fine earth bulk density (Gargiulo et al., 2016; Shi et al., 2012) or carbon content (Bornemann et al., 2011; Schiedung et al., 2017).

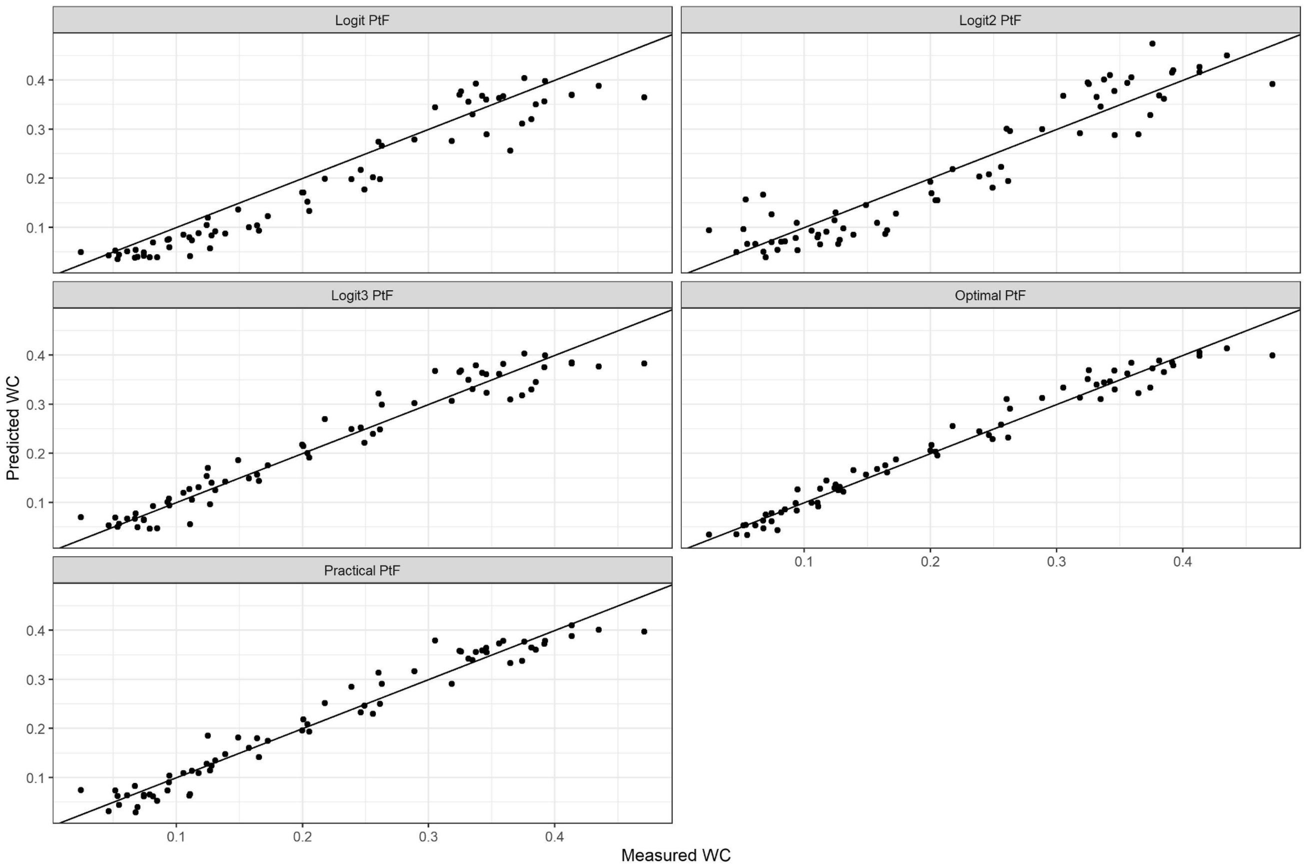

Fig. 7. Predicted total FC WC as a function of measured total FC WC.

There remains only three variables in the practical model (SSA, irrigation treatment and age of geomorphic surface) that are absent in logit3, which could explain the model's lower performance when compared to the practical PtF. When SSA was added to the logit3 PtF, the performance of the model was not notably different to the practical PtF. The SSA is a metric that may relate grain-scale properties to macro-scale physical and chemical properties of a porous medium (Petersen et al., 1996). Accordingly, Hillel (1980) suggested that SSA may become a more pertinent index for characterising a soil than the proportions of sand, silt and clay. Currently, SSA is more commonly used for determining soil WC at low matric potentials (Arthur et al., 2013; Chang and Cheng, 2018; Resurreccion et al., 2011), although our results suggest it could be relevant to FC estimates as well. In contrast, Petersen et al. (1996) found that SSA did not relate well with the WC at −10 kPa; however, they used different methods to estimate SSA, which can cause widely different results (de Jong, 1999; Petersen et al., 1996).

3.6. Implications and future work

Assuming RFs do not hold water or have no effect on water retention of the fine earth leads to non-negligible, systematic error in soil water storage estimates, as demonstrated by the performance of the logit PtF. Importantly, our results show that even low porosity greywacke (with a FC volumetric WC of 0.03–0.06, Robertson et al., 2021b) can have a substantial effect on prediction accuracy. Considering RFs besides greywacke can have FC WC of 0.20–0.67 cm^3 cm^{-3} (Gillespie, 2020; Schoeman et al., 1997; Tetegan et al., 2011), our results indicate the potentially significant error in current modelling methods that are used internationally (Román Dobarco et al., 2019a; Román Dobarco et al., 2019b).

We have identified depth and the volume proportion of RFs as important variables for reducing error when predicting FC WC of stony soils. Our results have potentially significant implications for developing better stony soil PtFs worldwide, as these variables are easy to measure (or estimate) and are either already a part of national and international datasets (Lilburne et al., 2012; Ribeiro et al., 2018; Shangguan et al., 2013), or are soon to be as part of the specifications for the GlobalSoilMap initiative (Arrouays et al., 2014). However, further research is required to determine the importance of these variables in stony soils formed in depositional settings contrasting to those of our study. For instance, the significant influence of depth we found may disappear where stony soils are formed in diamicts such as debris flows or glacial till. Similarly, the influence of the volumetric proportion of RFs is likely to vary with soil moisture content, RF lithology and weathering (Poesen and Lavee, 1994; Tetegan et al., 2011), requiring different calibrations for each. Further questions also exist around how this RF parameterisation interacts with predicting other soil water processes such as evapotranspiration, root water uptake and macropore/bypass flow. Results also indicate the potential for SSA as a useful predictor, especially as it is both cheap and quick to determine. Finally, our practical model offers an accurate method for predicting FC using information derived from a minimalistic field survey; however, to be used routinely in an operational way, the model needs to be tested using field-based assessments of soil texture and RF abundance instead of the lab measured values used in this study.

4. Conclusions

Results of this study demonstrate that hard sandstone RFs in Canterbury stony soils are not inert and can in fact cause significant error in FC WC predictions when the water held by RFs is not implicitly accounted for. However, the practical PtF we derived demonstrates that it is possible to accurately predict FC WC in stony soils, while only using explanatory variables that could be easily measured or estimated from a minimalistic field survey. This model also indicated the potential of SSA as an explanatory variable that is quick and cheap to determine. The logit model did not account for RF WC and tended to underestimate fine earth WC, resulting in a substantial bias in predictions for increments with high and low RF content. Alternatively, logit2 tended to overestimate fine earth WC in the lower increments, which by chance compensated for the neglected WC of RFs in the 40–60 cm increments, resulting in logit2 having a near-zero bias on average. However, incorporating depth and volumetric proportion of RFs as explanatory variables substantially improved prediction accuracy as demonstrated by the logit3 PtF. Our findings could have significant implications for the modelling of FC WC worldwide, as the effect of RFs (even those with much greater porosity than those measured in this study) are not currently accounted for in most PtFs. But, by including two variables (depth and volume proportion of RFs) that are already measured or estimated in most soil sampling projects, WC predictions may be significantly improved in stony soils. However, research must be repeated in soils that are not of alluvial origin and with RFs of varying weathering and lithology, to determine if the depth and the proportion of RFs remain important predictor variables.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

This research was funded by the Ministry of Business, Innovation and Employment's Endeavour Fund, through the Manaaki Whenua-led 'Next Generation S-map' research program, C09X1612, as well as the Ministry for Primary Industries Sustainable Farming Fund project 405305 'The Effect of Medium to Long-Term Irrigation on Soil Water Holding Properties', and support from Lincoln University. We would also like to thank the farmers throughout Canterbury for allowing sampling to take place on their farms; Andre Eger, Thomas Caspari and Nina Koele for help with field sampling; John Payne and Graeme Rogers for technical support; and the laboratory technicians at MWLR Soil Physics Laboratory for soil particle size distribution analysis. We also appreciate the valuable feedback from the reviewers of this paper. The authors declare no conflicts of interest.

Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.geoderma.2021.115346.

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