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Pedotransfer functions for Irish soils – estimation of bulk density (ρ_b) per horizon type

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Abstract

Soil bulk density is a key property in defining soil characteristics. It describes the packing structure of the soil and is also essential for the measurement of soil carbon stock and nutrient assessment. In many older surveys this property was neglected and in many modern surveys this property is omitted due to cost both in laboratory and labour and in cases where the core method cannot be applied. To overcome these oversights pedotransfer functions are applied using other known soil properties to estimate bulk density. Pedotransfer functions have been derived from large international datasets across many studies, with their own inherent biases, many ignoring horizonation and depth variances. Initially pedotransfer functions from the literature were used to predict different horizon types using local known bulk density datasets. Then the best performing of the pedotransfer functions, were selected to recalibrate and then were validated again using the known data. The predicted co-efficient of determination was 0.5 or greater in 12 of the 17 horizon types studied. These new equations allowed gap filling where bulk density data was missing in part or whole soil profiles. This then allowed the development of an indicative soil bulk density map for Ireland at 0–30 and 30–50 cm horizon depths. In general the horizons with the largest known datasets had the best predictions, using the recalibrated and validated pedotransfer functions.

1 Introduction

Soils are a vital global resource providing a range of ecosystem services, upon which we depend. Such services include the platform on which we produce food, fibre and raw materials, purifying and regulating water, cycling of carbon and nutrients, and providing a habitat for biodiversity (EU, 2002). To understand many of the processes on-going in soils that deliver these ecosystem services, we must quantify soil characteristics, as these vary considerably according to soil type. Bulk density (ρ_b) is defined as the oven-dry mass per unit volume of a soil (IUSS 20 Working Group, 2006).This is an integral

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soil property, as it not only describes the packing structure of soils (Dexter, 1988), but is essential for the measurement of soil carbon and nutrient stock assessment (Ellert and Bettany, 1995). Bulk density measures can also describe the permeability of a soil, whereby it defines drainage characteristics (Arya and Paris, 1981) and is used in pedotransfer functions that model soil hydraulic characteristics (Murphy et al., 2003; Van Alphen et al., 2001; Minasny, 2007). Bulk density can also indicate compacted layers resulting from machinery or animal trafficking (Saffih-Hdadi, 2009), which can then impact the nutrient availability in soils (Douglas and Crawford, 1998).

Furthermore bulk density (ρ_b) is a critical soil characteristic for soil carbon studies and modelling, it can indicate the amount/volume rather than the concentration of carbon at a given point. Soil organic carbon (SOC) pool stock calculation depends upon suitable data in terms of organic carbon content and soil bulk density, and on the methods used to upscale point data to comprehensive spatial estimates (Vanguelova et al., 2015). The lack of appropriate bulk density documentation is problematic for statistical confidence assessments. Historically, ρ_b measurements are commonly missing from databases for reasons that include omission due to sampling/budgetary constraints and laboratory mishandling/conflicting methodologies (Batjes, 2009). Pedotransfer functions (PTF) based on readily measured soil attributes, such as organic carbon and clay content, show strong potential to replace ρ_b measurements as their direct measurement are not feasible or lacking from historical records.

However, bulk density has been found to vary with depth (Leonavičiutė, 2000) and soil type (Manrique and Jones, 1991), while the use of generic pedotransfer functions, can result in large errors in the calculation of SOC stocks. In saying this, De Vos indicates there is a need for specific PTF to be calibrated and validated on a regional basis (De Vos et al., 2005). Others take this further and report that PTF should be developed for particular horizon types or designations (Suuster et al., 2011). Correlation with international datasets can be employed to generate PTF where local information is lacking. There is information available from large international soil survey databases (Hollis et al., 2006; Batjes, 2005, 2009), but in many cases bulk density is poorly documented. In these instances the use of splines or models of bulk density are then used with their own inherent variances, which can be problematic without large validation datasets (Lettens et al., 2005).

With the launch of the Irish Soil Information System (Irish SIS) and the publication of the 3rd edition of the Irish soil map, there is the opportunity to measure, interpolate and map bulk density values on a national scale. The latest soil map for Ireland has been published online by the Irish soil information system (Creamer et al., 2014).

The research presented in this paper will use new data generated by the Irish SIS to provide primary data for the calculation of PTF at the soil horizon level. Soil bulk density measurements were available for 15.9 % of the soil profiles described in Ireland in the last 40 years. In addition to this, PTF from the literature were used with known texture and organic carbon data, to develop the calculations for bulk density. These PTF were then recalibrated for Irish soil horizons, where ρ_b was measured. The PTF were then applied to the soil horizons with unknown ρ_b. This allowed the calculation of soil bulk density to a depth of 50 cm for all soil profiles described. Using the PTF, bulk density is now known at different horizon designations. This had led to an indicative map of soil bulk density in Ireland being developed.

2 Materials and methods

2.1 Soil profiles

From 2012 to 2014 the Irish SIS sampled 246 soil pits as part of its field survey. These pits were distributed across 16 counties in Ireland, Fig. 1. At each site a pit was excavated to approximately 1 m, where this was not possible, it was excavated to the depth of underlying bedrock preceding this. The pit face was at least one metre wide. In total there were 1028 soil horizons identified. Within these pits, 470 horizons were sampled for bulk density (ρ_b). The remainder could not be measured for bulk density as the

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stainless steel rings were unusable due to coarse fragments. Therefore these horizons required ρ_b predictions.

2.2 Legacy data

In addition, detailed descriptions of 560 soil profiles were available from legacy data collected under the An Foras Talúntais soil survey (AFT) conducted between the 1970s and 1990s. However, very few bulk density measurements were taken as part of this survey, but detailed descriptions of soil horizons did exist, along with analytical data for a number of soil parameters, such as texture and SOC. In total there were 2950 horizons described across 809 soil profiles located across the whole of Ireland, Fig. 1.

2.3 Field sampling

In the centre of each horizon, a smooth undisturbed vertical soil surface was prepared for ρ_b sampling. Three 50 mm × 50 mm stainless steel rings were hammered into place. Care was taken to just fill the ring and not compact the soil. The ring plus soil was then removed from the surface of the soil matrix with as little disturbance as possible using a flat sided trowel. Any excess soil was trimmed from the ring edges before being placed in a sealed plastic bag. Also if protruding coarse fractions were present, they were marked and retained for cutting in the laboratory. For other soil parameters (texture, SOC, pH, cation exchange capacity, Fe/Al content), within the same horizon 2 kg of soil was sampled with a trowel into plastic bags and then sealed.

2.4 Bulk density analysis

The laboratory method followed that of the method applied during the few sites collected during the An Foras Talúntais survey (Massey et al., 2014). This method corresponds to ISO 11272:1998 – Soil Quality Part 5: Physical methods Section 5.6 – Determination of dry bulk density. The primary difference between the ISO and An Foras Talúntais methodologies is that the ISO does not account for stone mass and

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volume in its core method, whereas the methodology applied here does include this Eq. (1).

To calculate bulk density (stone-free):

$$\rho_b\ (\mathrm{g\,cm^{-3}}) = (M_d - M_s)/(V - V_s) \tag{1}$$

where: M_d = Oven dry soil material weight (g), M_s = Oven dry stone weight (g), V = Volume of soil core ($\mathrm{cm^{-3}}$), V_s = Volume of stones (mL). The resulting ρ_b values were the mean of three field replicate samples.

2.5 Pedotransfer functions review and selection

Following a detailed review of the literature,22 pedotransfer functions (PTF) were collated (Alexander, 1980; Adams, 1973; Rawls and Brakensiek, 1985; Honeysett and Ratkowsky, 1990; Federer, 1983; Huntington, 1989; Manrique and Jones, 1991; Bernoux et al., 1998; Leonavičiutė, 2000; Kaur et al., 2002; Jeffrey, 1970; Harrison and Bocock, 1981; Tamminen and Starr, 1994). A first stage assessment was conducted using the Irish SIS data where ρ_b information was available for a range of soil horizon types. At this stage several ($n = 10$) PTFs were removed as negative and/or extremely low or high values were obtained and the PTF did not appear to suit Irish data sets. The best remaining 12 PTFs for the various horizon types were then selected for use in further investigation (Table 2). These PTFs were chosen from the particular papers due to their development using: high sample number ($n > 100$); sampling depth to at least 80 cm; wide range of soils covered and statistical evaluation (R^2). In most cases topsoils and subsoils were investigated and in others particular horizon types were investigated. For mineral soils eight PTFs were applied: Manrique and Jones (1991), Bernoux et al. (1998), Leonavičiutė (2000) (×4); Kaur et al. (2002) (×2). For organic soils four PTFs were applied: Jeffrey (1970), Harrison and Bocock (1981), Manrique and Jones (1991), and Tamminen and Starr (1994) (Table 2). As these PTF required soil organic carbon data, soil texture data and loss on ignition data, the methods below were applied to samples from the field campaign.

2.6 Soil organic carbon analysis

The soil was placed on aluminium trays and placed in an oven at 40 °C for four days. The dry weight was recorded and the soil sieved to 2 mm and stored. A LECO True-Spec CN elemental analyser was used to measure SOC. Concentrated hydrochloric acid was used to remove inorganic carbon. The method followed that of Massey et al. (2014), which is an adaptation of Organic Application Note of the analysis of Carbon and Nitrogen in Soil and Sediment (LECO Corporation). This method corresponds to ISO 10694: 1995 – Soil quality Part 3: Chemical methods Section 3.8 – Determination of organic and total carbon after dry combustion (elemental analysis). The soils in the AFT survey had organic carbon estimated by the Walkley-Black dichromate oxidation method as described by Jackson (1958) and modified for colorimetric estimation.

2.7 Soil texture analysis

The different particle sizes in the soil (sand, silt, clay) were determined via the pipette method. The premise of this method is based on Stokes Law where the relationship between particle grain size and settling velocity in a fluid medium is predictable. A subsample of 2 mm dried and sieved soil was initially treated with hydrogen peroxide to remove all organic matter. Then it was suspended in a dispersant, sodium hexametaphosphate. Then finally 25 mL of the suspension were removed at exact time periods following shaking to represent silt and then clay fractions. This method of Massey et al. (2014) followed the methodology stated by An Foras Talútais, National soil survey (1972). The work was conducted by NRM limited (Bracknell, Berkshire, United Kingdom) following USDA texture guidelines. An inter laboratory study was conducted to ensure continuity in the methodology between Teagasc and NRM. NRM carried out the analysis and Teagasc repeated the same procedure on 10 % of the samples to ensure accuracy in the method applied.

2.8 Loss on ignition

The soil organic matter content was estimated via loss on ignition (LOI) of any sample found to be over 10 % organic carbon via the elemental analyser or if the sample was labelled organic from the field. A subsample of the 2 mm dried and sieved soil was dried initially at 105 °C cooled and reweighed and then placed in a muffle furnace at 550 °C for 16 h. The difference in mass was equivalent to the organic matter content. This method is described in detail by Massey et al. (2014), which corresponds to BS EN 13039:2000 – Soil improvers and growing media – Determination of organic matter content and ash.

2.9 AFT and Irish SIS horizons

The horizon designations in the AFT survey were correlated to modern Irish Soil Information System definitions (Table 1). The AFT designations were based on the soil horizon classification of soil survey staff, USDA (1960). When the equivalent horizon designation was identified the newly derived PTF could be applied to all horizons of this type. The soil horizon designation Ah indicating a lack of cultivation had no equivalent in the AFT records. The AFT survey did not record a non-cultivated A horizon.

2.10 Evaluation of PTFs

The individual ρ_b values were grouped together based on horizon designation. Each individual observed ρ_b value was predicted by each of the eight PTF in the case of mineral soils and the four PTF in the case of organic soils. A polynomial regression equation was generated for observed versus predicted ρ_b within each horizon type per PTF. The coefficient of determination (R^2) was compared across the PTF (Fig. 2a and Table 4).

The same data points were then compared using complementary prediction quality indices (De Vos et al., 2005). Here the quality of the prediction was determined via

Eq. (2), the mean predicted error (MPE); Eq. (3), the standard deviation of the prediction error (SDPE); Eq. (4), the root mean squared prediction error (RMSPE); and Eq. (5) and the prediction coefficient of determination (R_p^2). These are defined as:

$$\mathrm{MPE} = \frac{1}{n}\sum_{i=1}^{n}(\widehat{\mathrm{Pb},i} - \mathrm{Pb},i) \tag{2}$$

$$\mathrm{SDPE} = \sqrt{\frac{1}{n-1}\sum\nolimits_{i=1}^{n}\left((\widehat{\mathrm{Pb},i} - \mathrm{Pb},i) - \mathrm{MPE}\right)^2} \tag{3}$$

$$\mathrm{RMSPE} = \frac{1}{n}\sum_{i=1}^{n}(\widehat{\mathrm{Pb},i} - \mathrm{Pb},i)^2 \tag{4}$$

$$R_\mathrm{p}^2 = \frac{[\mathrm{cov}\ \mathrm{Pb},i,\widehat{\mathrm{Pb},i}]^2}{\mathrm{var}(\mathrm{Pb},i) - \mathrm{var}\ \left(\widehat{\mathrm{Pb},i}\right)} \tag{5}$$

where Pb,i and $\widehat{\mathrm{Pb},i}$ are the observed and predicted ρ_b values, respectively; n the number of observations; and var and cov, variance and the covariance function, respectively. MPE allows the evaluation of the bias of the PTF. The SDPE shows the random variation of the predictions after correction for global bias. The RMSPE is the overall error of the prediction. R_p^2 is a measure of the strength of the linear relationship between measurements and predictions, and indicates the fraction of the variation that is shared between them. The PTF generating the various R_p^2 values were compared (Table 5).

2.11 Calibration of the PTF

Using the prediction quality indices, the PTF selected per horizon was determined based on the highest R_p^2 value (Table 6). Once, the PFT was selected, it was updated using Irish data. For this, all data was divided into 2 groups, using 80 % of the data for the calibration process and 20 % for the validation model. These 2 groups were randomly selected. The validation dataset is independent of the calibration dataset but both are representative of the same soils. This is due to both datasets having the same sampling and analysis methods used, therefore the validation can be considered internal.

A particular PTF was then recalibrated using 80 % of the observed data points, randomly selected to generate a new model equation for that particular horizon type. Coefficients of the selected PTF were updated using multiple regression analysis (Table 7).

2.12 Model validation

After the recalibration the validation process was applied, using 20 % of the observed data points, again randomly selected. In some cases there were too few data points when 20 % of the observations were extracted. In this instance no validation could be performed, this affected four horizons (Bs, Bt, C/Ck/Cr and E, Table 7).

2.13 Digital Soil Mapping (DSM) techniques

The application of PTF has facilitated the prediction of soil bulk density for each genetic horizon for a total of 809 soil profiles. The availability of this bulk density data allowed the development of maps derived upon these data points. Depths of the horizons were recorded, but these were not consistent across all sites as indicated earlier. Therefore, to obtain the bulk density at the different depths the horizon average was used (average of horizons that fall within the depth criterion).The horizon average was used for estimating bulk density at 0–30 and 30–50 cm depths (Fig. 4a and b). The DSM technique applied was a model which utilised the Universal Kriging method in R software. This involved the development of surface grids from the above profile bulk density data using spatial analyst interpolation.

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3 Results

3.1 Bulk density

The observed ρ_b values were grouped together based on horizon designation (Ap, Ap1, Ap2, Apg, Ah, O, E, AB, Bw, Bg, Bs, Bt, Btg, BC, BCg, C/Ck/Cr and Cg) and statistics applied in preparation for PTF application (Table 3).The minimum number of replicates per horizon type was seven for the Bs horizon and the maximum number of replicates per horizon was 111 for Ap. Horizons Ap1 and Ap2 are generally considered unique to Ap, this reflects the adoption of shallow till ploughing in some areas, however the bulk densities of both were similar, 1.044 and 1.072 g cm^{-3}, respectively. These designations were not unfounded as Ap horizons were generally lower (0.976 g cm^{-3}) when compared to Ap1 and Ap2 horizons. The largest bulk density was in Cg horizons (1.566 g cm^{-3}) and the lowest in the O horizons (0.329 g cm^{-3}). The Bt horizons had the lowest standard deviation and co-efficient of variation, 0.036 and 2.75 %, respectively. The O horizons had the largest co-efficient of variation at 11.854 %.

3.2 Application of pedotransfer functions

The selected eight mineral PTF and four organic PTF were applied to all horizon types (Table 4). The coefficient of determination for each PTF used, are presented in Table 4. Those highlighted in bold, indicate the highest R^2 value for a particular horizon type. This may span multiple PTF, for example horizon Ap, has an R^2 value of 0.57 using the Kaur, Kaur intrinsic and Manrique and Jones equations. The highest selected R^2 value from all the PTF was for horizon Bt at 0.99, this was for both Bernoux and Kaur PTFs. The lowest selected R^2 value for a specific horizon was the Bg with 0.32 using Manrique and Jones PTF. The highest R^2 value for O horizons was 0.49 using the Taminen and Starr PTF.

Using the Ap horizon as an example, the plot of observed versus predicted ρ_b values for all mineral PTFs are presented in Fig. 2a. For O horizons the plot of observed

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versus predicted ρ_b values are presented in Fig. 2b. In both cases the regression equations and coefficients of determination are included in the plot. In the case of the Ap horizon, the Manrique and Jones PTF has all values positive for the predictions. For Kaur many of the predicted data points are negative as are those for the Kaur intrinsic PTF. Coupled with the R^2 value of 0.57 Manrique and Jones appears to be the best fit PTF. The same principles were applied to the rest of the mineral horizon PTF. For the O horizons Taminen and Starr had the best R^2 value at 0.493, however this range contained negative values therefore the next highest R^2 value of 0.433 generated using Manrique and Jones was considered. Again on inspection this PTF also had generated negative values. The R^2 values of 0.251 for both Jeffrey and Harrison and Bocock were deemed too low to pursue even with all positive values. Taminen and Starr was finally selected as the PTF for further investigation.

3.3 Selection of the best PTF

The performance of the selected PTF were further scrutinised using the prediction quality indices. The first of the indices to be examined was the prediction coefficient of determination, R_p^2 , across the eight mineral and four organic PTF. In many cases where the R^2 was the same across two or more PTF (Table 4), there was a clear R_p^2 value, larger than the others (in bold, Table 5). For example Ap, where Manrique and Jones (0.53) is greater than Kaur and Kaur intrinsic at 0.48 and 0.42, respectively. The same situation occurred for horizon Ap1 (Leonavičiutė A) and Apg (Manrique and Jones). The best performing PTF based on R^2 value, changed for horizons Ap2, Ah, Bt, Btg, BC, BCg, Cg. C/Ck/Cr and E, due to a higher R_p^2 value with a different PTF. For horizons AB, Bw, Bg, Bs and O the original best performing PTF based on highest R^2 value, was still appropriate, displaying the highest R_p^2, value also.

In Table 6 other indices were applied (MPE, SDPE and RMSPE) to support the most appropriate PTF selection. In general, the results show a positive MPE indicating an overestimation of ρ_b values (Table 6). However, horizons Apg, Ah, Cg and O displayed a negative MPE indicating an underestimation of ρ_b values. The Bg horizon displayed the highest accuracy with a low MPE value of 0.055 g cm^{-3}, whereas the AB horizon had the poorest level of accuracy (0.538 g cm^{-3}).

RMSPE is the overall prediction error; this was highest with horizon O, 0.666 g cm^{-3}, and lowest for horizon E, 0.082 g cm^{-3}, (Table 6). The prediction coefficient of determination (R_p^2) had a large range from 0.142 (Ap2) to 0.957 (Bt) and a median of 0.516 (BC). This was indicating that for horizons Ap2, Bg and BCg there was low correlation and hence an unstable prediction. The SDPE value was converging to RMSPE value for horizons Ap, Apg, Bg, Cg and O, therefore overall predictive error was due to precision error (SDPE). In contrast the total error was due to accuracy in the case of AB horizons with the large difference between the SDPE value and RMSPE value (0.406 g cm^{-3}). There was no pattern where low or high levels of MPE, SDPE or RMSPE or combinations thereof, resulted in a higher R_p^2 value.

The observed and predicted ρ_b values are presented in a box and whisker plot in Fig. 3. These predicted values are calculated using the selected PTF based on R_p^2 values of Table 6. The horizons with low accuracy (MPE) are evident in the case of AB, Bs, Bt and C. Furthermore there is no overlap in the position of the interquartile ranges of the observed and predicted box and whisker plots. Those with good accuracy Apg, Bg, Cg and E are evident as the red (observed) and blue (predicted) median bars are closer in position. In most cases for deeper and normally denser horizons, the interquartile range of ρ_b values are generally greater in the predictions than the observed. The max and min spread of the data (between 0.2 to 0.3 g cm^{-3}) is much narrower than the observed data ranges for horizons Bs, Bt, Btg, BC, BCg and C.

3.4 Recalibration of the selected PTF

Having selected the best performing PTF for each horizon type using the prediction quality indices, 80 % of the observed dataset was randomly selected for the recalibration of the PTF. The recalibrated PTF are presented in Table 7. For Ap, Ap2, AB and

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Bg the Manrique and Jones intercept and coefficients have decreased due to lower densities in the dataset. The intercept and coefficients increased with this PTF for Apg, BC, C/Ck/Cr and Cg indicating higher densities in the data set. Leonavičiutė A (Ap1), Kaur intrinsic (Ah and Bt) and Leonavičiutė E (Bw), have decreased intercept and coefficients. Leonavičiutė B increased intercept and coefficients, in both the cases of recalibration for Btg and BC. Leonavičiutė E increased the coefficients and intercepts in the case of BCg and decreased in the case of E horizons.

The R_p^2 values have increased in most cases following recalibration (Table 7 compared to Table 6), especially in the case of Ah, Bs and BCg (0.254, 0.237 and 0.353) however, there was a slight decrease for Ag and Bg horizons (0.129 and 0.041).

3.5 Validation of the recalibrated PTF

Validation has improved the coefficient of determination once again (Table 7), where 20 % of the observed values were again randomly selected and R^2 generated. There have been increases in the R^2 validation values in comparison to the R_p^2 values of 0.3 or more for Ap2, AB, Bg, Cg, BCg and O. There was a large decrease for BC (0.323) and a small decrease for Ap1 and Btg (0.156 and 0.123). Except for horizon BC all other horizons have an R^2 of at least 0.47 or higher. Horizon BC with a low correlation (0.257) would have an unstable predictability. For horizons Bs, Bt, C and E there were not enough data points in the validation dataset of 20 % to generate any validation indices.

3.6 Indicative soil bulk density map

Having bulk density data measured per horizon allowed the prediction of ρ_b in horizons where there were no measurements. This allowed gap filling in the Irish SIS and AFT profile data. In combination with mapping units from the latest edition of the Irish soil map and the methodology described above, a ρ_b map of Ireland was produced (Fig. 4). These maps highlight that lower bulk densities are found at the surface (0–30 cm) which is consistent with expected findings in relation to soil types and management, due in principle to higher soil organic carbon in these soils. The bulk density ranges from < 0.79 to $> 1.1\,\mathrm{g\,cm^{-3}}$ (Fig. 4a) At increasing depths, 30–50 cm, higher bulk density values are likely to be found (< 1.0 to $> 1.4\,\mathrm{g\,cm^{-3}}$). In general the bulk densities are lower in mountainous and hill areas and higher in lowland areas for both depth ranges.

4 Discussion

4.1 Observed ρ_b values

The observed ρ_b values across all horizons have a mean of $1.187\,\mathrm{g\,cm^{-3}}$ with a standard deviation of $0.305\,\mathrm{g\,cm^{-3}}$. Removing the O horizon value of $0.329\,\mathrm{g\,cm^{-3}}$, the mean and standard deviation are 1.214 and $0.217\,\mathrm{g\,cm^{-3}}$, respectively. This mean value compares favourably to Manrique and Jones (1991) on a range of agricultural soils 1.2–$1.5\,\mathrm{g\,cm^{-3}}$. The ForSite study of DeVos et al. (2005) reported another comparable value of $1.23\,\mathrm{g\,cm^{-3}}$ for topsoil. This value also compares well to the subsurface soils of Harrison and Bocock (1991), $1.29\,\mathrm{g\,cm^{-3}}$, and forest soils of Taminen and Starr, $1.19\,\mathrm{g\,cm^{-3}}$.

Kiely et al. (2010), looking in particular at Irish soils to 50 cm depth found bulk densities for Brown Earths in the range of 1.02 to $1.22\,\mathrm{g\,cm^{-3}}$,Brown Podzolics 0.94 to $1.07\,\mathrm{g\,cm^{-3}}$, Gleys and Grey Brown Podzolics (Luvisols) 0.86 to $1.3\,\mathrm{g\,cm^{-3}}$ and Podzols 0.53 to $1.23\,\mathrm{g\,cm^{-3}}$. Reidy and Bolger (2013) reported ρ_b values of 1.018 to $1.063\,\mathrm{g\,cm^{-3}}$ on Gley soils in the Irish midlands to 30 cm depth. The generally higher levels in this study may be attributable to the greater depth studied and reported ρ_b increase with depth. This study's measured ρ_b values are well within the general ranges reported nationally and internationally. The O horizon value of $0.329\,\mathrm{g\,cm^{-3}}$, in this study appears to be greater than those reported in the literature. Wellock et al. (2011) report ρ_b values for Irish Raised, High and Low level blanket peats of 0.133, 0.118 and $0.125\,\mathrm{g\,cm^{-3}}$ and Kiely et al. (2010) report values of 0.15 to $0.25\,\mathrm{g\,cm^{-3}}$, for Irish peat soils. It should be noted that the O horizons in this present study included only horizons with greater than 12 % organic carbon. It is likely that these other studies, which indicate lower ρ_b values, are due to the peats having at least 40 % organic carbon content.

Looking at the mean values per horizon, the use of this approach appears justified with the large differences between surface horizons and sub surface horizons (Ap, 0.976 g cm^{-3}, and Cg, 1.566 g cm^{-3}, Table 3). The difference between each type of surface horizon is also notable, where O horizons are 0.329, and Ap1 and Ap2 (while close together at 1.044 and 1.072 g cm^{-3}) are different from Ap, reflecting differences in organic matter content and management, respectively. Therefore where possible predictions for soil bulk density should be at horizon level rather than topsoil or subsoil categorisation.

To support this thinking, De Vos et al. (2005) noted that because of differences in topsoil and subsoil ρ_b values, PTFs developed using topsoil parameters only, which are being used to indicate ρ_b values in the subsoil, may lead to an underestimation. For this reason they developed topsoil and subsoil PTFs. An extension of this logic would be to use horizon specific PTFs, as applied in this paper. Because it was found that there were clearly significant differences in the PTF used according to the horizon type and this should be recognised in studies applying ρ_b down a profile to a specific depth.

The practice of splitting the bulk density of a singular profile into horizons has other advantages, especially when modelling systems. Many studies note that high levels of SOC are found at the surface particularly 0–30 cm depth. However more SOC could be found in the 30–100 cm range where the soils are denser. Adhikari et al. (2014) modelled ρ_b values using quadratic splines, when different horizon data was not available. This is a method to reflect the changes of ρ_b in soil profiles by using discrete soil depths. It was noted that accurate quantification of SOC stocks required a depth function. Tranter et al. (2007) also included a depth function when describing PTF based on soil mineral packing structures and soil structure. However it should also be noted that

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the fitting quality of splines to profile data depends on smoothing parameters, which introduces another source of error (Malone et al., 2009). In this study the data has been directly measured across the various horizons which avoids this error.

4.2 Application of literature PTF

The decision was made to apply our dataset to PTF derived from the literature and then recalibrate. De Vos et al. (2005) indicated that the global predictive capacity of these functions appeared to be amenable to further improvement. Martin et al. (2009) stated that recalibration of existing PTF is worthwhile as the PTF itself defining more generally a function type, may be valid across several regions. However caution is required as parameters obtained under the given conditions can be too dependent on the dataset characteristics. Generating new PTF from limited data could be prone to propagation of errors. In the Khalil et al. (2013) study for particular Great Groups, in Ireland, there was only SOC data to 10 cm available. The SOC had to be predicted to 50 cm and this predicted value was used once again to predict ρ_b values to 50 cm. This process was then repeated to generate values to 100 cm.

Nevertheless compartmentalisation of bulk density data also has its merits, Heusher et al. (2005) who analysed 47 000 measurements in the USDA survey improved the ρ_b predictions of their soils by placing the soils into suborders and then applying modelling techniques. The R^2 value improved from 0.45 to 0.62 in this process. Similar results were found by Manrique and Jones (1991) when they developed and applied the predictions within soil orders. This highlights an area for further investigation with data from the Irish SIS.

4.3 Recalibration of literature PTF

When recalibrating the PTF, it allowed the refinement of the equations for the Irish scenario. To date this is the most comprehensive model of Irish soils using the largest available dataset, with soil profile, soil horizon and depth coverage. The use of 80 %

of the data points also followed the accepted De Vos et al. (2005) method. Where the categorisation into horizon PTF is justified and the R^2 values increased or are equalled for 14 out of the 17 horizons studied (Table 6).

The study of Xu et al. (2011) desired more data for deeper soils and greater site number (in the Irish context) to calibrate that studies PTF. They had used 0–10 cm soil depth carbon values to predict, firstly carbon content to 50 cm depth and then to predict soil bulk density to 50 cm depth. The use of sequential empirical regressions in developing PTF can propagate errors (Meersmans et al., 2008). The use of a singular PTF for peat and mineral soils in Xu et al. (2011) study is also unlikely to be useful once actual peat ρ_b and SOC estimations at depth are required. This present study had both the depth and sample number data to calculate different PTF for various horizon types. The data generated in this study will avoid the propagation of errors described above and allow more accurate SOC calculation.

4.4 Validation of the recalibrated PTF

De Vos et al. (2005) emphasised the need for recalibration and local validation. This would aid the decision making process with reference to the level of what prediction error is acceptable. Getting this right is crucial as it has been recognised that correction factors led to an increase in the Belgian SOC prediction by 22 %, which also affected their projections due to landuse change and climate change (Lettens et al., 2007). Although prediction errors between 10 and 20 % were deemed acceptable in the study of Prévost (2004). Huang et al. (2003) state that model acceptance would require between 10 and 20 % of the variance observed. For horizons with many replicates such as Ap ($n = 111$), the MPE falls within this criteria 0.067 g cm^{-3}, or 6.8 % of 0.976 g cm^{-3}. However this is not the case for many other horizon types which clearly need more replicates for example Bs ($n = 7$) MPE is 0.488 g cm^{-3}, or 44 % of 1.086 g cm^{-3}. Though, in most cases where a validation could be performed the predicted coefficient of variation was equalled or improved (R_v^2, Table 7).

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4.5 Mapping application

With the bulk density maps to 0–30 and 30–50 cm depth, the potential of these pedotranfer functions is realised. In Ireland there currently is no national map of soil carbon values, primarily due to the lack of bulk density data and also depth coverage. The National Soil Database project (2001-CD/S2-M2) measured 1365 points for organic carbon to 10 cm, however it did not measure bulk density. The SoilC project (Kiely et al., 2010) measured bulk density and organic carbon to 50 cm depth although this project was limited on number of sites ($n = 62$). Any studies deeper than 10 cm were in localised areas which did not allow extrapolation to the national area. Forest soils were covered in CARB*i*FOR 1 and CARB*i*FOR 2 projects, where soils were surveyed to 50 cm depth. ρ_b was measured but site number was restrictive ($n = 44$). However, in both cases mapping criteria were not developed for greater areas. Most SOC studies and inventories are confined to 30 cm soil depth but the amount of SOC stored below 30 cm is of relevance in many ecosystems (Adhikari et al., 2014).

The PTF developed in this study allows the estimation of national organic carbon coverage of all soil types to 1 metre depth with bulk density. This deficit of data was recognised with the initial development and is now further realised because of the recent availability of the Irish soil information system and its carbon data (Creamer et al., 2014). The same set of principles of method development of the PTF and mapping application could be applied to any national dataset lacking in bulk density coverage.

5 Conclusions

The ρ_b values reported for horizon type allowed a greater range of soils in the Irish SIS to have ρ_b values allocated in the cases where there are omissions and to depth (recommended 1 m). The same process was applied to the AFT samples that did not have ρ_b values measured in the field. This paper covers the methodology of producing soil horizon PTF given the measured data available. Related predictions are based on

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the best data available after screening for accuracy and precision of PTF; they were then recalibrated and eventually validated within the Irish scenario. The methodology enabled the researcher to return to the Irish SIS to produce a validated ρ_b map at two depths, 0–30 and 30–50 cm (details of validation of map are given in Simo et al., 2015). Now that a ρ_b value is available for the different soil depths, values could be attributed to each soil mapping unit using Irish SIS into the future. Potentially this data could then be combined with known carbon data to produce a soil carbon map to 1 m. The data could also be used to produce a drainage map for the country. Another area for potential use would be the PTF used in hydrology studies, which use bulk density values. Furthermore, where nutrient management is a concern in soils, areas prone to compaction can be identified via this map. The PTF produced are valid for some horizons (with large R^2 values) and have limited success with other horizons. It is hoped in time as the sample number of these rarer horizons increases that the accuracy of the prediction increases. In general the greater sample number the better the prediction and validation.

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Table 1. Irish SIS horizon designations used in this study and equivalent horizon titles used in the national soil survey by An Forais Talúntais.

Irish SIS	An Forais Talútais
O	O, Oh
Ap	A, A1
Ap1	A11
Ap2	A12, A13
Apg	A/C, A11g, A12g, A13g
Ah	N/A
AB	A/B, A3, A14g
Bw	B, B1, B2, B21, B21h, B22, B3
Bg	B1g,
Bs	Bsh,
Bt	Bth, Bts, Btc
Btg	Btgh, Btgs, Btgc
BC	BCtg, Bct, Bcg
BCg	B2ca, 2Bca, Bca1
Cg	A/Cg
C/Ck/Cr	C1, C2, C3
E	A2, A21, A22, A23m, II1, II2

Table 2. Published pedotransfer functions with corresponding authors used in this study. OC is organic carbon. ρ_b is bulk density in $\mathrm{g\,cm^{-3}}$.

Author(s)	Pedotransfer function
Manrique and Jones	$\rho_b = 1.660 - 0.318(\mathrm{OC})^{0.5}$
Bernoux et al.	$\rho_b = 1.398 - 0.0047(\mathrm{Clay}) - 0.042(\mathrm{OC})$
Kaur intrinsic	$\mathrm{Ln}(\rho_b) = 0.313 - 0.191(\mathrm{OC}) + 0.02102(\mathrm{Clay}) - 0.000476(\mathrm{Clay})^2 - 0.00432(\mathrm{Silt})$
Kaur et al.	$\rho_b = 1.506 - 0.266(\mathrm{OC}) + 0.004517(\mathrm{Clay}) - 0.00352(\mathrm{Silt})$
Leonavičiutė A	$\rho_b = 1.70398 - 0.00313(\mathrm{Silt}) + 0.00261(\mathrm{Clay}) - 0.11245(\mathrm{OC})$
Leonavičiutė B	$\rho_b = 1.07256 + 0.032732\ \ln(\mathrm{Silt}) + 0.038753\ \ln(\mathrm{Clay}) + 0.078886\ \ln(\mathrm{Sand}) - 0.054309\ \ln(\mathrm{OC})$
Leonavičiutė BC	$\rho_b = 1.06727 + 0.01074\ \ln(\mathrm{Silt}) + 0.08068\ \ln(\mathrm{Clay}) + 0.08759\ \ln(\mathrm{Sand}) + 0.05647\ \ln(\mathrm{OC})$
Leonavičiutė E	$\rho_b = 0.99915 - 0.00592\ \ln(\mathrm{Silt}) + 0.07712\ \ln(\mathrm{Clay}) + 0.09371\ \ln(\mathrm{Sand}) - 0.08415\ \ln(\mathrm{OC})$
Jeffrey	$\rho_b = 1.482 - 0.6786\ \log_{10}(\mathrm{LOI})$
Harrison and Bocock – topsoil	$\rho_b = 1.558 - 0.728\ \log_{10}(\mathrm{LOI})$
Harrison and Bocock – subsoil	$\rho_b = 1.729 - 0.769\ \log_{10}(\mathrm{LOI})$
Tamminen and Starr	$\rho_b = 1.565 - 0.2298\ (\mathrm{LOI})^{0.5}$

Table 3. Statistics of observed bulk density, ρ_b (g cm^{-3}) for each horizon type, used in the development of pedotransfer functions.

Hz type	*N*	Mean ρ_b Observed	Standard deviation	Co-efficient of variation	Min	Max	Variance
E	9	1.347	0.090	6.682	0.911	1.687	0.077
Ap	111	0.976	0.071	7.275	0.475	1.514	0.039
Ap1	28	1.044	0.061	5.843	0.386	1.289	0.035
Ap2	16	1.072	0.069	6.437	0.817	1.331	0.014
Apg	18	1.180	0.047	3.983	0.626	1.789	0.076
Ah	16	0.879	0.043	4.892	0.624	1.483	0.037
AB	12	1.014	0.075	7.396	0.881	1.373	0.020
O	20	0.329	0.039	11.854	0.196	0.777	0.032
Bw	52	1.147	0.094	8.195	0.758	1.844	0.053
Bg	56	1.381	0.080	5.793	0.902	1.762	0.035
Bs	7	1.086	0.058	5.341	0.710	1.353	0.052
Bt	8	1.307	0.036	2.754	0.907	1.501	0.058
Btg	15	1.521	0.072	4.734	1.131	1.770	0.033
BC	15	1.444	0.084	5.817	0.770	1.754	0.051
BCg	15	1.498	0.067	4.473	1.146	1.859	0.044
C/Ck/Cr	21	1.396	0.088	6.304	0.487	1.833	0.089
Cg	12	1.566	0.067	4.278	1.146	1.949	0.049

Table 4. Co-efficient of determination values (R^2) when comparing original bulk density values to predicted values for each horizon type, using the listed pedotransfer functions.

Author	Bernoux	Kaur	Kaur	Leonaviciuté				Manrique Jones	Jeffrey	Harrison and Bocock	Tamminen and Starr	*N*
HORIZON	(1998)	(2002)	(2002) intrinsic	(2000) (A)	(2000) (B)	(2000) (BC-C)	(2000) (E)	(1991)	(1970)	(1981) Topsoil	(1994)	
Ap	0.46	**0.57**	**0.57**	0.56	0.42	0.43	0.40	**0.57**				111
Ap1	0.57	**0.74**	0.60	**0.74**	0.54	0.52	0.52	0.70				29
Ap2	**0.48**	0.36	0.25	0.36	0.30	0.35	0.26	0.36				16
Apg	0.59	**0.69**	0.50	**0.69**	0.59	0.55	0.55	**0.69**				18
Ah	0.34	0.34	0.42	0.36	0.13	0.17	**0.43**	0.31				16
AB	0.34	0.59	0.38	0.58	0.60	0.59	0.55	**0.63**				12
Bw	0.09	0.32	0.21	0.35	0.33	0.10	**0.36**	0.28				52
Bg	0.21	0.22	0.04	0.19	0.25	0.19	0.25	**0.32**				56
Bs	0.36	0.64	0.43	**0.79**	0.50	0.65	0.57	0.31				7
Bt	**0.99**	**0.99**	0.96	0.96	0.82	0.84	0.78	0.96				8
Btg	0.57	0.59	0.21	0.40	0.65	0.18	0.63	**0.69**				15
BC	0.09	0.55	0.26	0.41	0.58	0.28	0.55	**0.59**				15
C/Ck/Cr	0.06	0.22	0.12	0.09	0.33	0.03	0.27	**0.34**				21
Cg	0.02	**0.71**	0.52	0.63	0.39	0.33	0.41	0.64				12
BCg	**0.41**	0.07	0.24	0.09	0.26	0.33	0.26	0.19				15
E	0.48	0.61	**0.78**	0.62	0.52	0.44	0.57	0.49				9
O								0.43	0.25	0.25	**0.49**	20

Table 5. Co-efficient of determination values (R_p^2) when comparing original bulk density values to predicted values for each horizon type, using complimentary prediction quality indices (De Vos et al., 2005).

Author	Bernoux	Kaur	Kaur	Leonaviciuté				Manrique and Jones	Jeffrey	Harrison and Bocock	Tamminen and Starr
HORIZON	(1998)	(2002)	(2002) intrinsic	(2000) (A)	(2000) (B)	(2000) (BC-C)	(2000) (E)	(1991)	(1970)	(1981) Topsoil	(1994)
Ap	0.43	0.48	0.42	0.47	0.41	0.45	0.38	**0.53**			
Ap1	0.43	0.62	0.56	**0.62**	0.50	0.30	0.50	0.60			
Ap2	0.02	0.06	0.08	0.06	0.02	0.04	0.03	**0.14**			
Apg	0.52	0.61	0.47	0.60	0.56	0.55	0.53	**0.64**			
Ah	0.01	0.10	**0.37**	0.10	0.01	0.05	0.00	0.07			
AB	0.46	0.54	0.20	0.52	**0.66**	0.45	0.60	0.59			
Bw	0.05	0.27	0.21	0.28	0.29	0.06	**0.32**	0.23			
Bg	0.12	0.20	0.00	0.19	0.15	0.08	0.17	**0.20**			
Bs	0.01	0.46	0.17	**0.55**	0.12	0.14	0.54	0.17			
Bt	0.61	0.59	**0.96**	0.58	0.50	0.37	0.51	0.69			
Btg	0.48	0.37	0.20	0.29	**0.53**	0.02	0.49	0.42			
BC	0.00	0.43	0.25	0.26	**0.52**	0.25	0.48	**0.50**			
C/Ck/Cr	0.05	0.22	0.11	0.08	**0.28**	0.01	0.25	0.26			
Cg	0.02	0.34	0.19	0.21	0.35	0.32	0.31	**0.47**			
BCg	0.01	0.07	0.00	0.09	0.15	0.02	**0.17**	0.06			
E	0.10	**0.53**	0.29	**0.52**	0.51	0.06	0.52	0.48			
O								0.00	0.24	0.24	**0.31**

Table 6. The mean predicted error (MPE, g cm $^{-3}$); the standard deviation of the prediction error (SDPE, g cm $^{-3}$); the root mean squared prediction error (RMSPE, g cm $^{-3}$); and the prediction coefficient of determination (R_p^2) using complimentary prediction quality indices (De Vos et al., 2005) for each horizon type and selected pedotransfer function type.

Horizon	Selected PTF	MPE	SDPE	RMSPE	R_p^2
Ap	Manrique and Jones	0.067	0.132	0.148	0.532
Ap1	Leonavičiutė A	0.246	0.137	0.280	0.619
Ap2	Manrique and Jones	0.110	0.117	0.158	0.142
Apg	Manrique and Jones	−0.058	0.174	0.179	0.640
Ah	Kaur (intrinsic)	−0.164	0.173	0.234	0.367
AB	Leonavičiutė B	0.538	0.151	0.557	0.660
Bw	Leonavičiutė E	0.425	0.206	0.471	0.318
Bg	Manrique and Jones	0.055	0.169	0.176	0.199
Bs	Leonavičiutė A	0.488	0.172	0.513	0.551
Bt	Kaur (intrinsic)	0.375	0.128	0.393	0.957
Btg	Leonavičiutė B	0.119	0.134	0.176	0.525
BC	Leonavičiutė B	0.232	0.189	0.295	0.516
C/Ck/Cr	Leonavičiutė B	0.275	0.158	0.315	0.276
Cg	Manrique and Jones	−0.085	0.159	0.175	0.471
BCg	Leonavičiutė E	0.173	0.262	0.307	0.169
E	Kaur	0.067	0.050	0.082	0.529
O	Tamminen and starr	−0.117	0.682	0.666	0.315

Table 7. Recalibrated pedotransfer functions (PTF) using Irish input data compared to measured bulk density. R_p^2R is the prediction coefficient of determination, R_v^2 is the validation coefficient of determination, bothbased on prediction quality indices (De Vos et al., 2005). ρ_b is bulk density (g cm $^{-3}$). OC is organic carbon.

Horizon	Original PTF	PTF recalibrated	R_p^2	R_v^2
Ap	Manrique and Jones	Db = 1.5228 − 0.2806 (OC∧0.5)	0.544	0.540
Ap1	Leonavičiutė A	Db = 1.26841 − 0.0010264 (silt) + 0.004514 (clay) − 0.092491 (OC)	0.709	0.553
Ap2	Manrique and Jones	Db = 1.3377 − 0.16927 (OC∧0.5)	0.137	0.931
Apg	Manrique and Jones	Db = 1.705925 − 0.342497 (OC∧0.5)	0.758	0.899
Ah	Kaur (intrinsic)	Ln(Db) = 0.228477 − 0.089759 (OC) + 0.0064201 (Clay) +0.0004778 (clay∧2) − 0.00963 (Silt)	0.621	0.744
AB	Manrique and Jones	Db = 1.3966572 − 0.256208 (OC∧0.5)	0.531	0.957
Bw	Leonavičiutė E	Db = −3.255 + 0.1517 (Ln(Silt)) + 0.4519 (Ln(Clay)) + 0.667 (Ln(Sand)) − 0.183 (Ln (OC))	0.472	0.560
Bg	Manrique and Jones	Db = 1.588 − 0.302 (OC∧0.5)	0.158	0.527
Bs	Leonavičiutė A	Db = 1.4809 − 0.0116 Silt + 0.02937 Clay − 0.64738 OC	0.788	NA
Bt	Kaur (intrinsic)	Ln(Db) = 0.208123 − 0.00139 Silt + 0.002082 Clay+0.000343(Clay∧2)−0.1867*OC	0.974	NA
Btg	Leonavičiutė B	Db = 1.241791 − 0.02586 Ln (Silt) − 0.01709 Ln (Sand) −0.07708 Ln (OC)	0.594	0.471
BC	Manrique and Jones	Db = 1.8618 − 0.839 (OC∧0.5)	0.580	0.257
C/Ck/Cr	Manrique and Jones	Db = 1.773479 − 0.832265 (OC∧0.5)	0.329	NA
Cg	Manrique and Jones	Db = 1.859853 − 0.477253 (OC∧0.5)	0.668	0.994
BCg	Leonavičiutė E	Db = 1.6969 + 0.2297 Ln (Silt) − 0.1102 Ln(Clay) − 0.1303 Ln (Sand) + Ln (OC)	0.522	0.987
E	Leonavičiutė E	Db = −9.74290 + 1.282390 Ln (Silt) + 0.6351 Ln (Clay) +1.222 Ln (Sand) − 0.30286 Ln (OC)	0.562	NA
O	Tamminen and starr	Db = 0.715618 − 0.05471 (LOI∧0.5)	0.453	0.821

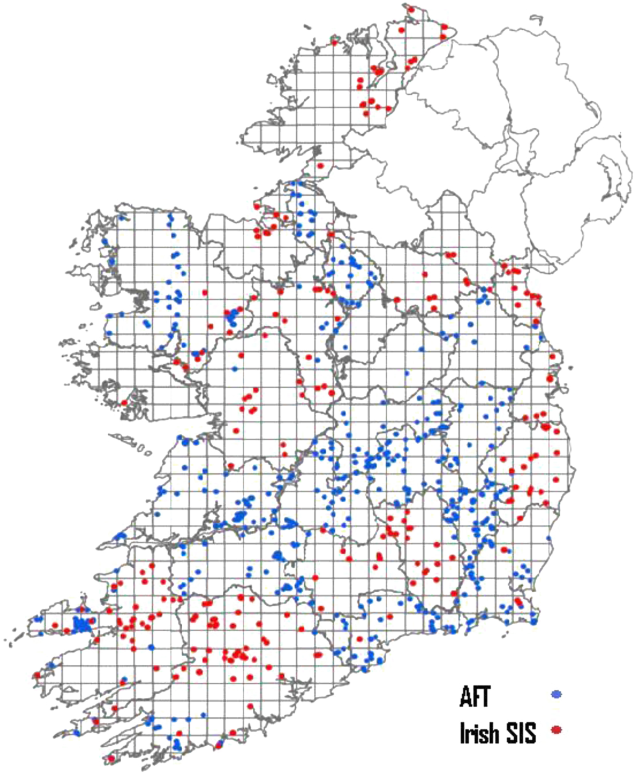

Figure 1. Location of Irish soil information system (Irish SIS) and An Forais Talútais (AFT) soil profile pits. The blue circles correspond to AFT and the red circles correspond to Irish SIS.

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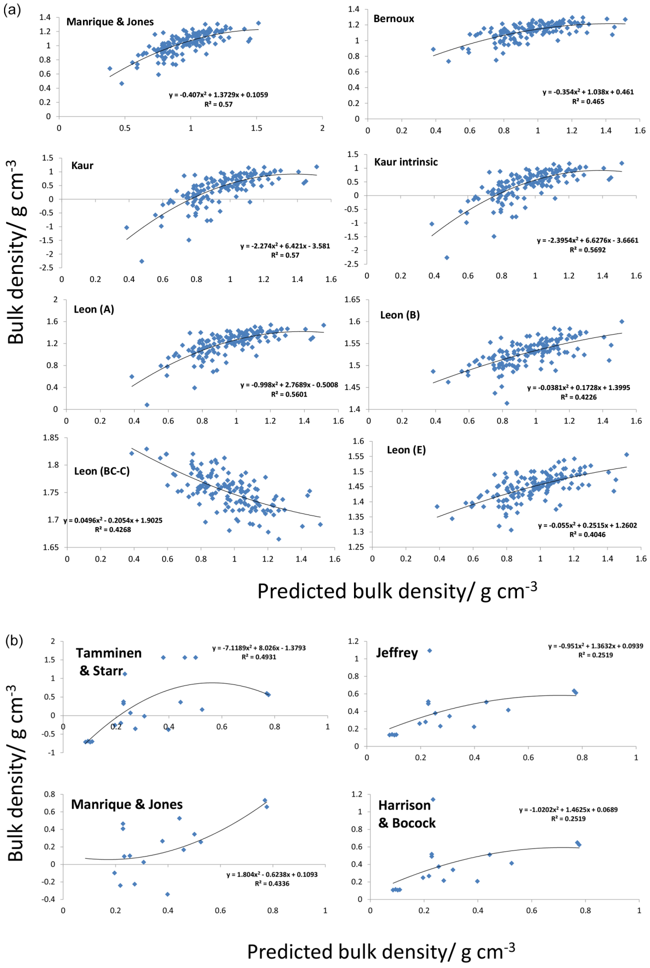
(a)
Bulk density/ g cm-3
Manrique & Jones
y = -0.407x² + 1.3729x + 0.1059
R² = 0.57
Bernoux
y = -0.354x² + 1.038x + 0.461
R² = 0.465
Kaur
y = -2.274x² + 6.421x - 3.581
R² = 0.57
Kaur intrinsic
y = -2.3954x² + 6.6276x - 3.6661
R² = 0.5692
Leon (A)
y = -0.998x² + 2.7689x - 0.5008
R² = 0.5601
Leon (B)
y = -0.0381x² + 0.1728x + 1.3995
R² = 0.4226
Leon (BC-C)
y = 0.0496x² - 0.2054x + 1.9025
R² = 0.4268
Leon (E)
y = -0.055x² + 0.2515x + 1.2602
R² = 0.4046
Predicted bulk density/ g cm-3
(b)
Bulk density/ g cm-3
Tamminen & Starr
y = -7.1189x² + 8.026x - 1.3793
R² = 0.4931
Jeffrey
y = -0.951x² + 1.3632x + 0.0939
R² = 0.2519
Manrique & Jones
y = 1.804x² - 0.6238x + 0.1093
R² = 0.4336
Harrison & Bocock
y = -1.0202x² + 1.4625x + 0.0689
R² = 0.2519
Predicted bulk density/ g cm-3

Figure 2. (a) Observed bulk density values for horizon Ap compared to prediction for original PTF formulae used indicating coefficient of variation equation and R^2 values. **(b)** Observed bulk density values for horizon O compared to prediction for original PTF formulae used indicating coefficient of variation equation and R^2 values.

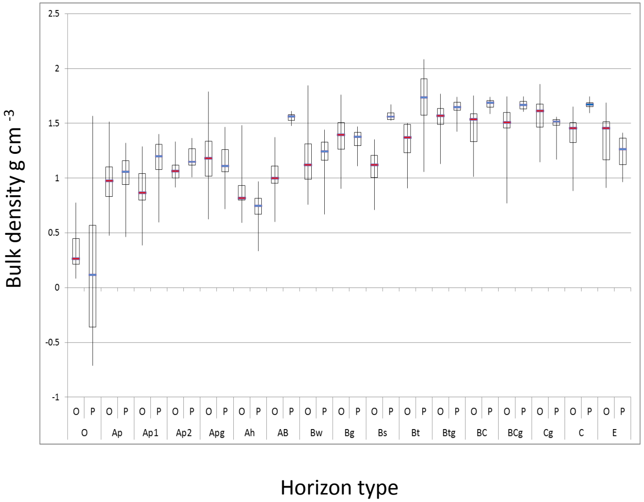

Figure 3. Observed bulk density (O) and predicted bulk density (P) g cm^{-3}, for each horizon type. Prediction based on selected PTF with best R_p^2R following prediction quality indices.

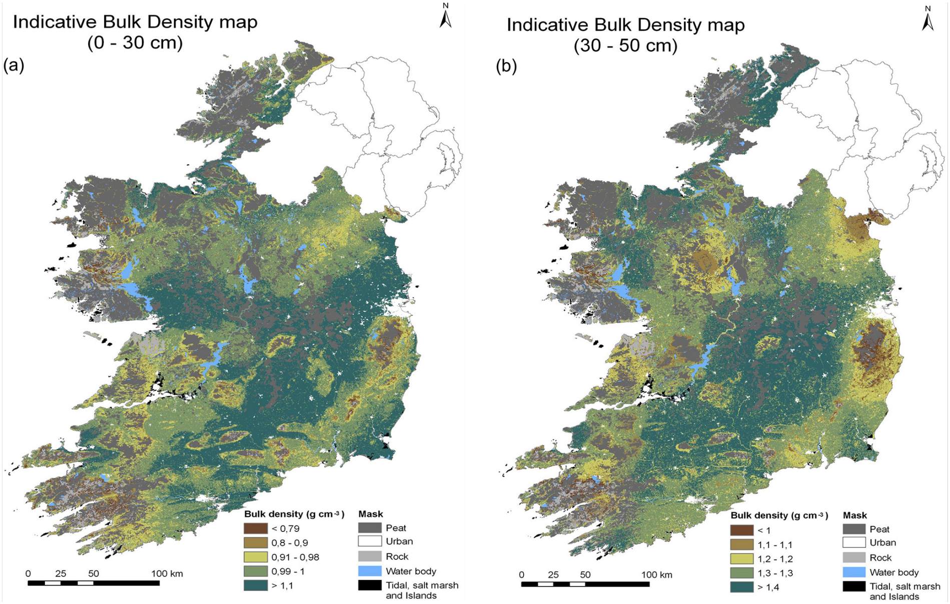

Figure 4. (a) Indicative soil bulk density distribution map for Ireland (0–30 cm, g cm^{-3}). **(b)** Indicative soil bulk density distribution map (30–50 cm, g cm^{-3}).

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