

# 1 **Pedotransfer functions for Irish soils - estimation of bulk** 2 **density ( $\rho_b$ ) per horizon type**

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## 7 **Summary**

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

## 24 **Introduction**

25 Soils are a vital global resource providing a range of ecosystem services, upon which we  
26 depend. Such services include the platform on which we produce food, fibre and raw  
27 materials, purifying and regulating water, cycling of carbon and nutrients, and providing a  
28 habitat for biodiversity (EU, 2002). To understand many of the processes on-going in soils  
29 that deliver these ecosystem services, we must quantify soil characteristics, as these vary  
30 considerably according to soil type. Bulk density ( $\rho_b$ ) is defined as the oven-dry mass per unit  
31 volume of a soil (IUSS 20 Working Group, 2006). This is an integral soil property, as it not  
32 only describes the packing structure of soils (Dexter, 1988), but is essential for the  
33 measurement of soil carbon and nutrient stock assessment (Ellert & Bettany, 1995). Bulk  
34 density measures can also describe the permeability of a soil, whereby it defines drainage  
35 characteristics (Arya, & Paris, 1981) and is used in pedotransfer functions that model soil  
36 hydraulic characteristics (Murphy *et al.*, 2003, Van Alphen *et al.*, 2001 and Minasny 2007).  
37 Bulk density can also indicate compacted layers resulting from machinery or animal  
38 trafficking (Saffih-Hdadi, 2009), which can then impact the nutrient availability in soils  
39 (Douglas and Crawford, 1998).

40 Furthermore bulk density ( $\rho_b$ ) is a critical soil characteristic for soil carbon studies and  
41 modelling, it can indicate the amount/volume rather than the concentration of carbon at a  
42 given point. Soil organic carbon (SOC) pool stock calculation depends upon suitable data in  
43 terms of organic carbon content and soil bulk density, and on the methods used to upscale  
44 point data to comprehensive spatial estimates (Vanguelova *et al.*, 2015). The lack of  
45 appropriate bulk density documentation is problematic for statistical confidence assessments.  
46 Historically,  $\rho_b$  measurements are commonly missing from databases for reasons that include  
47 omission due to sampling/budgetary constraints and laboratory mishandling/conflicting

48 methodologies (Batjes, 2009). Pedotransfer functions (PTF) based on readily measured soil  
49 attributes, such as organic carbon and clay content, show strong potential to replace  $\rho_b$   
50 measurements as their direct measurement are not feasible or lacking from historical records.  
51 However, bulk density has been found to vary with depth (Leonavičiūtė, 2000) and soil type  
52 (Manrique and Jones, 1991), while the use of generic pedotransfer functions, can result in  
53 large errors in the calculation of SOC stocks. In saying this, De Vos indicates there is a need  
54 for specific PTF to be calibrated and validated on a regional basis (De Vos *et al.*, 2005).  
55 Others take this further and report that PTF should be developed for particular horizon types  
56 or designations (Suuster *et al.*, 2011). Correlation with international datasets can be employed  
57 to generate PTF where local information is lacking. There is information available from large  
58 international soil survey databases (Hollis *et al.*, 2006; Batjes, 2005, 2009), but in many cases  
59 bulk density is poorly documented. In these instances the use of splines or models of bulk  
60 density are then used with their own inherent variances, which can be problematic without  
61 large validation datasets (Lettens *et al.*, 2005).

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

66 The research presented in this paper will use new data generated by the Irish SIS to provide  
67 primary data for the calculation of PTF at the soil horizon level. This was done using soil  
68 bulk density measurements were available for 15.9% of the soil profiles described in Ireland  
69 in the last 40 years. In addition to this, PTF from the literature were used with known texture  
70 and organic carbon data, to develop the calculations for bulk density. These PTF were then

71 recalibrated for Irish soil horizons, where  $\rho_b$  was measured. The PTF were then applied to the  
72 soil horizons with unknown  $\rho_b$ . This allowed the calculation of soil bulk density to a depth of  
73 50 cm for all soil profiles described. Using the PTF, bulk density is now known at different  
74 horizon designations. This has led to an indicative map of soil bulk density in Ireland being  
75 developed.

## 76 **Materials and methods**

### 77 *Soil profiles*

78 From 2012 to 2014 the Irish SIS sampled 246 soil pits as part of its field survey. The pits  
79 were selected by using an extensive auger survey of the Irish SIS. Pits were dug in areas  
80 where a high density of augers were found representing a particular soil type. From a  
81 practical position multiple pits were selected within a 10 km x 10 km area when possible.  
82 This allowed excavation costs to be reduced greatly. The pits were distributed across 16  
83 counties in Ireland, Figure 1. At each site a pit was excavated to approximately 1 m, where  
84 this was not possible, it was excavated to the depth of underlying bedrock preceding this. The  
85 pit face was at least one metre wide. In total there were 1028 soil horizons identified. Within  
86 these pits, 470 horizons were sampled for bulk density ( $\rho_b$ ). The remainder could not be  
87 measured for bulk density as the stainless steel rings were unusable due to coarse fragments.  
88 Therefore these horizons (528) required  $\rho_b$  predictions and pedotransfer functions were  
89 developed for this, detailed below.

### 90 *Legacy data*

91 In addition, detailed descriptions of 560 soil profiles were available from legacy data  
92 collected under the An Foras Talúntais soil survey (AFT) conducted between the 1960s and  
93 1990s (An Foras Talúntais Staff, 1963, 1969 and 1973; Conry 1987, Conry and Ryan 1967,

94 Conry et al., 1970; Diamond and Sills, 2011; Finch and Ryan, 1966; Finch et al., 1971; Finch  
95 and Gardiner, 1977; Finch et al., 1983; Finch and Gardiner, 1993; Gardiner and Ryan, 1964;  
96 Gardiner and Radford, 1980; Hammond and Brennan, 2003; Kiely et al., 1974). However,  
97 very few bulk density measurements were taken as part of this survey, but detailed  
98 descriptions of soil horizons did exist, along with analytical data for a number of soil  
99 parameters, such as texture and SOC. In total there were 2950 horizons described across 809  
100 soil profiles located across the whole of Ireland, Figure 1.

### 101 *Field sampling*

102 In the centre of each horizon, a smooth undisturbed vertical soil surface was prepared for  $\rho_b$   
103 sampling. Three 50 mm x 50 mm stainless steel rings were hammered into place. When  
104 possible, the rings were taken at 25 cm, 50 cm and 75 cm from the edge of the pit wall. Care  
105 was taken to just fill the ring and not compact the soil. The ring plus soil was then removed  
106 from the surface of the soil matrix with as little disturbance as possible using a flat sided  
107 trowel. Any excess soil was trimmed from the ring edges before being placed in a sealed  
108 plastic bag. Also if protruding coarse fractions were present, they were marked and retained  
109 for cutting in the laboratory. For other soil parameters (texture, SOC, pH, cation exchange  
110 capacity, Fe/Al content), within the same horizon 2 kg of soil was sampled with a trowel into  
111 plastic bags and then sealed.

### 112 *Bulk density analysis*

113 The laboratory method followed that of the method applied during the few sites collected  
114 during the An Foras Talúntais survey (Massey *et al.*, 2014). This method corresponds to ISO  
115 11272:1998 – Soil Quality Part 5: Physical methods Section 5.6 – Determination of dry bulk  
116 density. The primary difference between the ISO and An Foras Talúntais methodologies is

117 that the ISO does not account for stone mass and volume in its core method, whereas the  
118 methodology applied here does include this Eq. [1].

119 To calculate bulk density (stone-free):

$$120 \quad \rho_b \text{ (g cm}^{-3}\text{)} = (\text{Md} - \text{Ms}) / (\text{V} - \text{Vs}) \quad (1)$$

121 Where: Md = Oven dry soil material weight (g), Ms = Oven dry stone weight (g), V =  
122 Volume of soil core (cm<sup>3</sup>), Vs = Volume of stones (ml). The resulting  $\rho_b$  values were the  
123 mean of three field replicate samples.

#### 124 *Pedotransfer functions review and selection*

125 Following a detailed review of the literature, 22 pedotransfer functions (PTF) were collated  
126 (Alexander (1980); Adams (1973) Rawls & Brakensiek (1985); Honeysett & Ratkowsky  
127 (1990); Federer (1983); Huntington (1989); Manrique & Jones 1991; Bernoux *et al* 1998;  
128 Leonavičiūtė 2000; Kaur *et al* 2002; Jeffrey 1970; Harrison & Boccock 1981; Tamminen &  
129 Starr 1994). A first stage assessment was conducted using the Irish SIS data where  $\rho_b$   
130 information was available for a range of soil horizon types. At this stage several (n=10) PTFs  
131 were removed as negative and/or extremely low or high values were obtained and the PTF  
132 did not appear to suit Irish data sets. The best remaining 12 PTFs for the various horizon  
133 types were then selected for use in further investigation (Table 2). These PTFs were chosen  
134 from the particular papers due to their development using: high sample number (n > 100);  
135 sampling depth to at least 80 cm; wide range of soils covered and statistical evaluation ( $R^2$ ).  
136 In most cases topsoils and subsoils were investigated and in others particular horizon types  
137 were investigated. For mineral soils eight PTFs were applied: Manrique & Jones 1991;  
138 Bernoux *et al* 1998; Leonavičiūtė 2000 (x4); Kaur *et al* 2002 (x2). For organic soils four  
139 PTFs were applied: Jeffrey 1970; Harrison & Boccock 1981; Manrique & Jones 1991;

140 Tamminen & Starr 1994 (Table 2). As these PTF required soil organic carbon data, soil  
141 texture data and loss on ignition data, the methods below were applied to samples from the  
142 field campaign.

#### 143 *Soil organic carbon analysis*

144 The soil was placed on aluminium trays and placed in an oven at 40°C for four days. The dry  
145 weight was recorded and the soil sieved to 2 mm and stored. A LECO TrueSpec CN  
146 elemental analyser was used to measure SOC. Concentrated hydrochloric acid was used to  
147 remove inorganic carbon. The method followed that of Massey *et al.* (2014), which is an  
148 adaptation of Organic Application Note of the analysis of Carbon and Nitrogen in Soil and  
149 Sediment (LECO Corporation). This method corresponds to ISO 10694: 1995 – Soil quality  
150 Part 3: Chemical methods Section 3.8 – Determination of organic and total carbon after dry  
151 combustion (elemental analysis). The soils in the AFT survey had organic carbon estimated  
152 by the Walkley-Black dichromate oxidation method as described by Jackson (1958) and  
153 modified for colorimetric estimation. A comparison of archive samples using both methods  
154 was comparable with an  $R^2$  of 97%.

#### 155 *Soil texture analysis*

156 The different particle sizes in the soil (sand, silt, clay) were determined via the pipette  
157 method. The premise of this method is based on Stokes Law where the relationship between  
158 particle grain size and settling velocity in a fluid medium is predictable. A subsample of 2  
159 mm dried and sieved soil was initially treated with hydrogen peroxide to remove all organic  
160 matter. Then it was suspended in a dispersant, sodium hexametaphosphate. Then finally 25  
161 ml of the suspension were removed at exact time periods following shaking to represent silt  
162 and then clay fractions. This method of Massey *et al.* (2014) followed the methodology stated

163 by An Foras Talútais, National soil survey (1972). The work was conducted by an external  
164 laboratory following USDA texture guidelines. An inter laboratory study was conducted to  
165 ensure continuity in the methodology between Teagasc and the external lab, where 50 soil  
166 samples were analysed by both laboratories (85.4% of soil samples were in agreement in  
167 textural class.

#### 168 *Loss on ignition*

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

#### 176 *AFT and Irish SIS horizons*

177 The horizon designations in the AFT survey were correlated to modern Irish Soil Information  
178 System definitions (Table 1). The Irish SIS designations are similar to the World Reference  
179 Base (WRB) system except for O, AB and Cr horizons which are equivalent to H, BA and  
180 CR in the WRB. The AFT designations were based on the soil horizon classification of soil  
181 survey staff, USDA (1960). When the equivalent horizon designation was identified the  
182 newly derived PTF could be applied to all horizons of this type. The soil horizon designation  
183 Ah indicating a lack of cultivation had no equivalent in the AFT records. The AFT survey did  
184 not record a non-cultivated A horizon.

#### 185 *Evaluation of PTFs*

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

191 The same data points were then compared using complementary prediction quality indices  
 192 (De Vos *et al.*, 2005). Here the quality of the prediction was determined via Eq. [2], the mean  
 193 predicted error (MPE); Eq. [3], the standard deviation of the prediction error (SDPE); Eq. [4],  
 194 the root mean squared prediction error (RMSPE); and Eq. [5] and the prediction coefficient of  
 195 determination ( $R_p^2$ ). These are defined as:

196 [2]

$$197 \quad MPE = \frac{1}{n} \sum_{i=1}^n (\widehat{Pb}_i - Pb_i)$$

198 [3]

$$200 \quad SDPE = \sqrt{\frac{1}{n-1} \sum_{i=1}^n ((\widehat{Pb}_i - Pb_i) - MPE)^2}$$

201 [4]

$$202 \quad RMSPE = \sqrt{\frac{1}{n} \sum_{i=1}^n (\widehat{Pb}_i - Pb_i)^2}$$

203 [5]

204

$$205 \quad R_p^2 = \frac{[\text{cov}(Pb_i, \widehat{Pb}_i)]^2}{\text{var}(Pb_i) - \text{var}(\widehat{Pb}_i)}$$

206

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

#### 214 *Calibration of the PTF*

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

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

#### 225 *Model validation*

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

230 *Digital Soil Mapping (DSM) techniques*

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

240 Universal Kriging was the final model applied for the development of the Indicative bulk  
241 density maps. Covariables used within the Universal Kriging approach included a land use  
242 map (O'Sullivan et al., 2015), slope data and a Digital Elevation Model (DEM 20 m  
243 resolution). Land-use data was applied as this reflected the soil management types, in terms  
244 of compaction/poaching etc, which are major drivers of soil bulk density. The DEM provided  
245 information on altitude and slope degree, these data types were selected as they represent  
246 natural changes in bulk density as a result of the major topographical features and provide an  
247 indicator of the climatic influence on soils at high altitudes (colder, wetter more acidic  
248 conditions). The soil association map was not included in this analysis, as this map is also a  
249 predicted product, SIS Final Technical Report 5, which uses the co-variants described within  
250 the prediction (Mayr et al., 2015).

251 The mask is the result of a number of updates that were made to the original post-processing,  
252 which was verified with soil profile pit descriptions. This includes areas of Peat, Rock,

253 Alluvium, Water, Sand. A matrix was compiled based on the legend of Dunes, Tidal  
254 Marshes, and Urban areas (Creamer et al., 2014).

255 *Map validation methodology*

256 For the validation of the map, independent data was used from the SoilH project having 72  
257 locations sampled for bulk density (Kiely, 2015). The De Vos indexes (De Vos et al., 2005,  
258 covered in section 2.10 above) were applied to establish the prediction quality of the  
259 Universal Kriging of the indicative bulk density maps. The map validation methodology is  
260 covered in detail in the SIS Final Technical Report 18 (Simo et al., 2015).

261 *Mapping confidence*

262 The validation applied indicated low confidence for both bulk density maps (for 0-30 cm and  
263 for 30-50 cm, having an  $R^2 = 0,32$  and  $R^2 = 0,25$ , respectively). The main problem is that the  
264 data used for mapping bulk density was not taken with this purpose in mind. Bulk density is a  
265 soil property that it is strongly influenced by the management practices and the sampling  
266 point strategy could influence directly the map product. Some features of the distribution may  
267 reflect regional variations in land use and management practices as well as the underlying soil  
268 properties, and the analysis may be influenced by sampling density across land use types.  
269 Therefore, these maps should be considered as indicative maps, guarantees cannot be made  
270 that the map gives the full actual picture, hence the bulk density could vary in a particular  
271 location, thus the map legend shows ranges and not unique single values (Simo et al., 2015).

272

273

## 274 **Results**

### 275 *Bulk Density*

276 The observed  $\rho_b$  values were grouped together based on horizon designation (Ap, Ap1, Ap2,  
277 Apg, Ah, O, E, AB, Bw, Bg, Bs, Bt, Btg, BC, BCg, C/Ck/Cr and Cg) and statistics applied in  
278 preparation for PTF application (Table 3). The minimum number of replicates per horizon  
279 type was seven for the Bs horizon and the maximum number of replicates per horizon was  
280 111 for Ap. Horizons Ap1 and Ap2 are generally considered unique to Ap, this reflects the  
281 adoption of shallow till ploughing in some areas, however the bulk densities of both were  
282 similar,  $1.044 \text{ g cm}^{-3}$  and  $1.072 \text{ g cm}^{-3}$ , respectively. These designations were not unfounded  
283 as Ap horizons were generally lower ( $0.976 \text{ g cm}^{-3}$ ) when compared to Ap1 and Ap2  
284 horizons. The largest bulk density was in Cg horizons ( $1.566 \text{ g cm}^{-3}$ ) and the lowest in the O  
285 horizons ( $0.329 \text{ g cm}^{-3}$ ). The Bt horizons had the lowest standard deviation and co-efficient of  
286 variation, 0.036 and 2.75%, respectively. The O horizons had the largest co-efficient of  
287 variation at 11.854%.

### 288 *Application of pedotransfer functions*

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

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

### 310 *Selection of the best PTF*

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

320 best performing PTF based on highest  $R^2$  value, was still appropriate, displaying the highest  
321  $R_p^2$ , value also.

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

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

338 The observed and predicted  $\rho_b$  values are presented in a box and whisker plot in Figure 3.

339 These predicted values are calculated using the selected PTF based on  $R_p^2$  values of Table 6.

340 The horizons with low accuracy (MPE) are evident in the case of AB, Bs, Bt and C.

341 Furthermore there is no overlap in the position of the interquartile ranges of the observed and  
342 predicted box and whisker plots. Those with good accuracy Apg, Bg, Cg and E are evident as

343 the red (observed) and blue (predicted) median bars are closer in position. In most cases for  
344 deeper and normally denser horizons, the interquartile range of  $\rho_b$  values are generally greater  
345 in the predictions than the observed. The max and min spread of the data (between 0.2 to 0.3  
346  $\text{g cm}^{-3}$ ) is much narrower than the observed data ranges for horizons Bs, Bt, Btg, BC, BCg  
347 and C.

#### 348 *Recalibration of the selected PTF*

349 Having selected the best performing PTF for each horizon type using the prediction quality  
350 indices, 80% of the observed dataset was randomly selected for the recalibration of the PTF.  
351 The recalibrated PTF are presented in Table 7. For Ap, Ap2, AB and Bg the Manrique and  
352 Jones intercept and coefficients have decreased due to lower densities in the dataset. The  
353 intercept and coefficients increased with this PTF for Apg, BC, C/Ck/Cr and Cg indicating  
354 higher densities in the data set. Leonavičiūtė A (Ap1), Kaur intrinsic (Ah and Bt) and  
355 Leonavičiūtė E (Bw), have decreased intercept and coefficients. Leonavičiūtė B increased  
356 intercept and coefficients, in both the cases of recalibration for Btg and BC. Leonavičiūtė E  
357 increased the coefficients and intercepts in the case of BCg and decreased in the case of E  
358 horizons.

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

#### 362 *Validation of the recalibrated PTF*

363 Validation has improved the coefficient of determination once again (Table 7), where 20% of  
364 the observed values were again randomly selected and  $R^2$  generated. There have been  
365 increases in the  $R^2$  validation values in comparison to the  $R_p^2$  values of 0.3 or more for Ap2,

366 AB, Bg, Cg, BCg and O. There was a large decrease for BC (0.323) and a small decrease for  
367 Ap1 and Btg (0.156 and 0.123). Except for horizon BC all other horizons have an  $R^2$  of at  
368 least 0.47 or higher. Horizon BC with a low correlation (0.257) would have an unstable  
369 predictability. For horizons Bs, Bt, C and E there were not enough data points in the  
370 validation dataset of 20% to generate any validation indices.

### 371 *Indicative soil bulk density map*

372 Having bulk density data measured per horizon allowed the prediction of  $\rho_b$  in horizons  
373 where there were no measurements. This allowed gap filling in the Irish SIS and AFT profile  
374 data. In combination with mapping units from the latest edition of the Irish soil map and the  
375 methodology described above, a  $\rho_b$  map of Ireland was produced (Figure 4). These maps  
376 highlight that lower bulk densities are found at the surface (0-30 cm) which is consistent with  
377 expected findings in relation to soil types and management, due in principle to higher soil  
378 organic carbon in these soils. The bulk density ranges from  $< 0.79$  to  $> 1.1$   $\text{g cm}^{-3}$  (Figure 4a)  
379 At increasing depths, 30-50 cm, higher bulk density values are likely to be found ( $< 1.0$  to  $>$   
380  $1.4$   $\text{g cm}^{-3}$ ). In general the bulk densities are lower in mountainous and hill areas and higher  
381 in lowland areas for both depth ranges.

382

## 383 **Discussion**

### 384 *Observed $\rho_b$ values*

385 The observed  $\rho_b$  values across all horizons have a mean of  $1.187$   $\text{g cm}^{-3}$  with a standard  
386 deviation of  $0.305$   $\text{g cm}^{-3}$ . Removing the O horizon value of  $0.329$   $\text{g cm}^{-3}$ , the mean and  
387 standard deviation are  $1.214$  and  $0.217$   $\text{g cm}^{-3}$ , respectively. This mean value compares

388 favourably to Manrique & Jones (1991) on a range of agricultural soils 1.2-1.5 g cm<sup>-3</sup>. The  
389 ForSite study of DeVos *et al.* (2005) reported another comparable value of 1.23 g cm<sup>-3</sup> for  
390 topsoil. This value also compares well to the subsurface soils of Harrison and Bocoock (1991),  
391 1.29g cm<sup>-3</sup>, and forest soils of Taminen & Starr, 1.19g cm<sup>-3</sup>.

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

406 Looking at the mean values per horizon, the use of this approach appears justified with the  
407 large differences between surface horizons and sub-surface horizons (Ap, 0.976 g cm<sup>-3</sup>, and  
408 Cg, 1.566 g cm<sup>-3</sup>, Table 3). The difference between each type of surface horizon is also  
409 notable, where O horizons are 0.329, and Ap1 and Ap2 (while close together at 1.044 &  
410 1.072 g cm<sup>-3</sup>) are different from Ap, reflecting differences in organic matter content and

411 management, respectively. Therefore where possible predictions for soil bulk density should  
412 be at horizon level rather than topsoil or subsoil categorisation.

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

420 The practice of splitting the bulk density of a singular profile into horizons has other  
421 advantages, especially when modelling systems. Many studies note that high levels of SOC  
422 are found at the surface particularly 0 – 30 cm depth. However more SOC could be found in  
423 the 30 – 100 cm range where the soils are denser. Adhikari *et al.* (2014) modelled  $\rho_b$  values  
424 using quadratic splines, when different horizon data was not available. This is a method to  
425 reflect the changes of  $\rho_b$  in soil profiles by using discrete soil depths. It was noted that  
426 accurate quantification of SOC stocks required a depth function. Tranter *et al.* (2007) also  
427 included a depth function when describing PTF based on soil mineral packing structures and  
428 soil structure. However it should also be noted that the fitting quality of splines to profile data  
429 depends on smoothing parameters, which introduces another source of error (Malone *et al.*,  
430 2009). In this study the data has been directly measured across the various horizons which  
431 avoids this error.

432 *Application of literature PTF*

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

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

#### 450 *Recalibration of literature PTF*

451 When recalibrating the PTF, it allowed the refinement of the equations for the Irish scenario.  
452 To date this is the most comprehensive model of Irish soils using the largest available dataset,  
453 with soil profile, soil horizon and depth coverage. The use of 80% of the data points also  
454 followed the accepted De Vos *et al.* (2005) method. Where the categorisation into horizon

455 PTF is justified and the  $R^2$  values increased or are equalled for 14 out of the 17 horizons  
456 studied (Table 6).

457

458 The study of Xu *et al.* (2011) desired more data for deeper soils and greater site number (in  
459 the Irish context) to calibrate that studies PTF. They had used 0-10 cm soil depth carbon  
460 values to predict, firstly carbon content to 50 cm depth and then to predict soil bulk density to  
461 50 cm depth. The use of sequential empirical regressions in developing PTF can propagate  
462 errors (Meersmans *et al.* 2008). The use of a singular PTF for peat and mineral soils in Xu *et*  
463 *al.* (2011) study is also unlikely to be useful once actual peat  $\rho_b$  and SOC estimations at depth  
464 are required. This present study had both the depth and sample number data to calculate  
465 different PTF for various horizon types. The data generated in this study will avoid the  
466 propagation of errors described above and allow more accurate SOC calculation.

467

#### 468 *Validation of the recalibrated PTF*

469 De Vos *et al.*, 2005, emphasised the need for recalibration and local validation. This would  
470 aid the decision making process with reference to the level of what prediction error is  
471 acceptable. Getting this right is crucial as it has been recognised that correction factors led to  
472 an increase in the Belgian SOC prediction by 22%, which also affected their projections due  
473 to landuse change and climate change (Lettens *et al.*, 2007). Although prediction errors  
474 between 10 and 20 % were deemed acceptable in the study of Prévost (2004). Huang *et al.*  
475 (2003) state that model acceptance would require between 10 and 20 % of the variance  
476 observed. For horizons with many replicates such as Ap (n=111), the MPE falls within this  
477 criteria  $0.067 \text{ g cm}^{-3}$ , or 6.8% of  $0.976 \text{ g cm}^{-3}$ . However this is not the case for many other  
478 horizon types which clearly need more replicates for example Bs (n=7) MPE is  $0.488 \text{ g cm}^{-3}$ ,

479 or 44% of  $1.086 \text{ g cm}^{-3}$ . Though, in most cases where a validation could be performed the  
480 predicted coefficient of variation was equalled or improved ( $R_v^2$ , Table 7).

#### 481 *Mapping Application*

482 With the bulk density maps to 0-30 cm and 30-50 cm depth, the potential of these pedotransfer  
483 functions is realised. In Ireland there currently is no national map of soil carbon values,  
484 primarily due to the lack of bulk density data and also depth coverage. The National Soil  
485 Database project (2001-CD/S2-M2) measured 1365 points for organic carbon to 10 cm,  
486 however it did not measure bulk density. The SoilC project (Kiely *et al.*, 2010) measured  
487 bulk density and organic carbon to 50 cm depth although this project was limited on number  
488 of sites ( $n = 62$ ). Any studies deeper than 10 cm were in localised areas which did not allow  
489 extrapolation to the national area. Forest soils were covered in CARBiFOR 1 (Black and  
490 Farrell, 2006) and CARBiFOR 2 (CARBiFOR staff, 2015) projects, where soils were  
491 surveyed to 50 cm depth.  $\rho_b$  was measured but site number was restrictive ( $n = 44$ ). However,  
492 in both cases mapping criteria were not developed for greater areas. Most SOC studies and  
493 inventories are confined to 30 cm soil depth but the amount of SOC stored below 30 cm is of  
494 relevance in many ecosystems (Adhikari *et al.*, 2014).

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

**501 Conclusion**

502 The  $\rho_b$  values reported for horizon type allowed a greater range of soils in the Irish SIS to  
503 have  $\rho_b$  values allocated in the cases where there are omissions and to depth (recommended 1  
504 metre). The same process was applied to the AFT samples that did not have  $\rho_b$  values  
505 measured in the field. This paper covers the methodology of producing soil horizon PTF  
506 given the measured data available. Related predictions are based on the best data available  
507 after screening for accuracy and precision of PTF; they were then recalibrated and eventually  
508 validated within the Irish scenario. The methodology enabled the researcher to return to the  
509 Irish SIS to produce a validated  $\rho_b$  map at two depths, 0-30 cm and 30-50 cm (details of  
510 validation of map are given in Simo *et al.*, 2015). Now that a  $\rho_b$  value is available for the  
511 different soil depths, values could be attributed to each soil mapping unit using Irish SIS into  
512 the future. Potentially this data could then be combined with known carbon data to produce a  
513 soil carbon map to 1 metre. The data could also be used to produce a drainage map for the  
514 country. Another area for potential use would be the PTF used in hydrology studies, which  
515 use bulk density values. Furthermore, where nutrient management is a concern in soils, areas  
516 prone to compaction can be identified via this map. The PTF produced are valid for some  
517 horizons (with large  $R^2$  values) and have limited success with other horizons. It is hoped in  
518 time as the sample number of these rarer horizons increases that the accuracy of the  
519 prediction increases. In general the greater sample number the better the prediction and  
520 validation.

521

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707

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

<b>Irish SIS</b>	<b>An Forais Talúntais</b>
O	O, Oh
Ap	A, A1
Ap1	A11
Ap2	A12, A13
Ap3	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

710

711 **Table 2.** Published pedotransfer functions with corresponding authors used in this study. OC

712 is organic carbon.  $\rho_b$  is bulk density in  $\text{g cm}^{-3}$ .

713

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

714 **Table 3.** Statistics of observed bulk density,  $\rho_b$  ( $\text{g cm}^{-3}$ ) for each horizon type, used in the  
 715 development of pedotransfer functions.

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

716

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

Author	Bernoux (1998)	Kaur (2002)	Kaur intrinsic (2002)	Leonaviciūtė (2000)(A)	(2000)(B)	(2000)(BC-C)	(2000)(E)	Manrique & Jones (1991)	Harrison & Boccock (1981) Topsoil	Tamminen & Starr (1994)	N	
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	
Ap <sub>g</sub>	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	
B <sub>g</sub>	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	
Bt <sub>g</sub>	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	
C <sub>g</sub>	0.02	0.71	0.52	0.63	0.39	0.33	0.41	0.64			12	
BC <sub>g</sub>	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

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

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

722 **Table 6.** The mean predicted error (MPE, g cm<sup>-3</sup>); the standard deviation of the prediction  
 723 error (SDPE, g cm<sup>-3</sup>); the root mean squared prediction error (RMSPE, g cm<sup>-3</sup>); and the  
 724 prediction coefficient of determination ( $R_p^2$ ).using complimentary prediction quality indices  
 725 (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 & Jones	0.067	0.132	0.148	0.532
Ap1	Leonavičiutė A	0.246	0.137	0.280	0.619
Ap2	Manrique & Jones	0.110	0.117	0.158	0.142
Apg	Manrique & 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 & 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 & 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 & starr	-0.117	0.682	0.666	0.315

726 **Table 7.** Recalibrated pedotransfer functions (PTF) using Irish input data compared to  
 727 measured bulk density.  $R_p^2$  is the prediction coefficient of determination,  $R_v^2$  is the validation  
 728 coefficient of determination, both based on prediction quality indices (De Vos *et al.*, 2005).  $\rho_b$   
 729 is bulk density ( $\text{g cm}^{-3}$ ). OC is organic carbon.

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

730

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

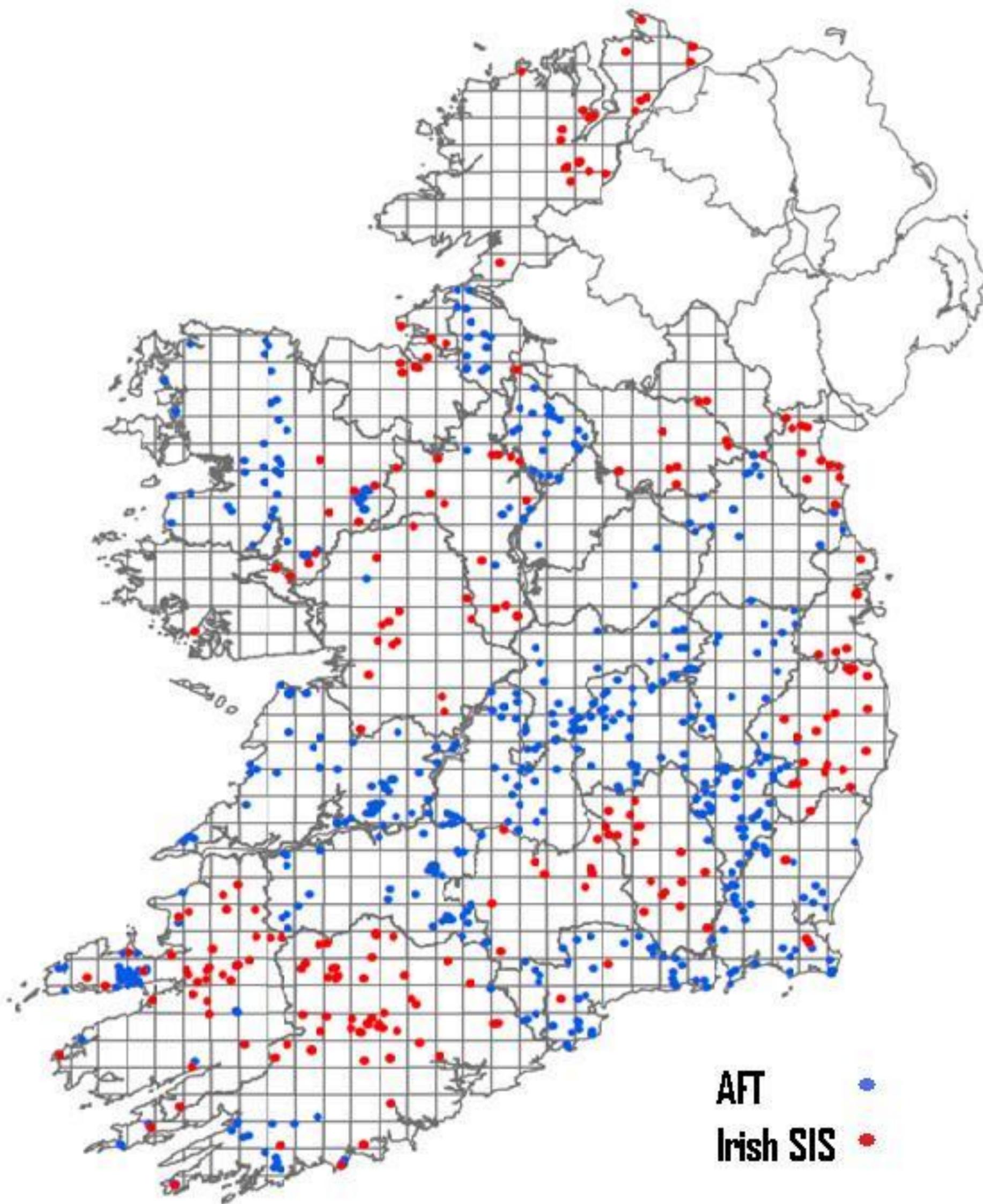
734 **Figure 2 a.** Observed bulk density values for horizon Ap compared to prediction for original  
735 PTF formulae used indicating coefficient of variation equation and  $R^2$  values.

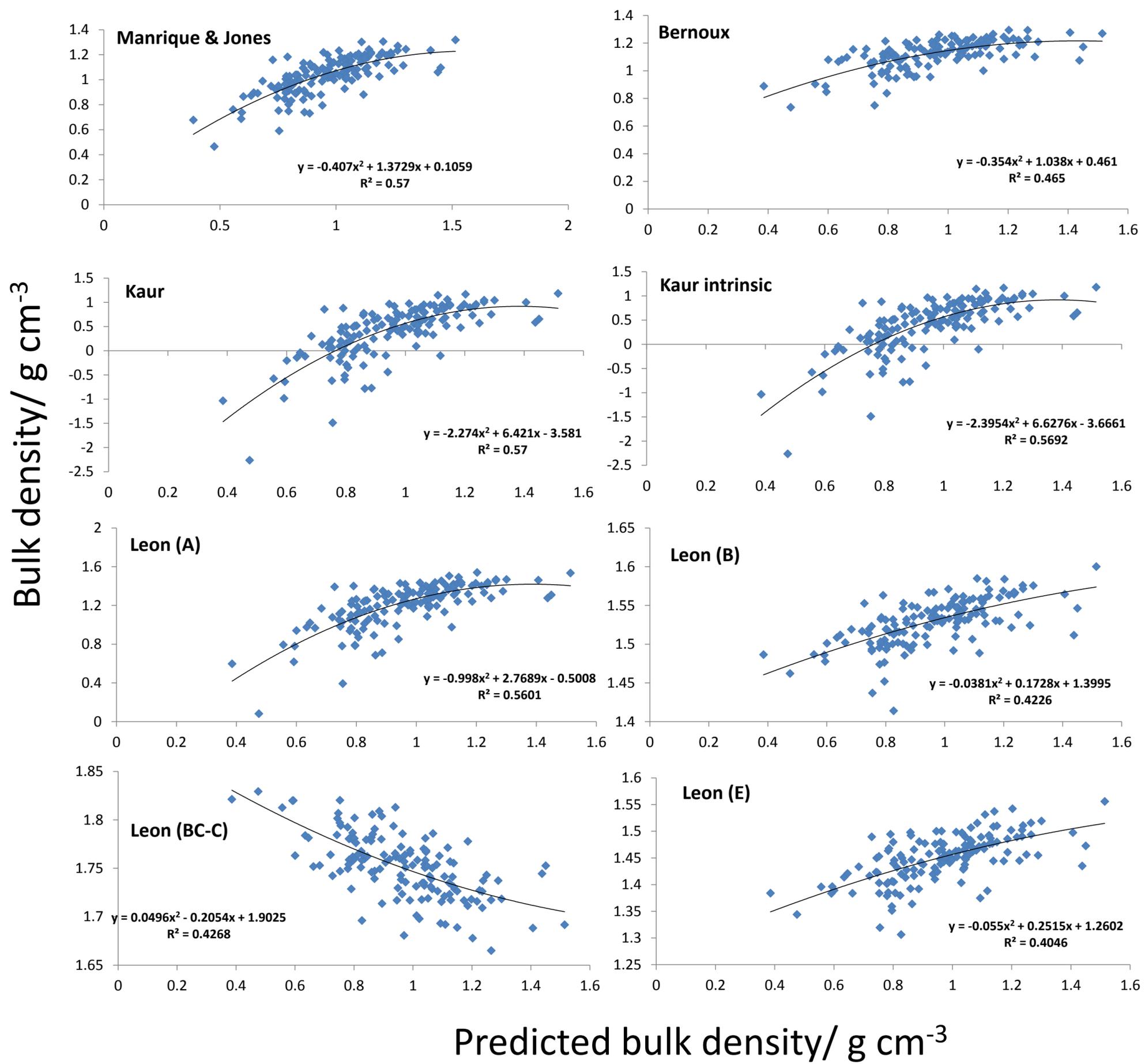
736 **Figure 2 b.** Observed bulk density values for horizon O compared to prediction for original  
737 PTF formulae used indicating coefficient of variation equation and  $R^2$  values.

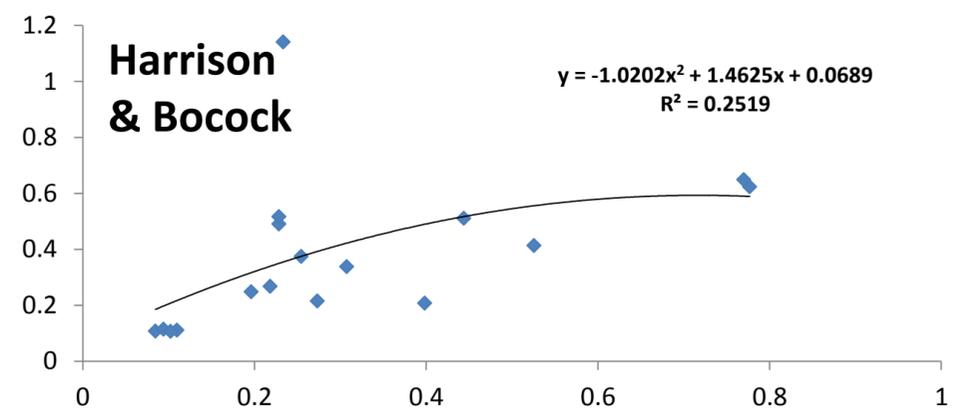
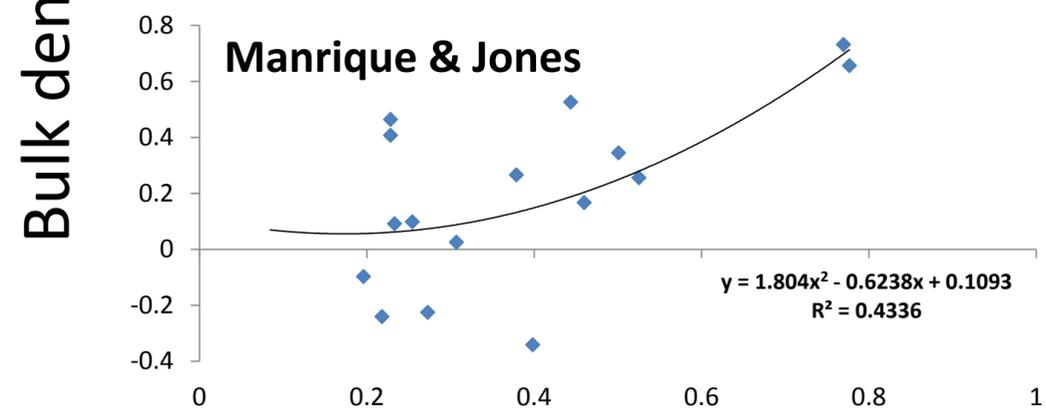
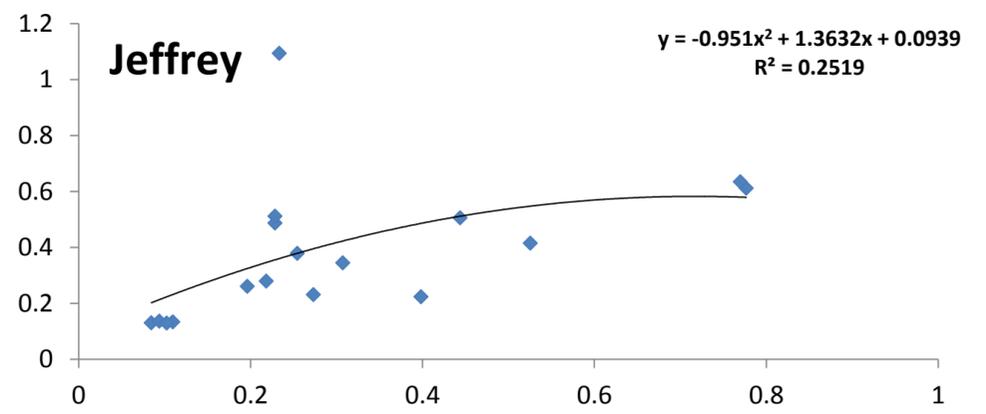
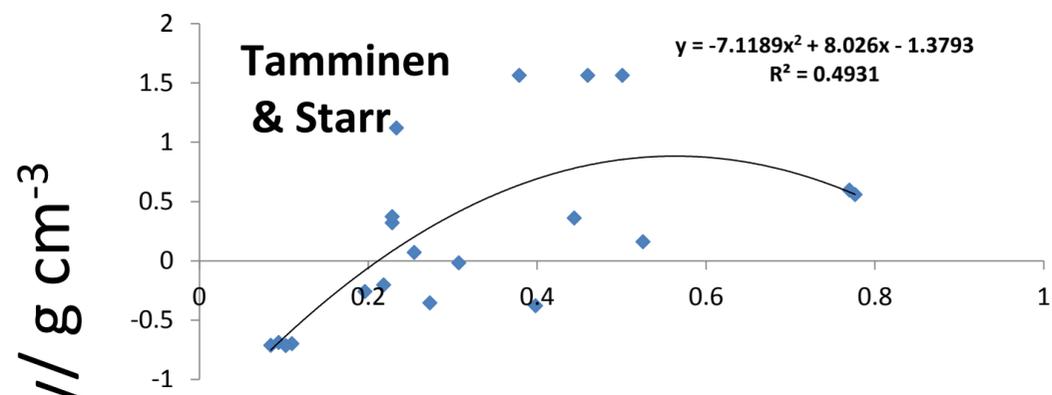
738 **Figure 3.** Observed bulk density (O) and predicted bulk density (P)  $\text{g cm}^{-3}$ , for each horizon  
739 type. Prediction based on selected PTF with best  $R_p^2$  following prediction quality indices.

740 **Figure 4a.** Indicative soil bulk density distribution map for Ireland (0-30 cm,  $\text{g cm}^{-3}$ ).

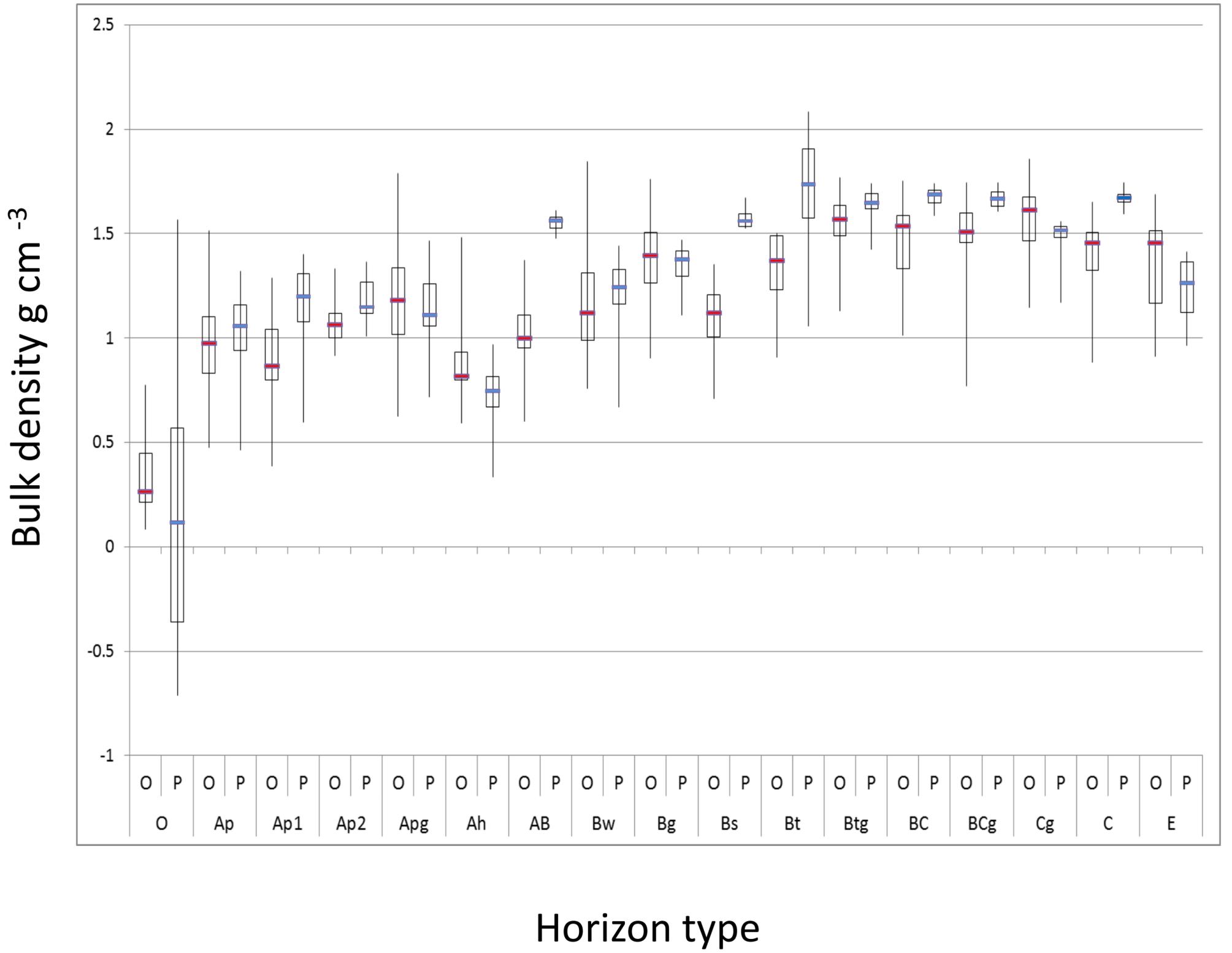
741 **Figure 4b.** Indicative soil bulk density distribution map (30-50 cm,  $\text{g cm}^{-3}$ ).



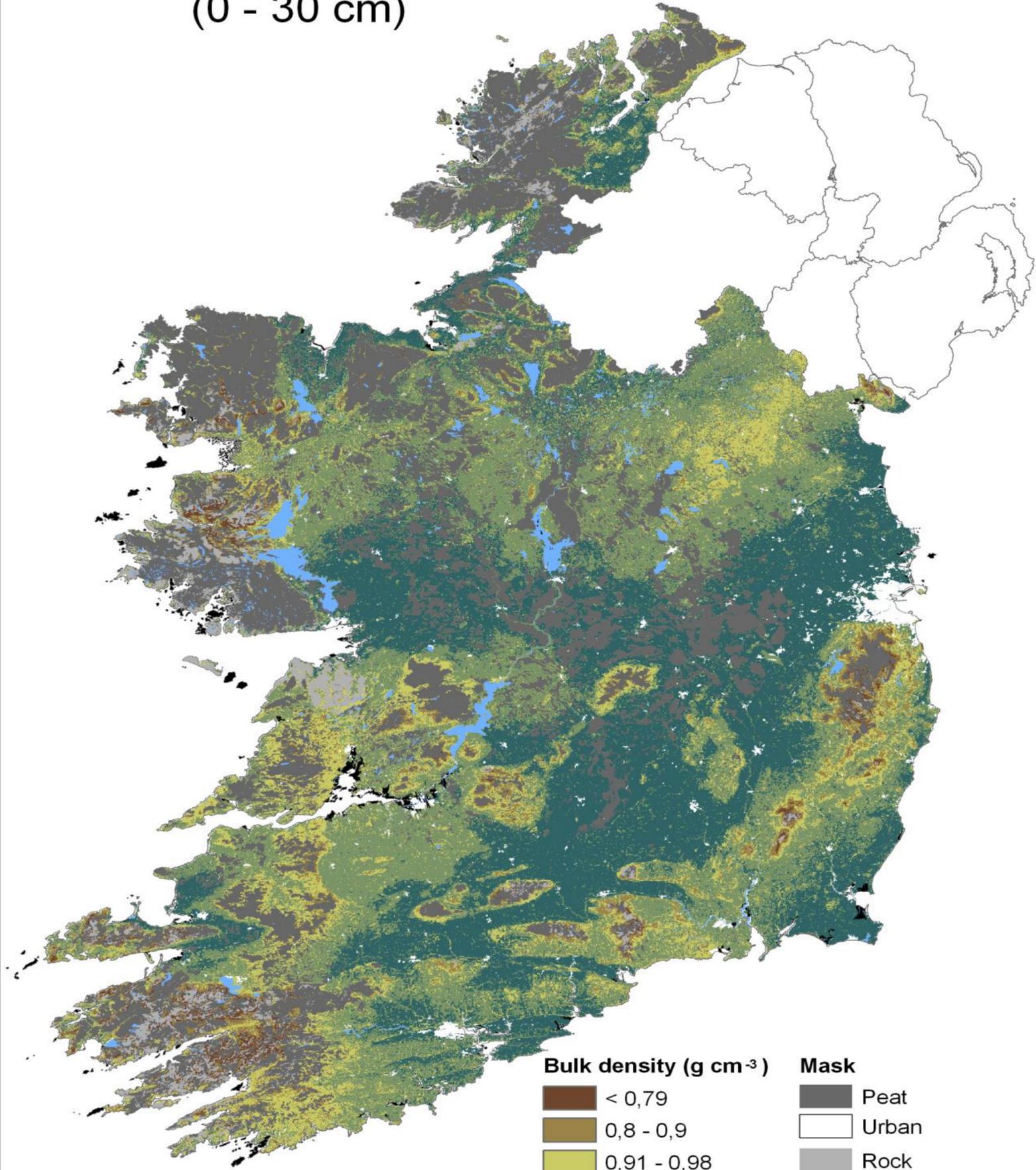




Predicted bulk density/ g cm<sup>-3</sup>



# Indicative Bulk Density map (0 - 30 cm)



0 25 50 100 km

### Bulk density (g cm<sup>-3</sup>)

- < 0,79
- 0,8 - 0,9
- 0,91 - 0,98
- 0,99 - 1
- > 1,1

### Mask

- Peat
- Urban
- Rock
- Water body
- Tidal, salt marsh and Islands

# Indicative Bulk Density map (30 - 50 cm)

