Response to reviewers and editors comments

As pointed out by all reviewers, it is nice to see that a lively debate about the correct calculation of SOC stock is underway. The reviewers and authors have pointed out some valid points, but despite the suggestion that the debate be closed (Referees 1 and 2), there remain a few points of clarification.

- 5 Chiefly, Poeplau et al. state in their paper that M4, which they use as the 'correct' standard for comparing, is 'the closest approximation to reality'. They also state in their response that M4 with equation 6 is the same as the IPCC standard. M4 is however, not statistically equivalent to the derived equation (viii) in our comment, which is illustrated by a comparison of the errors of their M4 compared with the derived equation 8 in our comment. This information has been added to P2 L25ff to demonstrate this point.
- 10 The authors are indeed correct in their assertion that this can be used for multiple depth samples, but they have not clarified the units to be used and this has left some confusion. Nevertheless, this was deleted from the manuscript (P2 L24) for the sake of brevity.

With regards the estimation of rock content from the profile, we have added a section to discuss rock content estimation P3 L17-23).

15 Lastly, further literature has been added to support the use of equation 8 for calculations of SOC stocks.

Comment on 'Soil organic stocks are systematically overestimated by misuse of the parameters bulk density and rock fragment content' (Poeplau *et al.*, 2017, SOIL, 3(1), 61-66).

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- 10 Poeplau et al [2017] recently outlined the systematic overestimation of soil organic carbon (SOC) stocks due to incorrect application of bulk density and rock fragment content in calculation of SOC stocks. Unfortunately, the method they propose to rectify this is associated with a greater error (due to assumption of rock density, extra calculation steps and propagation of errors) than the simpler mass balanced derived equation for SOC stock calculations, outlined below. Using a mass balance approach to C stocks we define:
- 15 $C_{Stock} = Mass Proportion_{c} \cdot \rho \cdot d$

(i)

Where C_{stock} is the amount of carbon stored in a given soil area (kg m⁻²) and depth, d (cm); Mass Proportion_C is the carbon content of the whole soil (g kg⁻¹) and ρ is the bulk density of the whole soil (g cm⁻³).

Using a mass balance approach on the Mass Proportion of C in the whole soil, we obtain:

 $MassProportion_{C} = C_{Content, fine} \cdot Mass Proportion_{fine} + C_{Content, coarse} \cdot Mass Proportion_{coarse}$ (ii)

- 20 Where $C_{Content,fine}$ is the mass proportion of C in the fine soil fraction (g kg⁻¹), Mass Proportion_{fine} is the mass proportion of the fine soil to the whole soil sample (g kg⁻¹) and $C_{Content, coarse}$ is the mass proportion of C in the coarse soil fraction (g kg⁻¹), Mass Proportion_{Coarse} is the mass proportion of the coarse soil to the whole soil sample (g kg⁻¹), generally referred to as the rock content. $C_{Content, coarse}$ is assumed to be negligible (i.e. = 0) in all methods, so that the equation (2) simplifies to:
 - $MassProportion_{C} = C_{Content, fine} \cdot Mass Proportion_{fine}$ (iii)
- 25 The Mass Proportion_{fine} is

$$MassProportion_{fine} = \frac{Mass_{fine}}{Mass_{Total}} = \frac{Mass_{fine}}{Mass_{fine} + Mass_{coarse}}$$
(iv)

$$= \frac{Mass_{fine} + Mass_{coarse} - Mass_{coarse}}{Mass_{fine} + Mass_{coarse}}$$
(v)
= 1 - Mass Proportion_{coarse} (vi)

Substituting equation (vi) into equation (iii) we obtain:

$$MassProportion_{C} = C_{Content, fine} \cdot (1 - Mass Proportion_{coarse})$$
(vii)

5 Substituting equation (vii) into (i) we obtain:

$$C_{Stock} = C_{Content, fine} \cdot (1 - Mass Proportion_{coarse}) \cdot \rho \cdot d \tag{viii}$$

This looks similar to equation (5) in Poeplau *et al.* [2017]. However, they use the volumetric proportion, not the mass proportion of rock fragments, which is mathematically incorrect. They also state that their equation (6) 'resembles' equation (viii). However, their M4 is actually a more convoluted and obtuse equivalent to the commonly known and applied equation

10 (viii) (Ellert and Bettany 1995; Goidts et al. 2009, Mikha et al. 2013; Orgill et al. 2013). This can be shown by combining equations (3) and (6) from Poeplau *et al*, which illustrates the redundancy of using the rock density to calculate SOC stocks because, as can be shown by combining equations (3) and (6) from Poeplau *et al*, the inclusion of rock density to calculate SOC stocks is unnecessary and redundant. -

Equation (viii) is also mathematically equivalent to calculations according to equations (7) and (8) in Poeplau et al. However,

- 15 the recommended use of the mass of fine fraction for the calculations by Poeplau *et al.* also has a greater potential error than using the mass proportion of rocks according to equation (viii). The advantage of using the rock mass to correct the stocks is that rocks are (nearly) entirely conserved during sieving, whereas fine soil mass is lost as dust during sieving, increasing uncertainty in the calculations. In contrast, M4 (equations (3) and (6)) of Poeplau *et al.* requires an estimation of rock density (they recommend assuming a rock density of 2.63 g cm⁻³) to calculate the bulk density of the fine soil sample as well as to
- 20 adjust for rock content. Rock density depends on parent material, with basalts having higher densities than granites, so that this assumption increases error and uncertainty (Hazelton and Murphy, 2016).

Unfortunately, the additional calculations required also increase the uncertainty of the estimate due to error propagation. Although mathematically equivalent, calculations according to their M4 are therefore less precise due to extra sources of error (derived from either analytical or assumed rock density as well as error propagation). As such, using equation (viii) above,

25 based on the C content of the fine soil, mass proportion of rocks and bulk density in the whole sample will yield the most precise estimate of C stocks.

With regards to eliminating the depth, d, from the calculations (equation (9) in Poeplau *et al.*), this is only applicable to samples taken as a whole which are then not subdivided further. Samples are frequently cut into smaller depth increments for depth explicit sampling, e.g. to investigate the depth distribution of SOC, so that equation (9) in Poeplau *et al.* is only of use in a

30 limited number of cases. In order to avoid possible errors due to the application of equation (9) for samples which have been subdivided into discrete depth increments, it seems more appropriate to retain the universally applicable equation (viii).

<u>Unfortunately</u>, the additional calculations required in M4 also increase the uncertainty of the estimate due to error propagation. This can be illustrated by calculating the error terms of both equations. The squared relative error of equation (viii) is:

$$\frac{\sigma_{\mathcal{C}_{stock}}^{2}}{\mathcal{C}_{stock}^{2}} = \frac{\sigma_{\mathcal{C}_{content,fine}}^{2}}{\mathcal{C}_{content,fine}^{2}} + \frac{\sigma_{Mass\ proportion_{Rock}}^{2}}{Mass\ proportion_{Rock}^{2}} + \frac{\sigma_{\rho_{sample}}^{2}}{\rho_{sample}^{2}} + \frac{\sigma_{Depth}^{2}}{Depth^{2}}$$

<u>With</u> Mass proportion_{Rock} = $\frac{Mass_{Rock}}{Mass_{Sample}}$ and $\rho_{Sample} = \frac{Mass_{Sample}}{Volume_{Sample}}$ we obtain:

$$5 \quad \frac{\sigma_{C_{stock}}^2}{c_{stock}^2} = \frac{\sigma_{C_{content,fine}}^2}{c_{content,fine}^2} + \frac{\sigma_{Mass_{Rock}}^2}{Mass_{Rock}^2} + 2\frac{\sigma_{Mass_{Sample}}^2}{Mass_{Sample}^2} + \frac{\sigma_{Volume_{Sample}}^2}{Volume_{Sample}^2} + \frac{\sigma_{Depth}^2}{Depth^2}$$

The squared relative error of M4 in Poeplau et al. is:

$$\frac{\sigma_{C_{stock}}^{2}}{C_{stock}^{2}} = \frac{\sigma_{C_{content,fine}}^{2}}{C_{content,fine}^{2}} + \frac{\sigma_{Volume\ proportion_{Rock}}^{2}}{Volume\ proportion_{Rock}^{2}} + \frac{\sigma_{\rho_{fine}}^{2}}{\rho_{fine}^{2}} + \frac{\sigma_{Depth}^{2}}{Depth^{2}}$$

<u>Using the equation 3 in Poeplau et al. for ρ_{fine} and with Volume proportion_{Rock} = $\frac{Volume_{Rock}}{Volume_{Sample}}$ we obtain:</u>

$$=\frac{\sigma_{C_{content,fine}}^{2}}{C_{content,fine}^{2}}+\frac{\sigma_{Volume_{Rock}}^{2}}{Volume_{Rock}^{2}}+\frac{\sigma_{Volume_{Sample}}^{2}}{Volume_{Sample}^{2}}+\frac{\sigma_{Mass_{Sample}}^{2}}{Mass_{Sample}^{2}}+\frac{\sigma_{Volume_{Sample}}^{2}}{Volume_{Sample}^{2}}+2\frac{\sigma_{Mass_{Rock}}^{2}}{Mass_{Rock}^{2}}+\frac{\sigma_{PRock}^{2}}{\rho_{Rock}^{2}}+\frac{\sigma_{Peth}^{2}}{Depth^{2}}$$

10 With
$$\rho_{Rock} = \frac{Mass_{Rock}}{Volume_{Rock}}$$
 the squared relative error of M4 in Poeplau et al. is therefore:

$$\frac{\sigma_{C_{content,fine}}^2}{C_{content,fine}^2} + 2\frac{\sigma_{Volume_{Rock}}^2}{Volume_{Rock}^2} + 2\frac{\sigma_{Volume_{Sample}}^2}{Volume_{Sample}^2} + \frac{\sigma_{Mass_{Sample}}^2}{Mass_{Sample}^2} + 3\frac{\sigma_{Mass_{Rock}}^2}{Mass_{Rock}^2} + \frac{\sigma_{Depth}^2}{Depth^2}$$

As can be seen, M4 has more sources of error than equation (viii). M4 is therefore statistically inferior and should be avoided. This is in line with applying the law of parsimony (Occam's razor) to the problem of SOC stock calculations, which states that

- 15 when presented with competing answers to a problem, one should choose the one which makes the fewest assumptions. Calculations according to their M4 are therefore less precise due to extra sources of error (derived from either analytical or assumed rock density as well as error propagation). As such, using equation (viii) above, based on the C content of the fine soil, mass proportion of rocks and bulk density in the whole sample will yield the most precise estimate of C stocks. With regards to eliminating the depth, d, from the calculations (equation (9) in Poeplau *et al.*, suggested by Wendt and Hauser,
- 20 2013), it would appear that the error of this method is lower still. However, this is deceptive, because the error associated with sampling a specific depth remains, so that the mathematical simplification does not eliminate the error term. Of key concern and not addressed here is the calculation of SOC stocks in stony soils, as here an accurate estimation of rock content is highly difficult. Estimating rock content from the profile face is highly error prone, because 2D surface areas are not representative of irregular 3D structures, such as rocks. Therefore, estimating rock content from the profile face is not

volumetric. Taking larger volumes of sample in very large cores to determine the bulk density of the whole soil would help to alleviate this issue, but would be associated with more field and laboratory work. A systematic study into this issue, similar to the systematic evaluation of sources of error when up-scaling to SOC analyses to landscape stocks (Goidts, van Wesemael & Crucifix, 2009) could help to resolve the issue.

5 In summary, Poeplau *et al.* have clearly demonstrated the need to adjust for coarse fragments >2 mm in SOC stock calculations. Unfortunately, their recommendation has added some confusion to the correct method of calculation of SOC stocks via the introduction of unfamiliar formulas. Whilst mathematically correct, their formulas are associated with larger errors than the standard equation and are not universally applicable, so present no clear advantage. As such, we recommend the use of equation (viii) for SOC stock calculations.

10 References

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