National Soil Carbon Network: Database calculations and quality assessment.

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This document contains information about the data contained in the NSCN database reports. The information in this document falls into 4 major groupings: 1) how the SOC values (g cm^{-2}) were computed for the layers and profiles; 2) subtle but important differences in the variables used to calculated SOC; 3) what these calculations and differences in terminology mean for assessing the quality of the calculated SOC values; 4) additional notes on SOC calculations that are specific to the Alaska Deep Soil C Project data reports.

1a. SOC Calculations: Layer

For any given layer, whether it is a horizon of known thickness or a uniformly sampled depth increment, the SOC pool size of that layer is calculated as:

*SOC = (%C * BD * Th) / 100*

Where, for each layer, *SOC* is the soil organic C pool size (g cm^{-2}); *%C* is the concentration of ***organic C*** (*e.g.*, method 6A1C; Burt, 2004) ***or total*** C (*e.g.*, method 6A2d; Burt, 2004), *BD* is the bulk density (g cm^{-3}), and *Th* is the thickness (cm).

1b. SOC Calculations: Profile

A profile is the sum of its component layers, which may have been sampled by horizon or depth. Profile SOC pool sizes in the database reports are reported to varying depths. For profiles less than 100 cm, the total SOC pool is calculated to the maximum sampled extent (*e.g.,* 40 cm or 86 cm) by summing the SOC contents of the profile's component layers. Profiles 100 cm in depth have their SOC pool sizes reported to that depth, and profiles sampled deeper than 100 cm have their SOC pool sizes computed to a fixed 100 cm depth:

$$SOC_{adj} = ((100 - layer\_top) / (layer\_bot - layer\_top)) * SOC$$

where SOC_{adj} is the adjusted calculation of SOC and *layer_top* and *layer_bot* are the top and bottom of the layer that is intersected by 100 cm.

2. SOC Calculations: Variables Used

As noted in section 1a, the %C values used to calculate SOC pool sizes in the database reports included both % organic carbon (OC) and % total carbon (C_tot). Whenever possible, C_tot was used, because it was the more commonly reported measurement, although in other cases OC was the only available measurement. In soils with high inorganic C contents, using C_tot for this calculation will overestimate the SOC pool size. Users may simply acknowledge this as a limitation (potential bias) in the dataset, address this problem by using %$CaCO_3$ data to calculate corrected OC values for samples reporting both C_tot and %$CaCO_3$, or use other approaches.

Similar variation exists in the forms of bulk density reported in the database. Whenever possible, SOC pool sizes were calculated using sample bulk densities, which describe the grams of oven-dry, 2mm-sieved, root free soil per cm^{-3} (bd_samp; sample bulk density). However, in some cases, bulk density was only available for unsieved soils, which frequently contain particles >2mm and roots >1mm (bd_tot; total bulk density). Still other SOC pool sizes in the database reports were calculated using whole soil bulk densities (bd_whole) taken directly from the USDA-NRCS National Cooperative Soil Characterization Database, which are derived, not measured, bulk density values. Some of these whole soil bulk densities were derived from in-the-field estimates of coarse fragment content, while others may have simply been gap-filled according to averaged or theoretical values. Further, the clod method for measuring bulk density, commonly used for USDA-NRCS samples, is known to be different compared to other methods such as coring. The end result of this variation in bulk density measurement and estimation techniques is the introduction of unquantified bias into the calculated SOC pool sizes in the database reports. Users with strict requirements may wish to filter the data in the reports and use only those that reported bulk density as bd_samp, while for other purposes using all SOC pool sizes regardless of the type of bulk density measurement may be sufficient.

3. Data Quality

It is the intent of the NSCN to provide an assessment of the 'quality' or risk of bias associated with each layer- or profile-level SOC pool size calculation in the National database reports. At this time, we plan to assign quality scores (letter grades) according to which C concentration and bulk density techniques were used. The rubric is outlined below, and shows that emphasis is placed on using OC as the C-reporting parameter, and bd_samp as the bulk density parameter. Reporting data in terms such as C_tot, the less precise bd_tot, or the estimated bd_whole terms will result in lower quality grades.

SOC pool size computed using	Quality score
oc, bd_samp	A
oc, bd_tot	B
c_tot, bd_samp	B
c_tot, bd_tot	B
oc, bd_whole	C
c_tot, bd_whole	C

*Layers missing C concentration, bulk density, or both are not currently shown in the National database reports. Database reports for the AK Deep Soil C Project, however, used modeled relationships to fill such data gaps; details on the calculations involved in that process are detailed in section 4 below.

4. Calculations Specific to the AK Deep Soil C Project Reports

The database reports produced by the Alaska Deep Soil C Project are populated by some data that were derived from modeled relationships between reported variables. In most cases, these modeled relationships were applied in order to derive bulk density from %C for individual samples. Other equations were applied to make minor adjustments so that %C and bulk density measurements from different methods, and their SOC calculations, were comparable. The propagated error from using these equations and adjustments for calculating SOC at the profile level remains unquantified. These calculations are described below, with text adapted from Appendix 1 of Johnson et al. (in review).

Gap-filling procedure

Negative exponential models that predict bulk density from %C were applied for missing data in all mineral soil horizons except arctic soils (Table 1 below). There were some rare cases when samples had bulk density data available but not %C and were gap-filled using a modified equation (Eq. 3b). Models of SOC or bulk density were better fit when the horizon designation was known (Eq. 4-6). When there was no horizon designation, and the horizon was only known to be organic (SOC_{O}) or mineral (BD_{min}), then general models were applied (Eq's. 3a, 9). Frozen mineral soil bulk density of mainly boreal profiles was predicted separately from the relation found from the %C and bulk density relation of similar soils, but was not distinguished by horizon designation (Eq. 7). In contrast to bulk density measurements of mineral soils, bulk density in organic soils was not well-predicted by non-linear models of %C. The best approach in this case proved to be the direct prediction of SOC content from horizon thickness, *Th*, using a weighted least squares regression and by horizon designation (Eq. 10-12).

Adjustment equations were applied to bulk density and organic carbon concentration measurements from the USDA-NRCS in order to make them comparable to other datasets. Bulk density measurements by the USDA-NRCS were done by the clod method, BD_{clod} (method 3B1; Burt, 2004) whereas all the other bulk densities in the AK database reports were measured by the cylinder method, BD_{core}. The clod method yields consistently higher values than the cylinder method (Van Remortel and Shields, 1993; Calhoun et al., 2001). To correct for this difference in mineral soils, the same equation used in VanRemortel and Shields (1993) was applied (Eq. 1). A similar correction equation has not been published for organic soils to our knowledge. Yet, we found that organic layer bulk densities measured by the clod method were between 1.4 and 5 times greater than by the core method (using a subset of data including black spruce stands only). Therefore, organic horizon bulk density measurements by the clod method were excluded and treated as if they were missing data. For organic carbon concentration, some NRCS data (26% of the total dataset) was measured only for organic carbon, $\%C_{org}$ (*e.g.*, method 6A1c; Burt, 2004). The rest of the dataset was measured for total carbon, $\%C_{tot}$ (methods 4H2a or 6A2d; Burt, 2004).Therefore, a relation was found so that in cases where only $\%C_{org}$ data was available, it was adjusted to more closely match $\%C_{tot}$ (Eq. 2).

In the arctic tundra many profiles were highly cryoturbated which requires specialized methods of calculating SOC content (*e.g.*, Michaelson et al., 1996). The 1-m SOC estimates for highly cryoturbated profiles in this study included only those with published values (Michaelson et al., 1996; Ping et al., 1997; Bockheim et al., 1999; Bockheim, 2007a,b) and therefore no bulk density predictions were necessary. Non-cryoturbated soils whether organic or mineral, frozen or unfrozen, were predicted by a separate relation specific to arctic soils (Eq. 13; see also Bockheim et al., 2003 for a similar equation).

Table 1. Gap-filling equations for the AK Deep Soil C Project database reports.

Equations	**adj. R2**
adjustment equations	
1. $BD_{adj} = BD_{core} = \frac{BD_{clod} - 0.068}{1.011}$	0.98
2. $\%C_{adj} = \%C_{tot} = 0.2107 + 0.8830 * \%C_{org}$	0.98
prediction equations for mineral soils	
3a. $BD_{\min} = 0.4189 + e^{-0.1868 * \%C_{tot}}$	0.64
3b. $\%C_{pred} = -\frac{\log(BD_{core} - 0.4223)}{0.1890}$	0.54
4. $BD_{A} = 0.3417 + e^{-0.1712 * \%C_{tot}}$	0.59
5. $BD_{B} = 0.4671 + e^{-0.1915 * \%C_{tot}}$	0.52
6. $BD_{C} = 0.6560 + e^{-0.2466 * \%C_{tot}}$	0.49
7. $BD_{frzn} = 0.3105 + e^{-0.1400 * \%C_{tot}}$	0.48
prediction equations for organic soils	
9. $SOC_{O} = 0.0085 + 0.0334 * Th$	0.47
10. $SOC_{Oi} = 0.0109 + 0.0183 * Th$	0.38
11. $SOC_{Oe} = 0.0269 + 0.0411 * Th$	0.59
12. $SOC_{Oa} = 0.0743 + 0.0354 * Th$	0.63
prediction equation for all arctic soils frozen or unfrozen; mineral, organic, or cryoturbated	
13. $BD = 0.0577 + e^{-0.0694 * \%C_{tot}}$	0.60

Data quality assessment for the AK Deep Soil C Database reports is based on the gap-filling equations described above, which were used to calculate the SOC values in the reports. See the rubric below:

SOC pool size computed using	Quality score
No gap-filling or adjustments*	A
Equations 1-2	B
Equations 3-13	C
Equations 1-2 and 3-13	C

*includes highly cryoturbated arctic tundra 1-m SOC estimates from publications

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