Validation of modelled soil organic carbon pools by DRIFT-PLS

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Can we assign a chemical fingerprint to modelled SOM pools by measuring spectral attributes of the bulk soil?

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Foreword

I am not a modeller

I am working on agricultural soils

Results from a long-term agricultural experiment will be presented

Hope that it will stimulate the discussion anyhow
Outline

Why validation at the pool level and how?

What is DRIFT-PLS?

The long-term experiment in Bad Lauchstädt, Germany

The CANDY soil organic matter model

Results and Discussion
Why validation at the pool level?

SOM-pools are related to different soil functions

Could help for model initialization

Short – to medium term response of SOM to climate/management depends much on labile/intermediate C,N
How validation at the pool level?

Making use of isotopic labelling experiments

Soil fractionation and comparison to modelled pools

Indirect modelling

...
Criteria for SOM pool / fraction

Pool: A compartment containing material that is chemically indistinguishable and equally accessible (Jenkinson et al. 1985)

Measured fraction equals modelled pools if it is unique and non-composite in its dynamics (Smith et al. 2002)

Experimentally derived soil fractions have different turnover rates are often chemically different

Are conceptual model pools characterised by chemically unique soil attributes?
**DRIFT-PLS** (diffuse reflectance infrared Fourier-transform spectroscopy with partial least squares regression)

**DRIFT-spectra** with high information density (organic and mineral composition of soil)

Multivariate statistics is applied to
1) relate spectral information to property measurements and
2) Reduce the dimension of the data set
= indirect modelling

**PLS**: *Calibration* and *Prediction*

Validation of modelled soil organic carbon pools by DRIFT-PLS
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PLS: Calibration and Prediction

DRIFT spectra + property data set (e.g., SOC-contents) → PLS factors; PLS loading and score vectors and weights → Residuals for x and y

Statistical Model to predict y-value

\[ y_{\text{pred}} = x \times \text{regression coeff.} \]
DRIFT-PLS

IR-PLS has been applied to:

predict various soil properties (texture, pH, CEC, OC, N, functional groups) (e.g. Janik and Skjemstad 1995a,b, McCarty et al. 2002, Rumpel et al. 2001; Leifeld 2006)

predict C in soil fractions
(Cozzolino & Maron 2006, Zimmermann et al. 2006)

→SOM fractions and functional groups can be predicted (uncertainty!)

This talk: Prediction of modelled C-pools
(pool size treated as measured soil property)
The static fertilisation long-term experiment in Bad Lauchstädt, Germany

Different fertiliser applications since 1902:

N=without fertilisation
NM=change from null to manuring in 1978
MN=change from manuring to null in 1978
M=Manuring since 1902

Haplic Chernozem (FAO), 22% clay
MAT 8.7°C
MAP 484 mm

Crop rotation: winter wheat, spring barley, sugar beet, potatoes

Validation of modelled soil organic carbon pools by DRIFT-PLS
The static fertilisation long-term experiment in Bad Lauchstädt, Germany

<table>
<thead>
<tr>
<th>Treatment</th>
<th>Soil Management</th>
<th>Yield$^2$</th>
<th>% SOC$^3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>N</td>
<td>No fertiliser since 1902</td>
<td>1.39</td>
<td>1.73</td>
</tr>
<tr>
<td>N→M</td>
<td>Manure$^1$ since 1978</td>
<td>3.54</td>
<td>2.18</td>
</tr>
<tr>
<td>M→N</td>
<td>No manure since 1978</td>
<td>2.71</td>
<td>2.16</td>
</tr>
<tr>
<td>M</td>
<td>Manure since 1902</td>
<td>3.68</td>
<td>2.38</td>
</tr>
</tbody>
</table>

$^1$ Manure: 15 t ha$^{-1}$ a$^{-1}$

$^2$ t ha$^{-1}$, summer barely 1994

$^3$ 2004, 0-20 cm; mean over 7 sampling dates between April - October
The CANDY model (Franko et al. 1995)

Crop model
Hydrological model
Management

Environmental drivers:
Temperature, WFPS,
Content clay+fine silt

Validation of modelled soil organic carbon pools by DRIFT-PLS
Carbon\(^1\) distribution among pools modelled by CANDY

Most of C is ‘inert C’

‘Inert’ \(\neq\) inert

Inner pool variance: mainly management-induced

‘Active’ and ‘stabilised’ SOC: Small contribution to total variance

\(^1\)C stocks in 0-30 cm
Validation of modelled soil organic carbon pools by DRIFT-PLS

SOC measured vs. SOC modelled by CANDY

$R^2 = 0.93$

rel. SEE $4.1\%$

Validation of modelled soil organic carbon pools by DRIFT-PLS
Validation of modelled soil organic carbon pools by DRIFT-PLS

SOC measured vs. SOC modelled by DRIFT-PLS:

- **R²**: 0.93
- **SEE**: 3.1%

SOC measured vs. SOC modelled by CANDY:

- **R²**: 0.90
- **SEE**: 4.9%

Previous page (SOC meas. vs. SOC modelled by CANDY):

- **R²**: 0.93; **SEE**: 4.1%

Validation of modelled soil organic carbon pools by DRIFT-PLS
Validation of modelled soil organic carbon pools by DRIFT-PLS

DRIFT-PLS modelling: Pools vs. other soil properties

\[ \text{SEP}\% = \left( \frac{\sum (y_{\text{pred.}} - y_{\text{meas.}})^2}{n_s - 1} \right) \frac{100}{y_{\text{mean}}} \]

Validation of modelled soil organic carbon pools by DRIFT-PLS
DRIFT-PLS modelling: Pools vs. other soil properties

Validation of modelled soil organic carbon pools by DRIFT-PLS

\[
1SE\text{P}(%) = \sqrt{\frac{\sum (y_{\text{pred.}} - y_{\text{meas.}})^2}{n_s - 1}} \times 100
\]

\[\text{mean}\]

\[\text{sep}\]

\[\text{soc}\]

\[\text{active C}\]

\[\text{stabilised C}\]

\[\text{inert C}\]

\[\text{plant residues}\]

\[\text{NMR functional groups}\]

\[\text{C in physico-chemical fractions}\]

\[\text{Soil organic carbon}\]

\[\text{modelled CANDY-pools}\]
Validation of modelled soil organic carbon pools by DRIFT-PLS

DRIFT-PLS modelling: CANDY-pool ‘stabilised C’

Predicted with cross-validation

Calibration model
Validation of modelled soil organic carbon pools by DRIFT-PLS

DRIFT-PLS modelling: Pools vs. other soil properties

Validation of modelled soil organic carbon pools by DRIFT-PLS
Validation of modelled soil organic carbon pools by DRIFT-PLS

Title:
DRIFT-PLS modelling: Pools vs. other soil properties

Diagram:
- SEP (% of mean value) vs. R2 (PLS calibration)
- Data points for:
  - NMR functional groups
  - C in physico-chemical fractions
  - Soil organic carbon
  - Modelling CANDY-pools
- Symbols for:
  - Stabilised C
  - Active C
  - Inert C
  - Plant residues

Subtitle:
Validation of modelled soil organic carbon pools by DRIFT-PLS
Can we assign a chemical fingerprint to modelled SOM pools by measuring spectral attributes of the bulk soil?

Chemical soil attributes can be modelled indirectly by DRIFT-PLS

Representation of total and inert C in CANDY by DRIFT-PLS: Reliable

Representation of all non-inert CANDY-pools by DRIFT-PLS: Flawed

No treatment effects

No temporal dynamics over the year

No single PLS model for the same pool in different treatments
Can we assign a chemical fingerprint to modelled SOM pools by measuring spectral attributes of the bulk soil?

Conceptual pool structure in CANDY does not reproduce important chemical attributes of SOM \textit{(take-home message)}

BUT: Is this an indication for a conceptually wrong model?
Validation of modelled soil organic carbon pools by DRIFT-PLS

Carbon distribution among treatments modelled by CANDY
DRIFT-PLS modelling: Pools vs. other soil properties

Validation of modelled soil organic carbon pools by DRIFT-PLS