Validation of modelled soil organic carbon pools by DRIFT-PLS

Jens Leifeld[1], Uwe Franko[2] and Elke Schulz[2]

1 Swiss Federal Research Station for Agroecology and Agriculture, Zürich, Switzerland

2 UFZ Centre for Environmental Research, Leipzig-Halle, Germany

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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)*

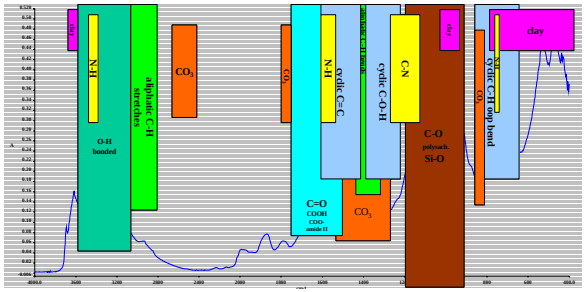
Measured fraction equals modelled pools if it is unique and non-composite in its dynamics *(Smith et al. 2002)*

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**

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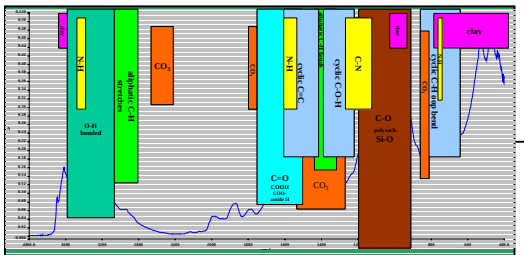
DRIFT-PLS

PLS: Calibration and Prediction



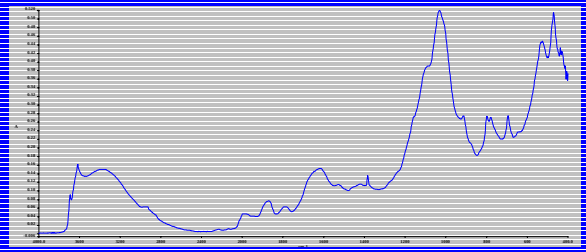
BL 097	15.1
BL 110	7.1
BL 098	3.6
BL 076	1.3
BL 089	479.1
BL 003	235.1
BL 011	175.8
BL 047	35.8
BL 013	17.1
BL 081	8.7
BL 039	3.2
BL 019	520.1
BL 015	255.1
BL 001	190.8
BL 044	20.5
BL 042	9.7
BL 091	4.9
BL 069	1.7
BL 043	412.1
BL 079	200.1
BL 108	148.9
BL 068	32.1
BL 038	15.4
BL 074	7.8
BL 063	2.9
BL 096	552.8
BL 059	271.1
BL 067	202.9

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_{pred} =  x *regression coeff.*

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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

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The static fertilisation long-term experiment in Bad Lauchstädt, Germany

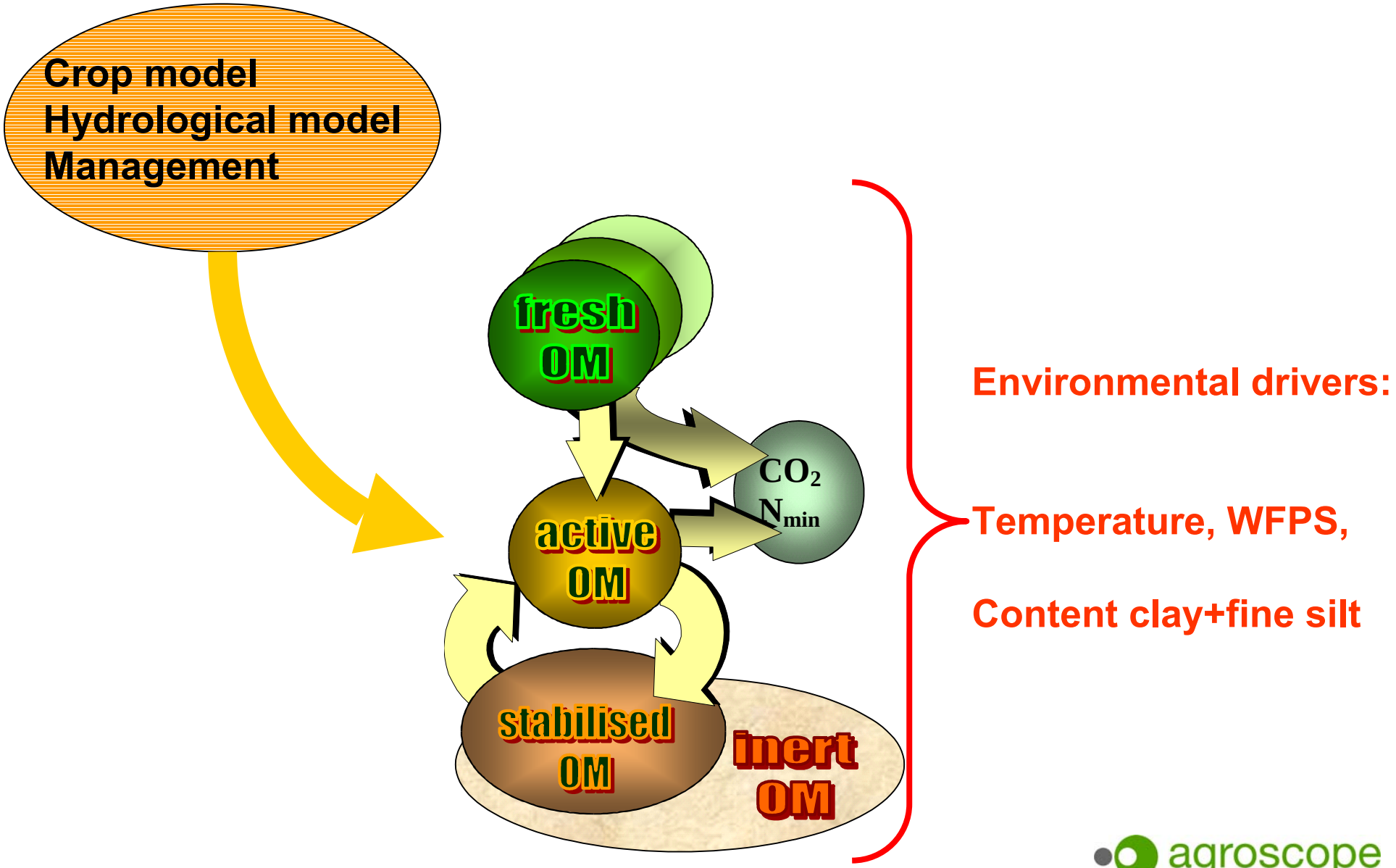
		Yield[2]	% SOC[3]
N	No fertiliser since 1902	1.39	1.73
N→M	Manure[1] since 1978	3.54	2.18
M→N	No manure since 1978	2.71	2.16
M	Manure since 1902	3.68	2.38

[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)*



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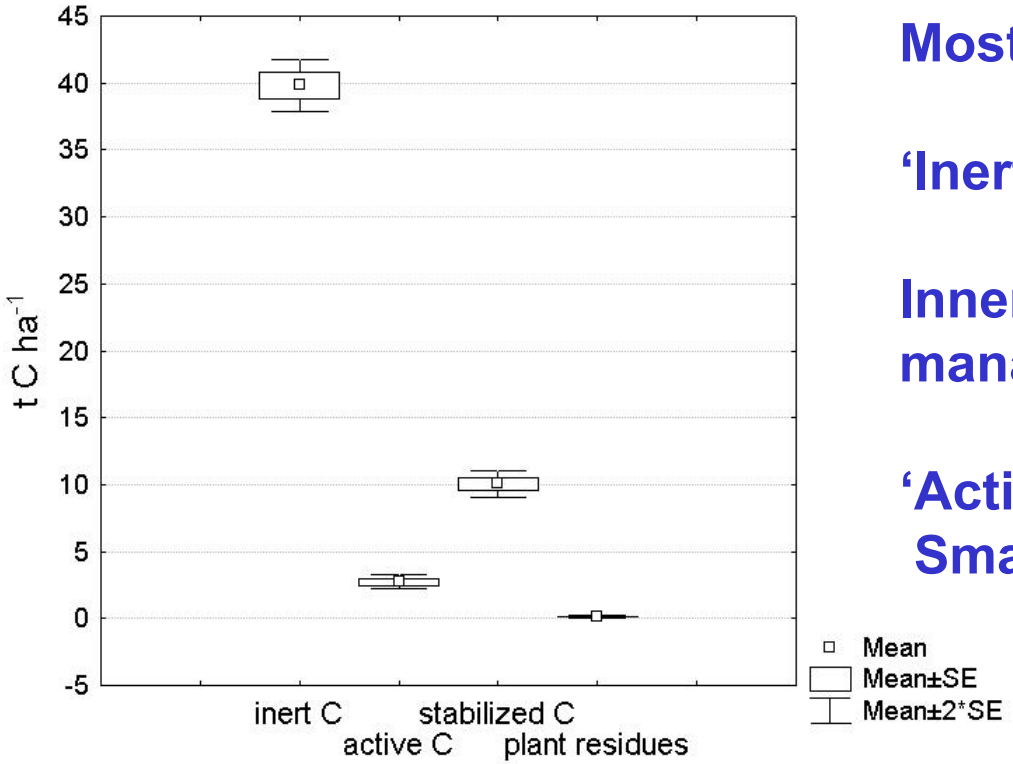
Carbon[1] distribution among pools modelled by CANDY



Most of C is 'inert C'

'Inert' ≠ inert

Inner pool variance: mainly management-induced

'Active' and 'stabilised' SOC: Small contribution to total variance

[1]C stocks in 0-30 cm

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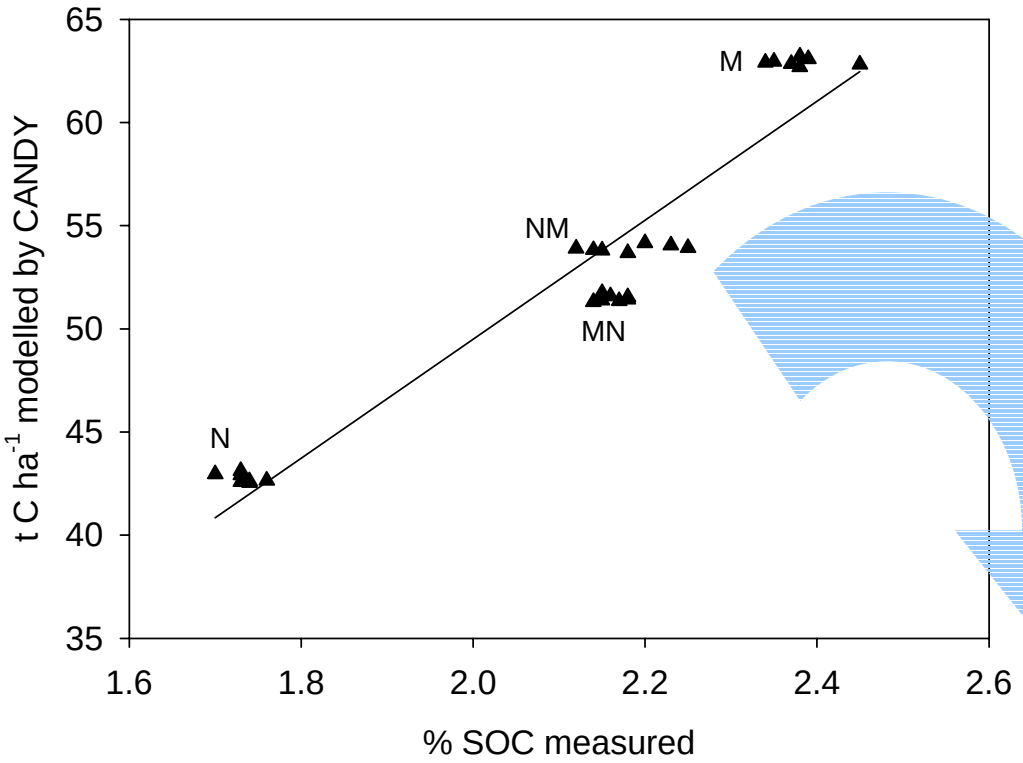
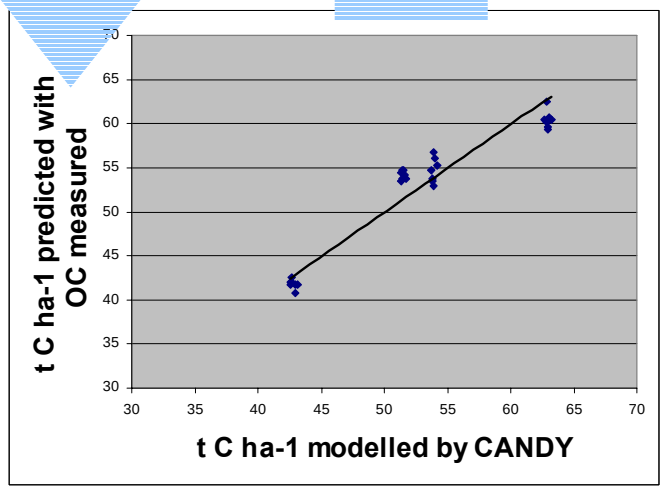
SOC measured vs. SOC modelled by CANDY



R^2 0.93

rel. SEE 4.1%[1]



$$^{1}SEE(\%) = \frac{\sqrt{\frac{\Sigma(y_{icalib.} - y_{imeas.})^2}{n_s - d.f.}}}{y_{mean}} \times 100$$

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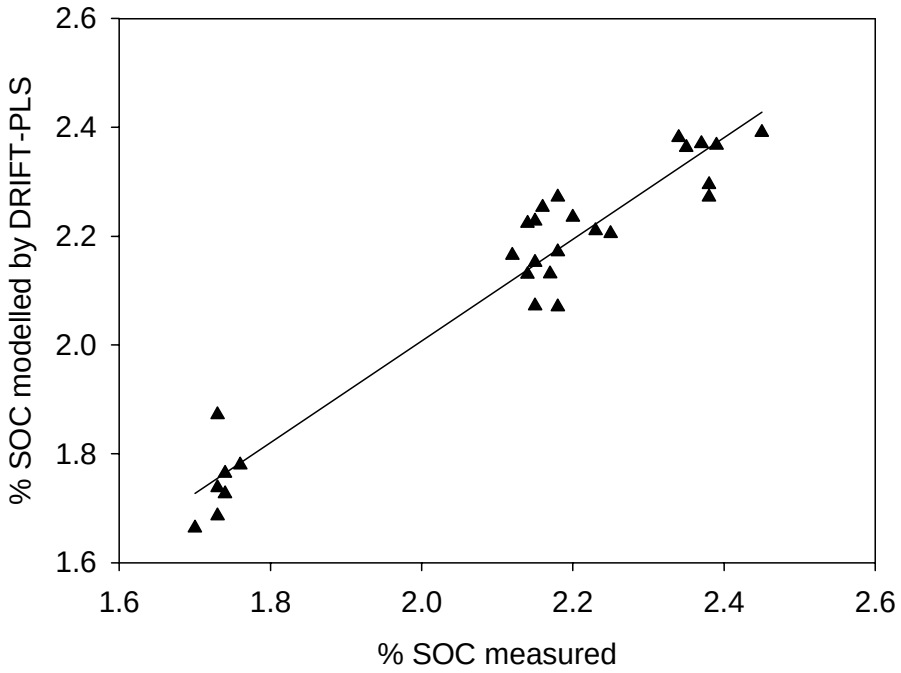
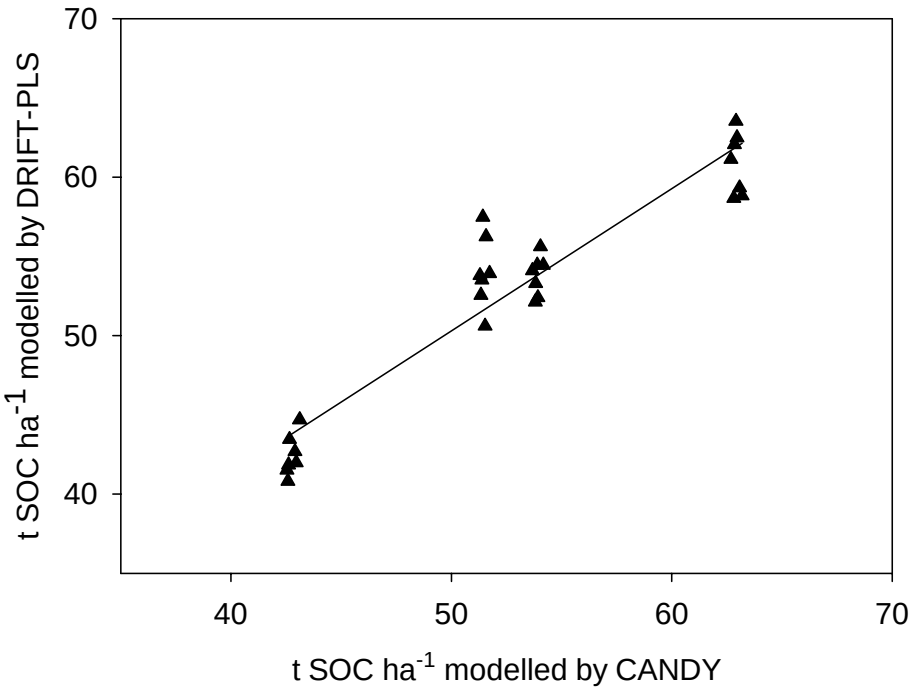
SOC modelled by DRIFT-PLS

SOC measured



R^2 0.93
SEE 3.1%

CANDY-SOC



R^2 0.90
SEE 4.9%

Previous page (SOC meas. vs. SOC modelled by CANDY):
R^2 = 0.93; SEE = 4.1%

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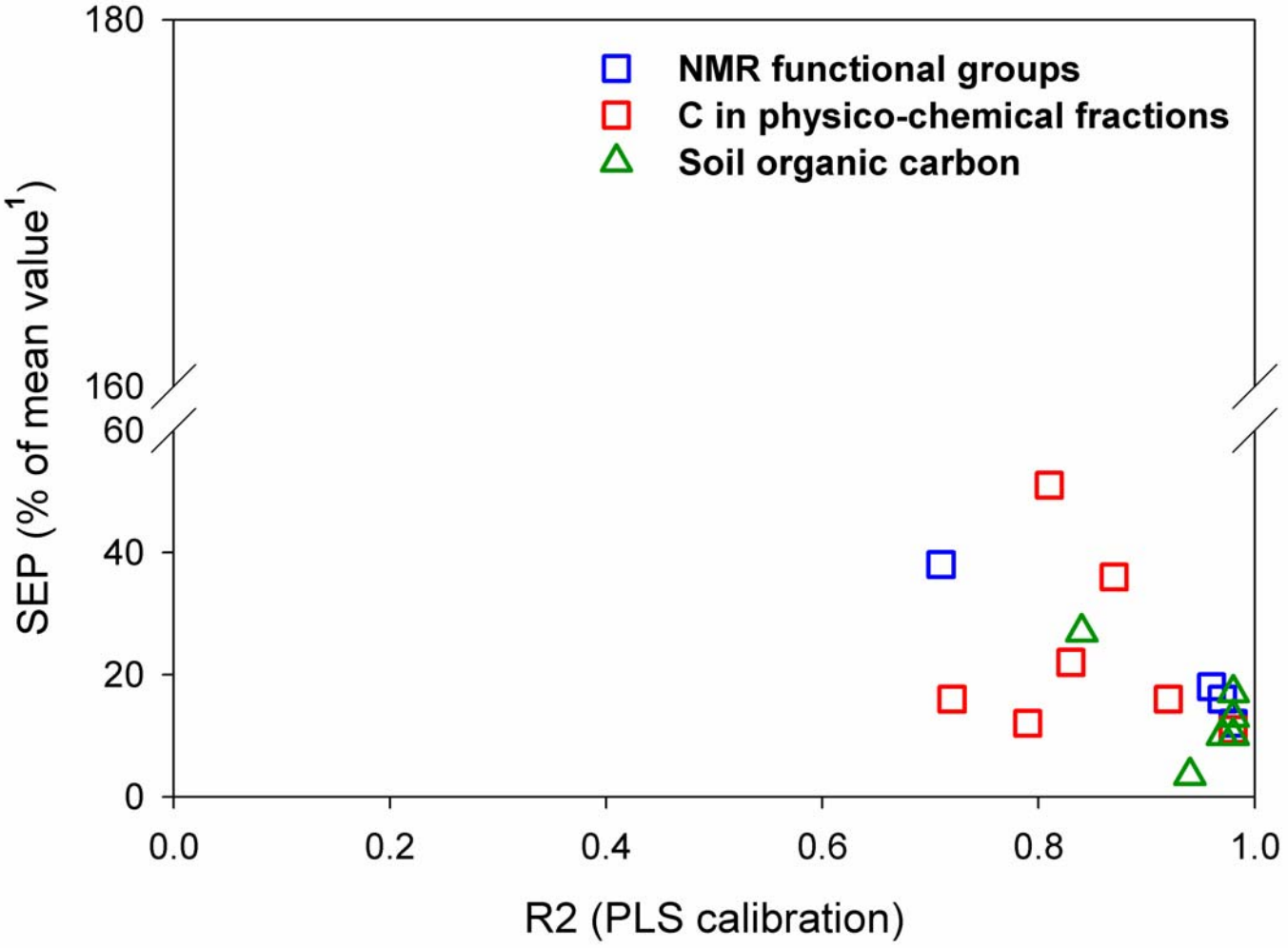
DRIFT-PLS modelling: Pools vs. other soil properties



$$^{1}SEP(\%) = \frac{\sqrt{\frac{\Sigma(y_{i\,pred.} - y_{i\,meas.})^2}{n_s - 1}}}{y_{mean}} \times 100$$

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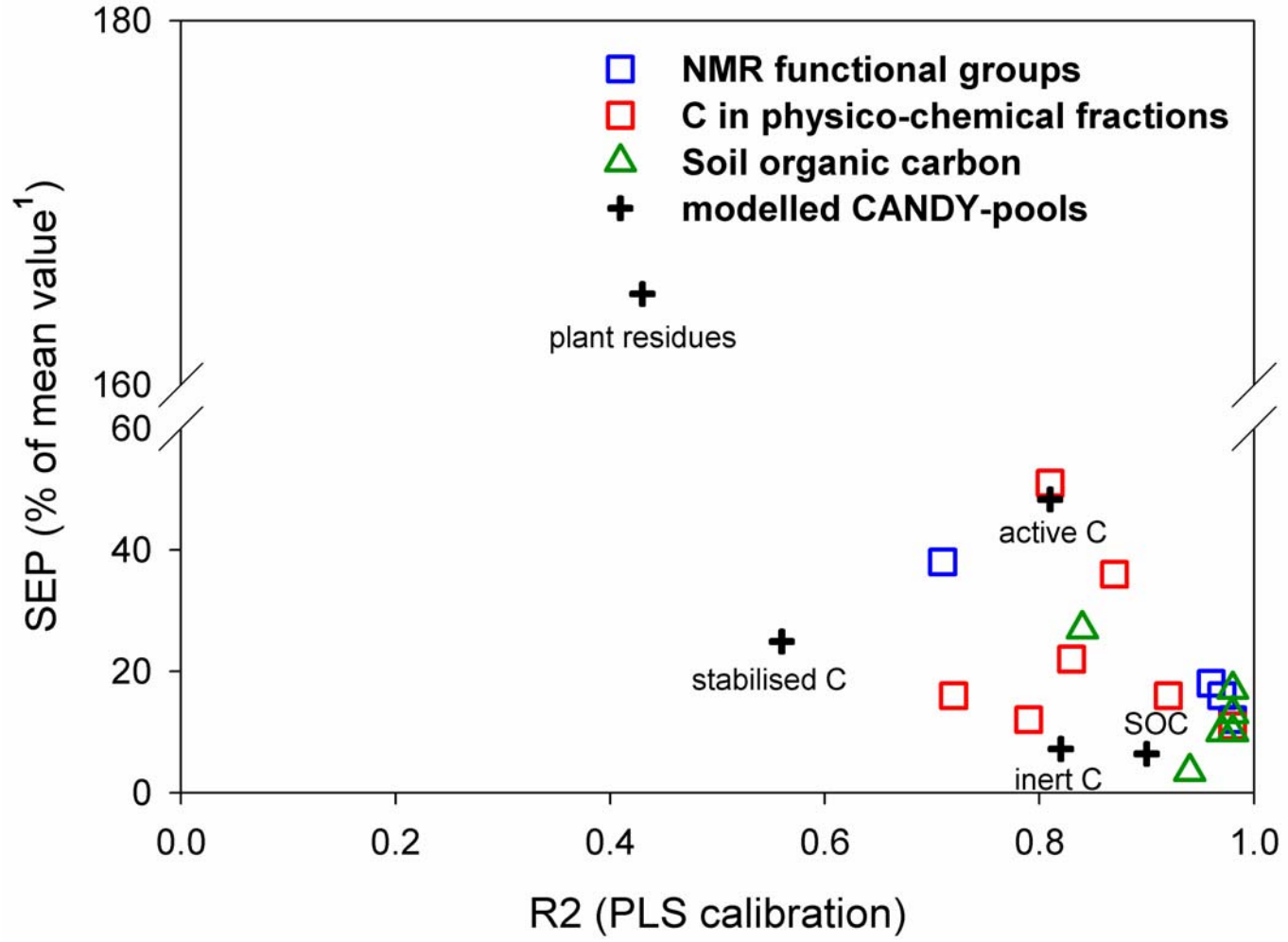
DRIFT-PLS modelling: Pools vs. other soil properties



$$^{1}SEP(\%) = \frac{\sqrt{\frac{\Sigma(y_{i\,pred.} - y_{i\,meas.})^2}{n_s - 1}}}{y_{mean}} \times 100$$

Validation of modelled soil organic carbon pools by DRIFT-PLS

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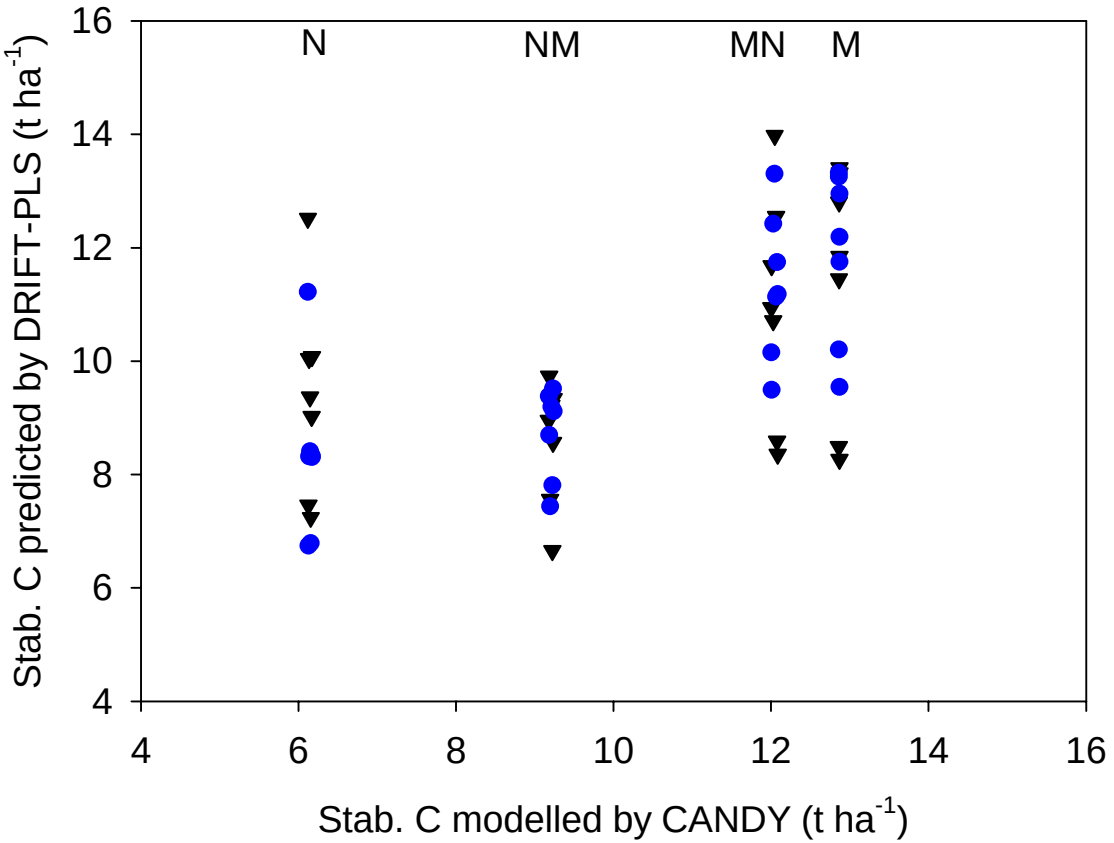
DRIFT-PLS modelling: CANDY-pool ‘stabilised C’



Predicted with cross-validation

Calibration model

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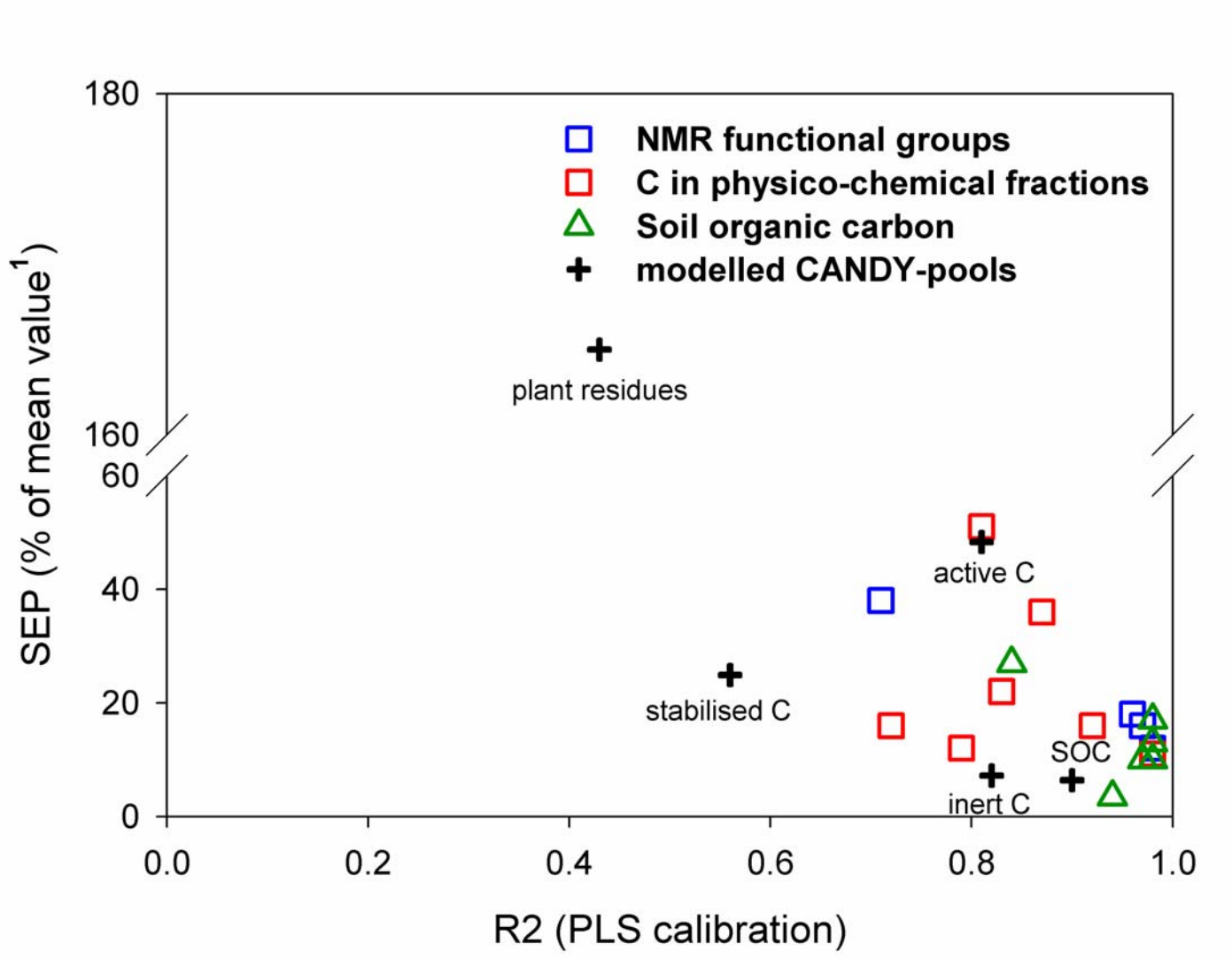
DRIFT-PLS modelling: Pools vs. other soil properties



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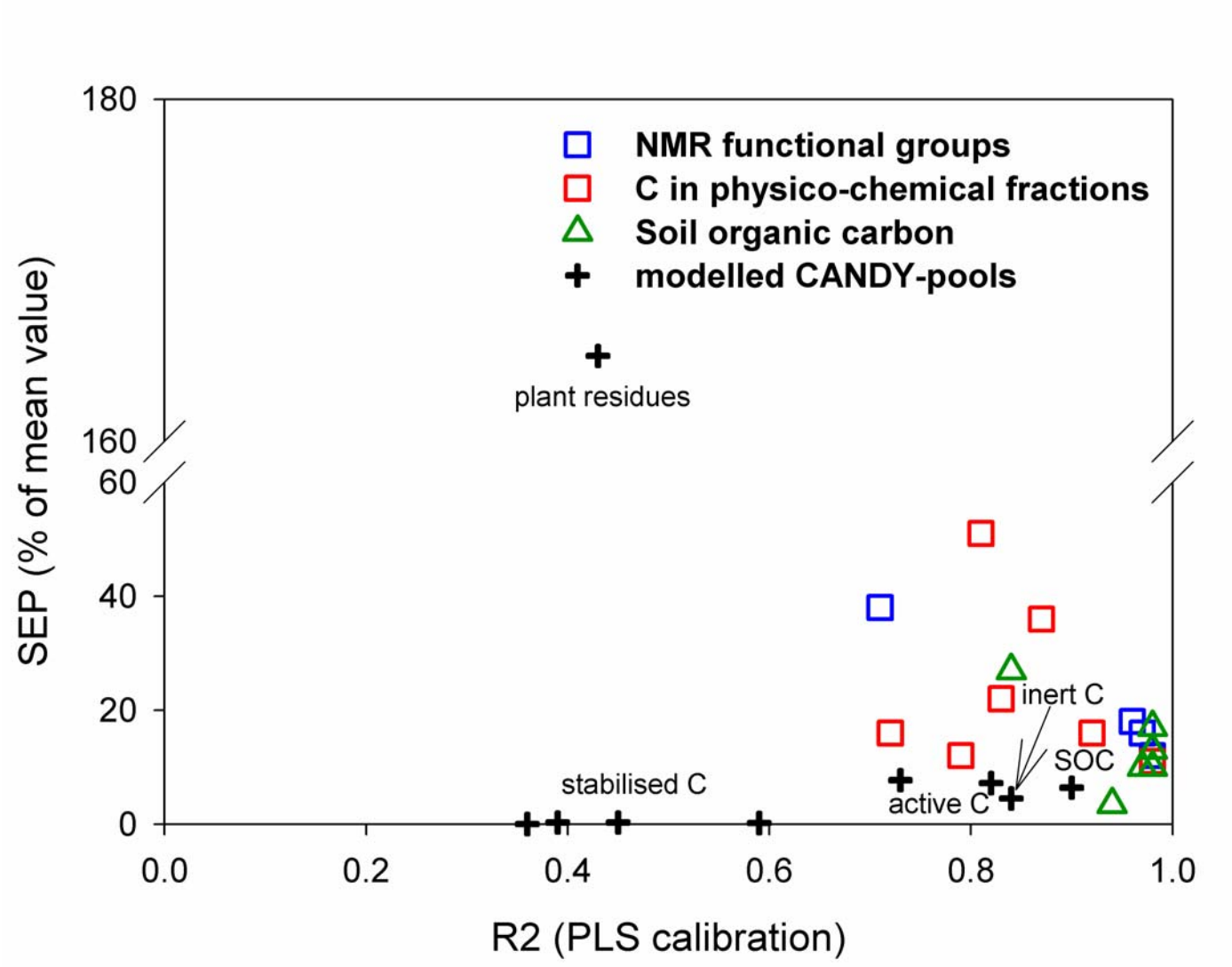
DRIFT-PLS modelling: Pools vs. other soil properties



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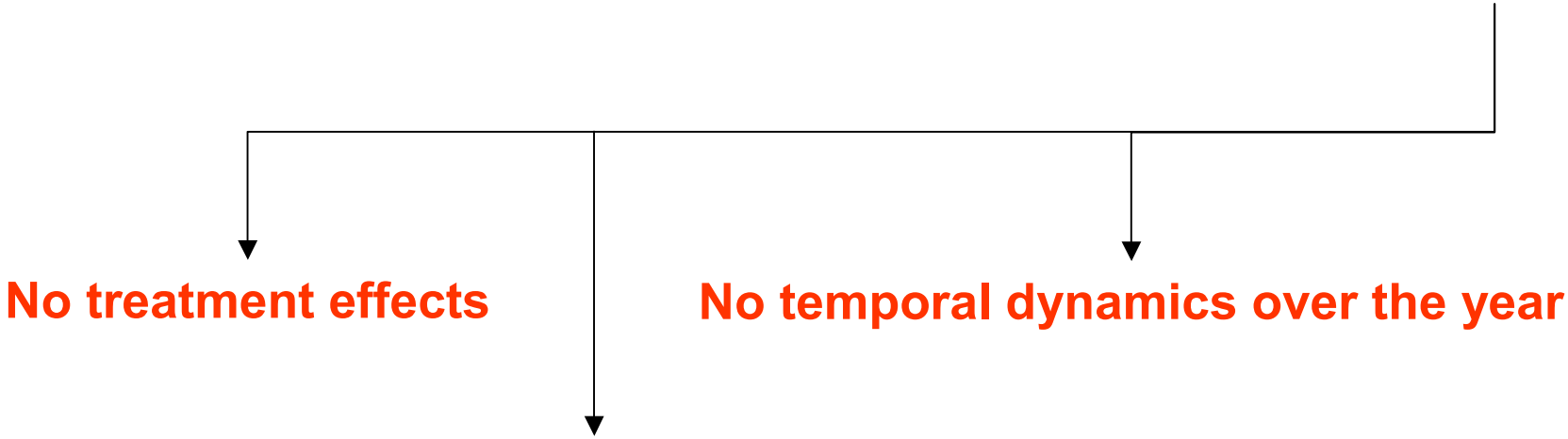
Can we assign a chemical fingerprint to modelled SOM pools by measuring spectral attributes of the bulk soil?

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



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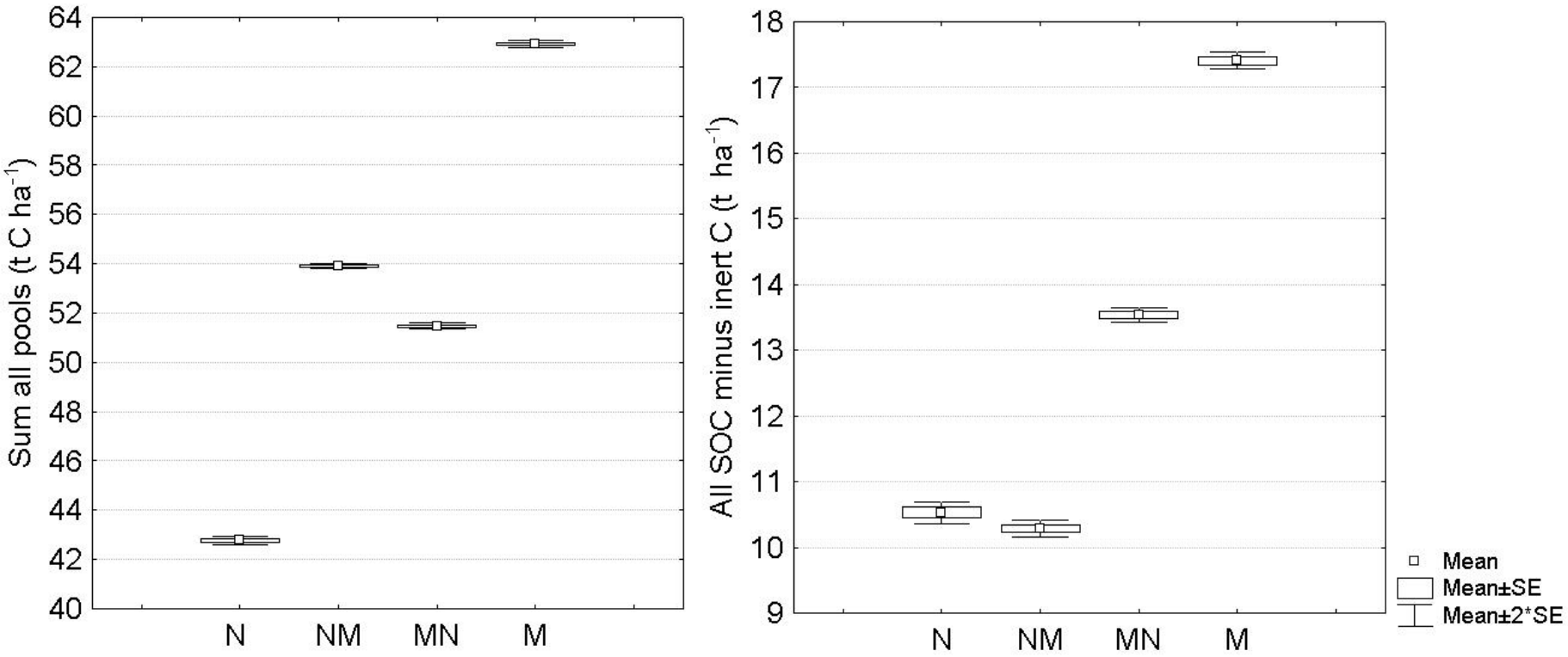
Can we assign a chemical fingerprint to modelled SOM pools by measuring spectral attributes of the bulk soil?

Conceptual pool structure in CANDY does not reproduce important chemical attributes of SOM *(take-home message)*

BUT: Is this an indication for a conceptually wrong model?

Carbon distribution among treatments modelled by CANDY



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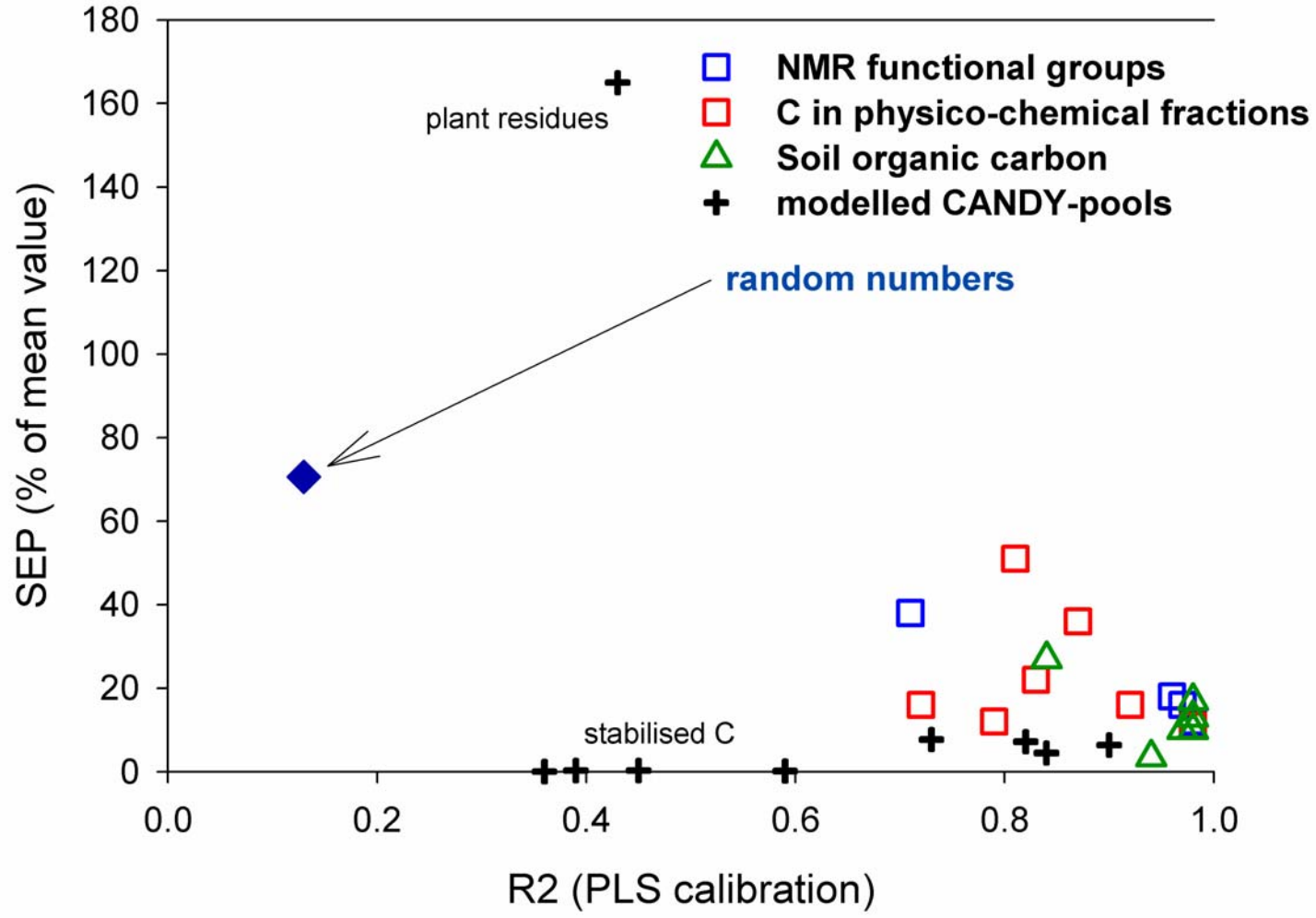
DRIFT-PLS modelling: Pools vs. other soil properties



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