



Uncertainty propagation in carbon modelling due to quantification of soil C fractions with MIR/PLS

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National Research
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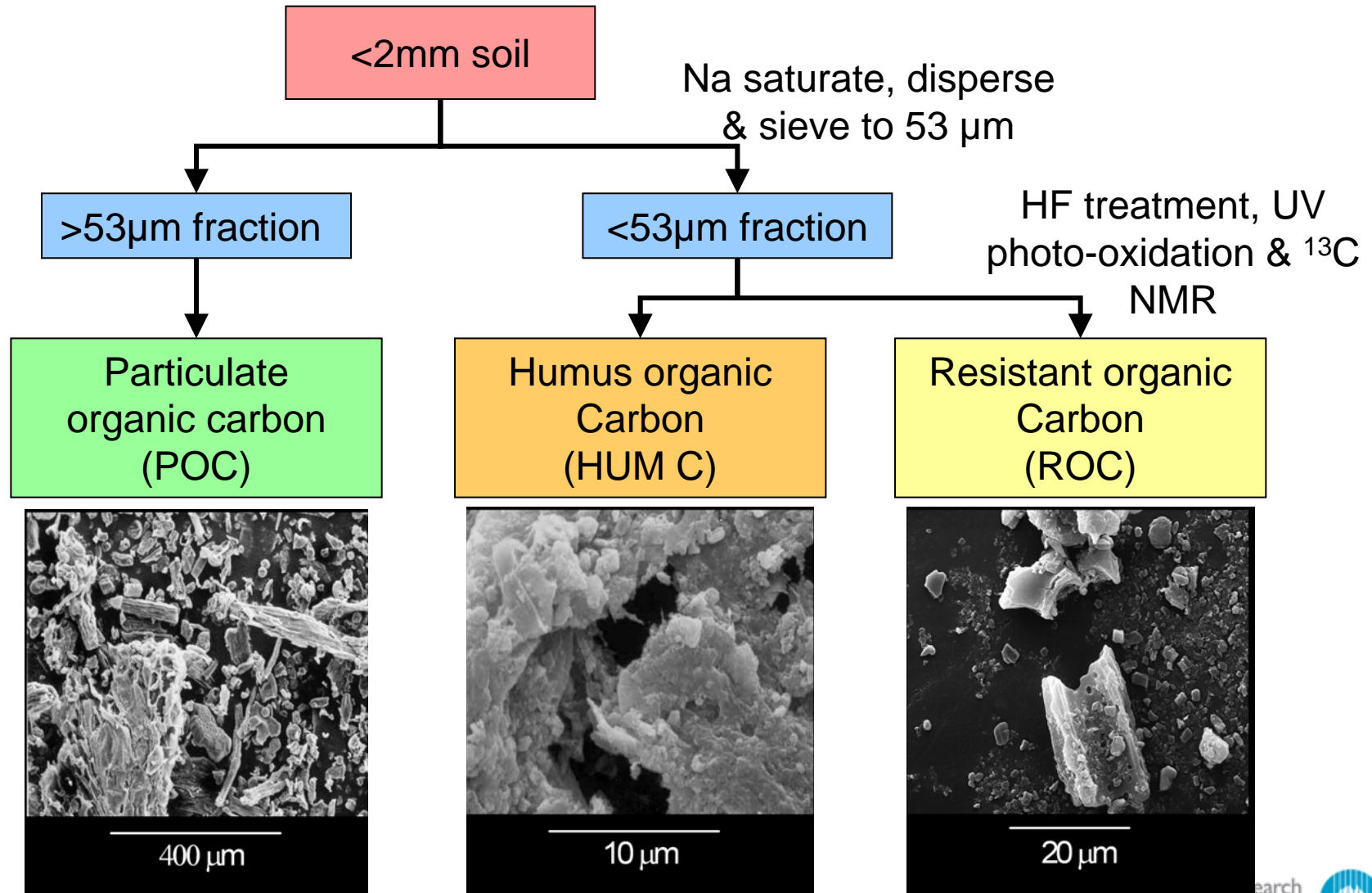
Outline

- Introduction to NCAS and soil carbon fractions
- Describe the MIR/PLS technique for predicting soil organic carbon content and allocation to fractions
- Defining the uncertainty (error) associated with the MIR/PLS predictions
- Examine the impacts of this uncertainty on outcomes of soil carbon modelling
- Conclusions

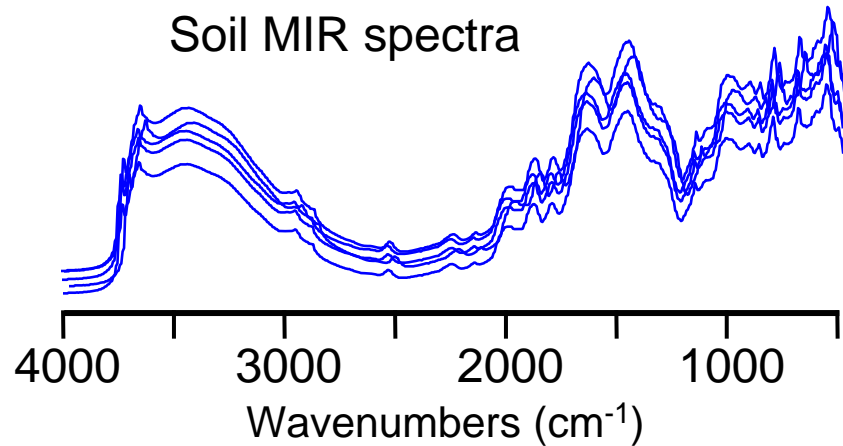
Introduction

- National Carbon Accounting System (NCAS) has been developed in response to Australia's UNFCCC reporting requirements
 - NCAS is an assemblage of a suite of different models
 - Soil carbon component is based on a variation of RothC
 - Calibrated to use measureable fractions (Skjemstad *et al.* 2004 AJSR 42 79)
- Measurement of fractions is expensive and time consuming
- A more cost effective and rapid method is being developed
 - Combines mid-infrared spectroscopy and a partial least squares statistical approach (MIR/PLS)
 - Implications on carbon modelling need to be defined

Quantifying soil organic carbon fractions used by NCAS



Predicting soil carbon content and allocation to fractions: the MIR/PLS process



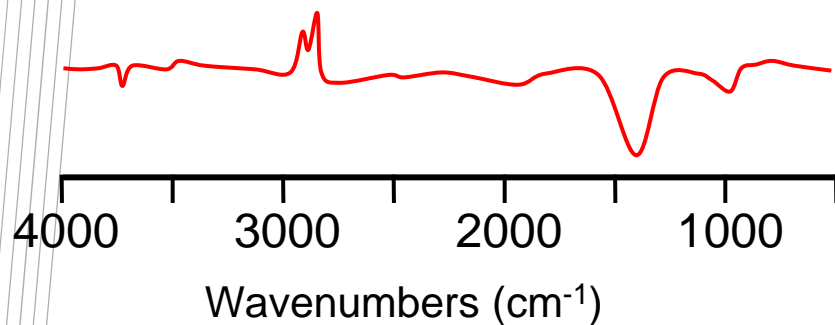
Analytical data

Soil 1	21.4
Soil 2	11.8
Soil 3	19.5
Soil 4	21.9
Soil 5	10.1



Partial Least Squares analysis

Loadings spectra

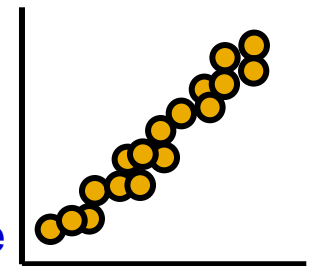


MIR/PLS predictions

Soil 1	20.3
Soil 2	12.5
Soil 3	16.2
Soil 4	19.6
Soil 5	12.5

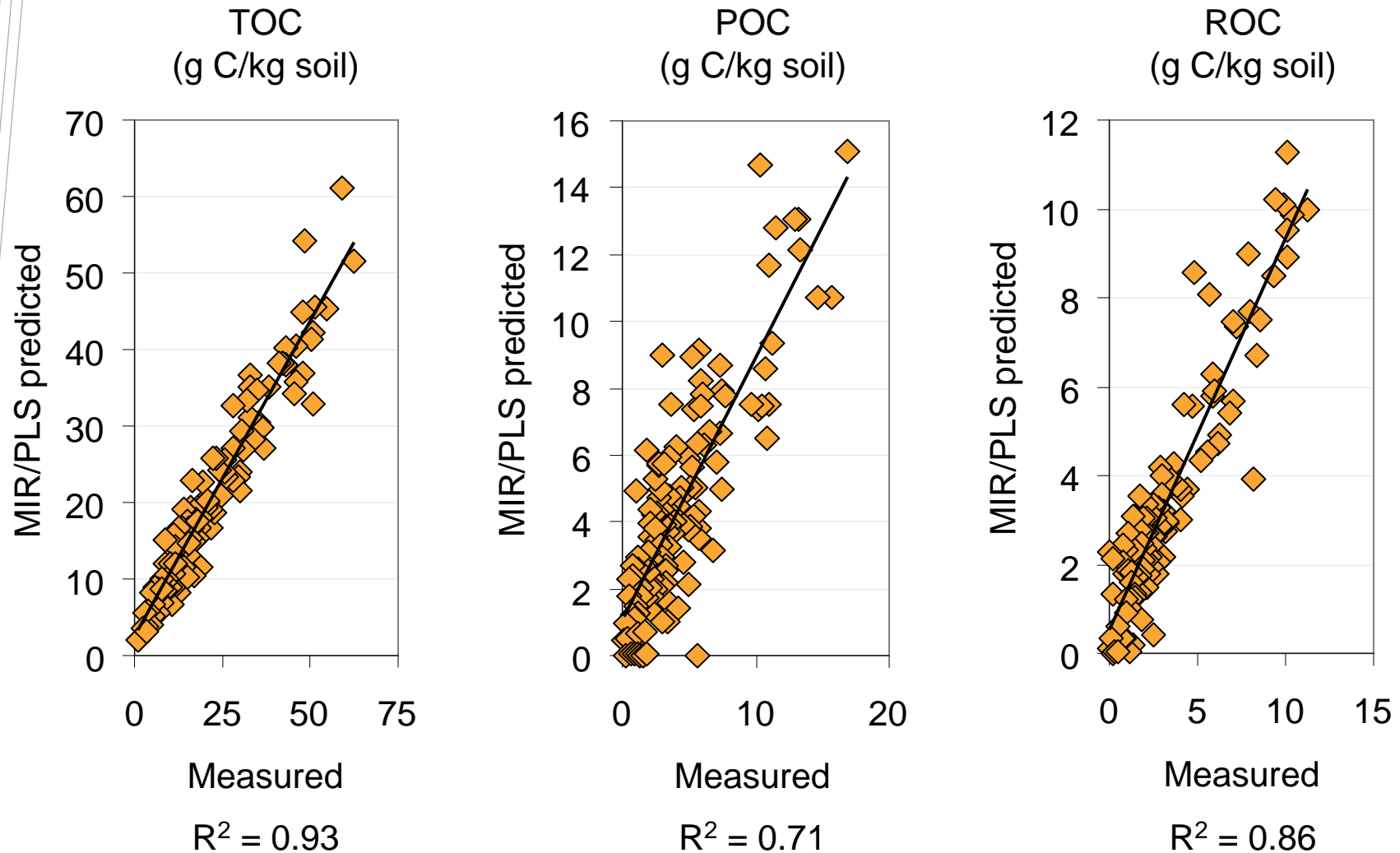


MIR/
PLS
value



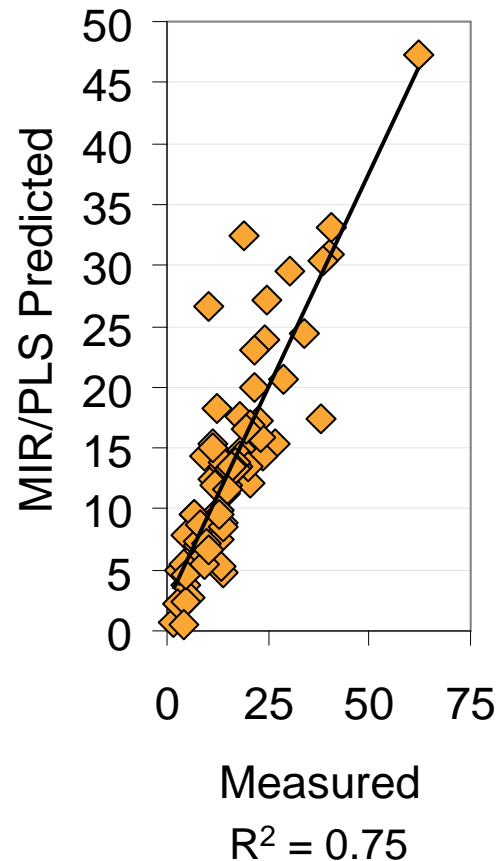
Measured value

Predicting the amount of total organic carbon and the allocation to POC and Char C



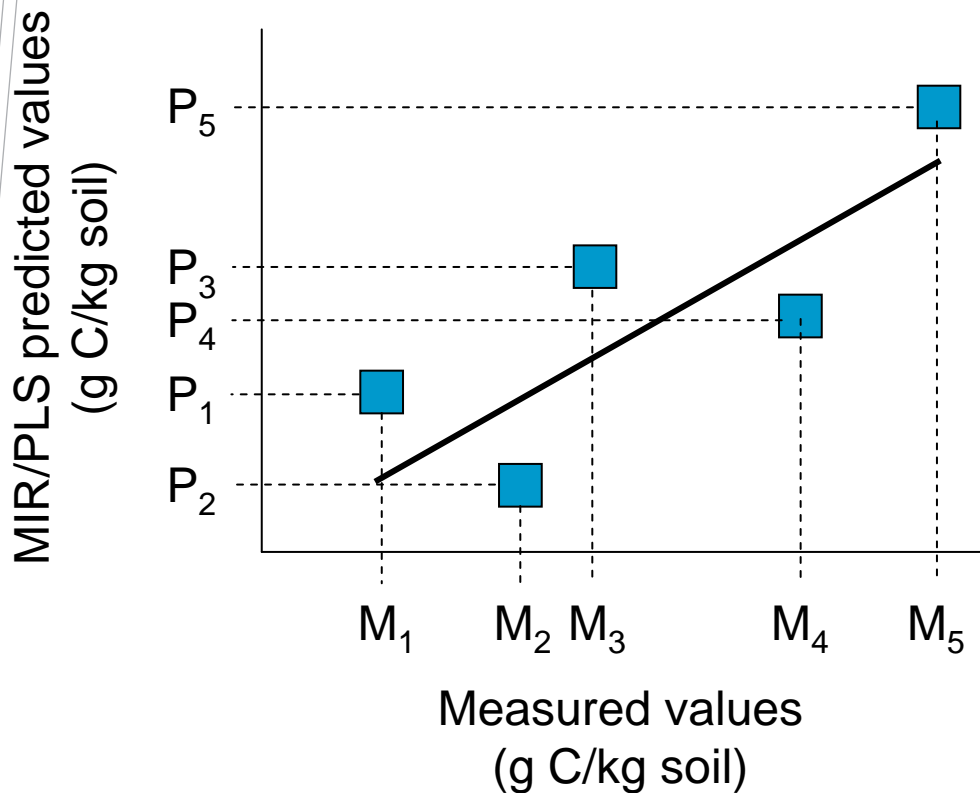
Quantifying the allocation of carbon to the Humus fraction

- Allocation of organic carbon to the Humus fraction is calculated by difference
 - $\text{HUM C} = \text{TOC} - \text{POC} - \text{ROC}$



Implication: all errors in predictions of TOC, POC and ROC accumulate in the HUM C fraction

Defining the error associated with MIR/PLS predictions



Error associated with MIR/PLS predictions

$$E_1 = (P_1 - M_1)$$

$$E_2 = (P_2 - M_2)$$



$$E_n = (P_n - M_n)$$

Assuming homogeneity of errors over all P_i
- standard deviation of E_i provides an indication of MIR/PLS error for set of samples

Standard deviations of the differences between predicted and measured values

Carbon Fraction	Standard deviation of $(P_i - M_i)$
	(g C/kg soil)
TOC	4.25
POC	1.92
ROC	1.07
HUM C	5.34

Typical approach to modelling within RothC

- Define the agricultural production system and soil characteristics
- Define initial allocation of carbon to pools (measurement or MIR/PLS prediction)

Measured/estimated
soil C pool Sizes
(Mg C/ha)

POC = 13.9

HUM C = 34.8

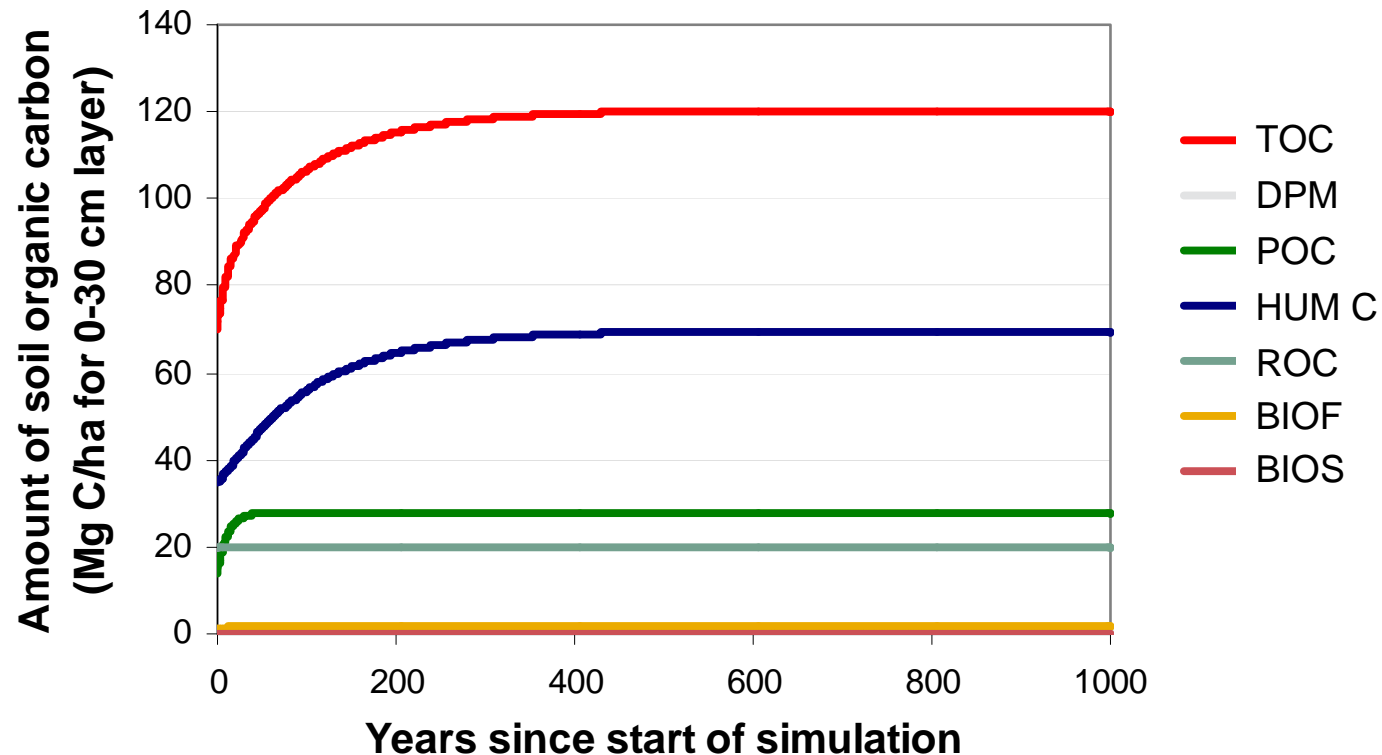
ROC = 20.0

DPM = 0.44

BIOF = 0.83

BIOS = 0.10

TOC = 70.16

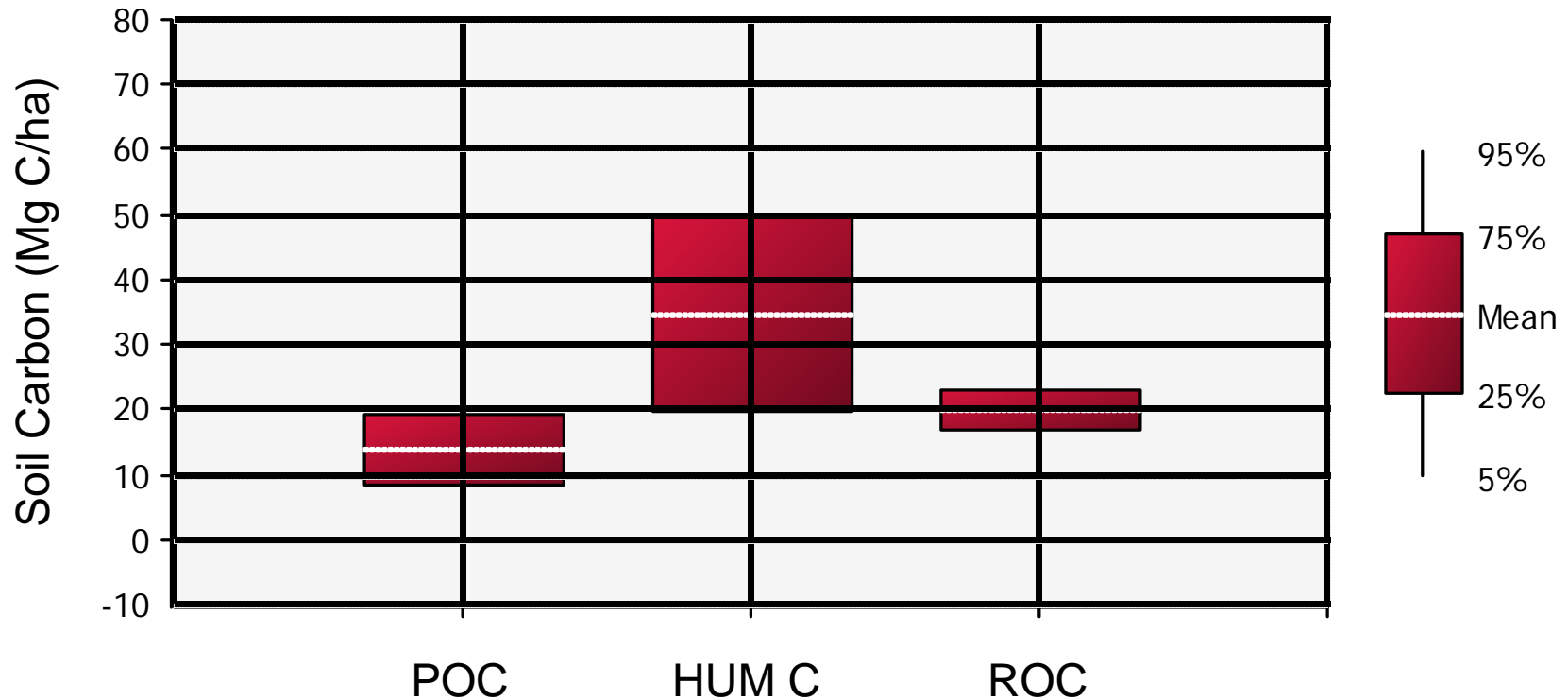


Standard deviations of the differences between predicted and measured values

Carbon Fraction		Standard deviation
	(g C/kg soil)	BD=1.4 Mg m ⁻³ , D=30 cm (Mg C/ha)
TOC	4.25	17.85
POC	1.92	8.08
ROC	1.07	4.48
HUM C	5.34	22.43

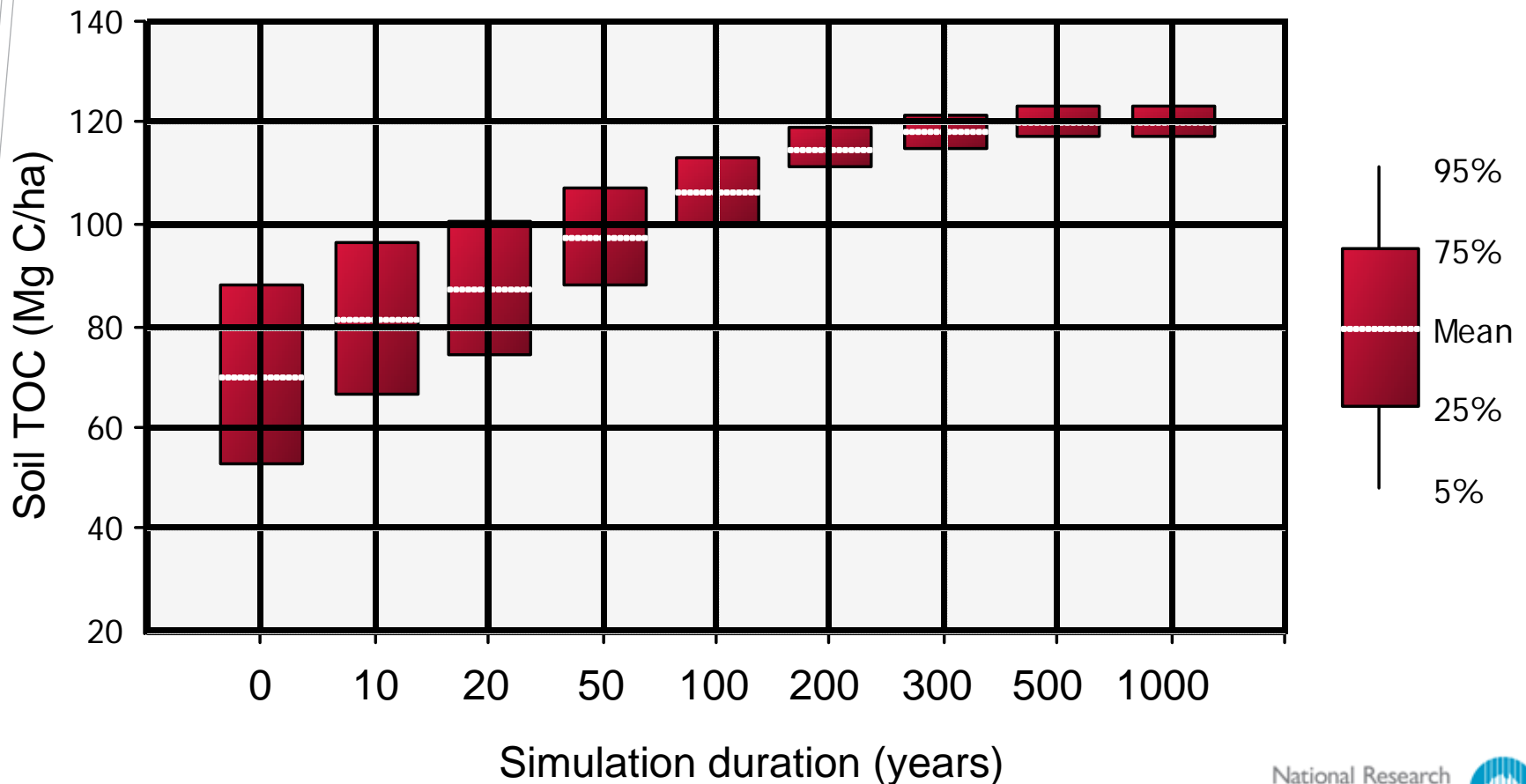
Potential variability in the soil carbon fractions

- Derive probability distributions for soil carbon fractions using Latin Hypercube sampling of normal distributions
 - Mean = amount of C in a fraction, Stdev = $S_{\text{pred-meas}}$ with 1000 draws



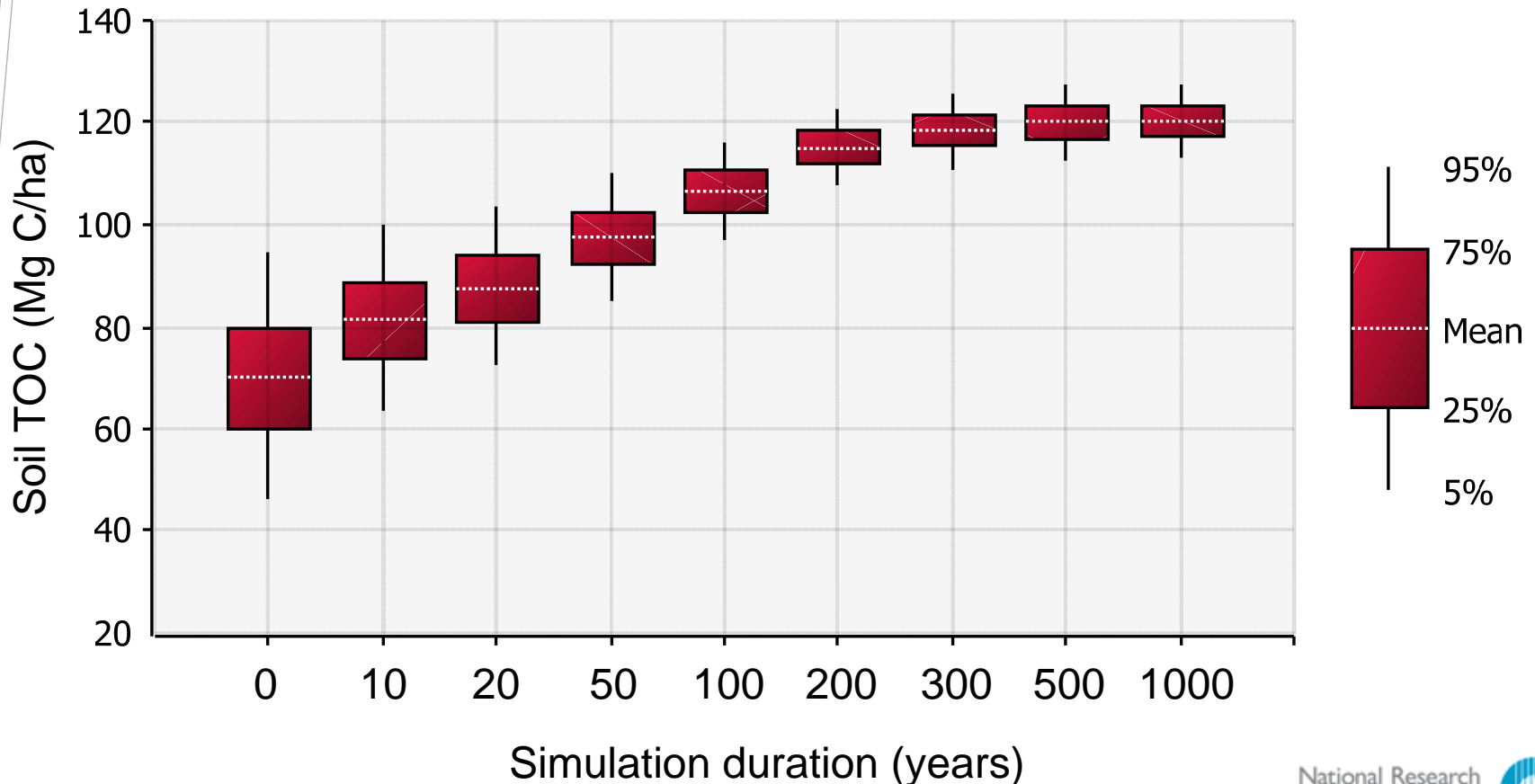
Propagation of error through the model

- Latin hypercube sampling of POC, HUM C and ROC distributions with correlations defined (1000 iterations)



Propagation of error through the model – reduce the standard deviation of the HUM C to 2.0

- Latin hypercube sampling of POC, HUM C and ROC distributions with correlations defined (1000 iterations)



Conclusions

- Set of soil samples used for MIR/PLS predictions was diverse
 - More accurate analyses may be possible through the derivation of soil type specific calibrations
 - A new soil carbon research program will provide the samples required
- The largest prediction errors were associated with the HUM C fractions
 - This error should be reduced by direct measurement of the HUM C fractions and completion of carbon balance calculations
- Need to compare MIR/PLS prediction errors with other sources of error to define their significance
 - Laboratory fractionation methodology
 - Spatial variability within soil sampling units

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Thank you

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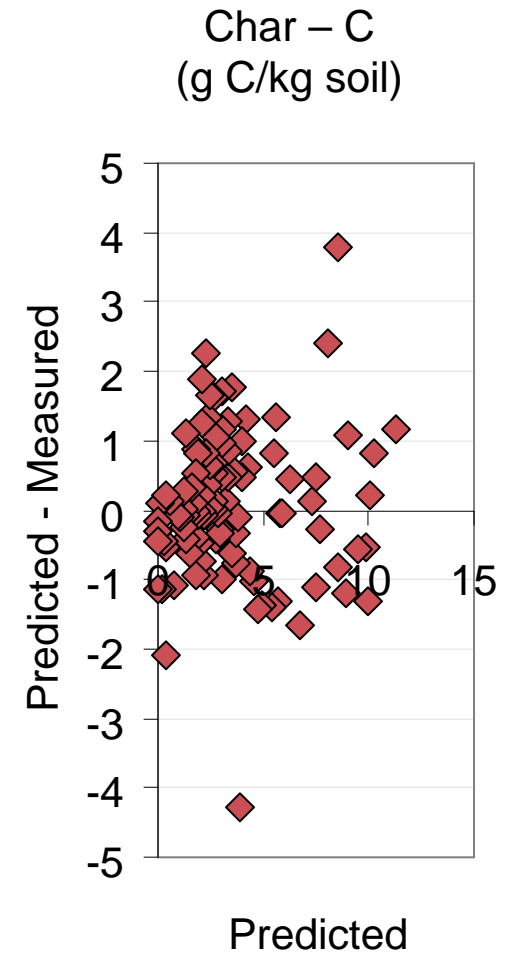
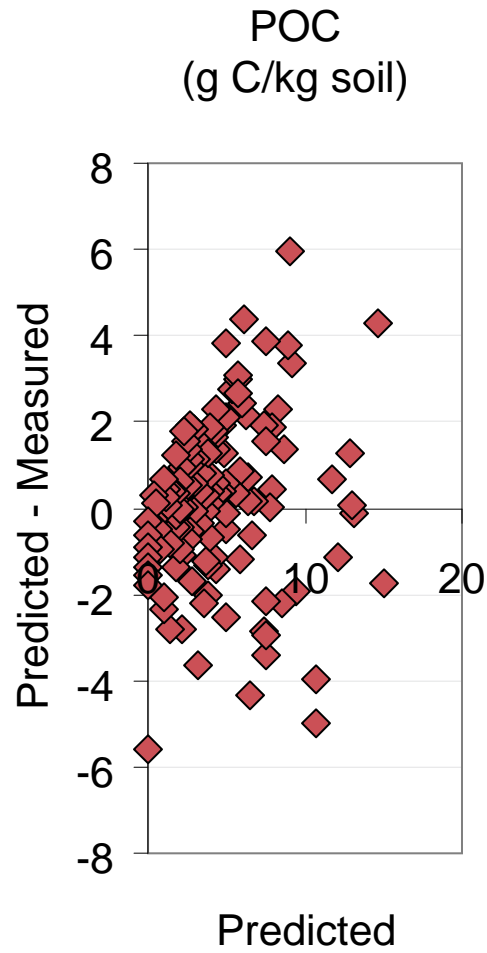
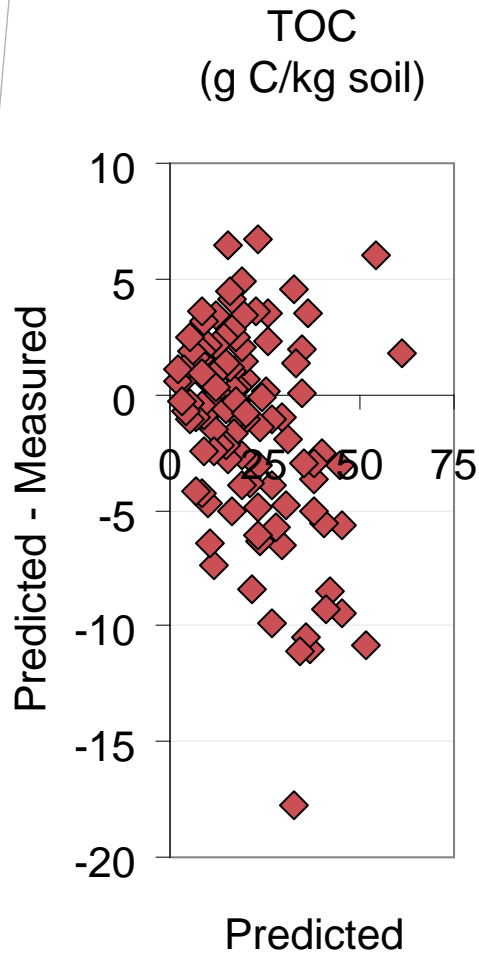
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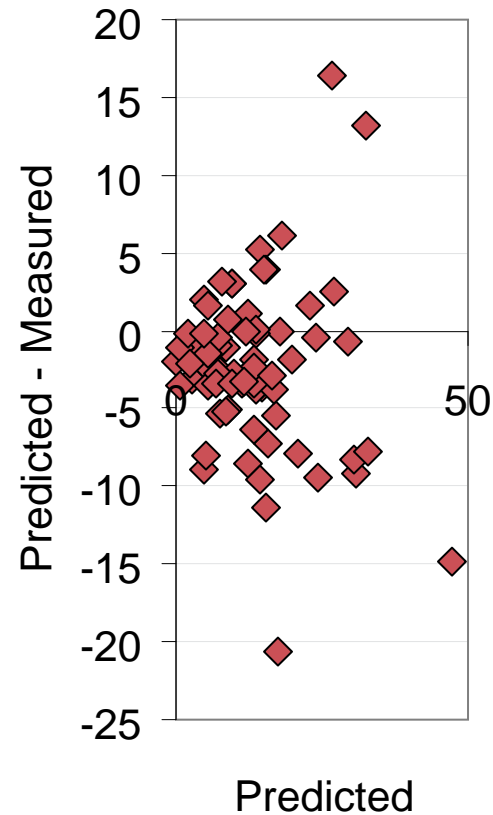
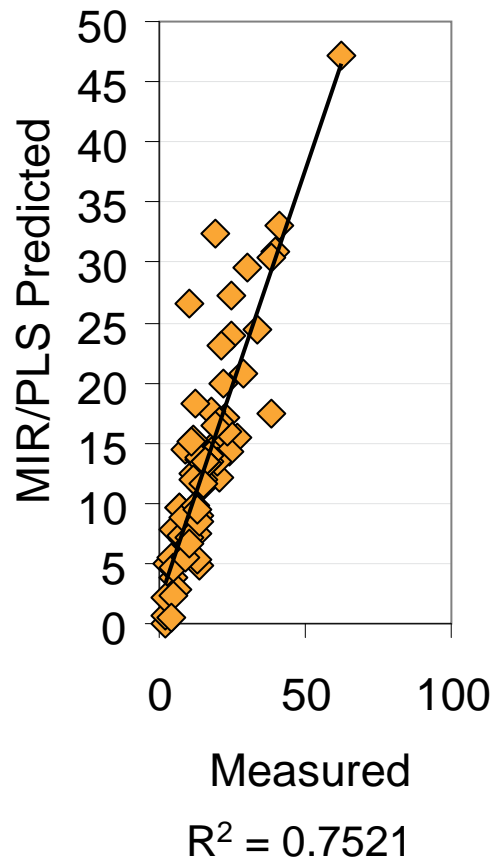
Errors of MIR/PLS prediction (predicted – measured)



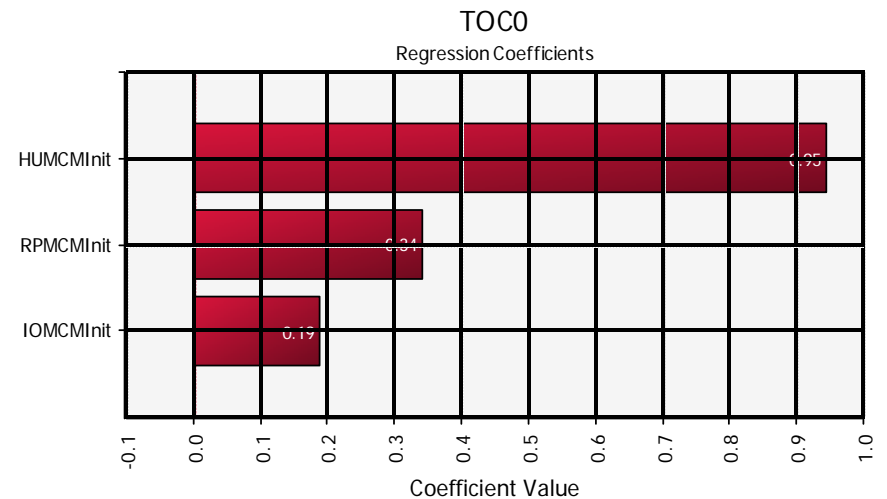
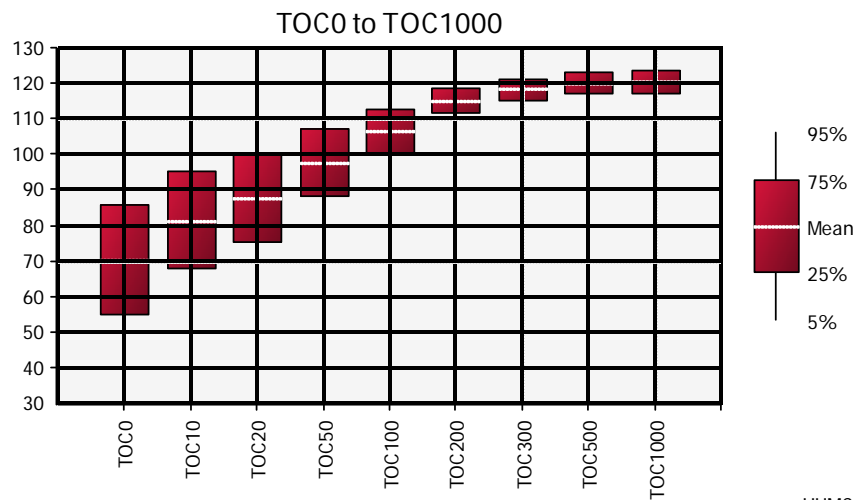
Humus fractions

- Calculated by difference for both measured and predicted data

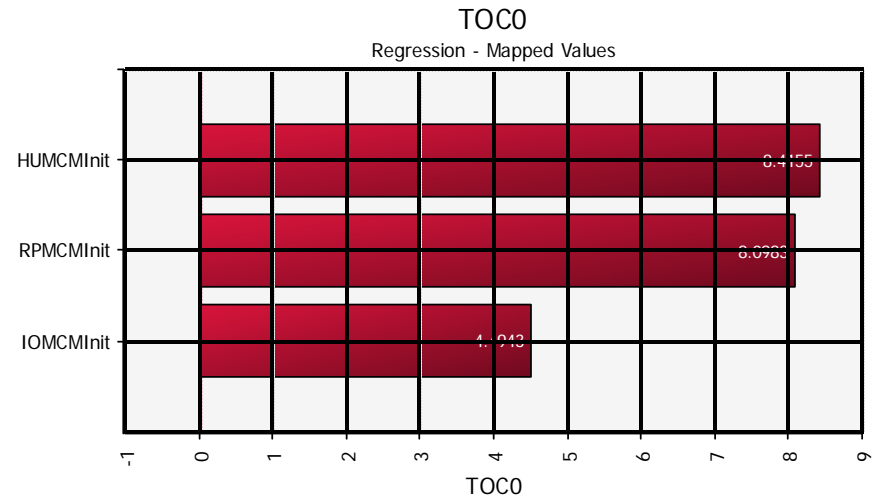
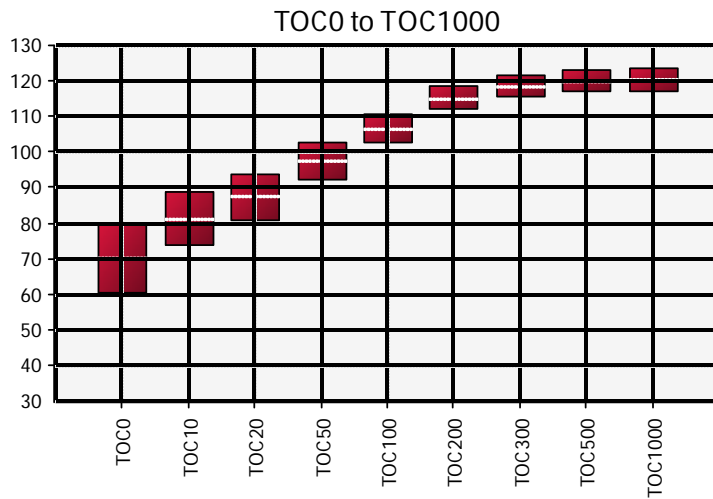
$$\text{Humus C} = \text{TOC} - \text{POC} - \text{Char C}$$



Propagation of error through the model (no correlations)



Revised humus error



Propagation of error through the model

