Predicting radiocaesium transfer in the agricultural foodchain

Neil Crout
Environmental Science
School of Biosciences
University of Nottingham

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Predicting the transfer of radiocaesium from organic soils to plants using soil characteristics

J. P. Absalom[a], S. D. Young[a], N. M. J. Crout[a,*], A. Sanchez[b], S. M. Wright[b], E. Smolders[c], A. F. Nisbet[d], A. G. Gillett[a]

[a]*School of Biological Sciences, University of Nottingham, Sutton Bonington Campus, Loughborough, Leicestershire, LE12 5RD, UK*

[b]*Institute of Terrestrial Ecology, Grange-Over-Sands, Cumbria, LA11 6JU, UK*

[c]*Laboratory of Soil fertility and Soil Biology, Faculty of Applied Biological and Agricultural Sciences K.U.Leuven, K. Mercierlaan, 92, B 3001 Heverlee, Belgium*

[d]*National Radiological Protection Board, Chilton, Didcot, Oxfordshire, OX11 ORQ, UK*

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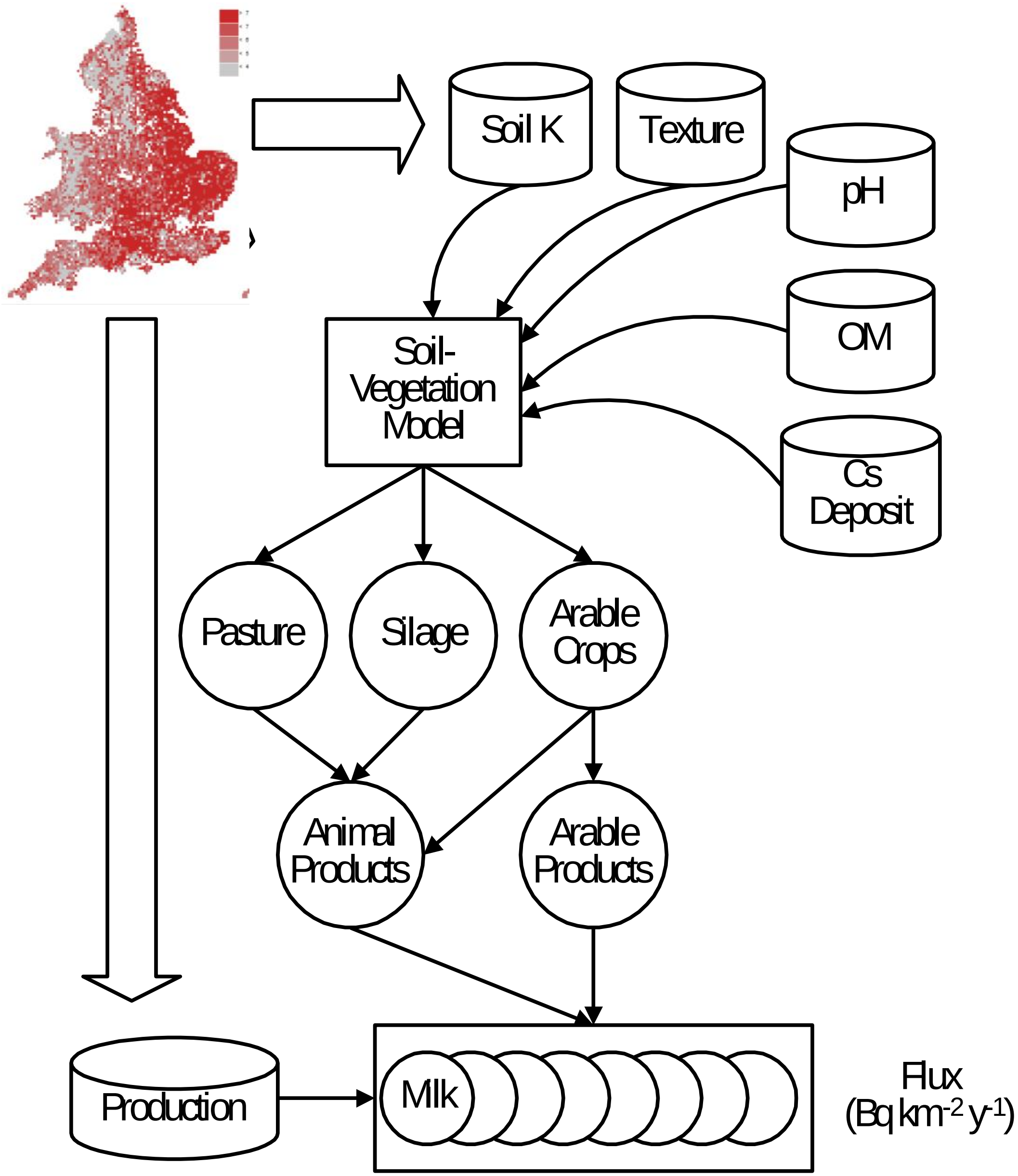
A reviewers comment

‘….horribly empirical….’

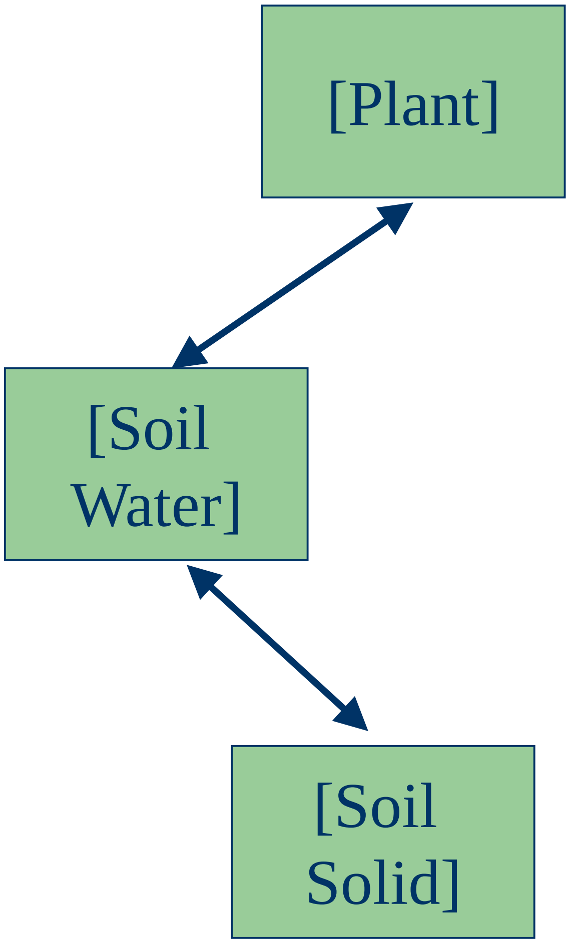
Motivation

- Estimating transfer over large areas
- Spatial soils data existed but lacked detail
- Devise a model that used simple soil characteristics to estimate uptake to crops?
- Link to production, estimate 'flux'



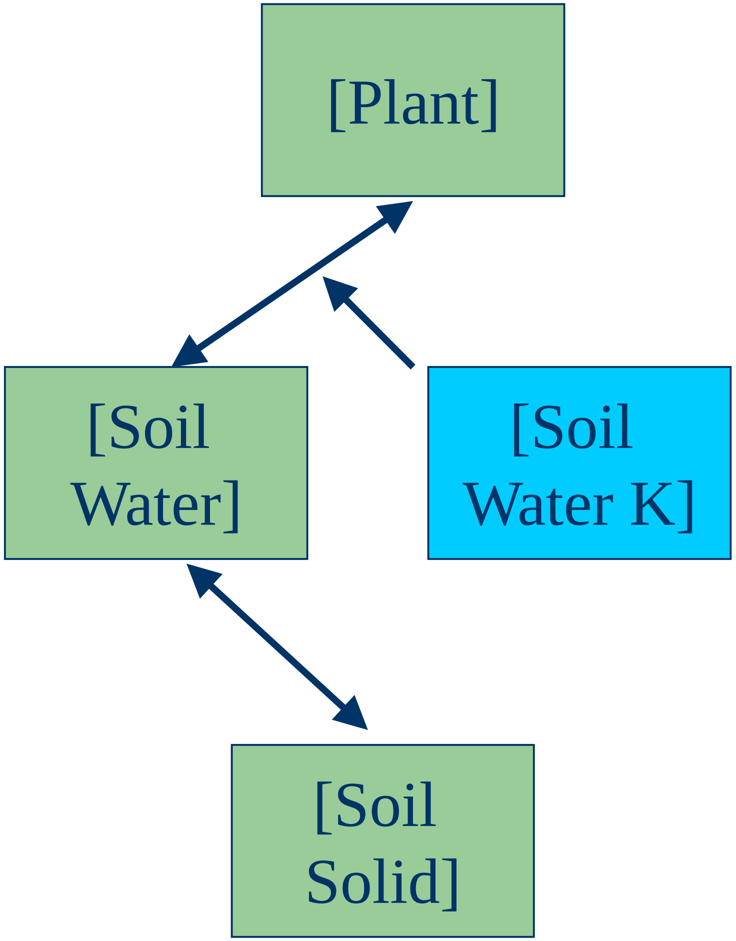
Central Idea…

- Could partition Cs distribution between solid and liquid
- But, mechanistically Cs uptake related to potassium
- So, more realistic to allow for potassium interaction

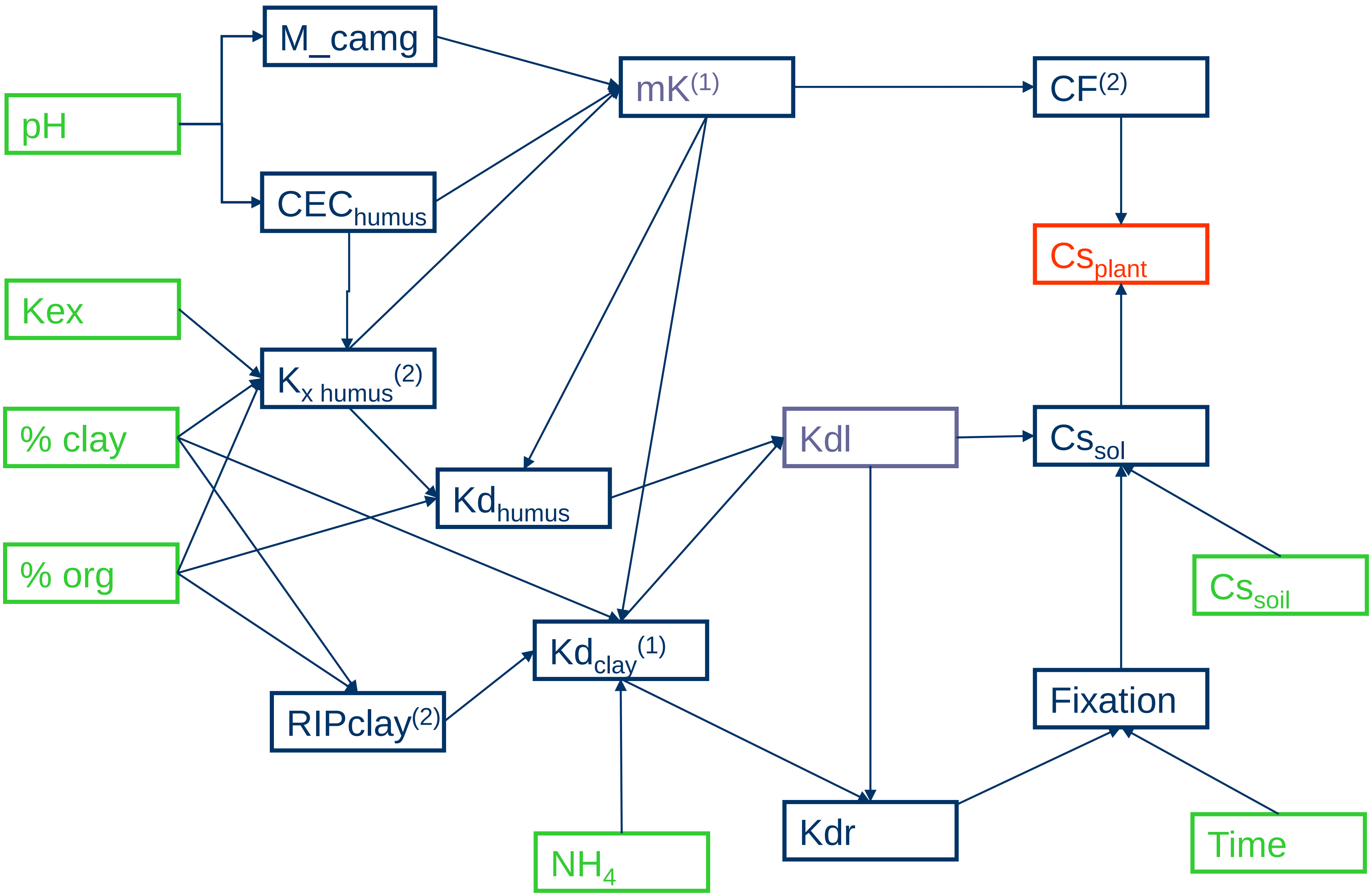


Central Idea…

- So include soil water K
- But, mechanistically soil water K related to exchangeable K
- Interacts with Ca and Mg, related to pH
- and so on and so on and so on......



Schematically



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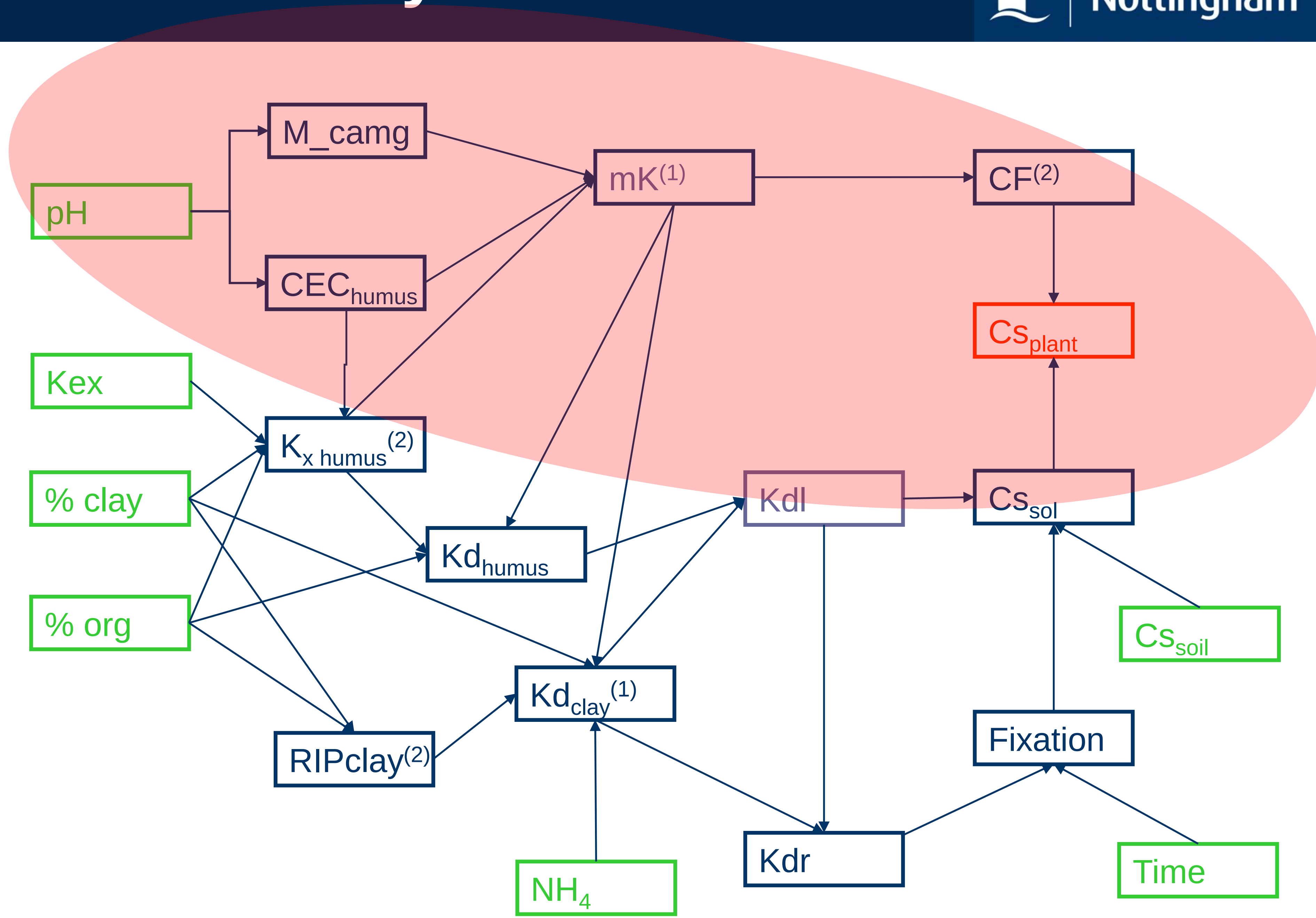

Plant Cs

$$Cs_{plant} = \mathrm{CF} \times Cs_{sol}$$

- *CF* imagined as plant specific constant (i.e. plant concentration related to the plant accessible Cs)
- *Cs*$_{sol}$ – soil solution concentration of Cs

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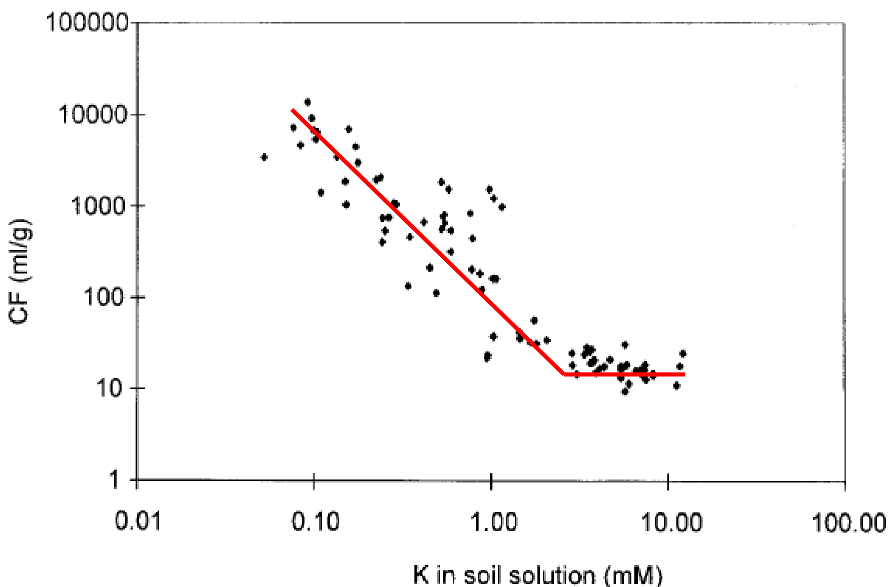

$$\log(CF) = a_1 - a_2 log(m_K)$$

Smolders et al, 1997

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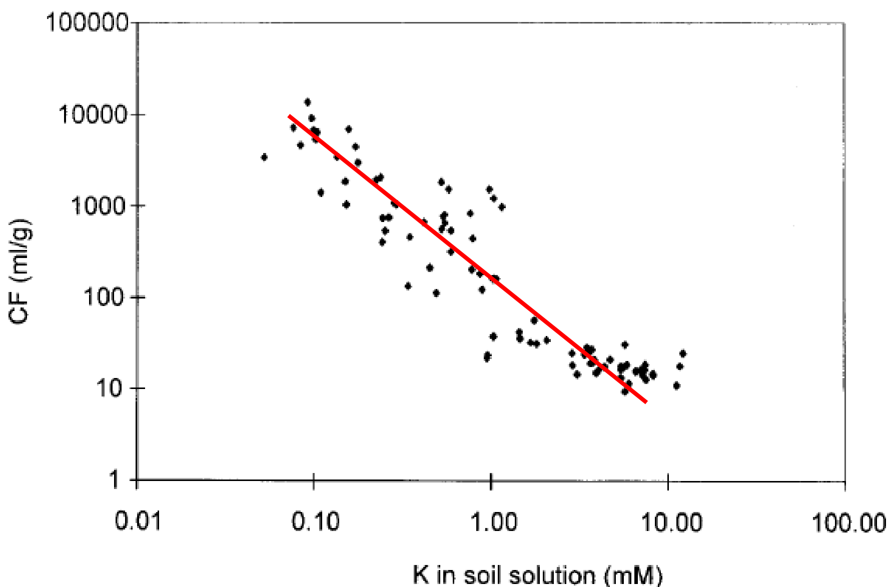

Smolders et al, 1997

$$\log(CF) = a_1 - a_2 log(m_K)$$

Plant concentration linear with Cs_{sol}

CF reduces as m_K increases
(K competes for uptake)

m_K – solution potassium

- Exchangeable K was available spatially
- Exchangeable cations dominated by Ca and Mg
- Distribution of exchangeable K equivalent to distribution of Ca+Mg
  - subject to relative selectivity (Gapon coefficient, k_G)
  - Stoichiometry

$$m_k = \frac{K_{ex}\sqrt{m_{Ca+Mg}}}{k_G\left(CEC - K_{ex}\right)}$$

  - Leading to relationships to organic and mineral CEC
- Now we need m_{Ca+Mg}

m_K – solution potassium –m_{Ca+Mg}?

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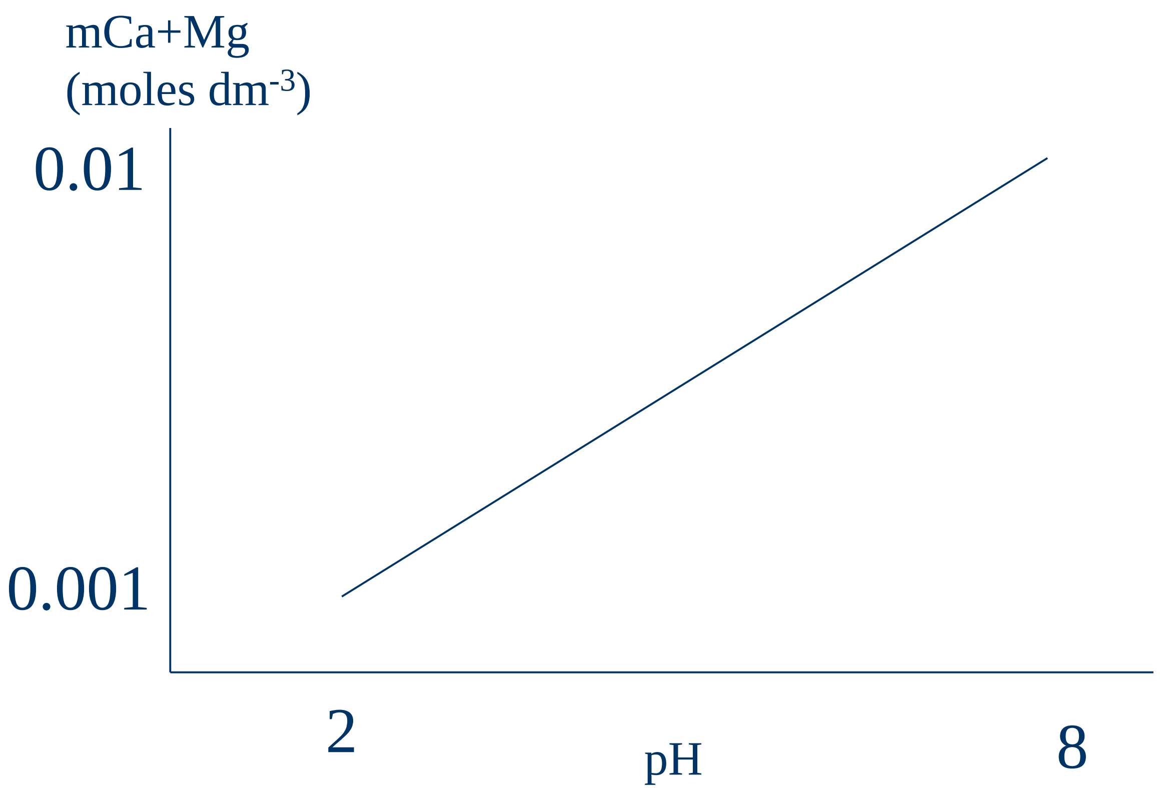
Ca increases as pH increases

$$\log(m_{Ca+Mg}) = a_4 pH - a_3$$



‘..seems about right..’

m_K – solution potassium –*CEC?*

$$CEC = CEC^{clay}\theta_{clay} + CEC^{org}\theta_{org}$$

$$= CEC^{clay}\theta_{clay} + (a_5 + a_6 pH)\theta_{org}$$

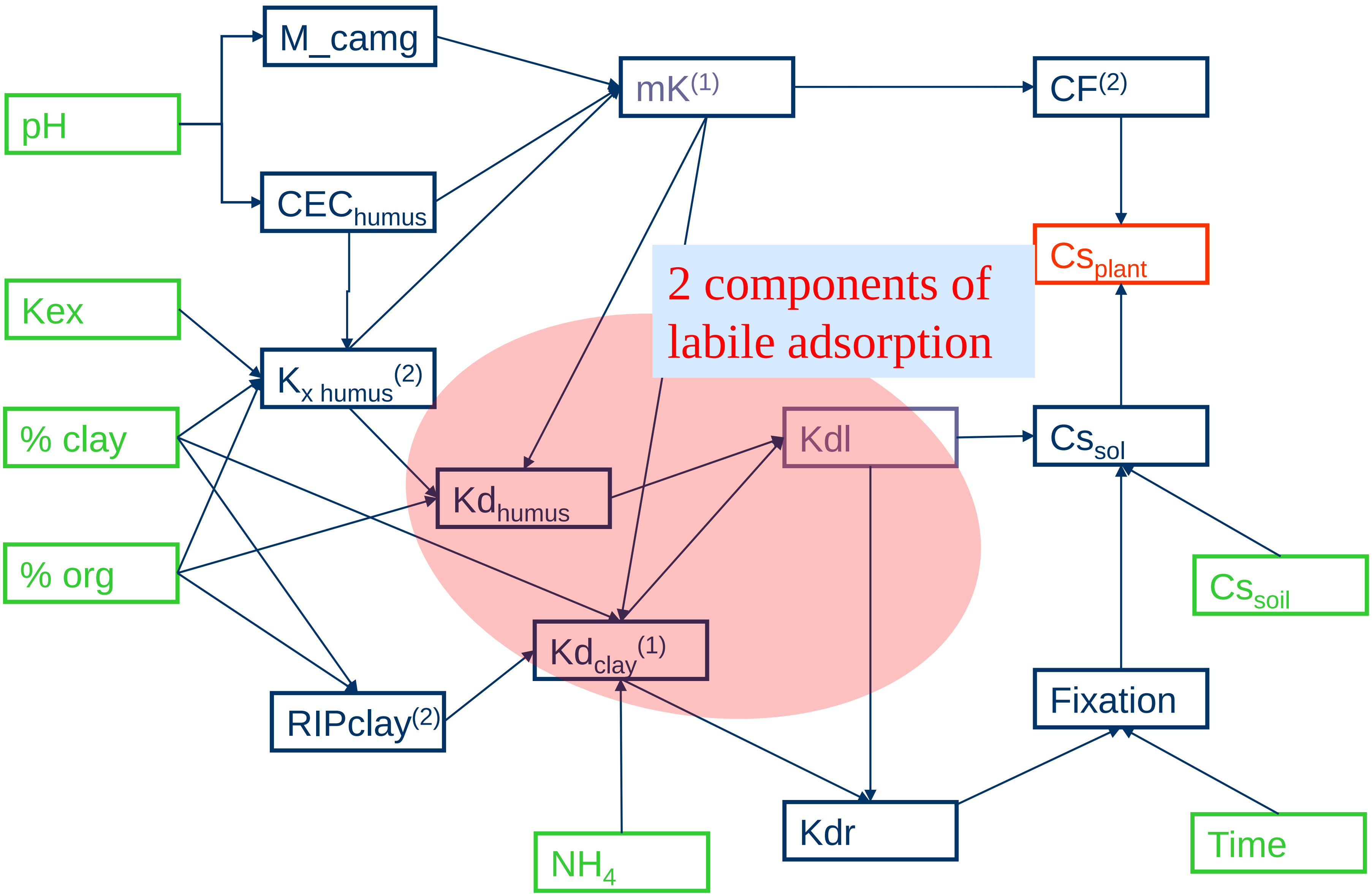
Helling, C. S., Chesters, G., & Corey, R. B. (1964). Contribution of organic matter and clay to soil cation-exchange capacity as affected by the pH of the saturating solution 1. *Soil Science Society of America Journal*, *28*(4), 517-520.

m_K – solution potassium

- Some mechanistic thinking
- Mixture of unknown and previously estimated model parameters

$$m_k = f\left(K_{ex}, pH, \theta_{org}, \theta_{clay}\right)$$

Schematically



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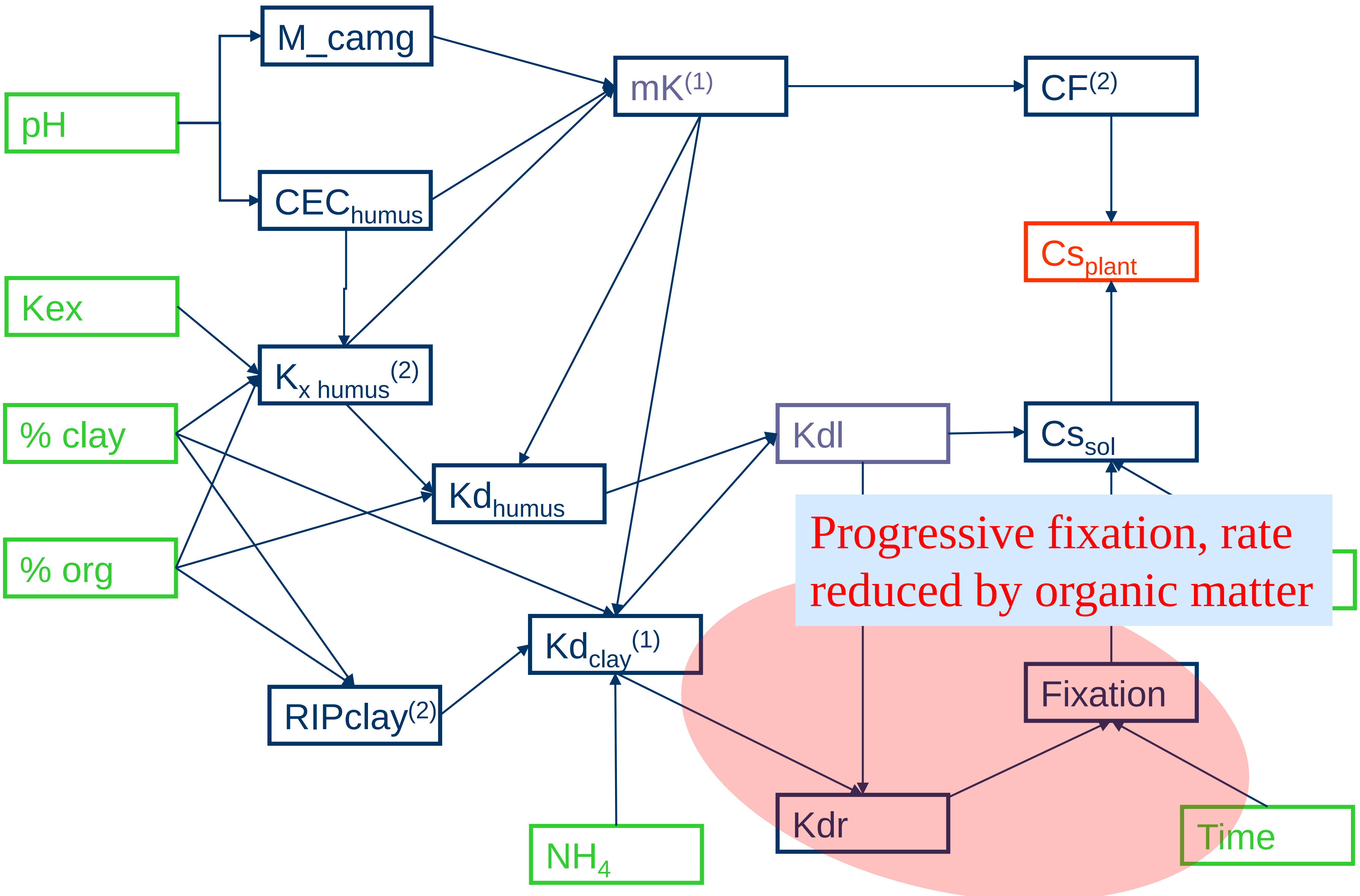
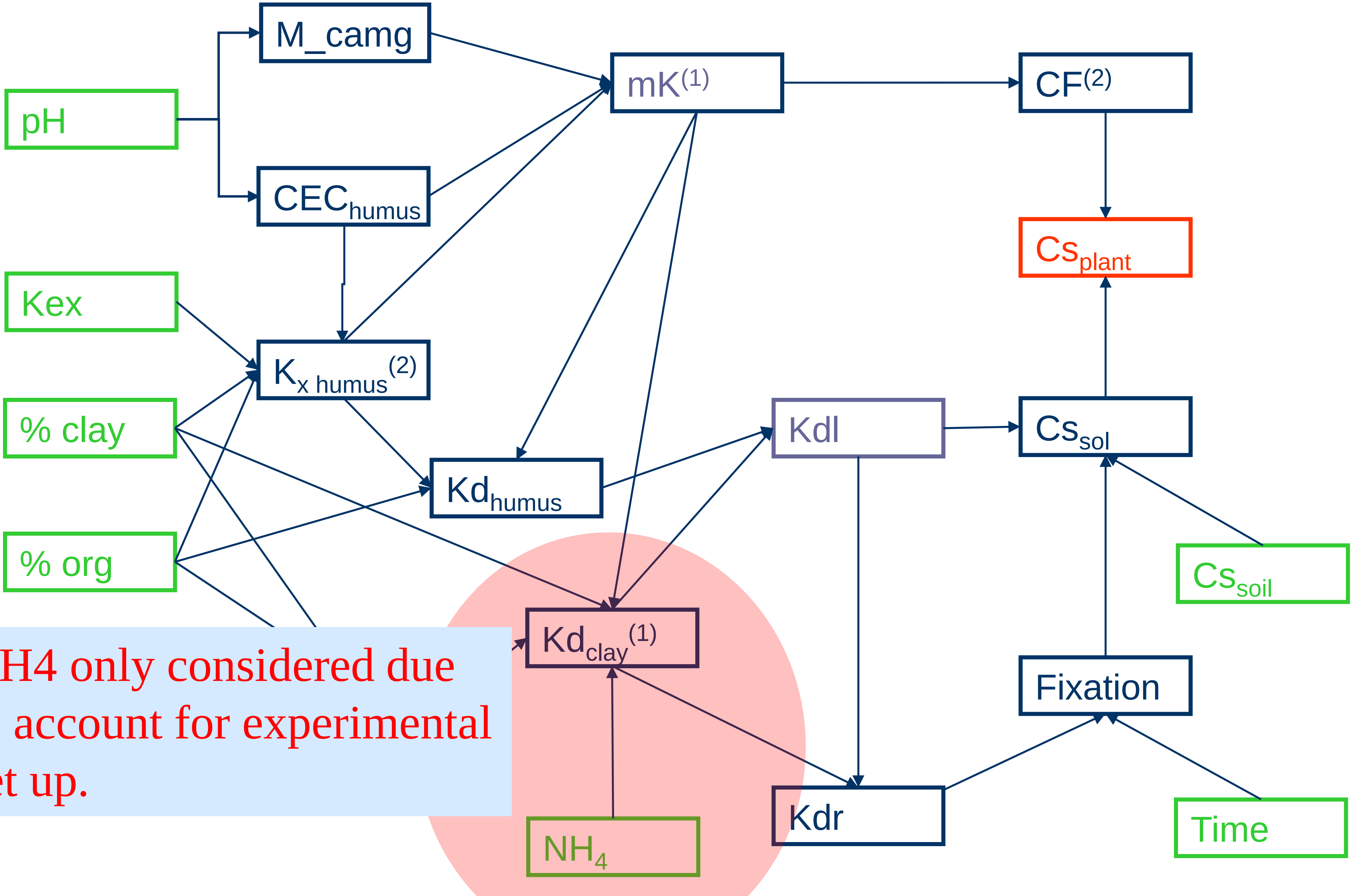


Schematically

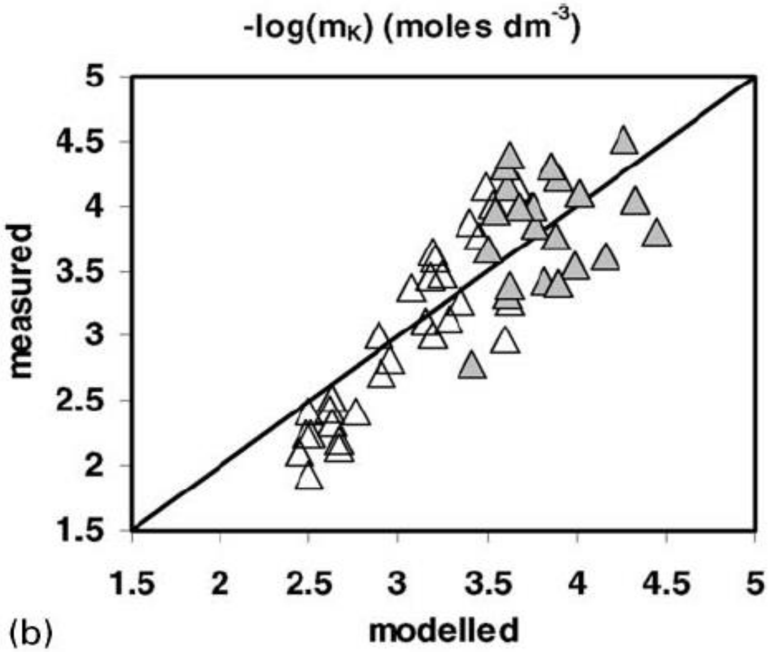


NH4 only considered due to account for experimental set up.

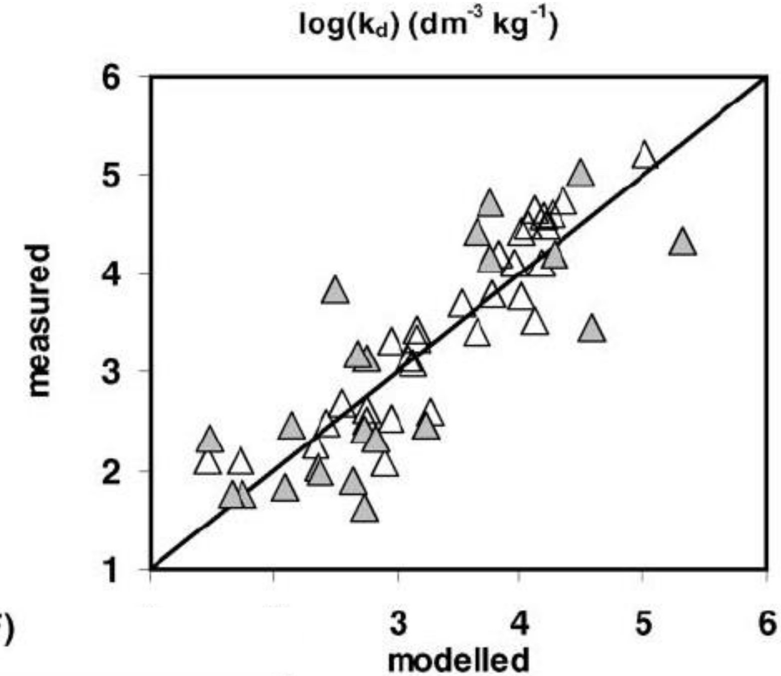
Data Sets…

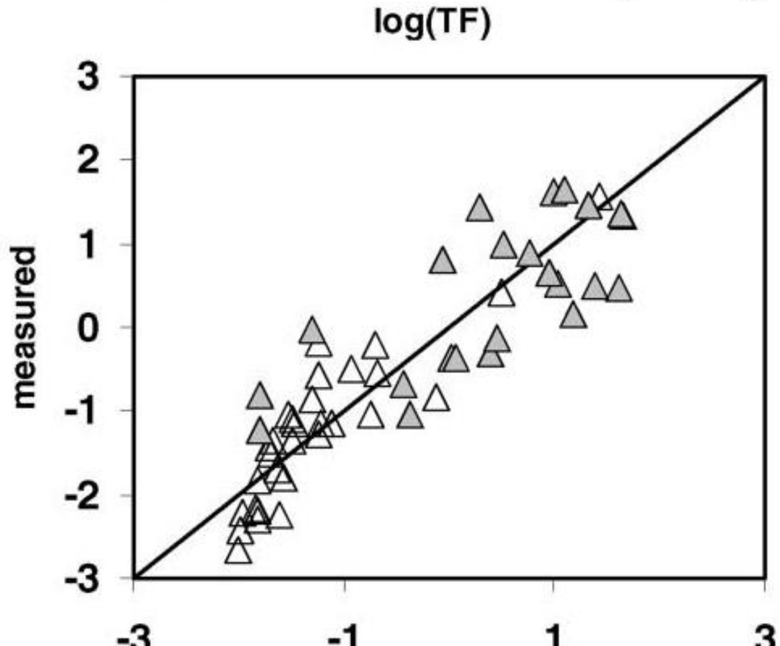
- Smolders et al 1997
  - Mineral soils, spiked with Cs, measurements of mk, kd, TF.
- Sanchez et al 2000
  - Organic soils
  - Same measurements as Smolders et al
- Short time scales (<100d)
- 53 soils considered (Belgium, England)

Fitted empirically – 3 key components

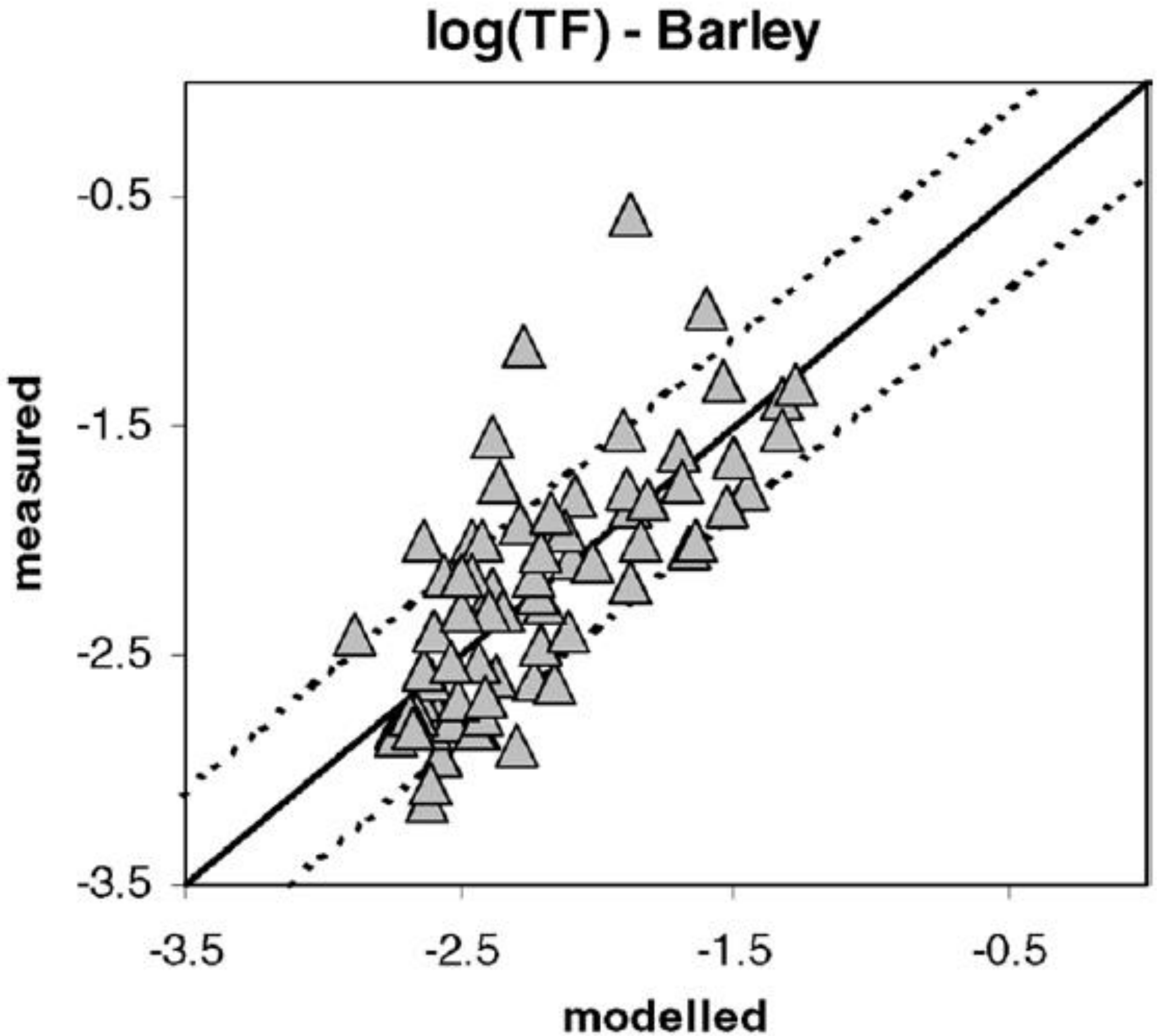


(b)





Independent Data



Nisbet et al, 1999

Food-chain comparisons

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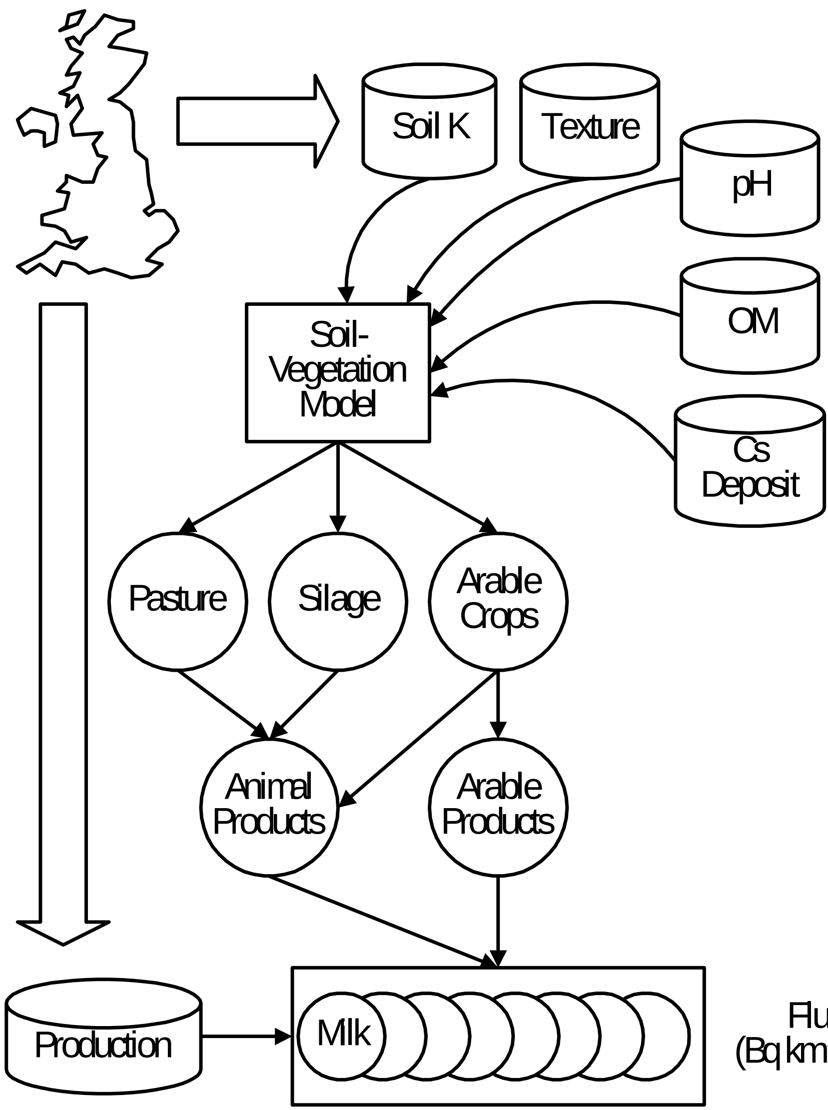
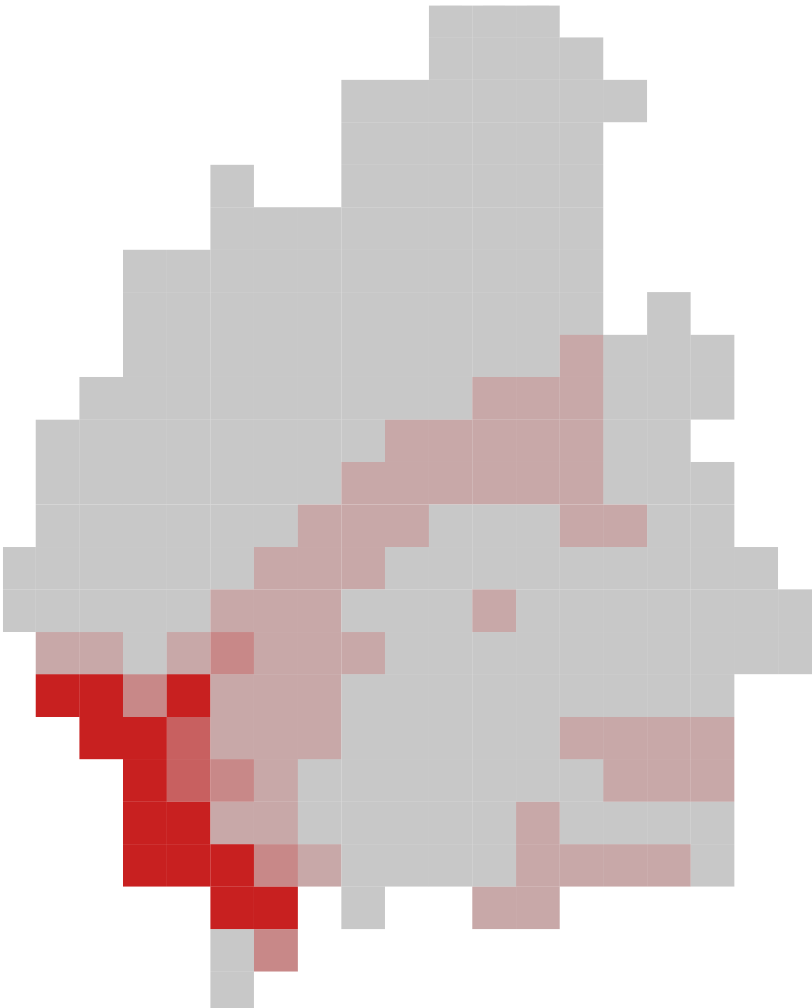
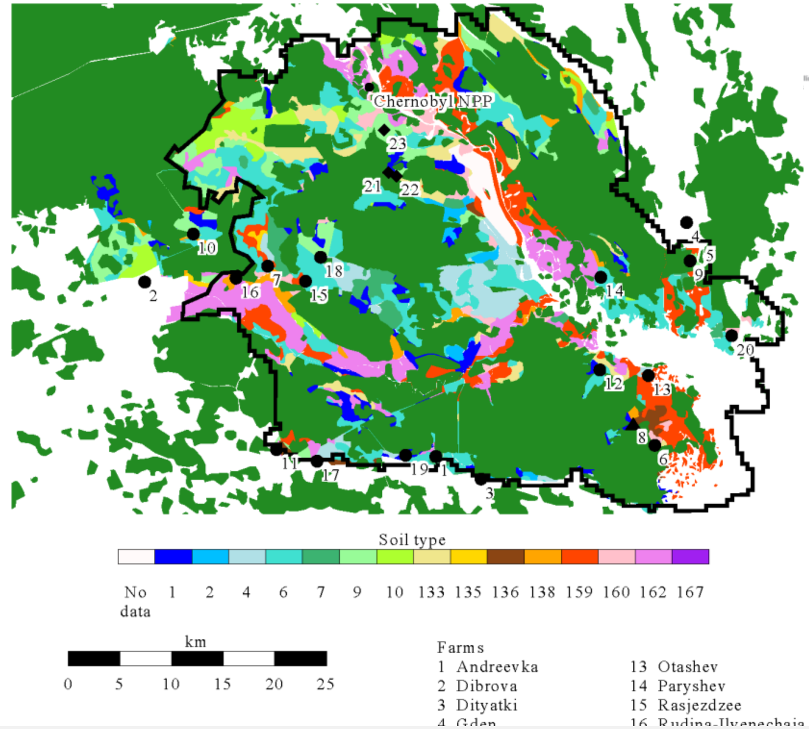
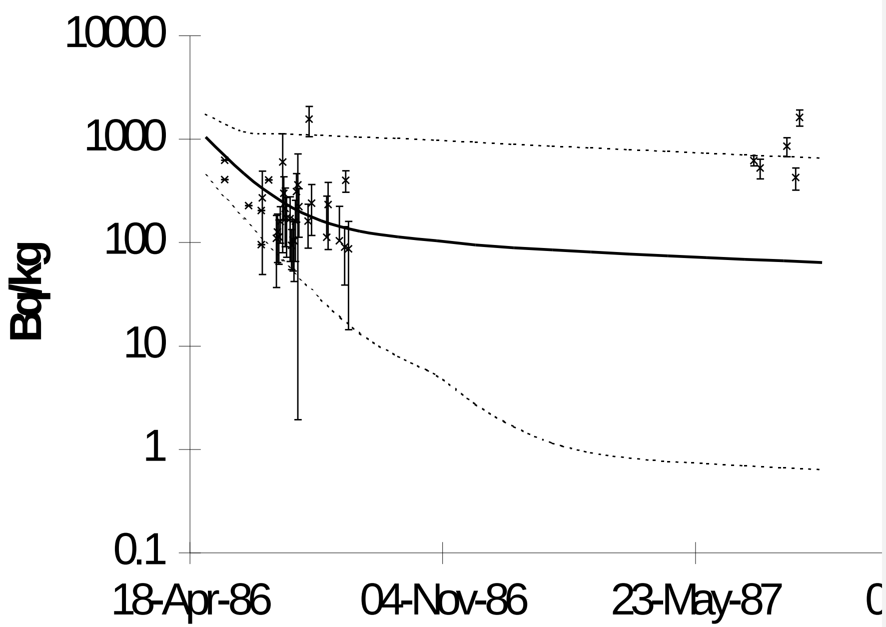


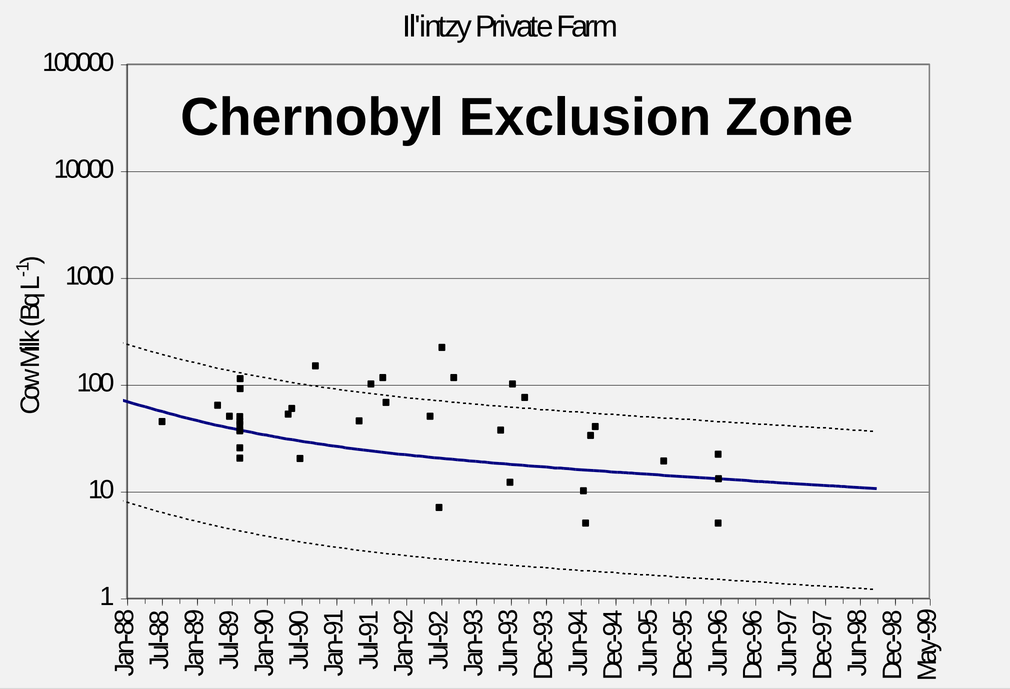


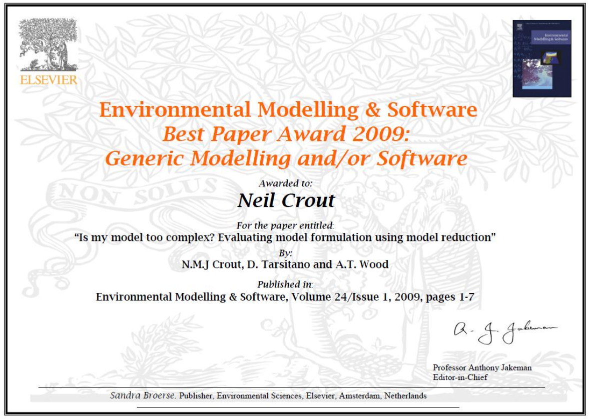


Lamb Concentrations in Clwyd



Chernobyl Exclusion Zone

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Best Paper Award 2009:
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Awarded to:
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For the paper entitled
"Is my model too complex? Evaluating model formulation using model reduction"

By:
N.M.J Crout, D. Tarsitano and A.T. Wood

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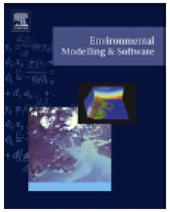

Is my model too complex? Evaluating model formulation using model reduction

N.M.J. Crout [a,b,*], D. Tarsitano [a,b], A.T. Wood [a,b]

[a] School of Biosciences, University of Nottingham, Nottingham NG7 2RD, UK
[b] School of Mathematical Sciences, University of Nottingham, Nottingham NG7 2RD, UK

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Bayesian evaluation

A B S T R A C T

While mechanistic models tend to be detailed, they are less detailed than the real systems they seek to describe, so judgements are being made about the appropriate level of detail within the process of model development. These judgements are difficult to test, consequently it is easy for models to become over-parameterised, potentially increasing uncertainty in predictions. The work we describe is a step towards addressing these difficulties. We propose and implement a method which explores a family of simpler models obtained by replacing model variables with constants (model reduction by variable replacement). The procedure iteratively searches the simpler model formulations and compares models in terms of their ability to predict observed data, evaluated within a Bayesian framework. The results can be summarised as posterior model probabilities and replacement probabilities for individual variables which lend themselves to mechanistic interpretation. This provides powerful diagnostic information to support model development, and can identify areas of model over-parameterisation with implications for interpretation of model results. We present the application of the method to 3 example models. In each case reduced models are identified which outperform the original full model in terms of comparisons to observations, suggesting some over-parameterisation has occurred during model development. We argue that the proposed approach is relevant to anyone involved in the development or use of process based mathematical models, especially those where understanding is encoded via empirically based relationships.

This project

Revised Model…

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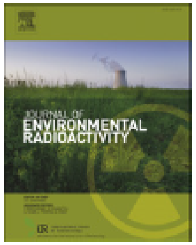

Evaluating and reducing a model of radiocaesium soil-plant uptake

D. Tarsitano, S.D. Young, N.M.J. Crout*

School of Biosciences, University of Nottingham, University Park, Nottingham, NG7 2RD, UK

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Plant
Reduction

A B S T R A C T

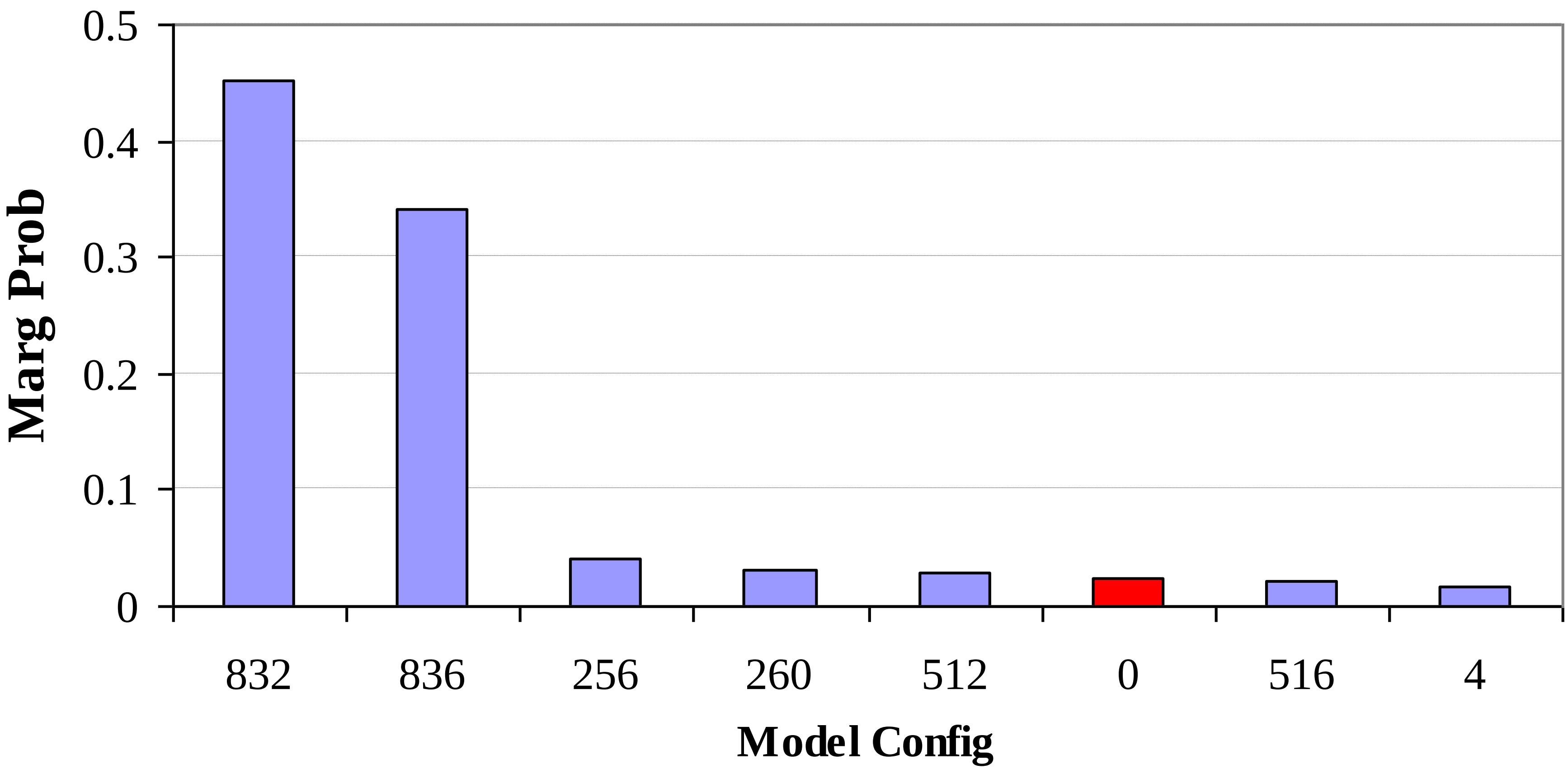
An existing model of radiocaesium transfer to grasses was extended to include wheat and barley and parameterised using data from a wide range of soils and contact times. The model structure was revised and evaluated using a subset of the available data which was not used for model parameterisation. The resulting model was then used as a basis for systematic model reduction to test the utility of the model components. This analysis suggested that the use of 4 model variables (relating to radiocaesium adsorption on organic matter and the pH sensitivity of soil solution potassium concentration) and 1 model input (pH) are not required. The results of this analysis were used to develop a reduced model which was further evaluated in terms of comparisons to observations. The reduced model had an improved empirical performance and fewer adjustable parameters and soil characteristic inputs.

Additional Data Sets…

Source	N	Crop	pH (median; range)	OM (% median; range)	TF (median; range)
Smolders et al, 1997	20	Grass	5.1 (4.6-7.0)	6.1 (3.5-34)	0.061 (0.0022-2.6)
Sanchez et al, 1999	33	Grass	2.8 (2.4-6.0)	75 (12.6-96.5)	3.41 (0.060-43.6)
Nisbett et al, 1999	152	Barley	6.1 (5.0-8.4)	4.2 (1.5-58.5)	0.0083 (0.0014-0.27)
	130	Wheat	6.3 (4.2-8.4)	3.9 (0.6-18.4)	0.0075 (0.0002-0.16)
Sanchez et al, 2001	57	Grass	6.1 (4.8-7.1)	11 (4.3-59.0)	0.073 (0.016-4.8)

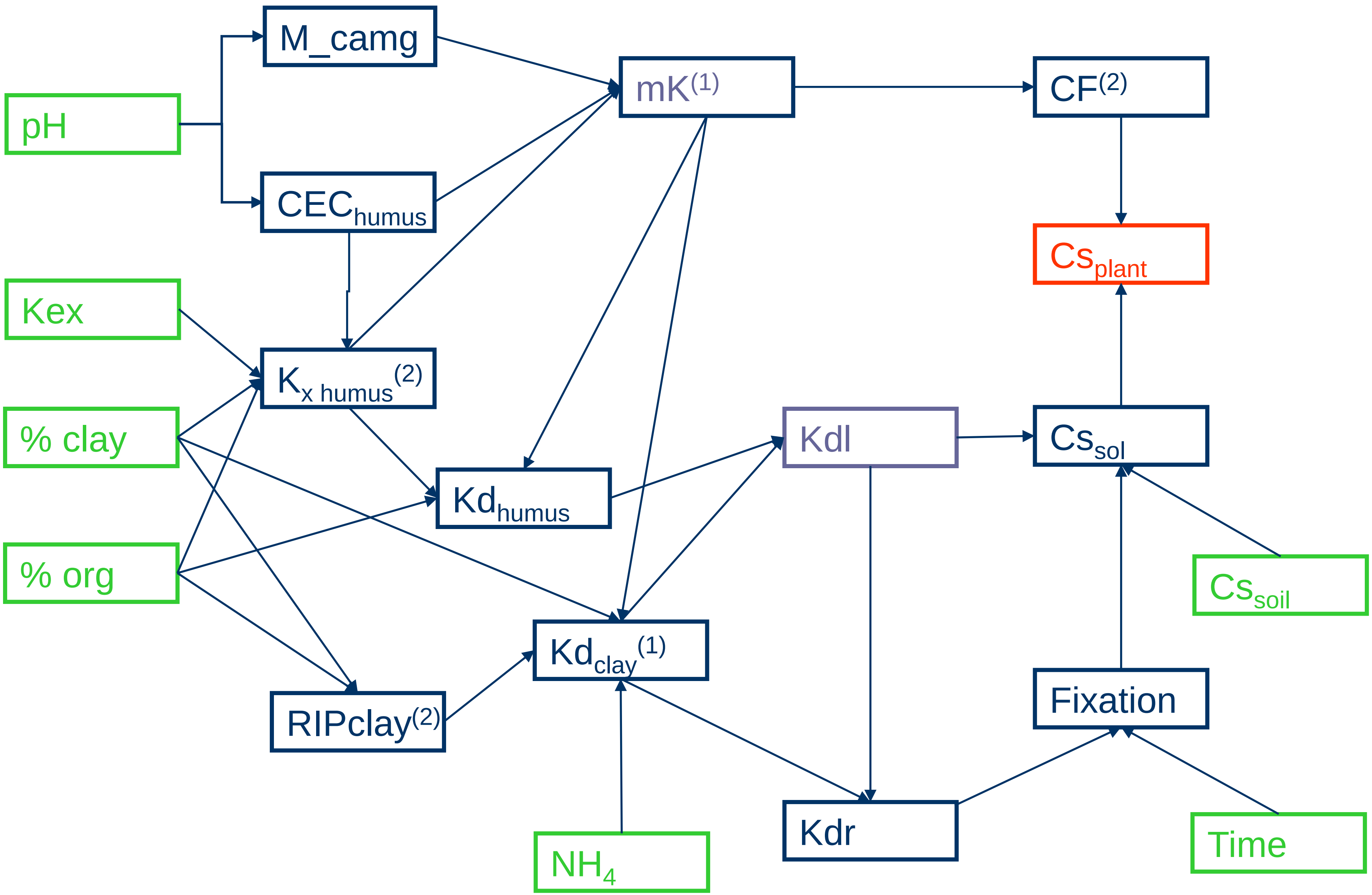
- Used these data to re-parameterise Absalom 2001 (AbsalomX)
- Reduce the model i.e. ‘falsify the model structure’

Model performance

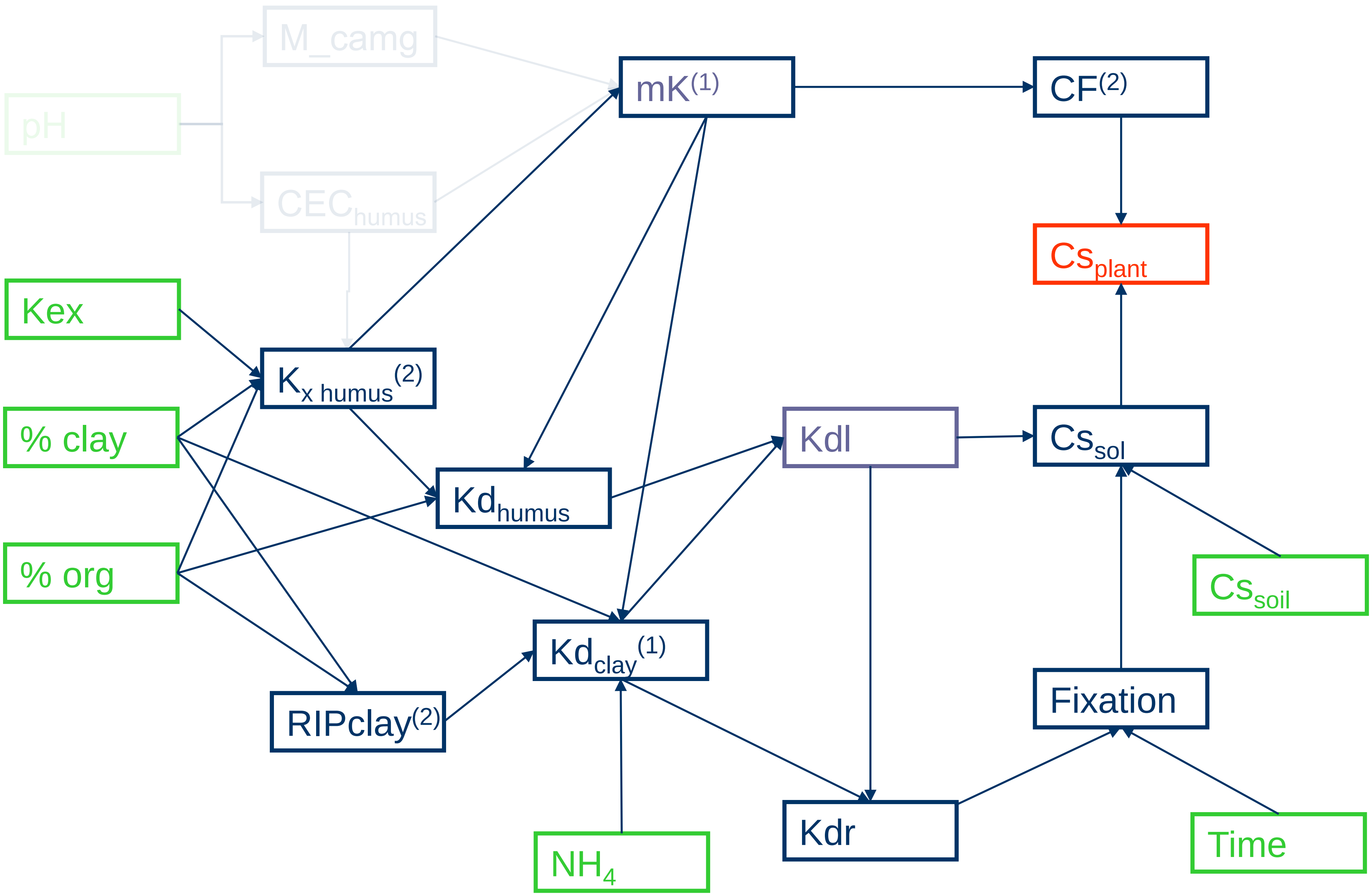


Redundancy removed...

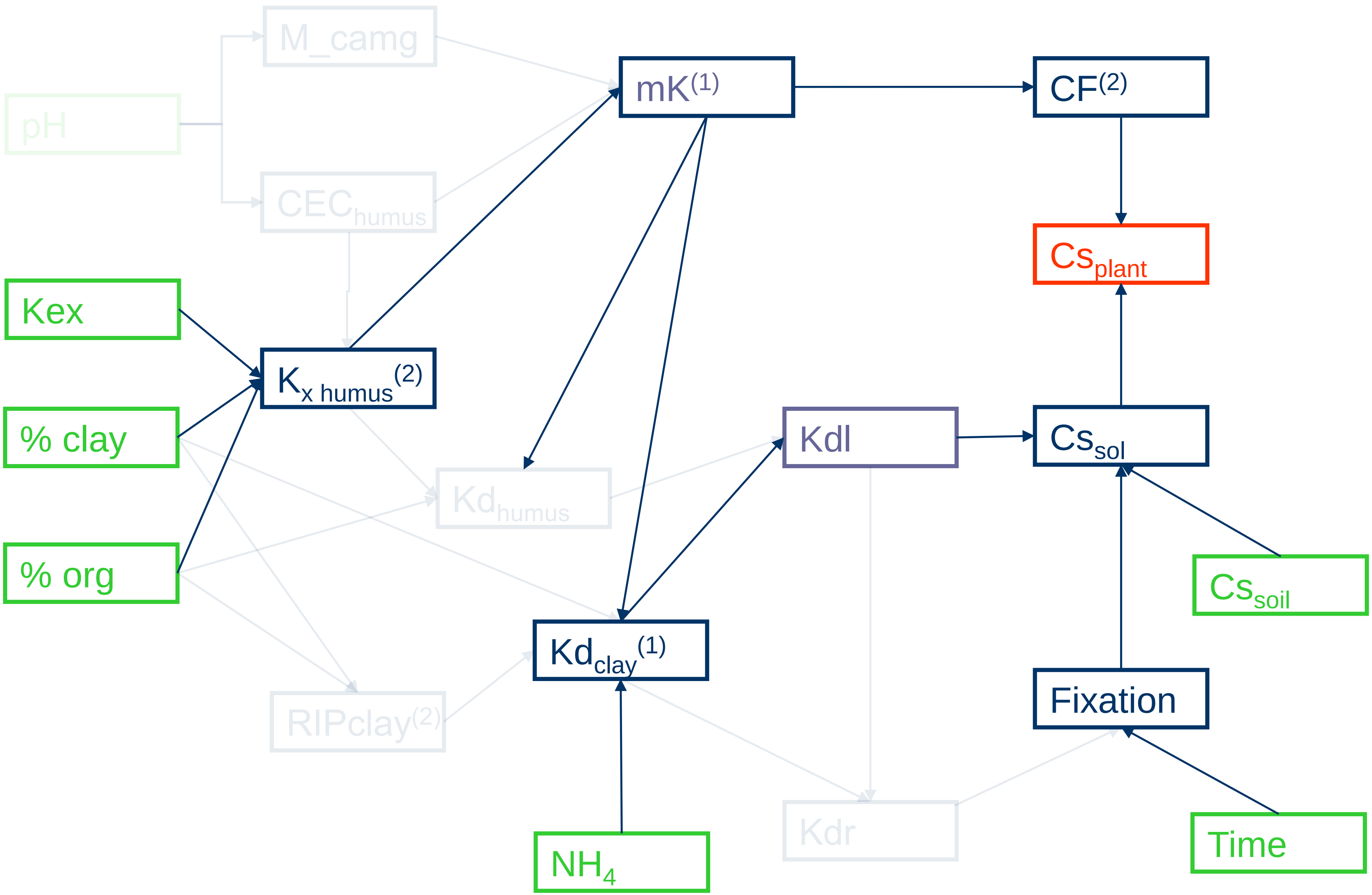
Full Model (as published 2001)



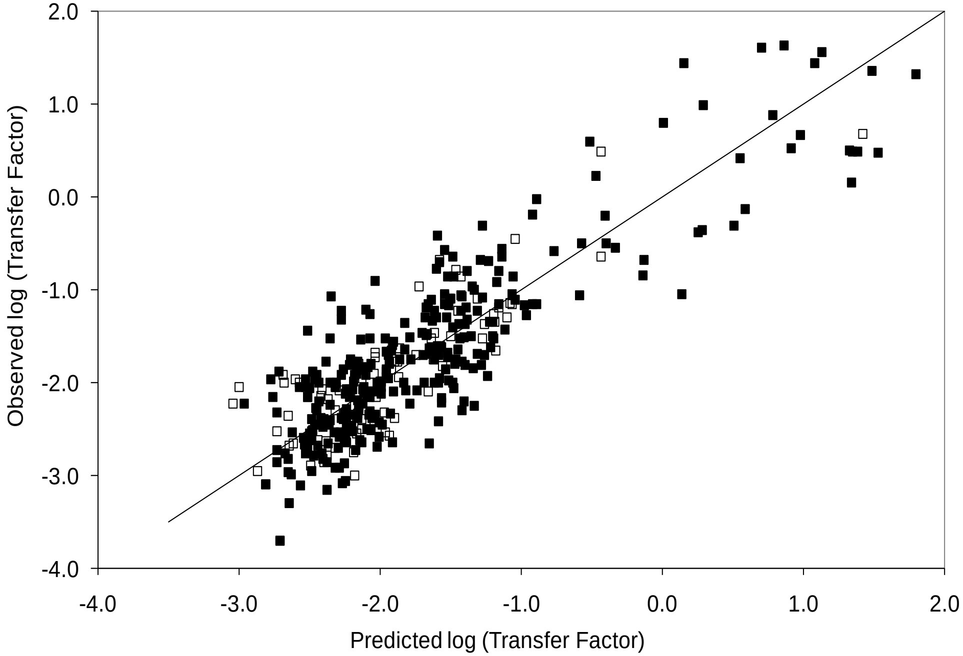
This works ‘better’



And so does this…

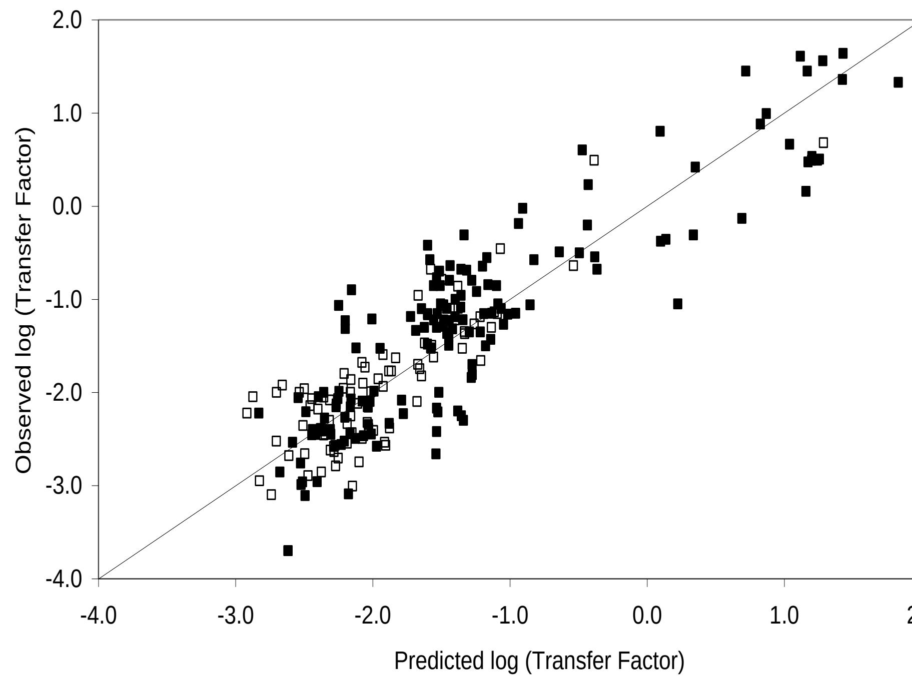


Comparing…



Absalom-X

Reduced Model
Tarsitano 2011

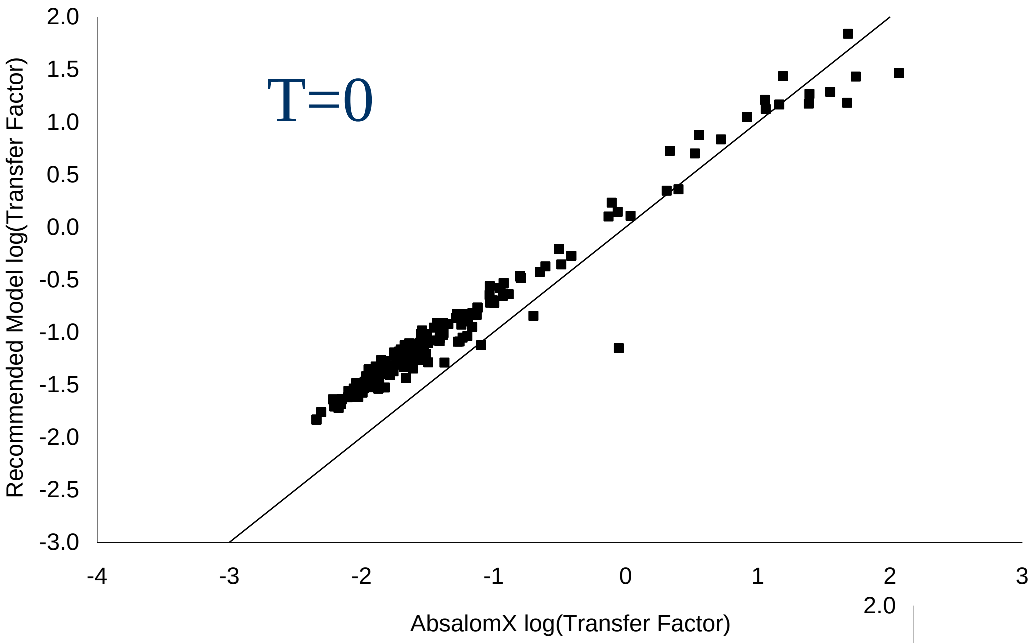


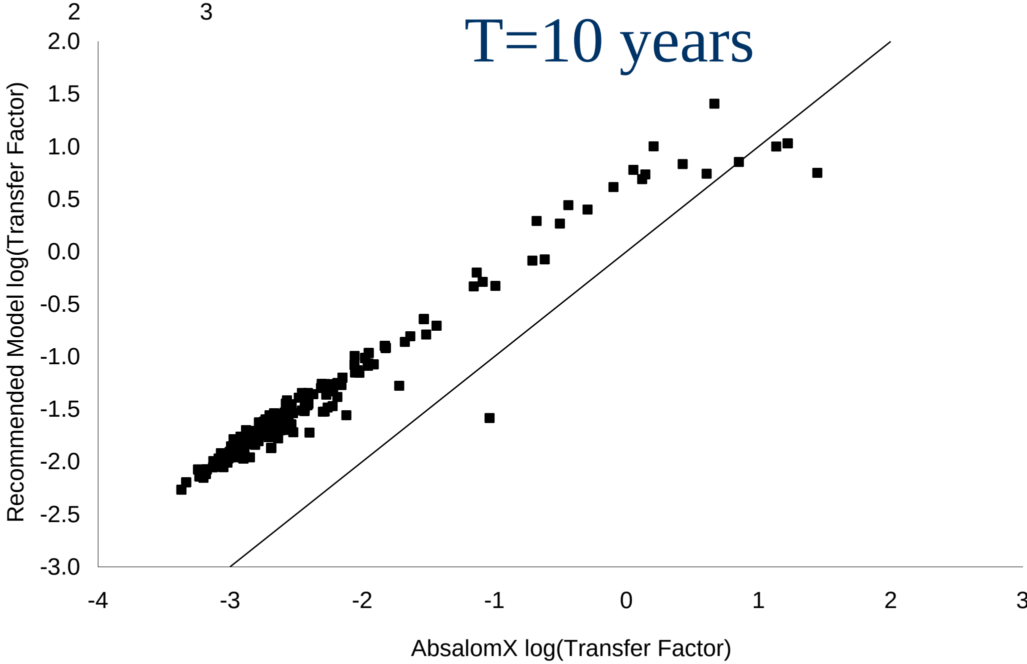
Model Statistics

	Parameterisation					Evaluation					
	RSS	AIC	ln(IML)	Nash	MAE	PSS	Nash	MAE			
								Overall	Grass	Barley	**Wheat**
Absalom2001	n/a	n/a	n/a	n/a	n/a	183.4	-3.76	1.26	n/a	n/a	**n/a**
AbsalomX	91.46	569.1	-324.3	0.747	0.379	14.14	0.689	0.34	0.37	0.26	0.35
Reduced	**85.04**	**541.1**	**-314.7**	**0.765**	**0.362**	**14.14**	**0.688**	**0.32**	**0.35**	**0.26**	**0.37**

- Reduced model fits marginally better
  - and has 1 fewer input required (pH)
- Evaluation outcomes are very similar
- Model behaviour is different
  - Time dependency is quite different

Comparisions





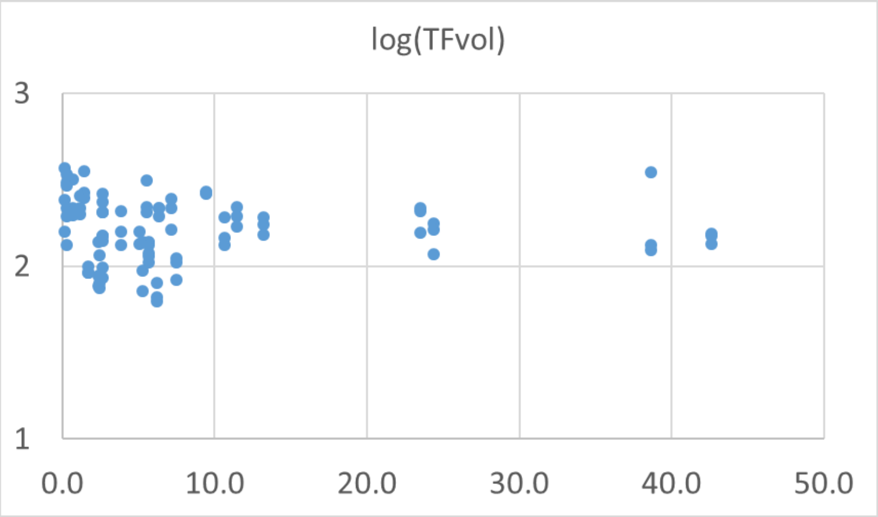
Final Thoughts – 'TREE' Project

Agrostis Capillaris

Lolium Perenne

- 'Modern' system
- Diverse group of soils (UK/Ukrainian)
- Spiked with stable isotope (Se, TC, I, U)
- Incubated (30 months)
- Contaminated soil used for plant uptake studies
- Lots of models….

Plants explore soil by volume not mass…



Se $TF_{available}$ calculated as

$$TF_{available} = \frac{[Plant](\mu g\ kg^{-1})}{[Soil_{available}](\mu g\ L^{-1})}$$

- c. 30% variation attributable to mass<>volume
- in the Cs work mass was used
  - would be interesting to re-parameterise using volume?

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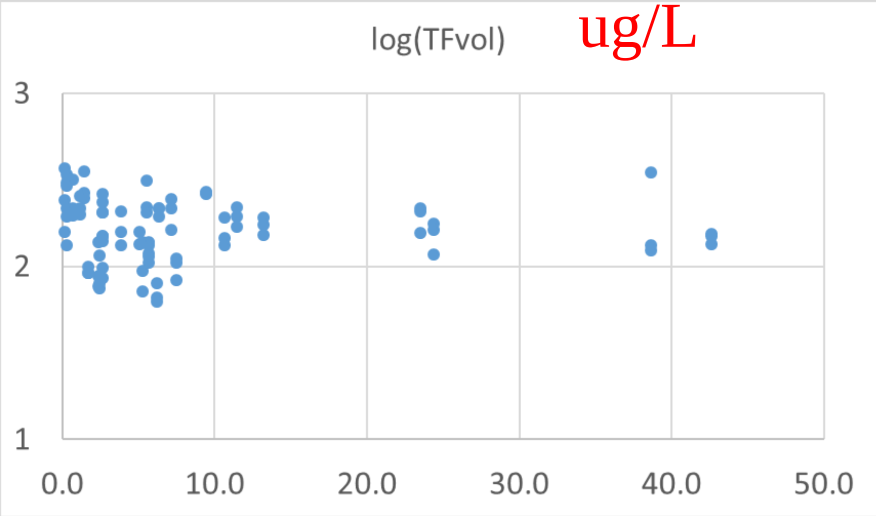

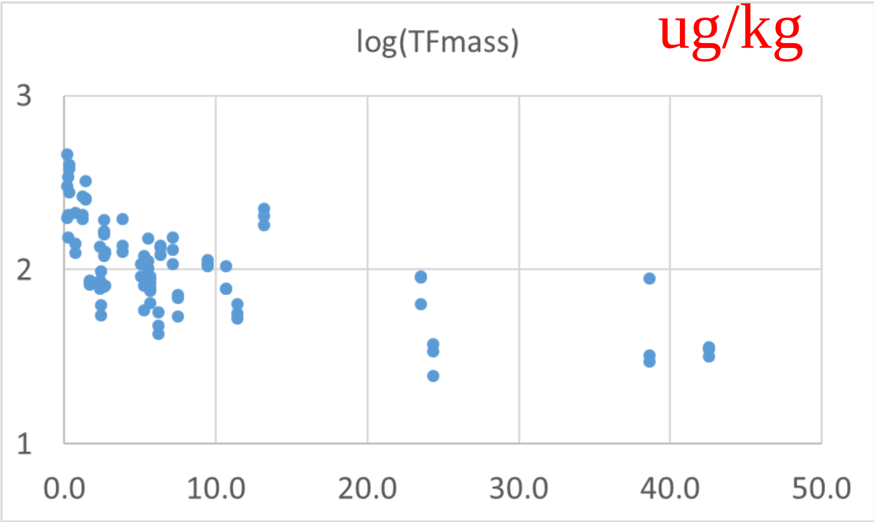

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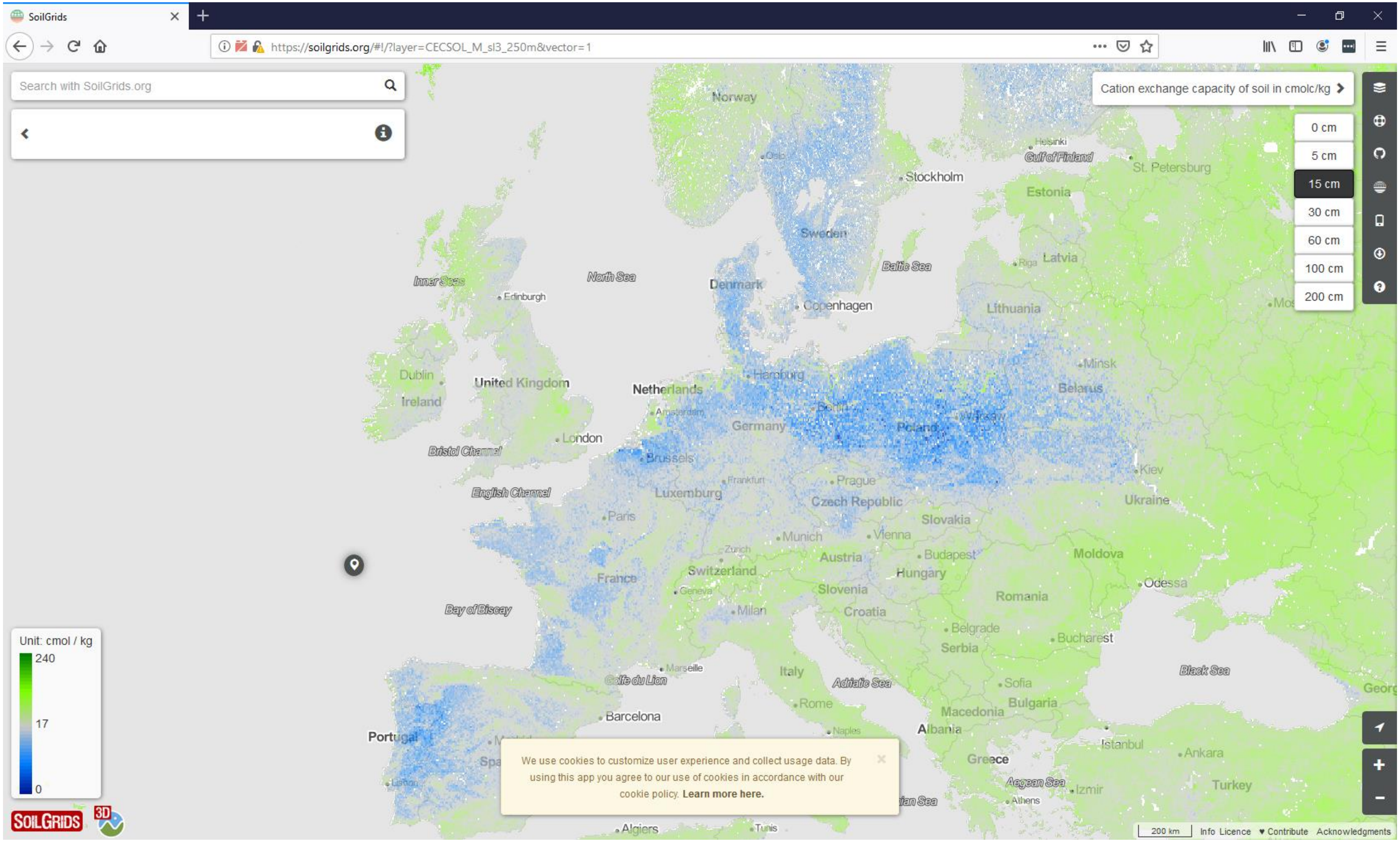
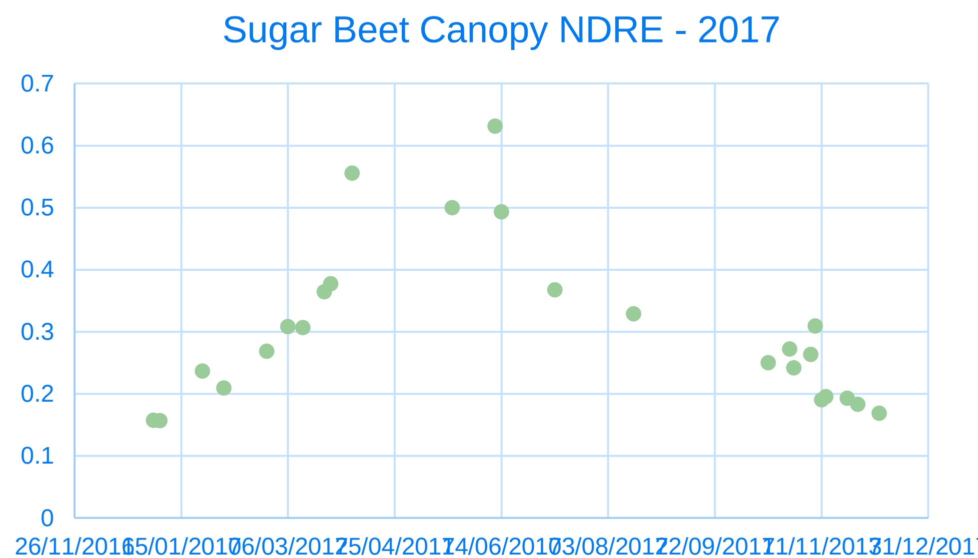
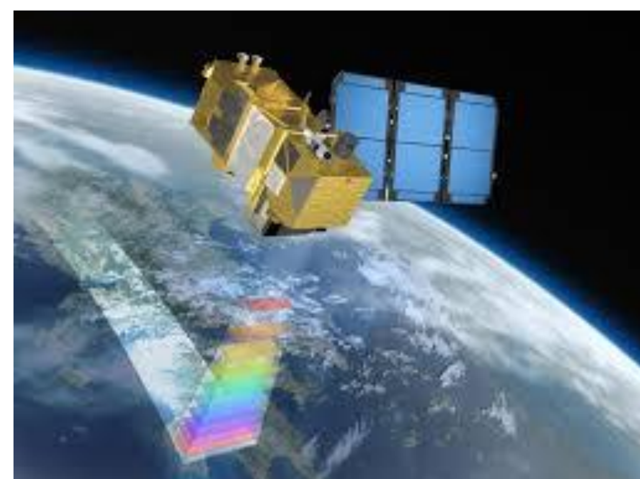
Final Thoughts…



Agricultural Practice Data?



- Ground cover – canopy size
- Crop Spotting
- Optical and radar
- Data assimilation…



Do Process-Based Models have a role…?

- ‘Horribly empirical’?
  - Maybe…
- Empirical equations with a mechanistic structure
  - Some of the ‘mechanistic thinking’ not supported by more modern analysis
- Geographical basis of soils data is limited
  - dominated by northern (and central Europe, Tarsitano 2011)
- In 2019 we would have a different
  - Data starting point
  - Basis of TF calculation
  - Experimental system