Predicting radiocaesium transfer in the agricultural foodchain

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

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Received 9 October 1999; received in revised form 17 March 2000; accepted 20 March 2000
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
● 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

\[ M_{\text{camg}} \]

\[ \text{pH} \]

\[ \text{CEC}_{\text{humus}} \]

\[ K_{\text{x humus}}^{(2)} \]

\[ \text{Kex} \]

\[ \% \text{ clay} \]

\[ \% \text{ org} \]

\[ K_{\text{d humus}} \]

\[ K_{\text{d clay}}^{(1)} \]

\[ \text{RIP}_{\text{clay}}^{(2)} \]

\[ \text{Kd}_{\text{clay}}^{(1)} \]

\[ \text{mK}^{(1)} \]

\[ \text{Kdl} \]

\[ \text{Time} \]

\[ \text{NH}_4 \]

\[ \text{Kdr} \]

\[ \text{Cs}_{\text{soil}} \]

\[ \text{Cs}_{\text{plant}} \]

\[ \text{CF}^{(2)} \]

\[ \text{RIP}_{\text{clay}}^{(2)} \]
Plant Cs

\[ CS_{\text{plant}} = CF \times CS_{\text{sol}} \]

- \( CF \) imagined as plant specific constant (i.e. plant concentration related to the plant accessible Cs)
- \( CS_{\text{sol}} \) – soil solution concentration of Cs
Plant Cs

\[ C_{S_{\text{plant}}} = CF \times C_{S_{\text{sol}}} \]

- \( CF \) imagined as plant specific constant (i.e. plant concentration related to the plant accessible Cs)
- \( C_{S_{\text{sol}}} \) – soil solution concentration of Cs

\[ \log(CF) = a_1 - a_2 \log(m_K) \]

Smolders et al, 1997
Plant Cs

\[ C_{S_{\text{plant}}} = CF \times C_{S_{\text{sol}}} \]

- \( CF \) imagined as plant specific constant (i.e. plant concentration related to the plant accessible Cs)
- \( C_{S_{\text{sol}}} \) – soil solution concentration of Cs

\[ \log(CF) = a_1 - a_2 \log(m_K) \]

Plant concentration linear with \( C_{S_{\text{sol}}} \)

\( CF \) reduces as \( m_K \) increases (K competes for uptake)

Smolders et al, 1997
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 $m_{Ca+Mg}$
Ca increases as pH increases

\[ \log(m_{Ca+Mg}) = a_4 \cdot pH - a_3 \]

‘..seems about right..’
\[ CEC = CEC^{\text{clay}} \theta_{\text{clay}} + CEC^{\text{org}} \theta_{\text{org}} \]

\[ = CEC^{\text{clay}} \theta_{\text{clay}} + (a_5 + a_6 pH) \theta_{\text{org}} \]

Some mechanistic thinking

Mixture of unknown and previously estimated model parameters

\[ m_k = f(K_{ex}, pH, \theta_{org}, \theta_{clay}) \]
Schematically

- pH
- Kex
- % clay
- % org
- M_camg
- CEC_{humus}
- K_{x\ humus}^{(2)}
- K_{d\ humus}
- K_{d\ clay}^{(1)}
- RIT_{clay}^{(2)}
- mK^{(1)}
- CF^{(2)}
- K_{dr}

2 components of labile adsorption

- Cs_{sol}
- Cs_{plant}
- Cs_{soil}

Fixation

Time
Schematically

- Schematically

- pH
- CEC_{humus}
- K_{ex}
- % clay
- % org
- M_{camg}
- mK^{(1)}
- CF^{(2)}
- K_{d_{humus}}
- K_{d_{clay}}^{(1)}
- RIP_{clay}^{(2)}
- NH_{4}
- K_{d_{soil}}
- Cs_{plant}
- Cs_{sol}

- Progressive fixation, rate reduced by organic matter
- Fixation
- Time
- RIP_{clay}^{(2)}
- K_{d_{clay}}^{(1)}
- K_{d_{humus}}
- CEC_{humus}
- mK^{(1)}
- CF^{(2)}
- pH

- Schematically

- pH
- CEC_{humus}
- K_{ex}
- % clay
- % org
- M_{camg}
- mK^{(1)}
- CF^{(2)}
- K_{d_{humus}}
- K_{d_{clay}}^{(1)}
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- K_{d_{soil}}
- Cs_{plant}
- Cs_{sol}

- Progressive fixation, rate reduced by organic matter
- Fixation
- Time
- RIP_{clay}^{(2)}
- K_{d_{clay}}^{(1)}
- K_{d_{humus}}
- CEC_{humus}
- mK^{(1)}
- CF^{(2)}
- pH

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

- $-\log(m_K)$ (moles dm$^{-3}$)

- $\log(k_d)$ (dm$^{-3}$ kg$^{-1}$)

(b) measured vs modelled

- $\log(TF)$

- measured vs modelled

- measured vs modelled

- $-\log(m_K)$ vs $\log(k_d)$
Independent Data

Nisbet et al, 1999
Food-chain comparisons

[Diagram showing the flow of soil K, Cs deposit, OM, and pH through production processes of soil-vegetation model, leading to arable crops, pasture, and slage, which in turn lead to animal products and arable products. These processes result in milk production with flux (Bq km⁻² y⁻¹).]
This project has received funding from the Euratom research and training programme 2014-2018 under grant agreement No 662287.

Lamb Concentrations in Clwyd

Chernobyl Exclusion Zone

Cow Milk (Bq L⁻¹)
Is my model too complex? Evaluating model formulation using model reduction

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ARTICLE INFO

Article history:
Received 5 December 2007
Received in revised form 6 June 2008
Accepted 13 June 2008
Available online 24 July 2008

Keywords:
Model reduction
Model complexity
Over-parameterisation
Structural error
Structural uncertainty
Bayesian evaluation

ABSTRACT

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.
Evaluating and reducing a model of radiocaesium soil-plant uptake

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ARTICLE INFO

Article history:
Received 4 August 2010
Received in revised form 29 November 2010
Accepted 30 November 2010
Available online 12 January 2011

Keywords:
Radiocaesium
Model
Evaluation
Soil
Plant
Reduction

ABSTRACT

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.

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

- 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)

- pH
- CEC_{humus}
- K_{ex}
- % clay
- % org
- K_d_{humus}
- K_d_{clay}\^{(1)}
- R^I P_{clay}\^{(2)}
- M_{camg}
- mK\^{(1)}
- CF\^{(2)}
- K_d_{l}
- Cf_{plant}
- Cs_{sol}
- Cs_{soil}
- Fixation
- Time
- K_d_{r}
- NH_4
This works ‘better’
And so does this…
Comparing…

Absalom-X

Reduced Model
Tarsitano 2011
### Model Statistics

<table>
<thead>
<tr>
<th>Parameterisation</th>
<th>Evaluation</th>
<th>MAE</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>RSS</td>
<td>AIC</td>
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<tr>
<td>Absalom2001</td>
<td>n/a</td>
<td>n/a</td>
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<tr>
<td>AbsalomX</td>
<td>91.46</td>
<td>569.1</td>
</tr>
<tr>
<td>Reduced</td>
<td>85.04</td>
<td>541.1</td>
</tr>
</tbody>
</table>

- 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
Comparisons

T=0

T=10 years
Final Thoughts – ‘TREE’ Project

- ‘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….

*Agrostis Capillaris*

*Lolium Perenne*
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?
Plants explore soil by volume not mass...

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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