Impact of distribution heterogeneity of microorganisms and 2,4-D on biodegradation processes in soil: Experiment & Modelling

Pinheiro M., Garnier P., Martin Laurent F., Rapaport A., Beguet J.
and Vieublé-Gonod L.

Grignon, France
 Difficulty of predicting pesticide fate in soil at macroscale, implication of processus at smaller scales?

Soil = complex environment
- *Heterogeneous distribution of soil microorganisms and their activities* 

  *Organised in mm to cm hotspots* (Morris et al; 1999, Vieublé Gonod et al; 2003)

Biodegradation of pesticides in soil will be driven by
- Presence of degrading microorganisms.
- Accessibility of pesticides for microorganisms (Dechesne & al, 2011)
- Availability (retention) of pesticides (Vieublé al, 2006)
- Local conditions ($\text{H}_2\text{O, T, O}_2$) (Monard & al 2012, Schroll & al, 2010)
Objective

- Role of accessibility between a model pesticide (2,4-D) and microorganisms on fate of 2,4-D
- Impact of different distributions

Experimental work

Modeling work
Control of localisation:

4 treatments

- Soil microorganisms
- Pesticide 2,4-D

Non co-localised co-localised homogeneous Sterilised control
Core construction:

- 2,4-D
- Microorganisms

Compaction

Incubation:
- BD=1,3g/cm³
- pF 2,5
- T: 20°C
- 2,4-D: 1,87µg/g soil
• Measures at:
  cm scale (core)
  mm scale (cubes) → cartography

<table>
<thead>
<tr>
<th>14C</th>
<th>Pesticide fate</th>
</tr>
</thead>
<tbody>
<tr>
<td>14CO2</td>
<td>CaCl2 soluble fraction</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>12C</th>
<th>Microbial populations</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>2,4-D Degraders</td>
</tr>
<tr>
<td></td>
<td>Tfda</td>
</tr>
</tbody>
</table>
Core scale: 2.4-D Mineralisation

Experimental results

Strong influence of initial localisation on 2,4-D mineralisation at the core scale

- Non Co-localised distribution
- Co-localised distribution
- Homogeneous distribution
Core scale $^{14}$C Mass Balance after 14 days:

Homogeneous vs heterogeneous distribution: $\uparrow$ $^{14}$CO$_2$, $\downarrow$ soluble $^{14}$C
Co-localised vs non colocalised distribution: $\uparrow$ distance = $\uparrow$ soluble $^{14}$C, $\downarrow$ $^{14}$CO$_2$, $\downarrow$ non extractable residues

Strong influence of initial localisation on fate of 2,4-D at the core scale
Presence of microorganisms \(\rightarrow\) \(\downarrow\) soluble fraction of \(^{14}\text{C}\)
Presence of microorganisms \(\rightarrow\) \(\uparrow\) non extractable residues
\(\Rightarrow\) strong influence of initial localisation on fate of 2,4-D at the mm scale
**Experimental results**

**mm scale**

**Day 14**

**CaCl₂**

**NER**

**Tfda**

Presence of microorganisms $\rightarrow$ soluble fraction of $^{14}$C

Presence of microorganisms $\rightarrow$ non extractable residues

$\Rightarrow$ strong influence of initial localisation on fate of 2,4-D at the mm scale
mm scale

Presence of microorganisms $\rightarrow$ ↓ solvent fraction of $^{14}$C
Presence of microorganisms $\rightarrow$ ↑ non-extractable residues
$\Updownarrow$ strong influence of initial localisation on fate of 2,4-D at the mm scale
Biological Model:

- **14CO₂**
  - 1-y
  - μmax, ks

- **14C Soluble**
  - kd
  - kd2

- **14C Adsorbed**
  - kr

- **14C NER abiotic**

- **14C Microbial waste**
  - 1-X
  - mt

- **14C Biomass**
  - y

- **14C NER biotic**

- **14C total**

9 parameters
Matrix model:

Graphical representation of matrices are comparable to experimental maps.

Representation of soil column by 3D matrices of MS, MA.....

Each model compartment = 3D matrix (MS, MA, ...).

1 cube = coordinates (i, j, k) = possibility to spatialize each model compartment.
Modeling method:

• Parameters optimisation on modelmaker and the matrix model:

  1. Calibration of biotic parameters on homogeneous system (ModelMaker) \( \mu_{\text{max}}, k_s, Y, X, m_t \)

  2. Calibration of abiotic parameters on separated system (matrix model) Diffusion, \( K_d, K_d^2, K_r \)

• Validation of the matrix model on colocalised system:

  ❏ One set of parameters can simulate the three experiments?
Core scale modeling:

Comparison of experimental and simulated mass balance:

**Experimental data**

**Simulation**

- EF = 0.99, $R^2 = 0.99$
- EF = 0.87, $R^2 = 0.99$
- EF = 0.89, $R^2 = 0.99$
mm scale modeling:

Experimental Maps

Simulated Maps

Day 14

| EF: 0.72 | EF: 0.88 |

| 1.89  | 1.47  | 1.26  | 0.84  | 0.42  | 0.21  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  |
| 1.47  | 0.42  | 0.84  | 0.83  | 0.63  | 0.42  | 0.21  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  |
| 1.26  | 0.84  | 0.83  | 0.63  | 0.42  | 0.21  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  |
| 0.84  | 0.63  | 0.63  | 0.42  | 0.21  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  |
| 0.42  | 0.42  | 0.21  | 0.21  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  |
| 0.21  | 0.21  | 0.21  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  |

| 0.33  | 0.28  | 0.23  | 0.14  | 0.07  | 0.03  | 0.01  | 0.01  | 0.00  | 0.00  | 0.00  | 0.00  |
| 0.13  | 0.10  | 0.07  | 0.03  | 0.01  | 0.01  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  |

| 0.86  | 0.39  | 0.51  | 0.60  | 0.32  | 0.14  | 1.60  | 15.49 | 1.05  | 0.08  | 0.06  | 0.01  |
| 0.85  | 0.59  | 0.54  | 0.44  | 0.22  | 0.09  | 0.20  | 1.45  | 0.27  | 0.05  | 0.02  | 0.01  |
| 0.62  | 0.56  | 0.44  | 0.28  | 0.13  | 0.06  | 0.07  | 0.08  | 0.07  | 0.03  | 0.01  | 0.00  |
| 0.33  | 0.28  | 0.23  | 0.14  | 0.07  | 0.03  | 0.02  | 0.02  | 0.02  | 0.01  | 0.01  | 0.00  |
| 0.13  | 0.10  | 0.07  | 0.03  | 0.01  | 0.01  | 0.01  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  |

Experimental Maps

Simulated Maps

EF: 0.72

EF: 0.88
Conclusion

- Strong influence of localization of \( \mu \)org and 2,4-D (and so accessibility) on pesticide fate:
  2,4-D mineralisation
  Formation of biotic and abiotic non extractable residues

Key factor = 2,4-D diffusion

- Predominant role of microorganisms in the formation and localisation of NER at a mm scale

- Good adequation between experimental and modeling results at a mm to cm scale

- Importance of microscale processes on macroscale fate of pesticides
- Impact of agricultural practices & tillage on pesticide fate
Thank you for your attention!

Cecile Nobile is the best & most beautiful woman I’ve ever met in the world. Thank God!