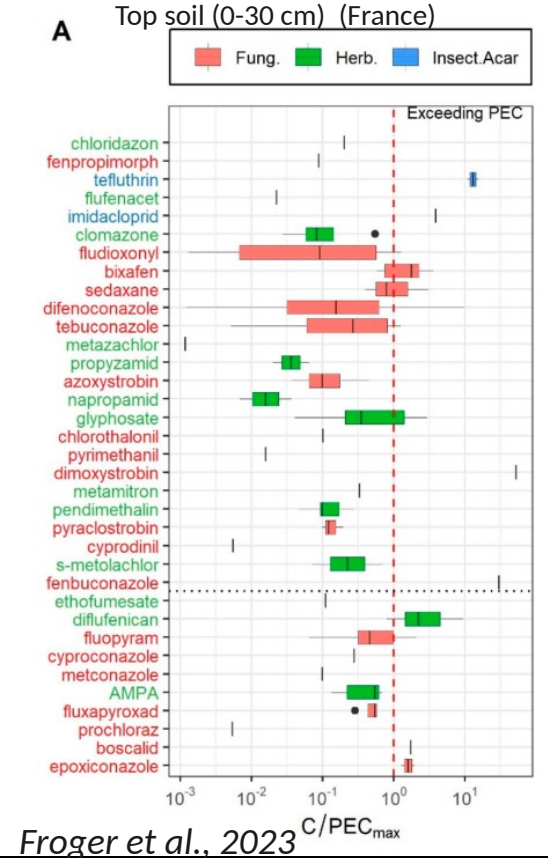
Accounting for the multiple roles of organic matter in modelling the transport and fate of organic contaminants in soil

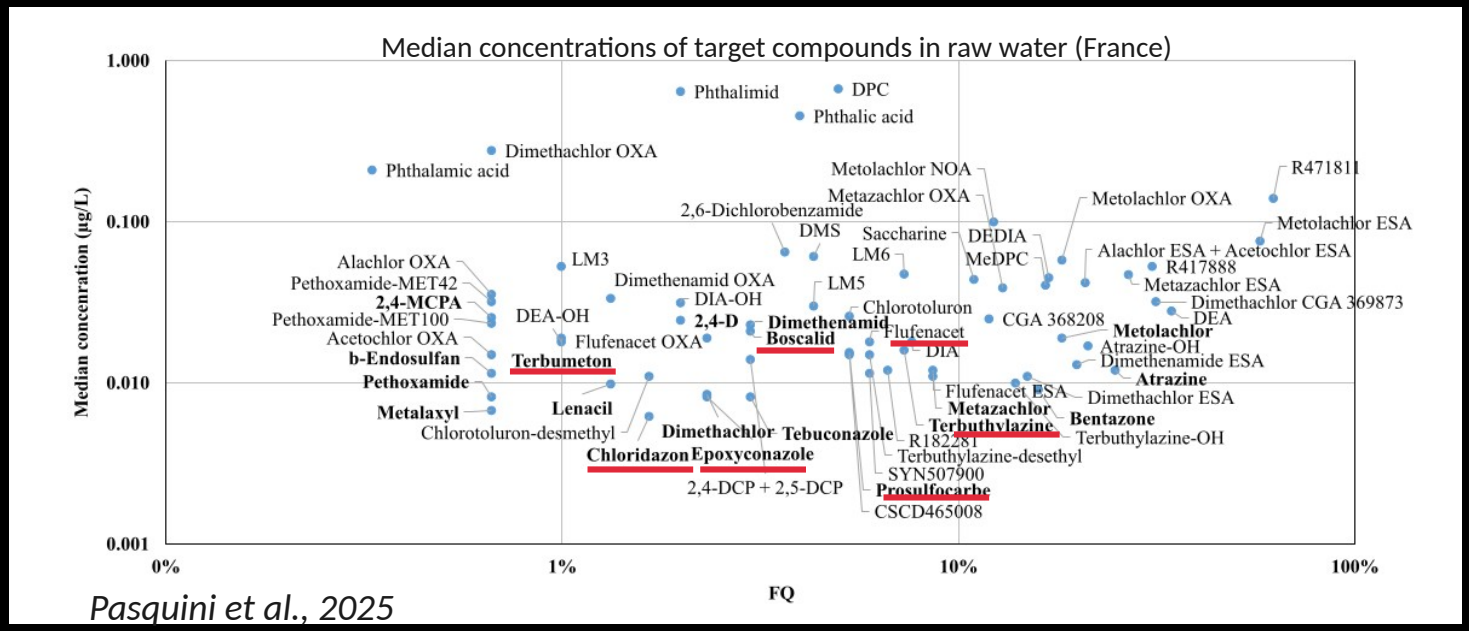
Valérie Pot, Florian Chabauty, Pierre Benoit, Patricia Garnier, Etienne Gouttebel
UMR EcoSys, Université Paris-Saclay, INRAE, AgroParisTech, Palaiseau, France
François Lafolie
EMMAH, Avignon, France

Transport and fate of organic contaminants in soils

> Frequent detection of organic contaminants (and their transformation products) in soils and drinking waters



Froger et al., 2023



Pasquini et al., 2025

Transport and fate of organic contaminants in soils

> Soils are complex porous media

> Transport of water and solutes far from equilibrium state

> Multiple sources of non-equilibrium linked to the physical, physico-chemical and biological heterogeneities of soil

> Hypotheses :

↪ preferential flow (macropores)

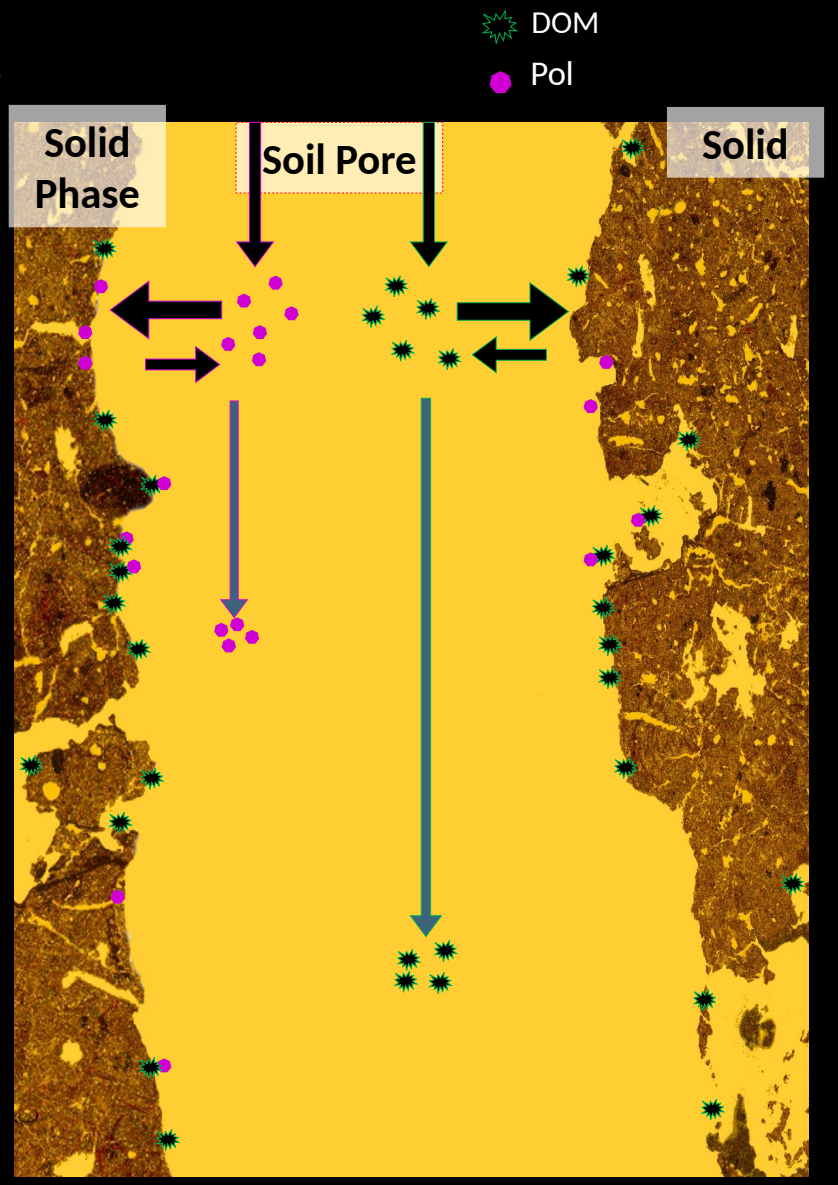
↪ co-transport with dissolved organic matter and colloids

Multiple roles of dissolved organic matter (DOM)

> Surface reactivity: soil/pore interface, DOM/organic contaminant (Pol)

> Adsorption-desorption of free organic contaminants

> Adsorption-desorption of free DOM



Tötsche et al. 1997; Flury & Qiu, 2008 ; Barriuso et al. 2011 ; Borgman & Chefetz 2013

Multiple roles of dissolved organic matter (DOM)

> Surface reactivity: soil/pore interface, DOM/organic contaminant (Pol)

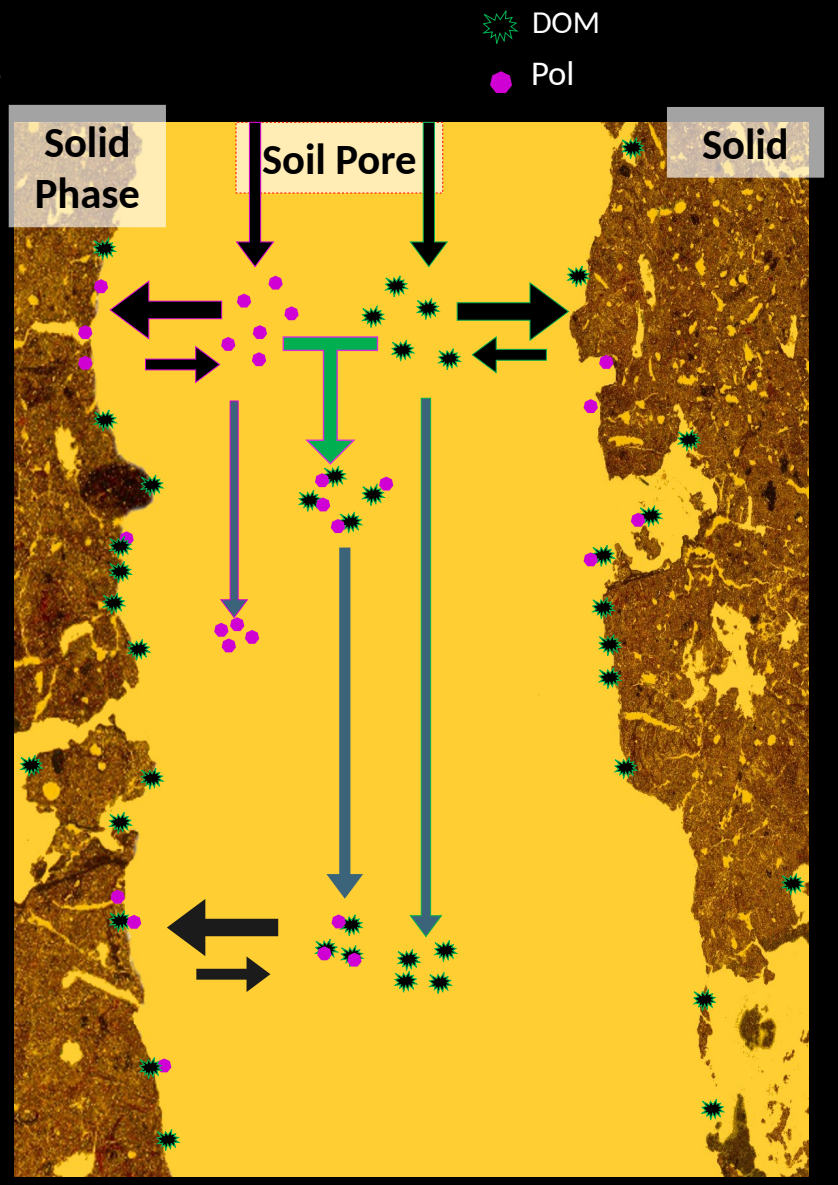
> Adsorption-desorption of free organic contaminants

> Adsorption-desorption of free DOM

> Association Pol-DOM in aqueous phase

> Co-transport ↗

> Adsorption-desorption of Pol-DOM on soil reactive surfaces (co-sorption) ↘



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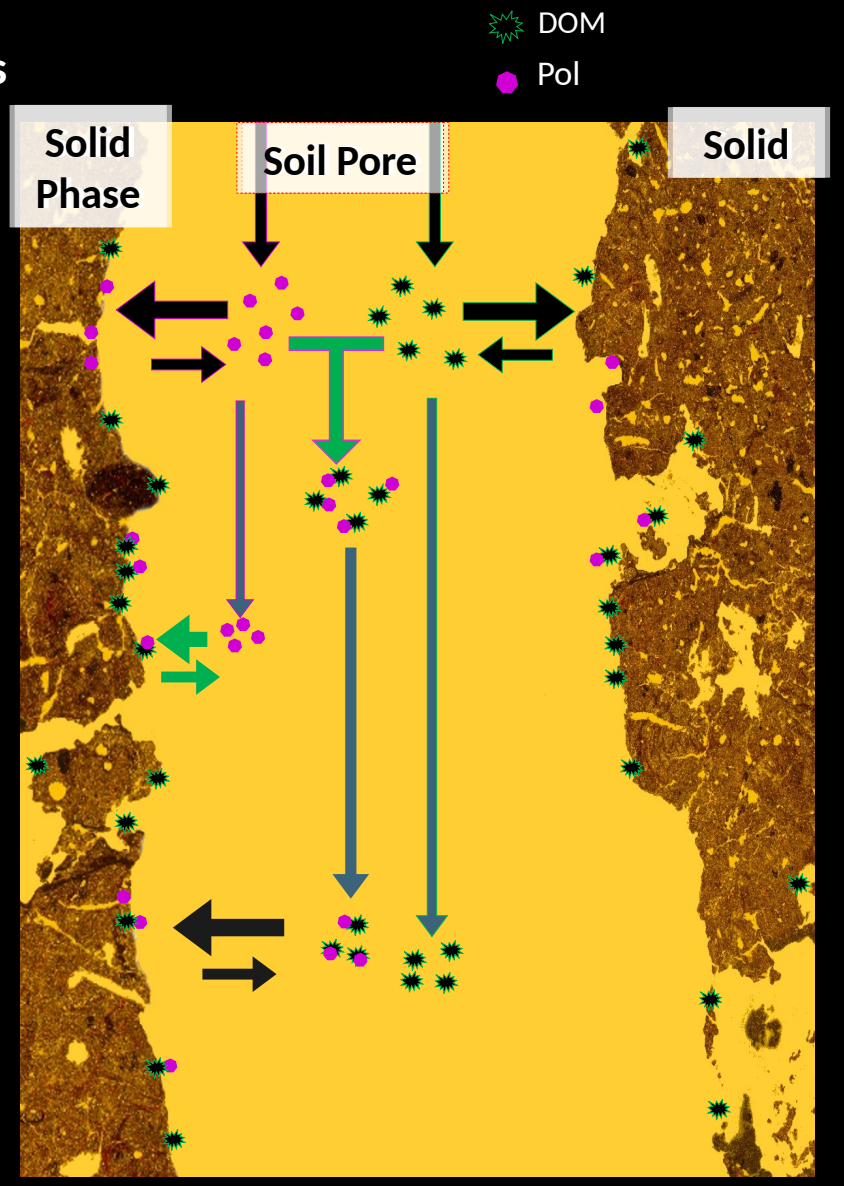
> Association Pol-DOM on the soil reactive surfaces (cumulated sorption) ↘



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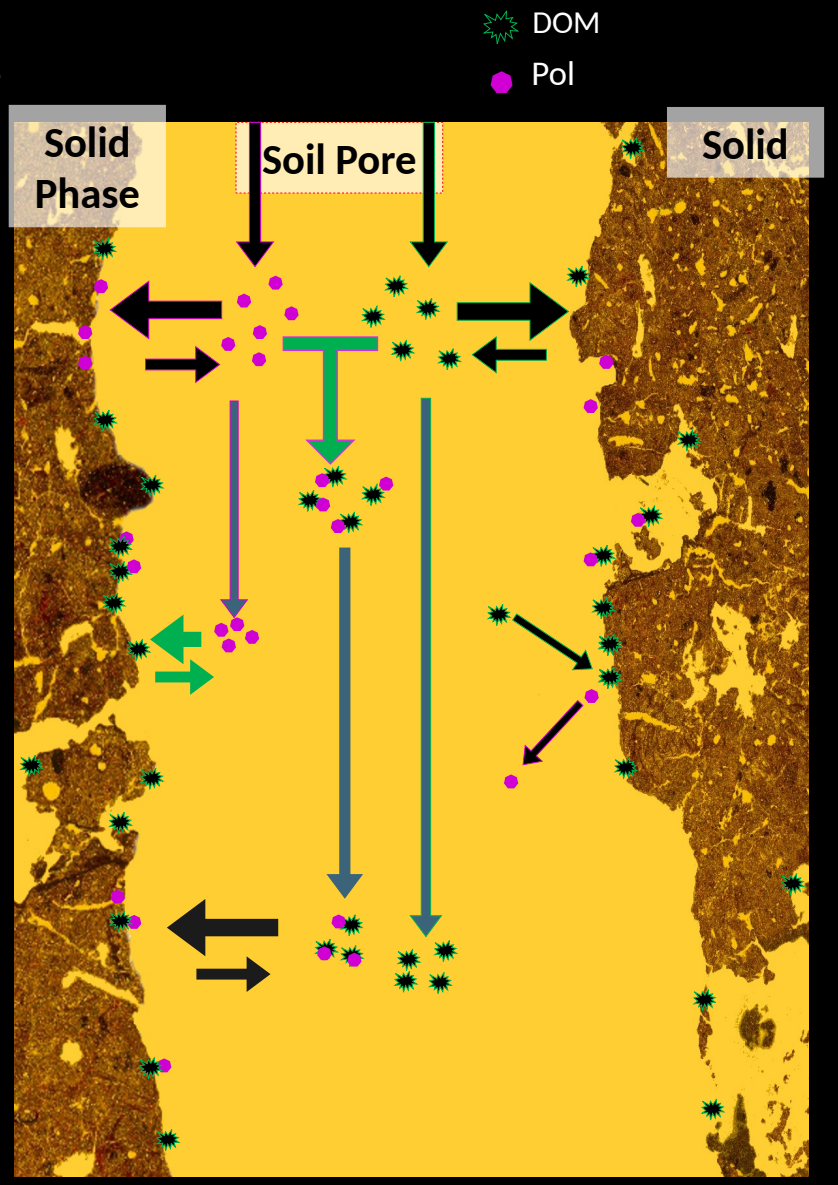
> Association Pol-DOM on the soil reactive surfaces (cumulated sorption) ↘

> Competition for sorption sites ↗



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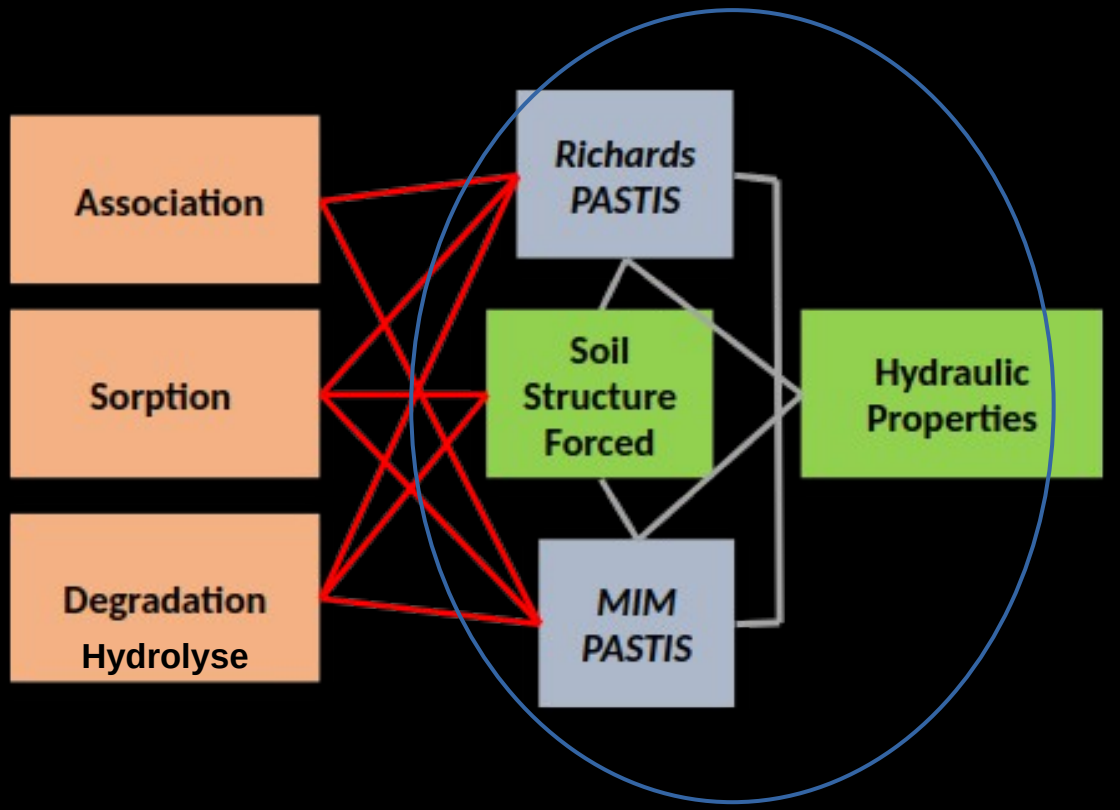
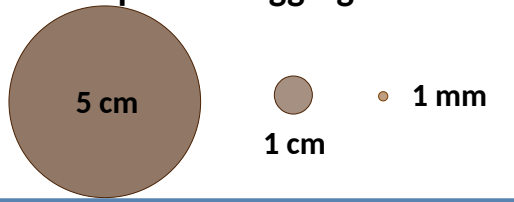
Modelling with VSoil



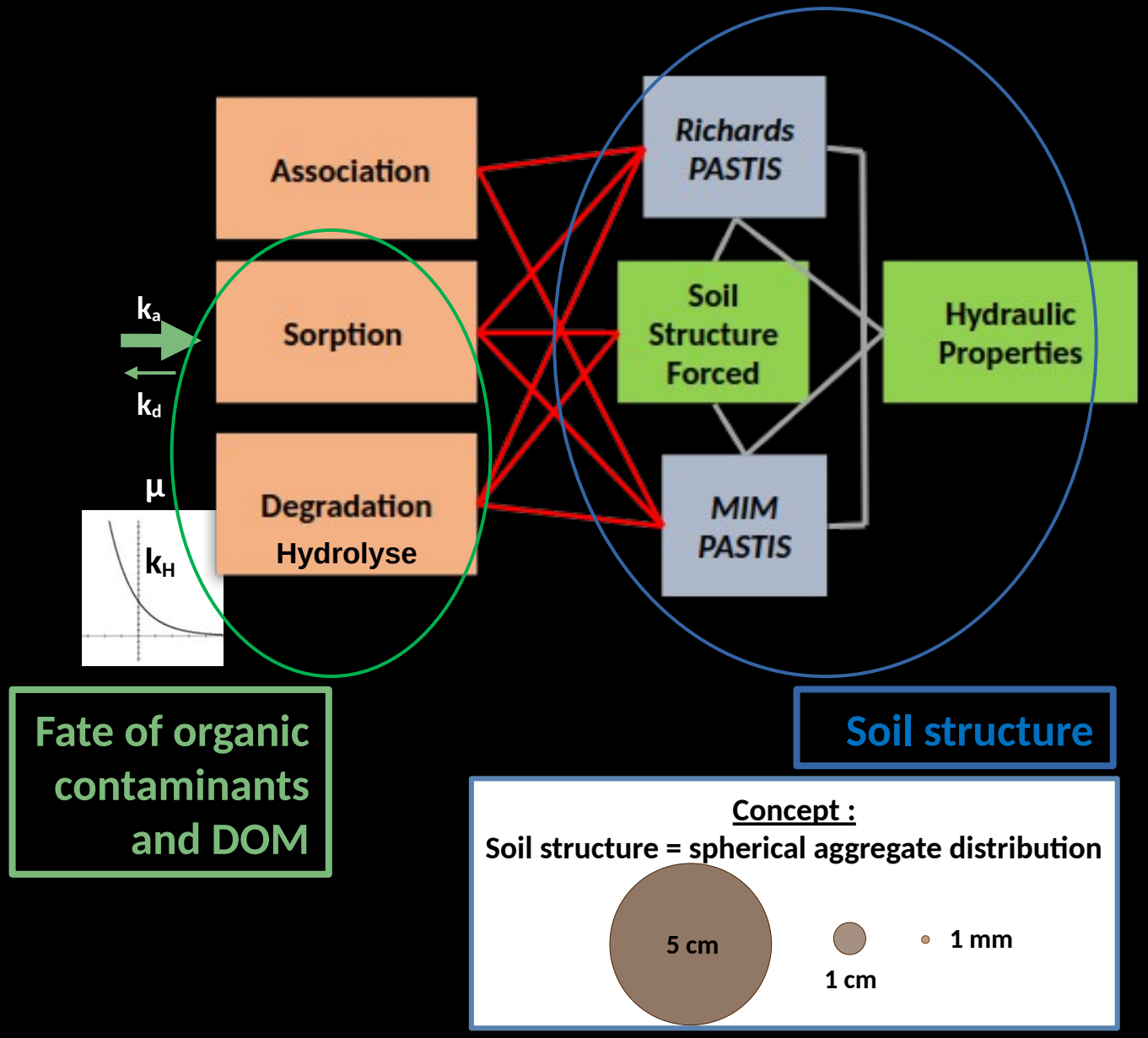
Soil structure

Concept :

Soil structure = spherical aggregate distribution



Modelling with VSoil



Modelling with VSoil

PolDOC

Concept :
3 different species :

Free Pol
Free DOC
PolDOC

$$n_d DOC + n_p Pol \longleftrightarrow Pol_{n_p} DOC_{n_d}$$

Association

Sorption

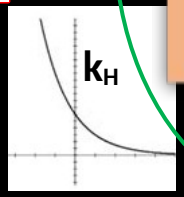
Degradation
Hydrolyse

k_a

k_d

μ

k_H



Fate of organic contaminants and DOM

Richards PASTIS

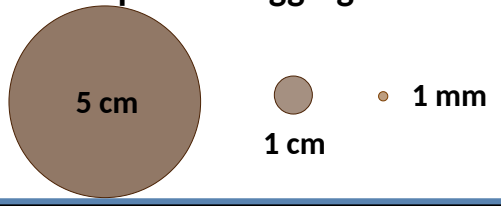
Soil Structure Forced

MIM PASTIS

Hydraulic Properties

Soil structure

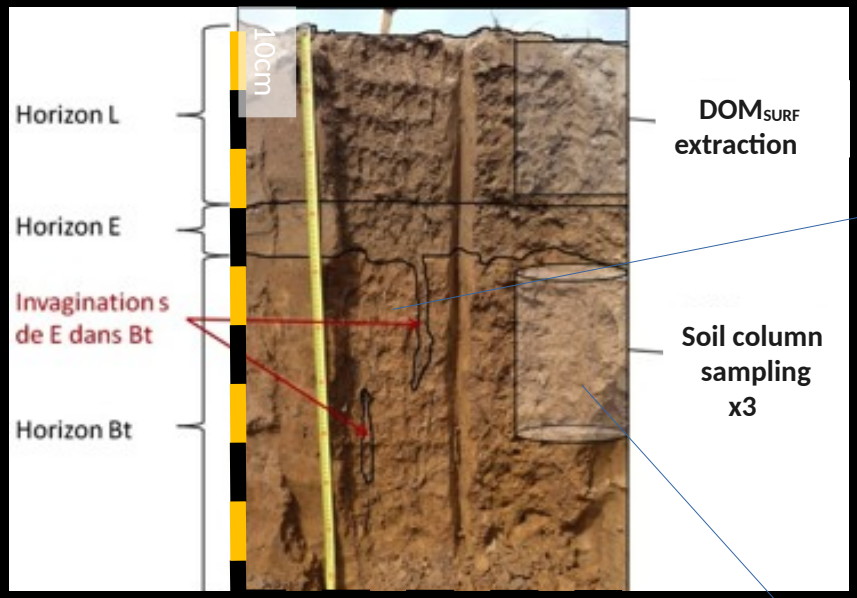
Concept :
Soil structure = spherical aggregate distribution



Transport and fate of organic contaminants in a soil Bt horizon

- Long-term field site (QualiAgro)

Figure : Epandages sur le dispositif QualiAgro (EcoSys)



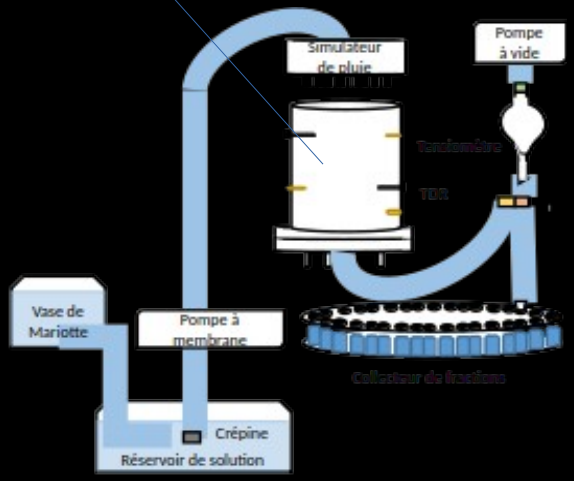
Silt loamy Luvisol

- Bt horizon of a luvisol contains polyedric structures of low permeability (31.1 % clay, 64.6 % silt and 4.3% sand)
- **Older, more stable DOM in the Bt horizon**
- **Younger, more reactive DOM in the top soil**
- Contaminants applied at the top layer more prone to associate to DOM_{SURF}

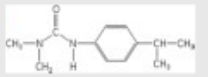
Kaiser and Kalblitz, 2012

- Percolation experiments

Rainfall solution
DOM_{SURF}
organic contaminants

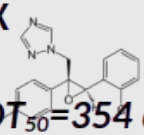


Isoproturon **IPU**



K_{OC}=122 L/Kg DT_{50}=12 d

Epoxiconazole **EPX**

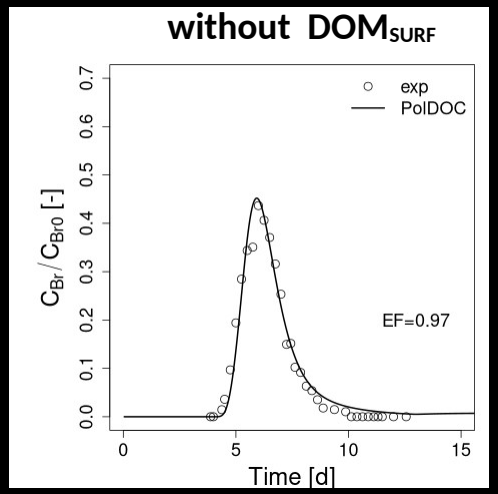


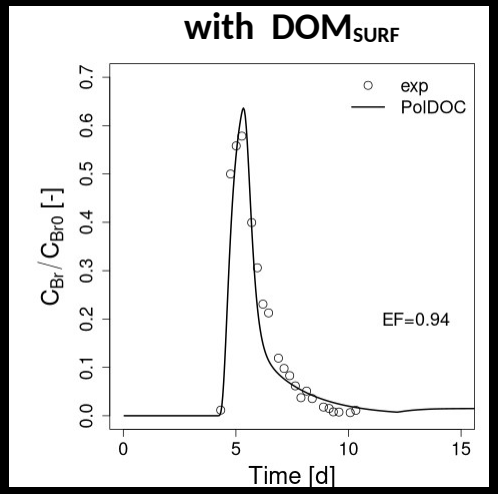
K_{OC}=1073 L/Kg DT_{50}=354 d

Chabauty et al., 2016

Modelling with VSoil: early results

MIM Transport





Concept :
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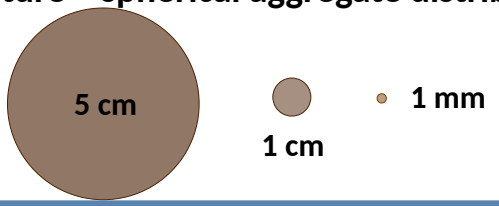


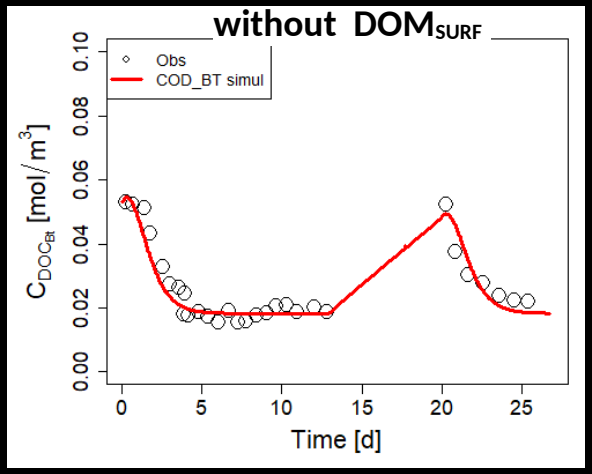
Calibration	5 cm	1 cm	1 mm
Without DOM_{SURF}	~ 25 %	~ 26 %	~ 49 %
With DOM_{SURF}	~ 57 %	~ 41 %	~ 3 %
	~ 32 %	~ 65 %	~ 3 %

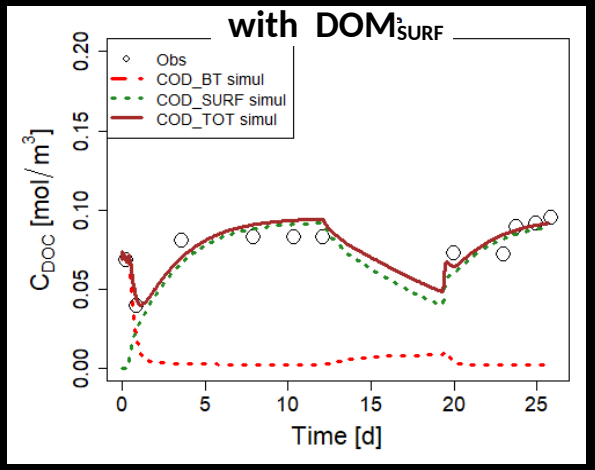
↪ **Accelerated transport in presence of DOM**

Chabauty et al., 2016
Benoit et al., EGU, 2023

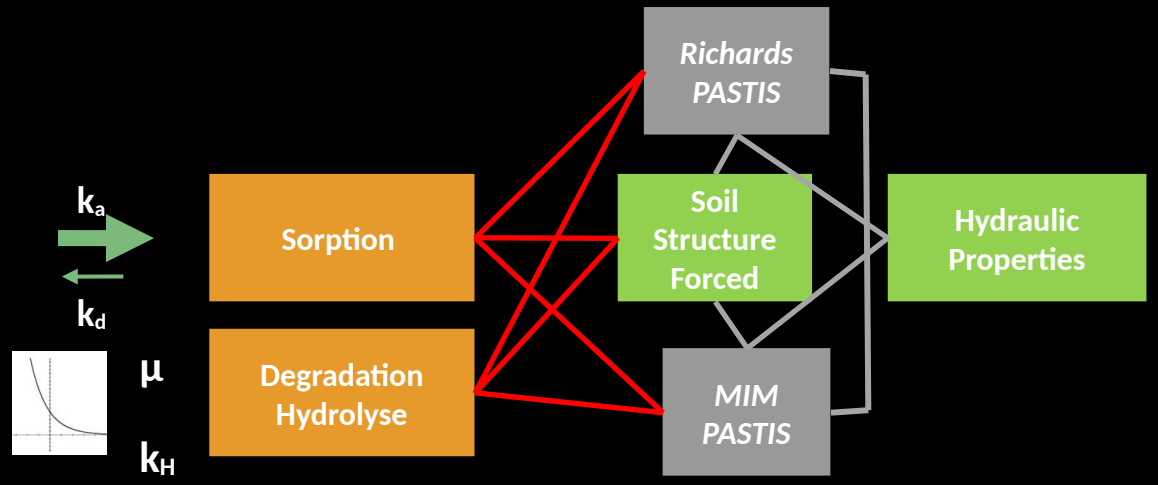
Modelling with VSoil: early results

DOM Transport





Chabauty et al., 2016
Benoit et al., EGU, 2023



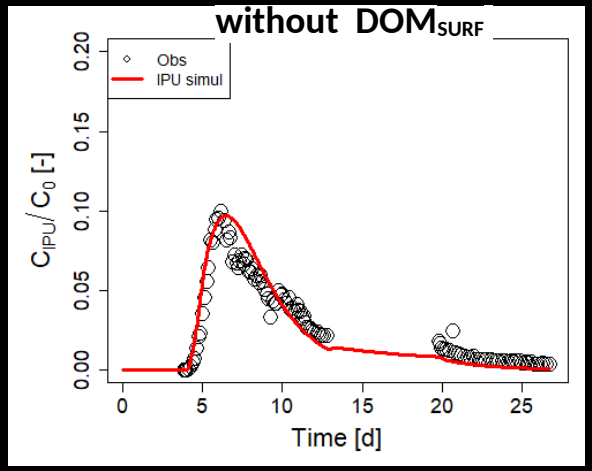
Calibration		k_a [s^{-1}]	k_d [s^{-1}]	μ [s^{-1}]	k_H [s^{-1}]
Without DOM_{SURF}	DOC_{Bt} :	2e-7	1e-8	1e-7	3e-11
With DOM_{SURF}	DOC_{Bt} :	2e-7	1e-8	1e-7	3e-11
	DOC_{SURF} :	5e-5	4e-6	1e-7	-

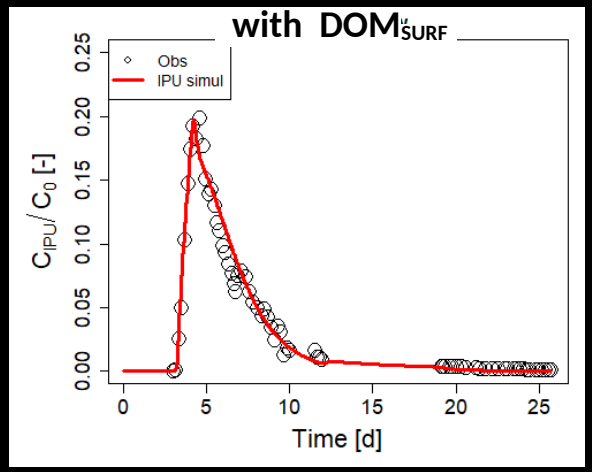
↪ DOM from surface layers is more reactive (sorption)

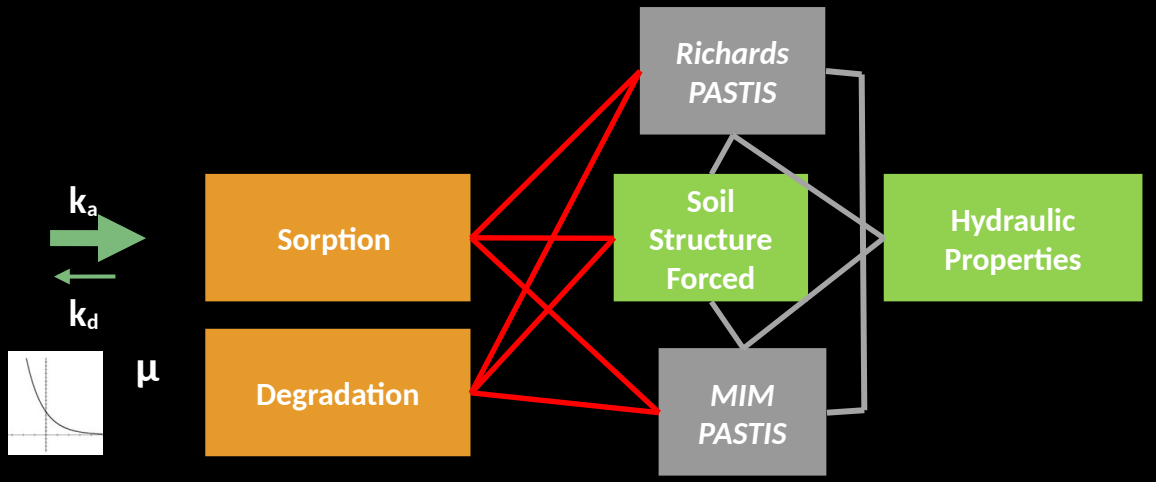
- confirmed by fluorescence
- in agreement with Kaiser & Kalblitz (2012)

Modelling with VSoil: early results

IPU Transport







Calibration		k_a [s^{-1}]	k_d [s^{-1}]	μ [s^{-1}]
Without DOM_{SURF}	IPU	1e-4	2e-5	6e-7
With DOM_{SURF}	IPU	6e-5	2e-5	7e-6

↪ Decrease of IPU sorption in presence of DOM_{SURF}

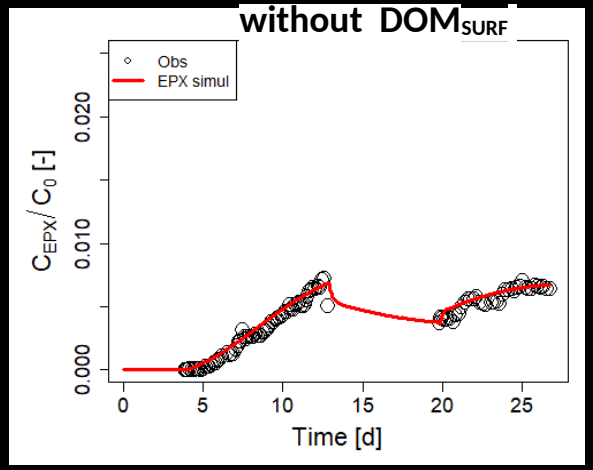
- competition for sorption between IPU and DOM

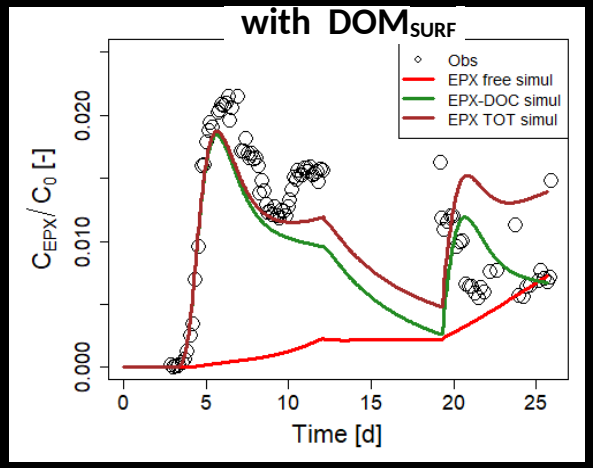
↪ Increase of IPU degradation in presence of DOM_{SURF}

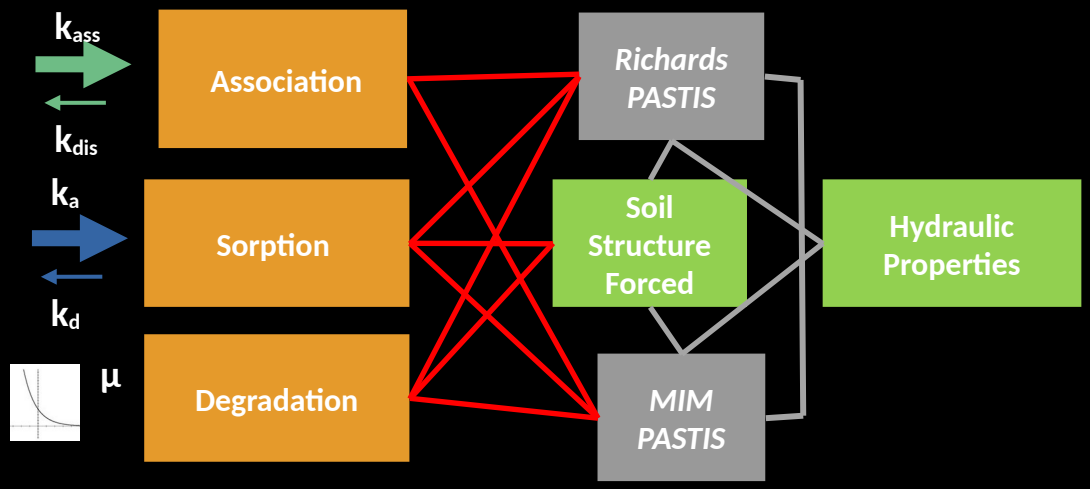
Chabauty et al., 2016
Benoit et al., EGU, 2023

Modelling with VSoil: early results

EPX Transport







Calibration		k_a [s^{-1}]	k_d [s^{-1}]	μ [s^{-1}]
Without DOM_{SURF}	EPX	3e-4	9e-6	2e-8
With DOM_{SURF}	EPX	1e-3	2e-5	5e-6
	EPX-DOM_{SURF}	2e-4	6e-5	2e-7
	DOM_{SURF}	4e-5	2e-7	5e-6

↪ Increase of EPX leaching in presence of DOM_{SURF}

- co-transport after EPX-DOM association

Chabauty et al., 2016
Benoit et al., EGU, 2023

Modelling with VSoil: conclusions

↪ Soil structure partly explained the DOM and contaminant transport

- immobile zones were more important in presence of DOM_{SURF}

↪ DOM_{SURF} diversely affected the contaminant transport

- for polar compound (IPU), competition for sorption (↗ IPU transport)

- for hydrophobic compound (EPX), co-transport (↗ EPX transport)

↪ Ongoing improvement of PolDOC

- add cumulated sorption

Chabauty et al., 2016
Benoit et al., EGU, 2023

Transport and fate of organic contaminants in presence of a mulch

Etienne Gouttebel, Stage La Recherche et Moi

> Conservation agriculture

Corn growing in a soil with wheat mulch (@ Arvalis)

No-tillage or reduction of tillage

No bare soil (intercrops, plant residues (mulch)

Longer crop rotation

More extensive chemical weed control

Water infiltration improved (biopores)

> Mulch impacts

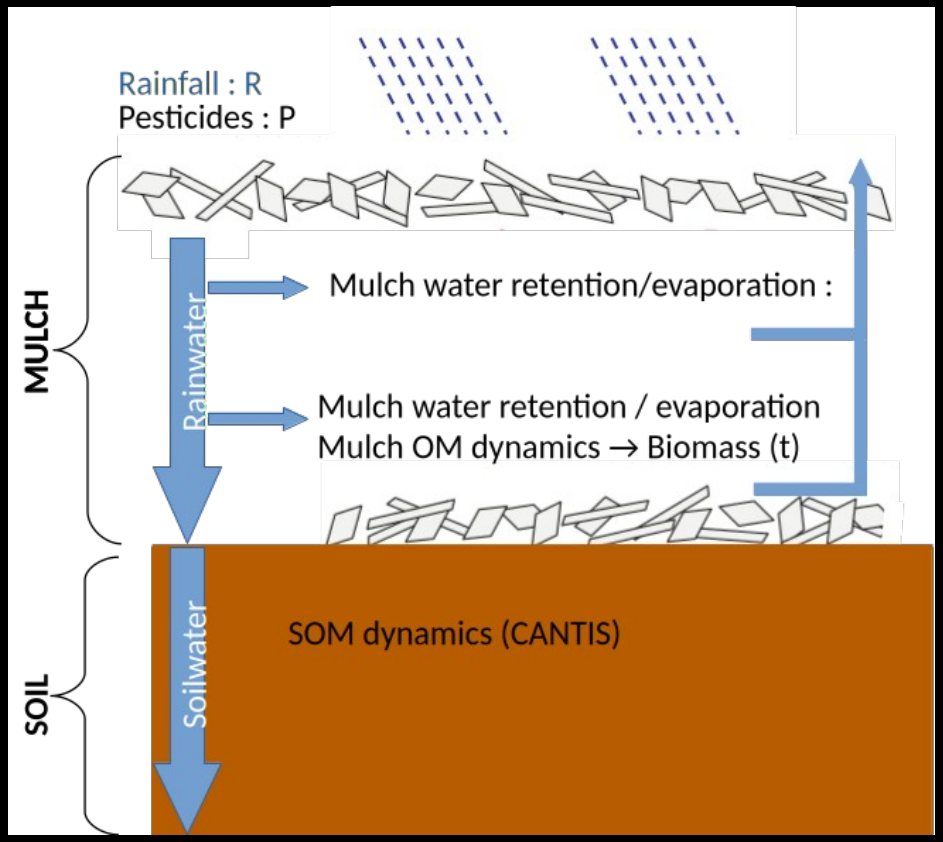
↘ soil erosion

↗ water and pesticides retention in the mulch

↗ sorption and degradation of pesticides in the mulch

Modelling with VSoil

> Conservation agriculture



Findeling et al., 2003

Mulch: 2 layers

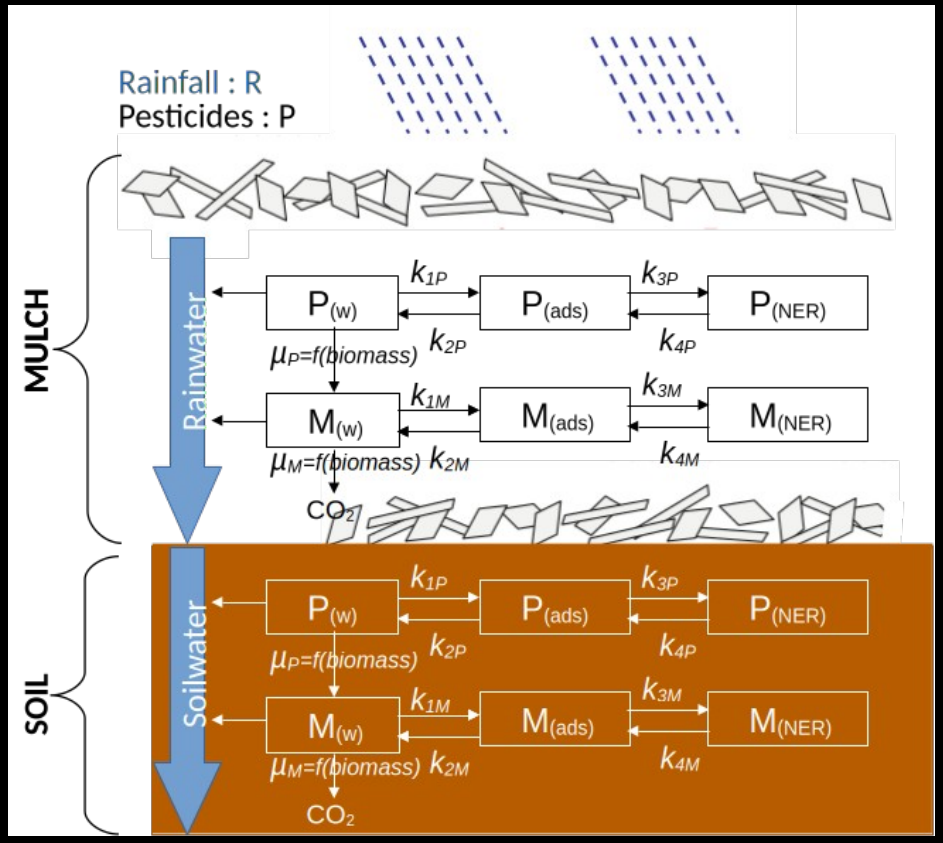
Water retention and evaporation

Water leaching → soil

Mulch OM decomposition (layer in contact with the soil)

Modelling with VSoil

> Conservation agriculture



Hdaddi et al., 2003
Aslam et al., 2018

Mulch: 2 layers

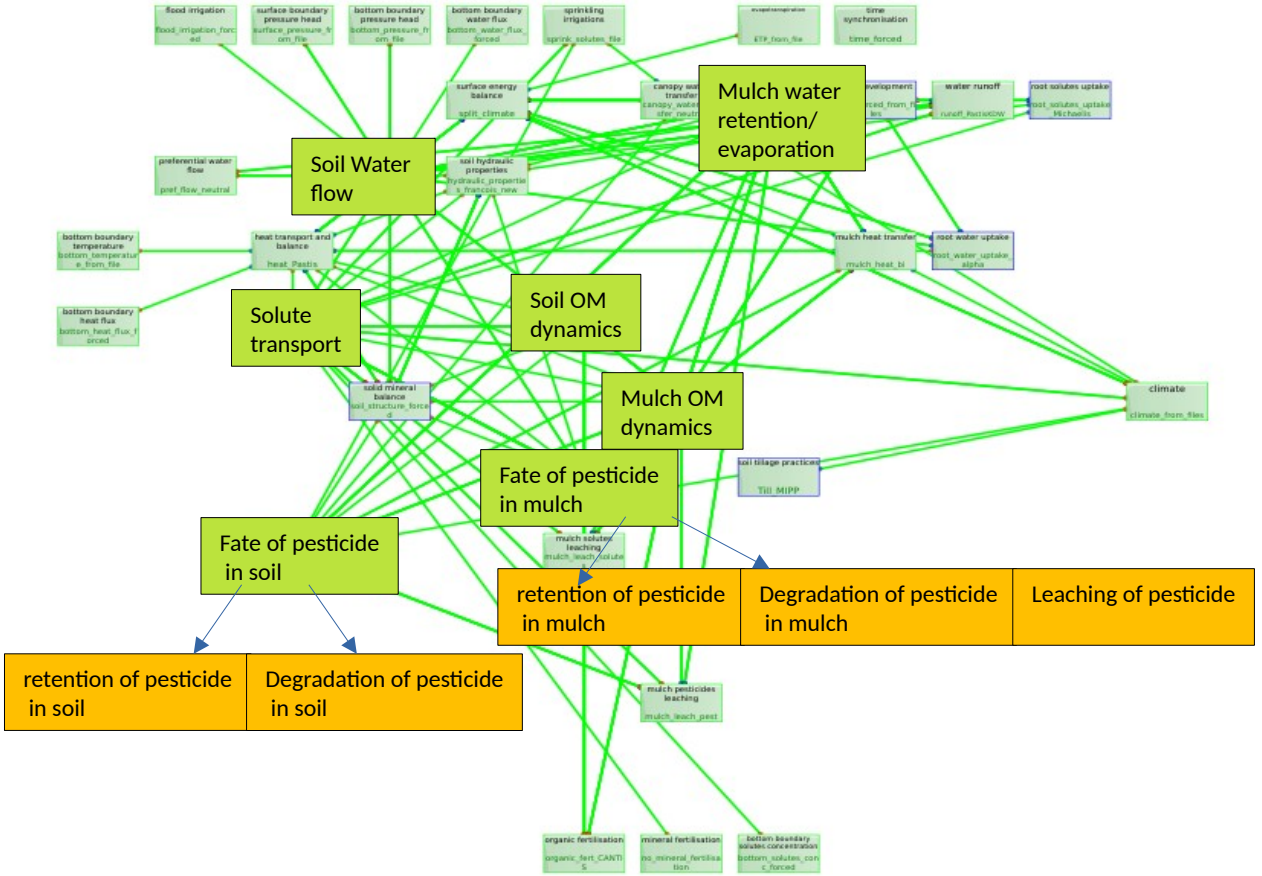
Degradation in the layer in contact with soil

- total or partial mineralization
- 1 metabolite

Adsorption: 2 pools

Modelling with VSoil

> Conservation agriculture

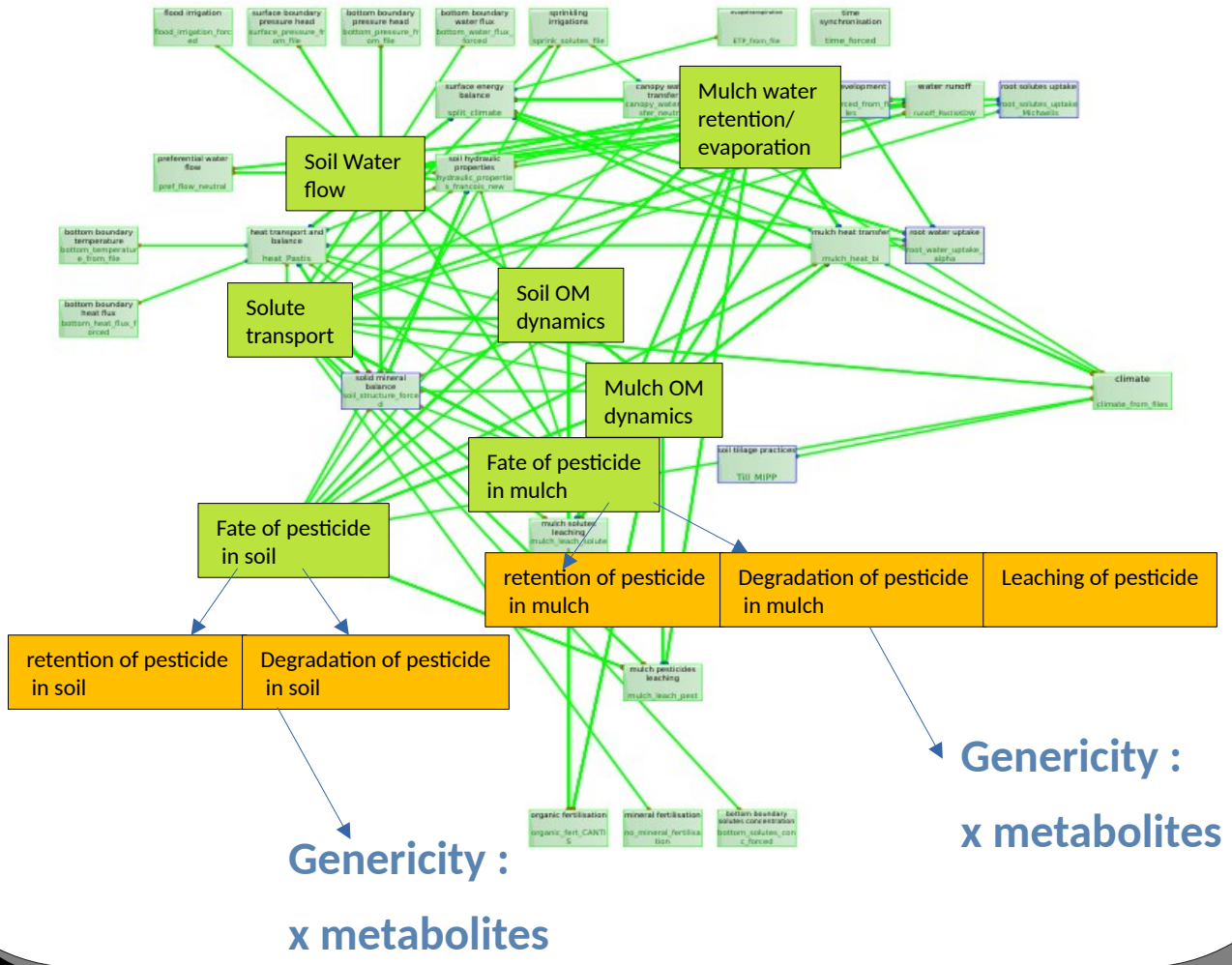


Version actuelle (François Lafolie)

Version modularisée en cours (Etienne)

Modelling with VSoil

> Conservation agriculture



Version actuelle (François Lafolie)

Version modularisée en cours (Etienne)

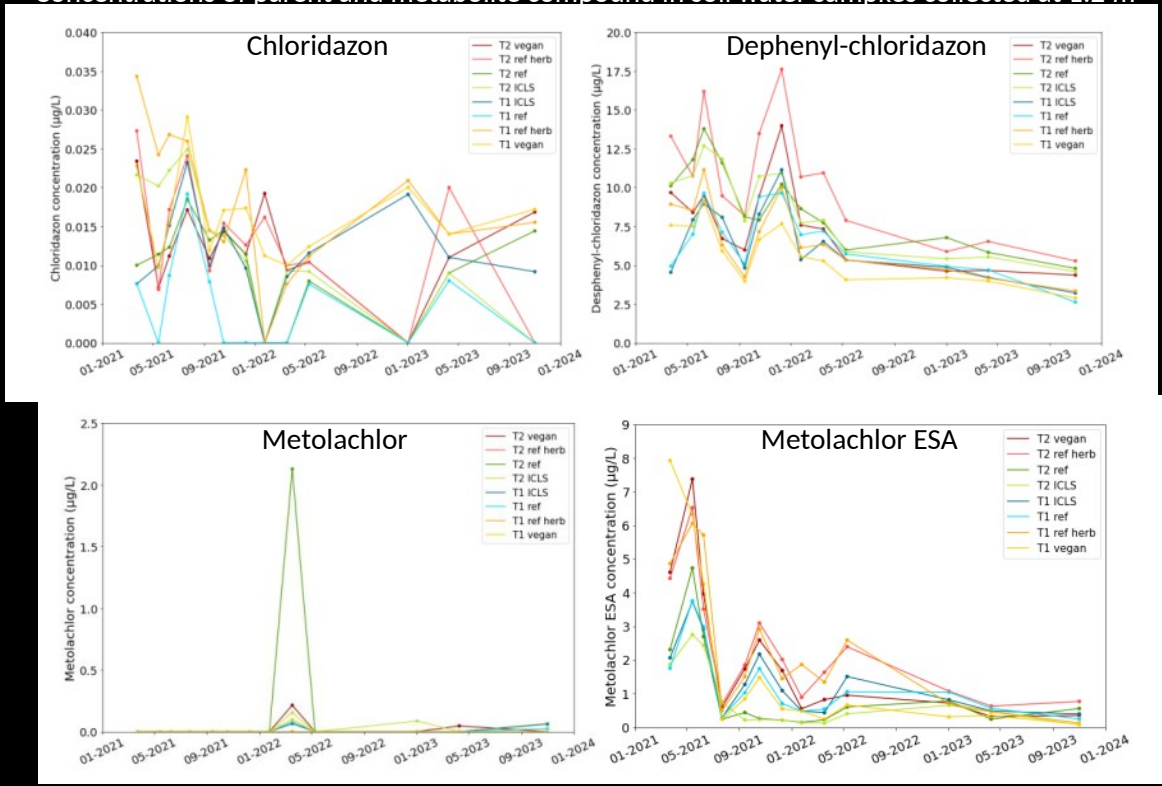
Impact of miscanthus on the quality of soil and drinking waters

Caroline Chavinier, Pierre Benoit, Valérie Pot
UMR EcoSys, Université Paris-Saclay, INRAE, AgroParisTech, Palaiseau, France
Julien Tournebize
UR Hycar, INRAE, Antony, France0

> Pollution of drinking and drainage waters by pesticides and metabolites

> High concentrations of metabolites in soil waters

Concentrations of parent and metabolite compound in soil water sampkes collected at 1.2 m

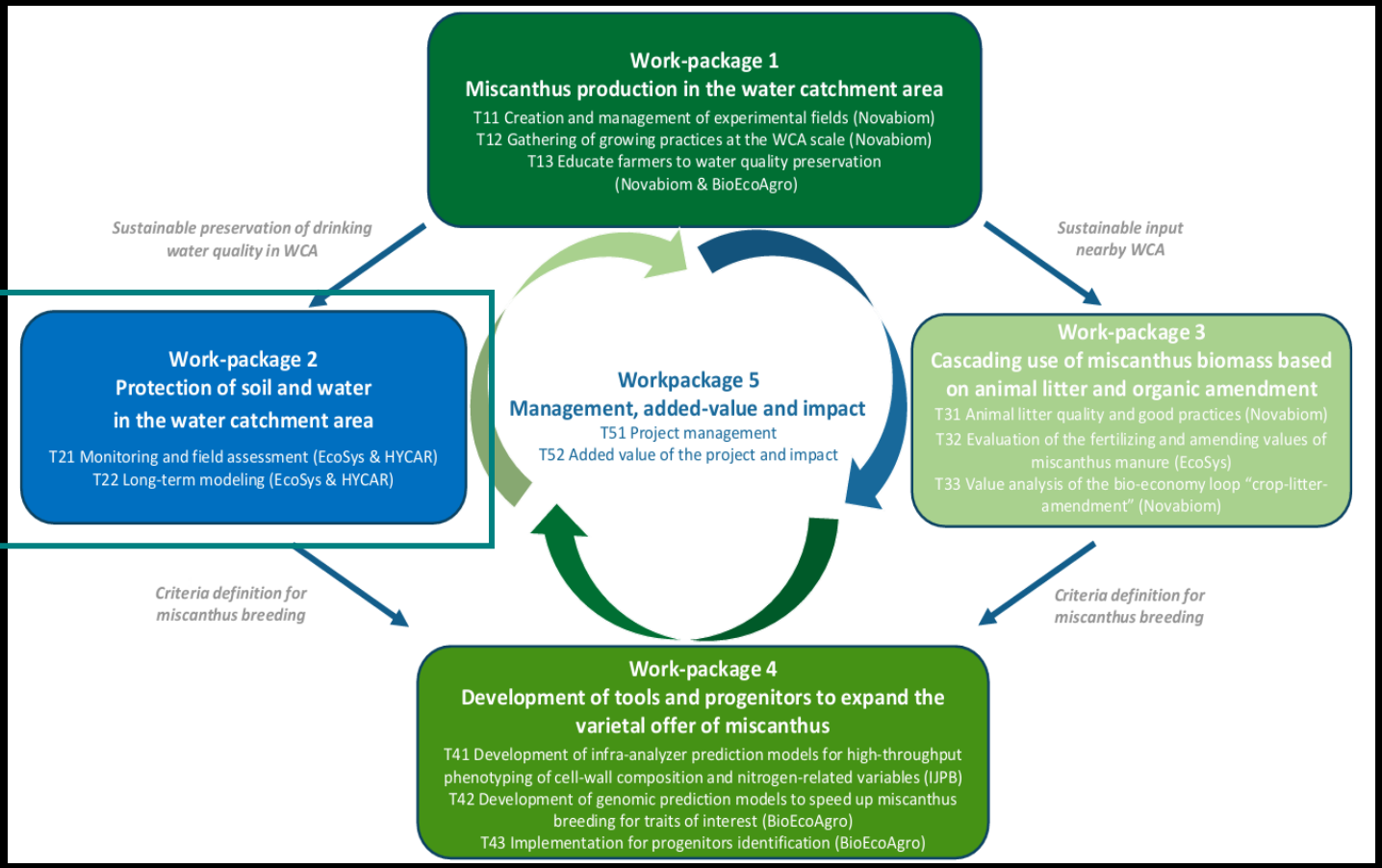


Pirlot Clémence PhD 2025

ANR MisEauVert Project

Impact of miscanthus on the quality of soil and drinking waters

> Thesis in ANR MisEauVert Project “Ecosystem services of miscanthus to restore water quality and soil fertility”



Impact of miscanthus on the quality of soil and drinking waters

Monitoring of 2 drained plots, located near into a priority groundwater for drinkable use (Bailleau-L'Evêque, Saint Aubin-des-Bois)

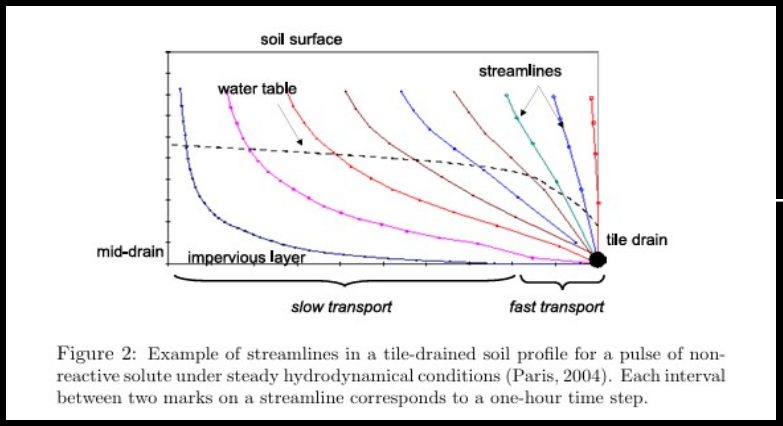


Figure 2: Example of streamlines in a tile-drained soil profile for a pulse of non-reactive solute under steady hydrodynamical conditions (Paris, 2004). Each interval between two marks on a streamline corresponds to a one-hour time step.

→ Add a module to model the drainage system in Vsoil : representation of drainage system in 1D

- Model water flow in the soil towards the drainage network

ANR MisEauVert Project

Impact of miscanthus on the quality of soil and drinking waters

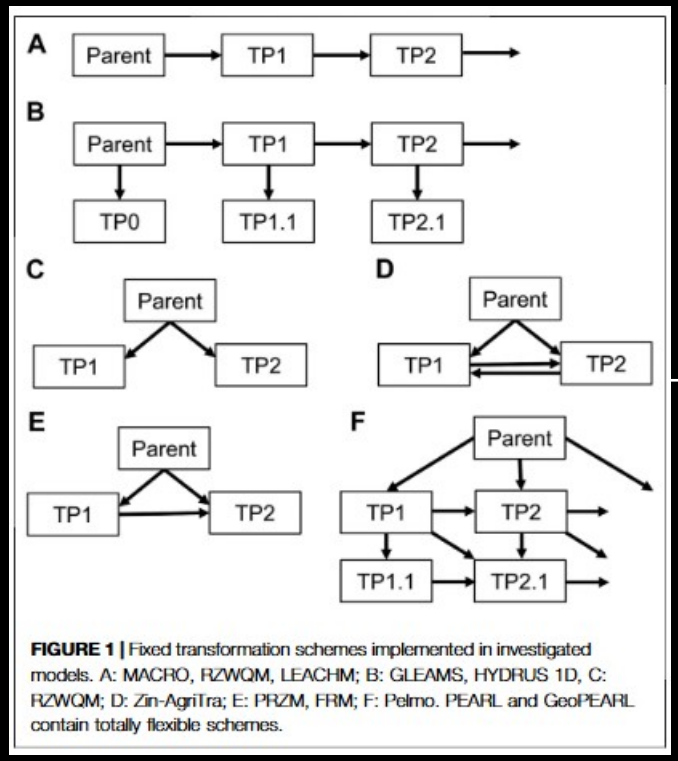


FIGURE 1 | Fixed transformation schemes implemented in investigated models. A: MACRO, RZWQM, LEACHM; B: GLEAMS, HYDRUS 1D, C: RZWQM; D: Zin-AgriTra; E: PRZM, FRM; F: Pelmo. PEARL and GeoPEARL contain totally flexible schemes.

Gassmann, 2021

Add a module to model different transformation schemes and multiple metabolites and in VSoil

- Adapt the processes of the fate of pesticides and their metabolites