Towards a quantification of the interactions between soil architecture and microbial dynamics under a dynamical soil architecture

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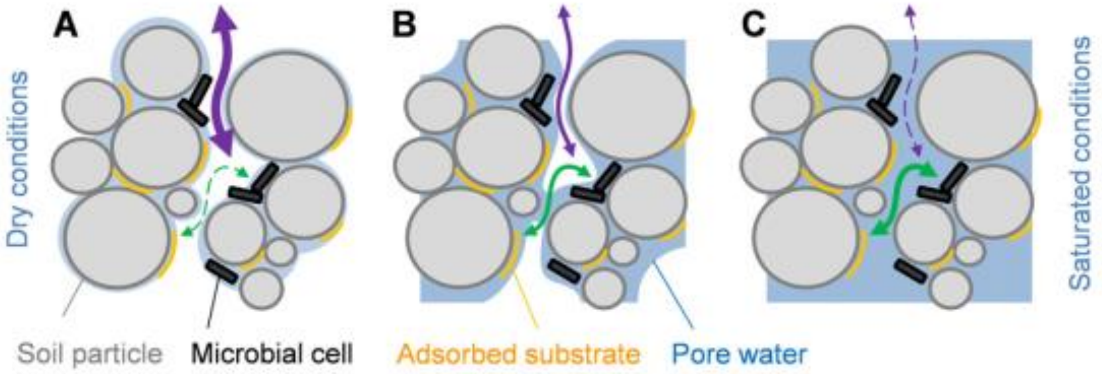
EGU General Assembly 2023 Session SSS6.1 - Soil structure, its dynamics and its relevance to soil functions: feedbacks with soil biology and impacts of climatic conditions and soil management

Quantify and predict C stock evolution in soil

unravelling soil microbial response to changing environmental conditions

→ complexity of processes involved in soil microbial response

- physical processes (diffusion)
  - → spatial accessibility of resources
  - → O_2 limitation



- physiological processes:
  - → C allocation patterns (respired, stored)
  - → microbial turnover (necromass), metabolites
- biochemical processes:
  - → labile substrates, organo-mineral associations
- ecological processes:
  - → soil food webs (predation), engineers (bioturbation → spatial accessibility)

Moyano et al., 2013
Schimel et al., 2018
Davidson & Janssens, 2006
Haggerty et al., 2022

Soil microbe response to changing environmental conditions

→ different predictions of carbon stocks under warming:
- traditional biogeochemical models: reduced soil C stocks
- models including explicit microbial dynamics: wider range of responses

→ parametrization of explicit microbial dynamics remains challenging (CUE dynamics)

→ understand processes at the scale of soil microhabitats:
- 2D/3D imaging tools (3D soil architecture and spatial accessibility)
- pore-scale modelling as a flexible tool (processes)

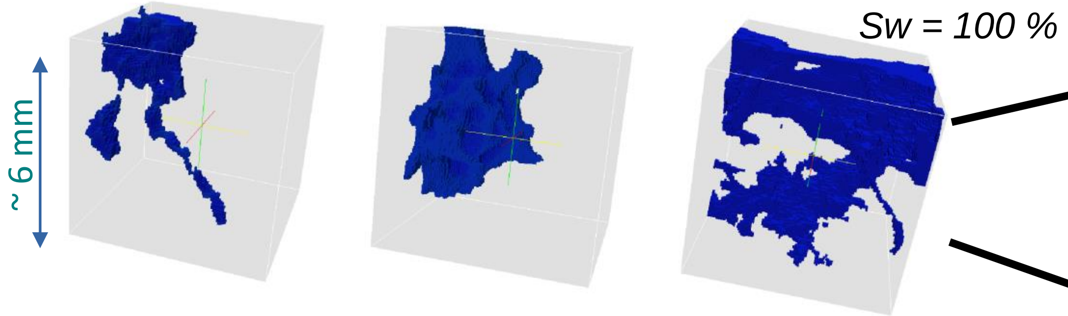
Wieder et al., 2013 ; Haggerty et al., 2022 ; Koenig et al., 2020; Pot et al., 2022

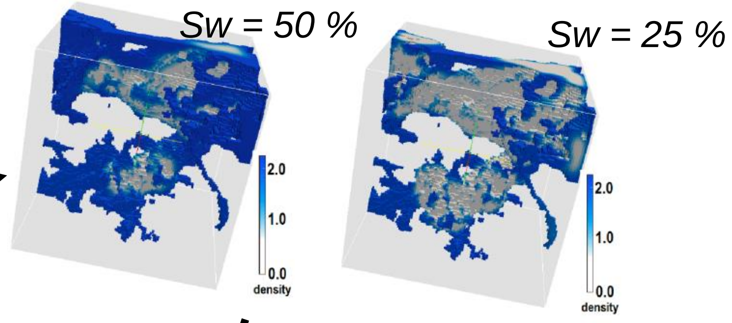
Elucidating the role of physical and physiological processes

→ complete factorial design (modelling scenarios)

µCT image (68 µm voxel resolution) of undisturbed soil sample (Albeluvisol)

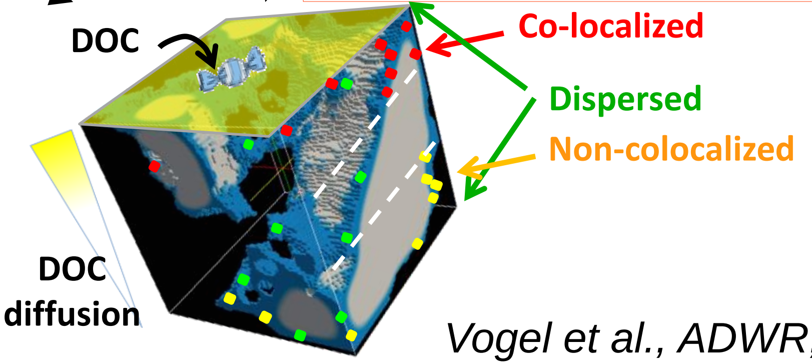
Three different water saturations





Three subsamples of different levels of heterogeneity (PSD, connectivity, tortuosity, SSA, anisotropy)

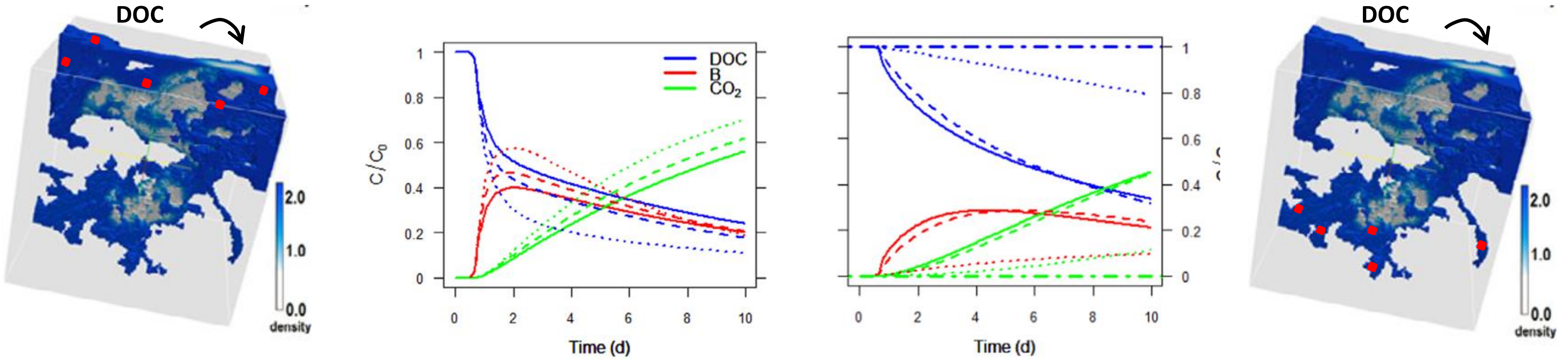
Three different bacteria localizations



Vogel et al., ADWR, 2015

Elucidating the role of physical and physiological processes

Higher spatial accessibility *Lower spatial accessibility*

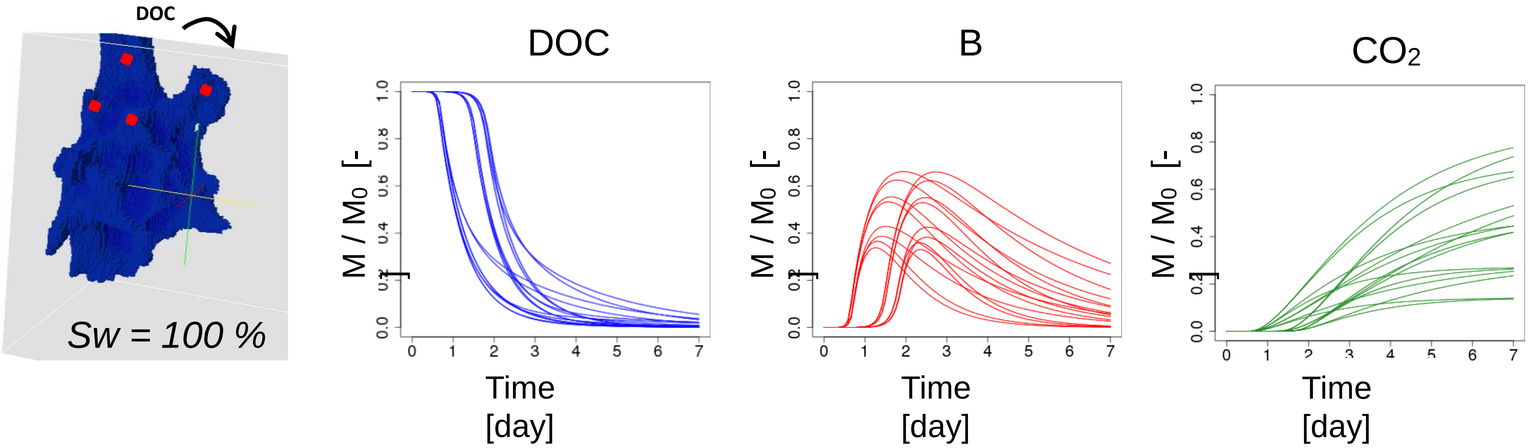


Vogel et al., ADWR, 2015

→ balance between DOC concentration and diffusional mixing

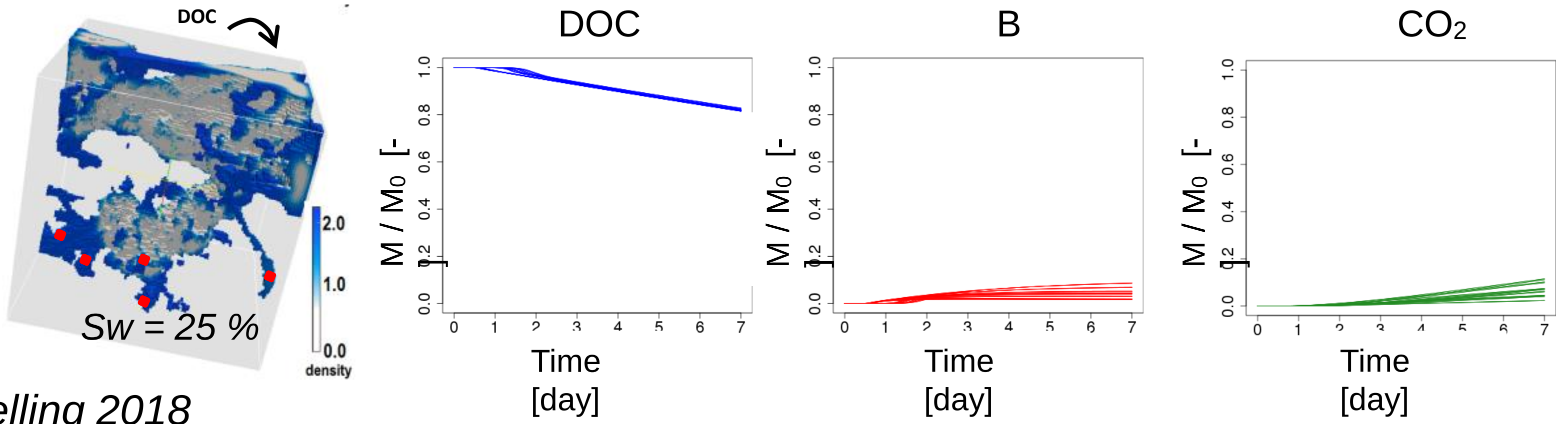
Elucidating the role of physical and physiological processes

Optimal spatial accessibility



→ under optimal spatial accessibility physiological processes modulate soil microbial response, whereas under limited spatial accessibility C uptake remains low

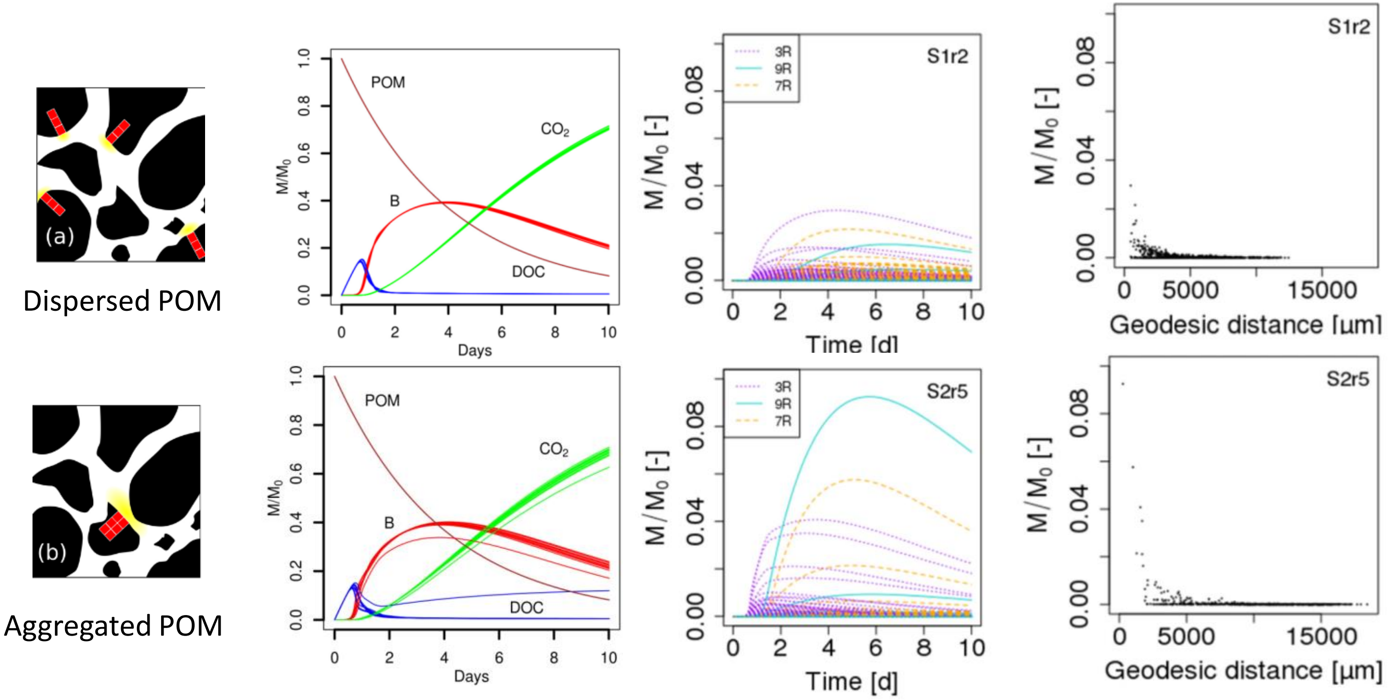
Lowest spatial accessibility



Vogel et al., Ecol Modelling 2018

Search indicators of the role of spatial accessibility?

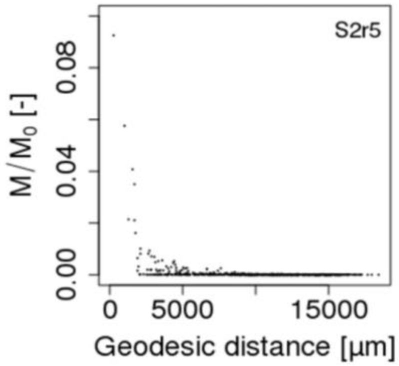
230 x 3 microbial spots (random) – 3R, 9R, 7R *Arthrobacter sp.*



→ geodesic distance

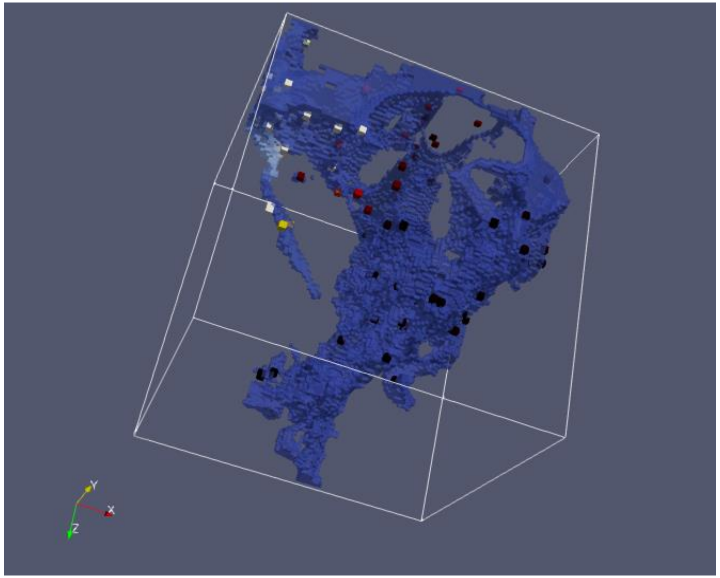
Portell et al., Front Microbiol 2018

Search indicators of the role of spatial accessibility?



→ geodesic distance x physiology

3R *Arthrobacter sp.*



Portell et al., Front Microbiol 2018

Search indicators of the role of spatial accessibility?

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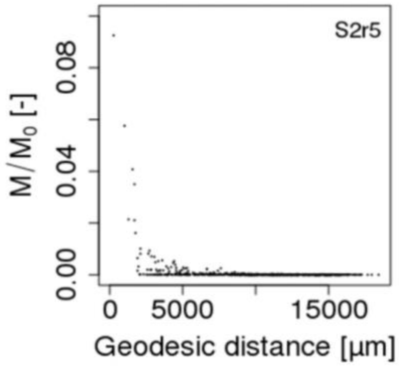

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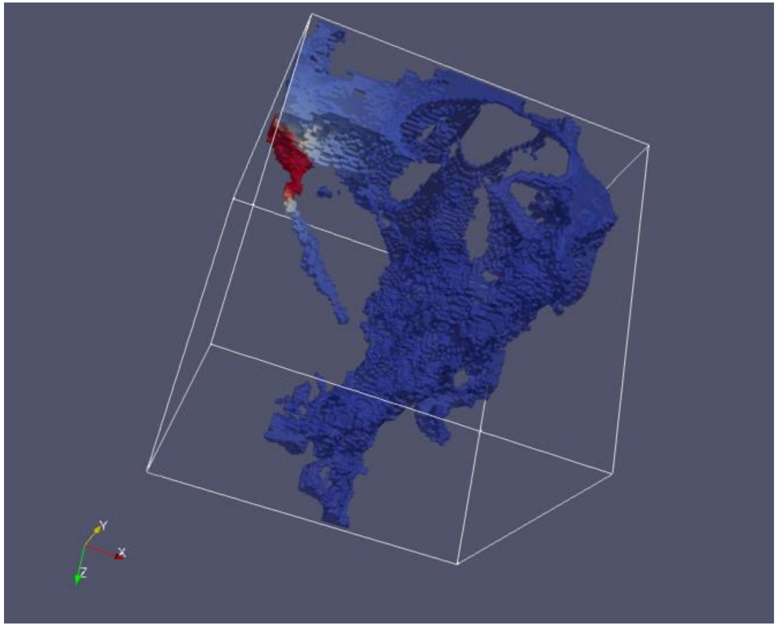

Portell et al., Front Microbiol 2018

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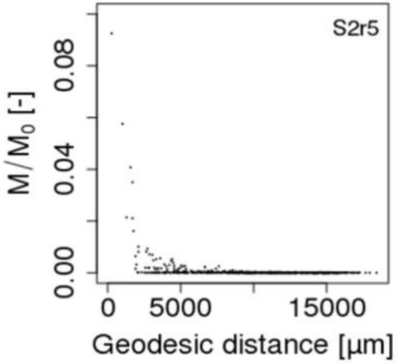
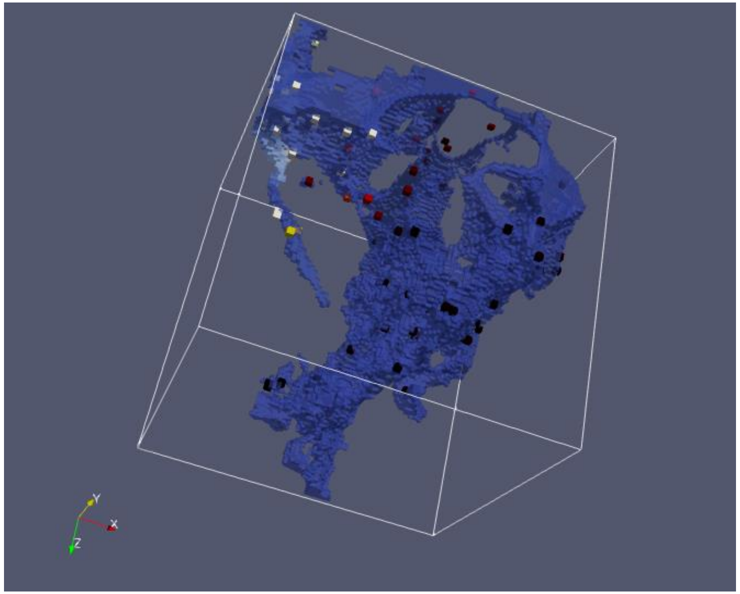
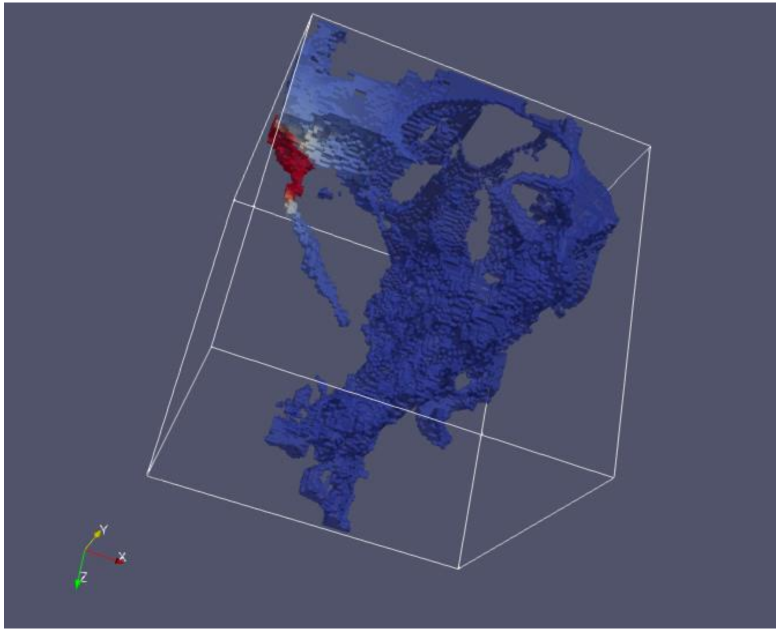


→ geodesic distance x physiology

3R *Arthrobacter sp.*



9R *Arthrobacter sp.*



Portell et al., Front Microbiol 2018

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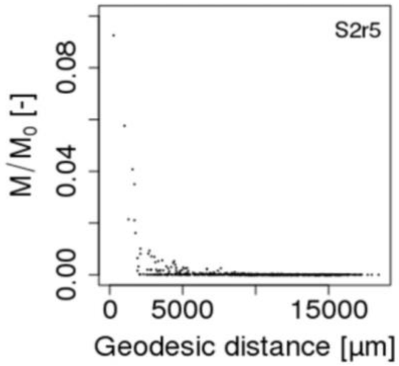

→ geodesic distance x physiology

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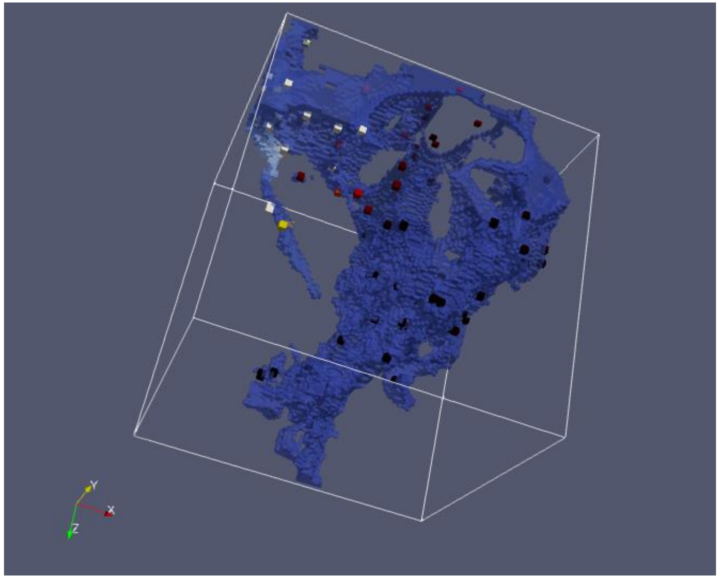

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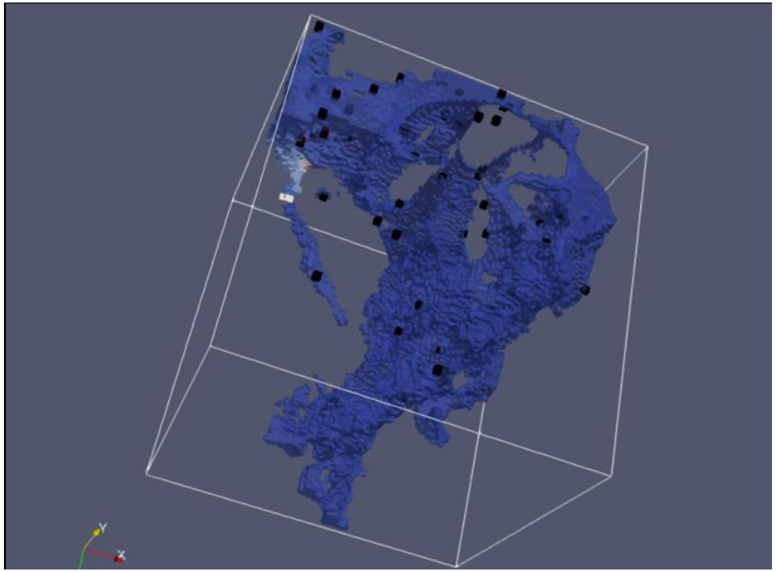


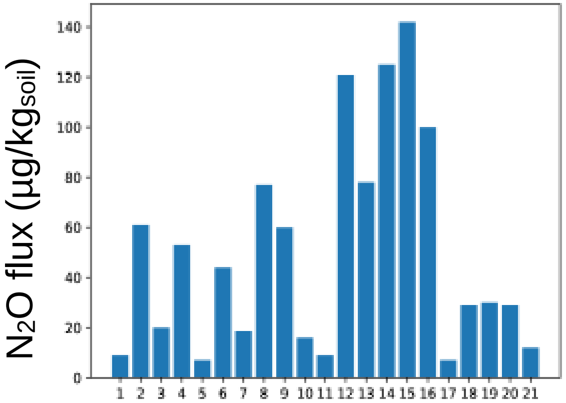
Portell et al., Front Microbiol 2018

Search indicators of the role of spatial accessibility?

→ geodesic distance: a good candidate?

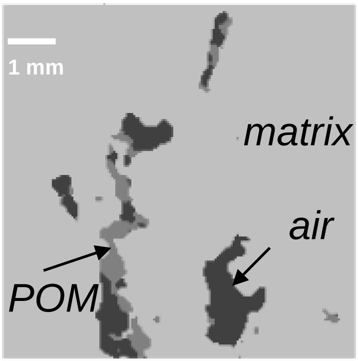
Parry et al., Eur J Soil Sci 1997
Rawlins et al., Soil 2016
Rohe et al., Biogeosciences 2021

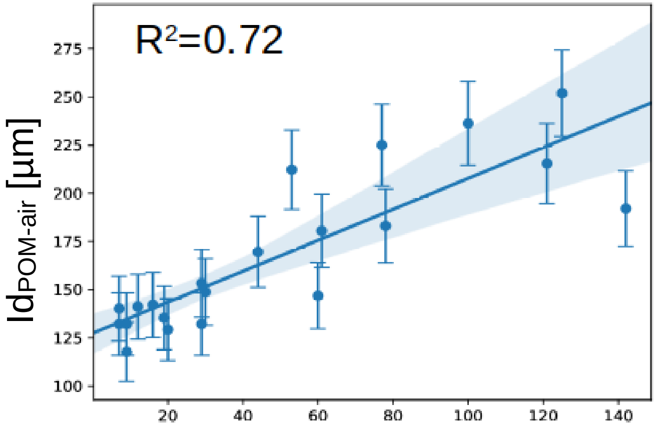
N_2O emissions



21 intact (silt-sandy) soil cores
(5 cm diameter)

µCT image (32 µm voxel resolution)





→ Indicator based on the geodesic distance between clusters of POM and air-filled pores

Ortega-Ramirez et al., Geoderma 2023

Towards a dynamical soil architecture – how-to?

→ Indicators could be introduced in statistical functions (CUE)
- to account for the role of spatial accessibility (macroscopic C turnover models)

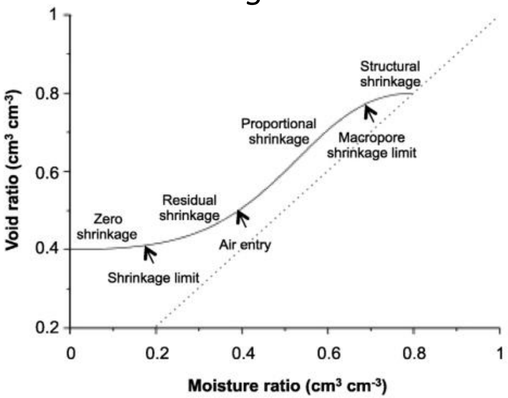
→ Robustness of these indicators (static soil architecture)

→ highly dynamic:
- water content (diffusion pathways)
- expansion/creation of pores, retraction/closure of pores (abiotic/biotic factors)
- relocation of C resources (roots, meso/macrofaune)

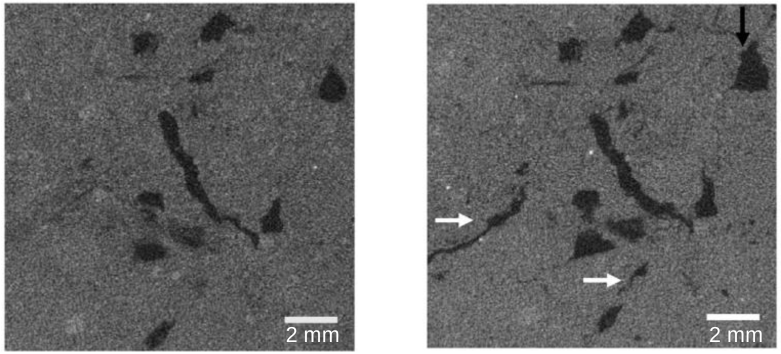
Qauntification of soil architecture dynamics

→ from macroscopic to microscopic measurements

Shrinkage curve

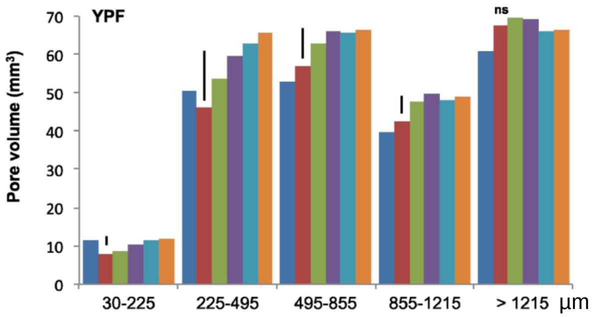


µCT image: 30 µm voxel resolution



Structural phase

Proportional phase



Bottinelli et al., Geoderma, 2016

0 min

after rain
81 min

drainage
120 min

Lissy, PhD, 2019
Sammartino et al., VZJ 2015

→ dynamics of macropores could be reproduced in pore-scale models by morphological operations (opening, dilation)

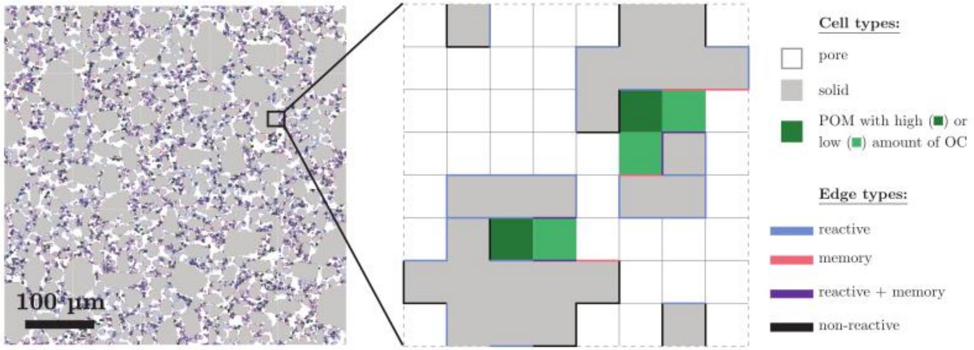
Including a dynamical soil architecture in pore-scale models

→ 2D model of spatial reorganization of solid particles (intra-particle binding forces):

- production of sticky agents
- CA jumping rules

Crawford et al., 2012 ; Ray et al., 2017

Zech et al., 2022



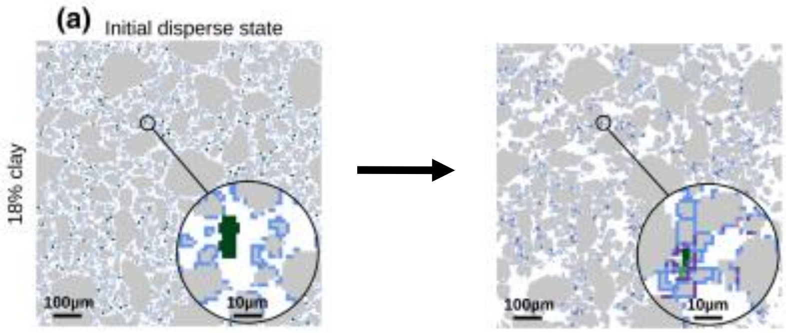


figure adapted from Zech et al., 2022

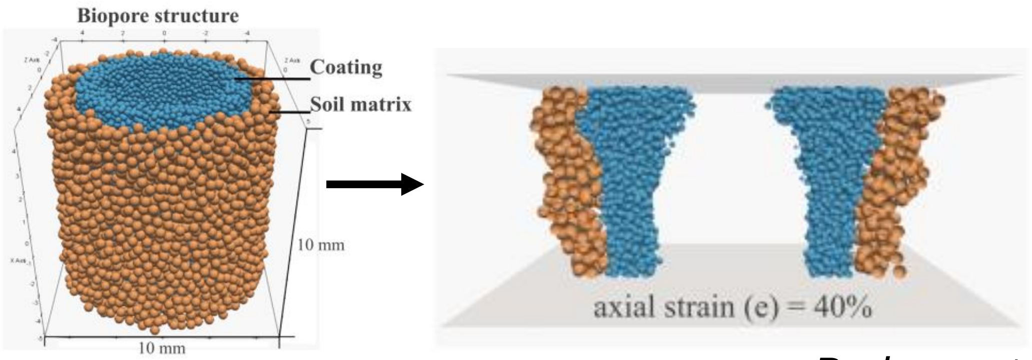
→ dynamical POM decomposition rates related to spatial location (occluded)

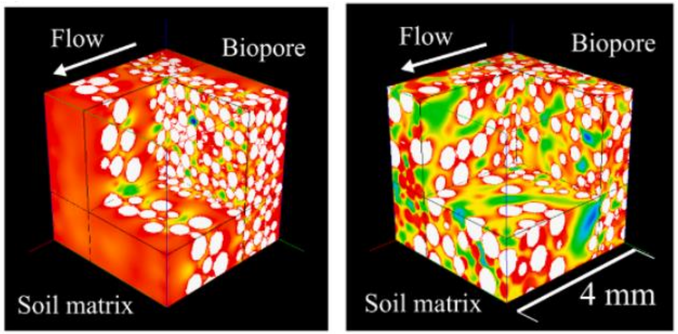
→ CO_2 production

Including a dynamical soil architecture in pore-scale models

→ describing friction and cohesion forces between particles using contact laws: 3D DEM model (granular media)

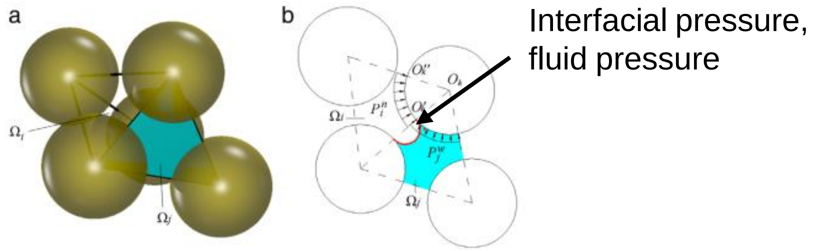
Smilauer et al., 2015





Barbosa et al., 2022

→ unsaturated conditions: hydro-mechanic coupling – 2PFV-DEM model



Yuan & Chareyre 2017

→ elasto-plastic deformation

→ calibration for soils

Conclusions

→ 3D imaging of soils allow to quantify the interactions between soil architecture and microbial dynamics

→ pore-scale models allow to disentangle the physical and physiological processes in the soil microbial response

→ spatial indicators to quantify spatial accessibility and contribute to explain soil microbial response

→ spatial indicators could be introduced in statistical functions to modulate CUE to account for the role of spatial accessibility (macroscopic C turnover models)

→ several approaches to include soil architecture dynamics have been developped and should be used to assess the robustness of such indicators

Assessing the multiple effects of dissolved organic matter on the transport of organic pollutants in subsoil horizons through a modular modeling approach

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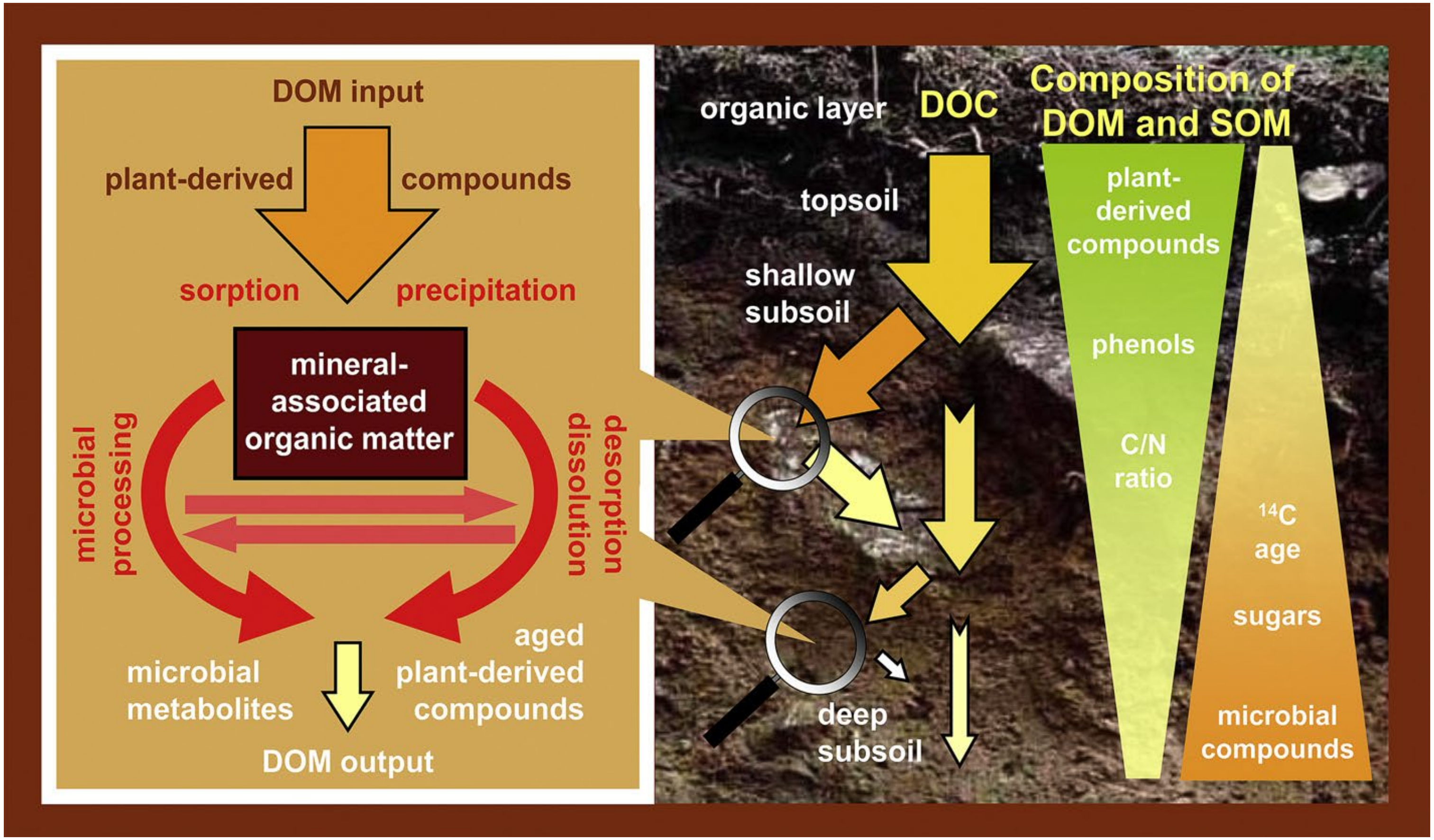
EGU General Assembly 2023 Session HS8.1.3 - Emerging contaminants and PFAS in soil-groundwater systems. Fate, risks, remediation and mitigation

Introduction

Importance of DOM cycle in soils



Kaiser & Kalbitz, 2012

Rationale

Multiple roles of dissolved organic matter (DOM) in the transport of trace organic contaminants

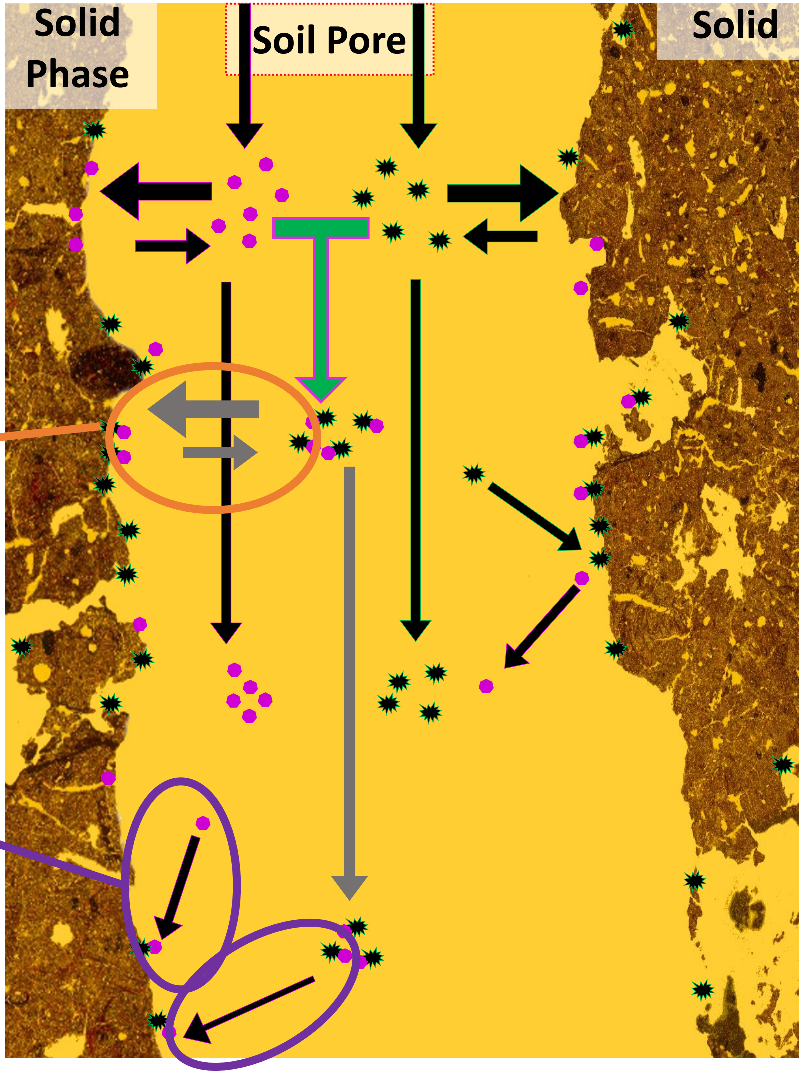
- Adsorption-desorption of free contaminant
- Adsorption-desorption of DOM
- Association DOM-contaminant in solution

- Co-Transport
- Competition for sorption sites

Increased velocity

- Cumulative sorption
- Co-Sorption

Decreased velocity



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

Rationale

Do we need a new model ?

- **DOM production, sorption and transport in soils** *Tipping et al (1988, 2012) ; Michalzik et al (2012)*
- **Co-transport of contaminants and colloids** *Simunek et al. (2006) ; Flury & Qiu (2008)*
- **Interactions DOM and Organic Contaminants** *Magee et al (1991) ; Smilek et al (2015)*
- **Co-sorption and cumulated sorption** *Tostsche et al. (1996) ; Wehrer & Tosche (2005)*

To help elucidating the multiple roles of DOM and accounting for DOM quality/reactivity and dynamics

PolDOC model implemented in the VSoil modeling platform

- modularity of the platform to couple
  - **available 1D water flow and solute transport** models
  - **novel reactivity modules** for **organic contaminants** and **DOM**
- **sink/source terms in the transport equation** used to account and characterize the interactions between contaminants, DOM and the soil solid phase

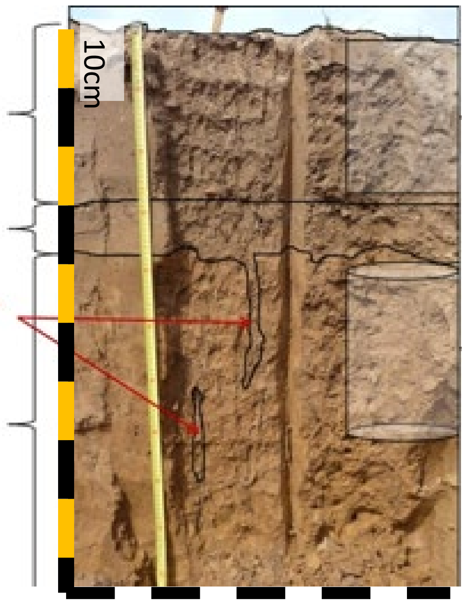
https://www6.inrae.fr/vsoil/

The Pol DOC Model

Main hypotheses

- 1D Richards' equation with **mobile and immobile** waters ***(Lafolie, 1991)***
- **Four solutes are transported** : native Bt DOM (DOC_{Bt}), topsoil DOM (DOM_{SURF}), free contaminant (C_{POL}), contaminant-topsoil DOM association (C_{POL}-DOM_{SURF})
  - Pollutants are applied at the soil surface
  - DOM_{SURF} – more aromatic - phenolic compounds
  - DOM_{Bt} more carbohydrates and nitrogen-rich compounds - highly degraded compounds and smaller compounds
    - involved into mineral-association in mineral horizons ***(Guggenberger & Zech, 1994 ; Kaiser et al., 2004 ; Kaiser & Kalbitz, 2012)***
    - less expected to associate with organic pollutant
- **Physicochemical and biological processes** are described by **sink/source terms** (Γ)

Experimental data



(Albeluvisol, WRB FAO, 2008)

Surface Soil Sampling

Bt Horizon Sampling

Undisturbed soil core - Bt horizon

Soil		pH	OC (g kg^{-1})	CEC (cmol+kg^{-1})	Clay	Silt	Sand
						(g kg^{-1})	
Ap hz (0–28 cm)	Control	7.0	10.2	8.6	146	790	64
	Amended	6.9	15.8	9.8	147	784	69
E hz (35–50 cm)		7.3	3.7	9.2	219	724	58
Bt hz (60–90 cm)		7.5	2.3	14.9	311	646	43
IC hz (140–160 cm)		7.6	1.6	13.9	238	702	41

Chabauty et al., 2016

Unsaturated Column Experiment

- with organic contaminants
- bromide tracer
- flow interruption (10 d)
- with or without DOM in the inflow

Experimental data

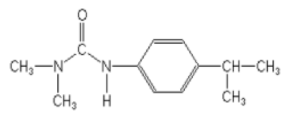
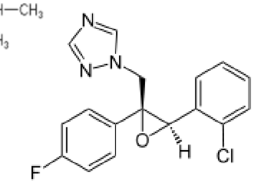
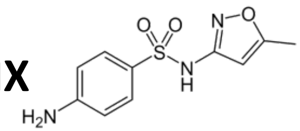
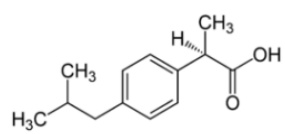
Environ Sci Pollut Res
DOI 10.1007/s11356-015-5938-9

CrossMark

RESEARCH ARTICLE

Transport of organic contaminants in subsoil horizons and effects of dissolved organic matter related to organic waste recycling practices

Florian Chabauty[1] · Valérie Pot[1] · Marjolaine Bourdat-Deschamps[1] · Nathalie Bernet[1] · Christophe Labat[1] · Pierre Benoit[1]

		Log K_{ow}	K_{oc} (L/kg)	DT 50 (d)
Isoproturon **IPU**		*2.5[a]*	*122[a]*	*12[a]*
Epoxiconazole **EPX**		*3.3[a]*	*1073[a]*	*354[a]*
Sulfamethoxazole **SMX**		*0.9*	*1.2*	*59*
Ibuprofen **IBP**		*4.9*	*nd*	*nd*

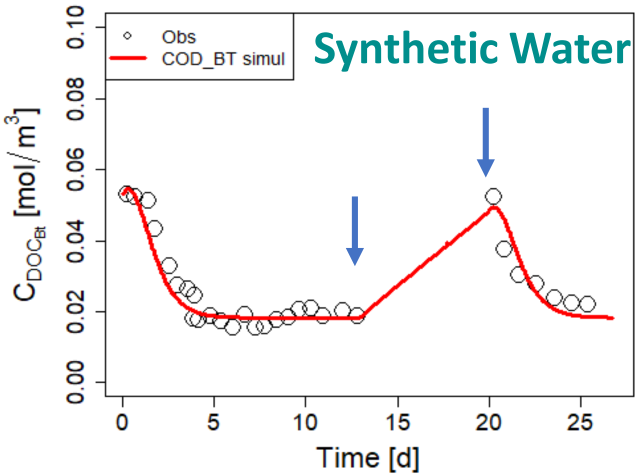
Breakthough curves

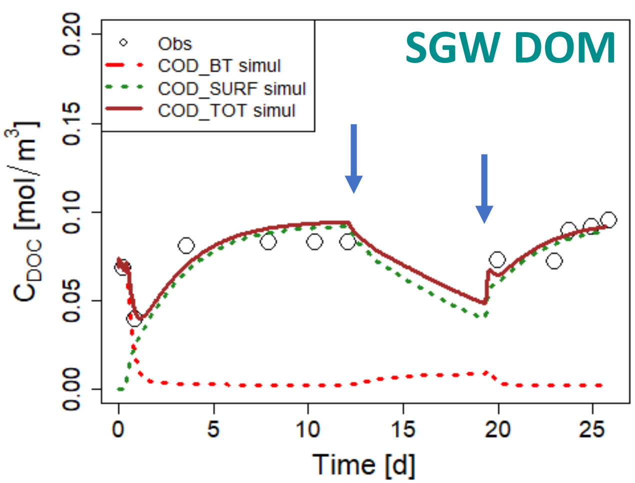
Without DOM **Control Soil DOM** **Compost Amended Soil DOM (SGW DOM)**

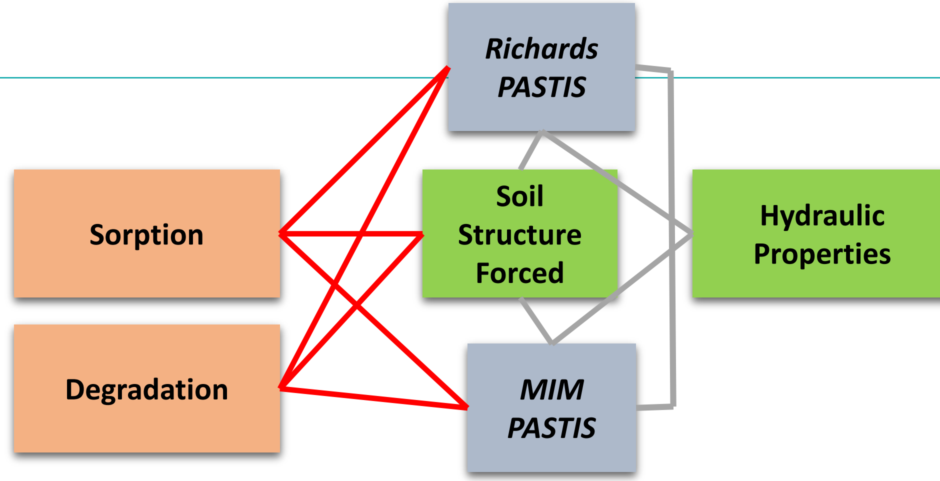
Chabauty et al., 2016

Results

DOM Transport







- Two pools of DOM with different sorption parameters

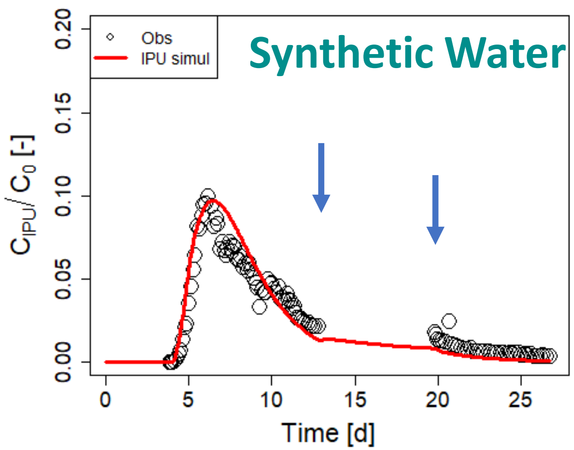
		$k_{a,m*}$	$k_{d,m}$	k_h	μ
		(s^{-1})			
Synthetic	**DOC_{Bt}**	4.10^{-8}	1.10^{-8}	3.10^{-11}	2.10^{-7}
Compost Amended Soil	**DOC_{Bt}**	4.10^{-8}	1.10^{-8}	3.10^{-11}	5.10^{-6}
	DOC_{SURF}	3.10^{-5}	1.10^{-5}	0	5.10^{-6}

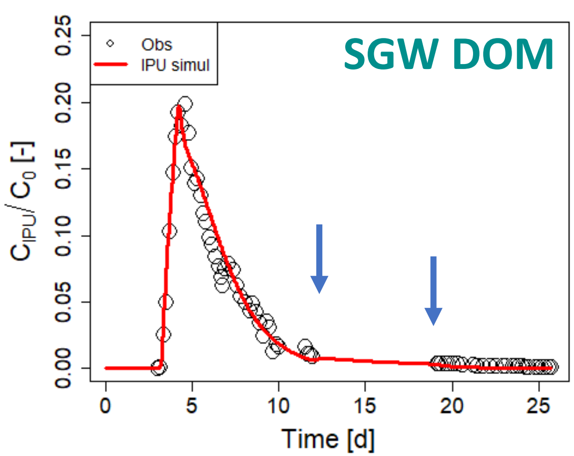
- DOM from surface soil more reactive in sorption
  - Confirmed by fluorescence
  - In agreement with Kaiser & Kalbitz (2012)

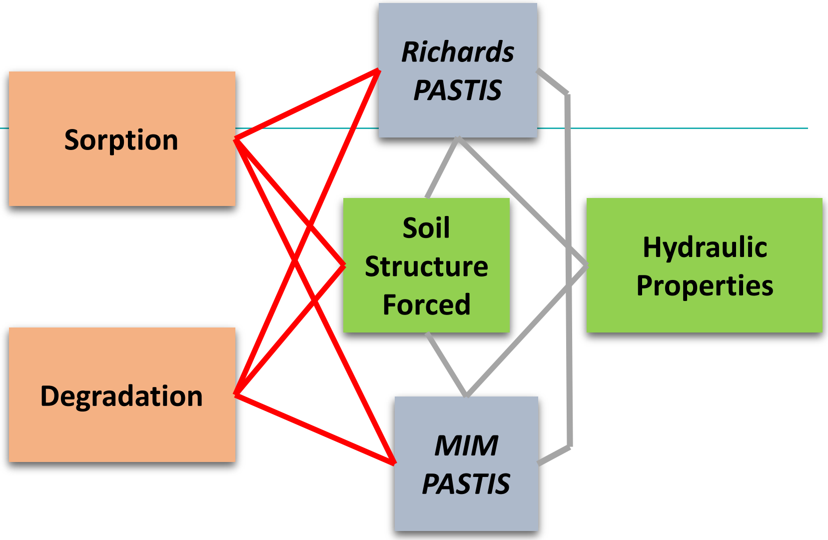
Results

Contaminant Transport

Isoproturon





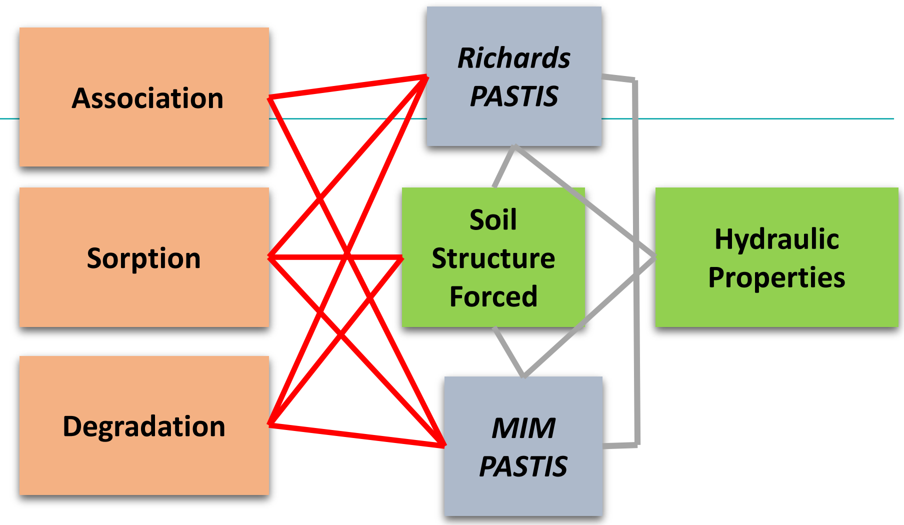


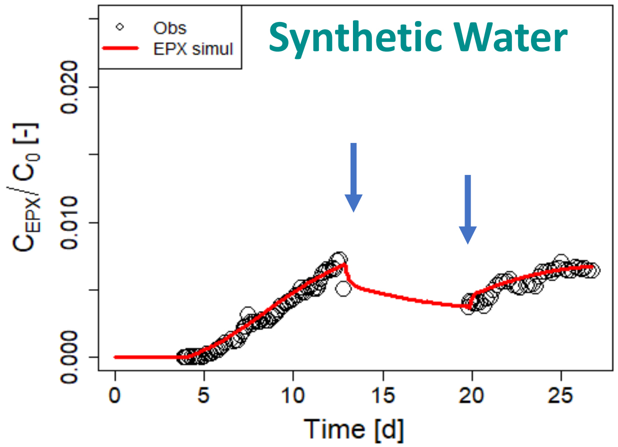
	Synthetic Water	Compost Amended Soil DOM
$k_{a,POLm*}$ (s^{-1})	$1.0\ 10^{-4}$	**$6.0\ 10^{-5}$**
$k_{d,POLm}$ (s^{-1})	$1.8\ 10^{-5}$	**$1.5\ 10^{-5}$**
μ (s^{-1})	$6,7.10^{-7}$	**$7.0\ 10^{-6}$**

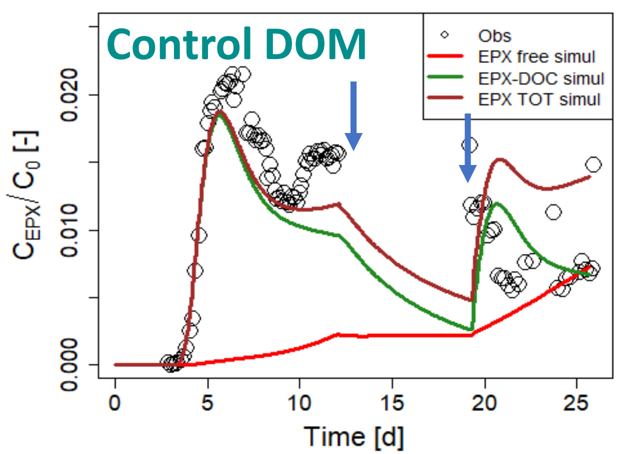
Results

Contaminant Transport

Epoxiconazole







	Synthetic	Control Soil DOM		
	EPX	EPX	EPX-DOC_{SURF}	DOC_{SURF}
$k_{a,i,m}$ (s^{-1})	3.0 10^{-4}	**1.0 10^{-3}**	**1.5 10^{-4}**	**4.0 10^{-5}**
$k_{d,i,m}$ (s^{-1})	9.0 10^{-6}	**2.0 10^{-5}**	**6.0 10^{-5}**	**2.0 10^{-7}**
μ (s^{-1})	2.3 10^{-8}	**5.0 10^{-6}**	**5.0 10^{-6}**	**5.0 10^{-6}**
k_{ass} (s^{-1})	-	**1.0 10^{-4}**	-	-
k_{dis} (s^{-1})	-	-	**5.0 10^{-6}**	-

Conclusions

- Physical non-equilibrium transport conditions were identified and quantified with PolDOC

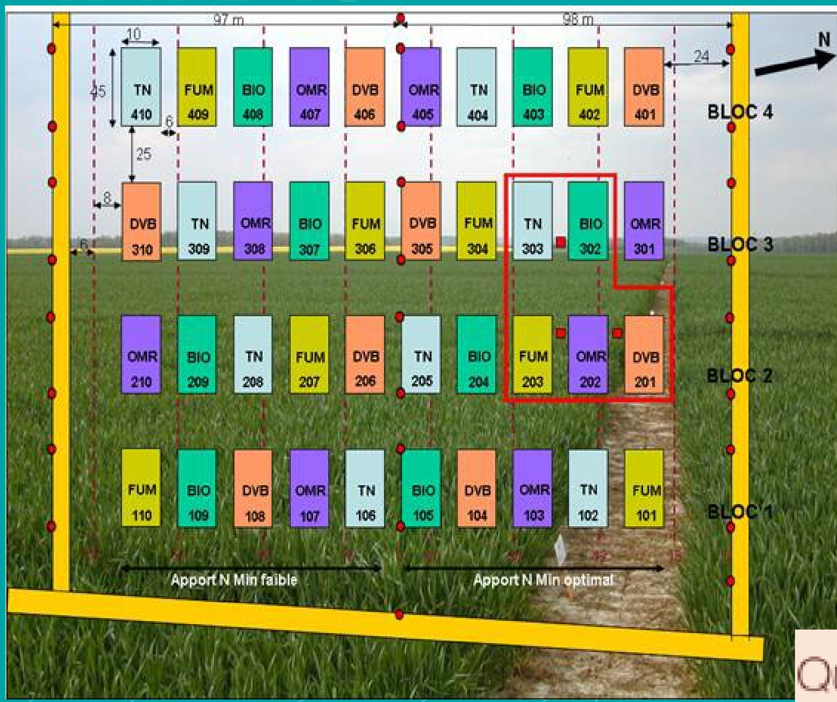
- Model showed that the Bt mineral horizon acted as a sink to partly retain DOM_{SURF}

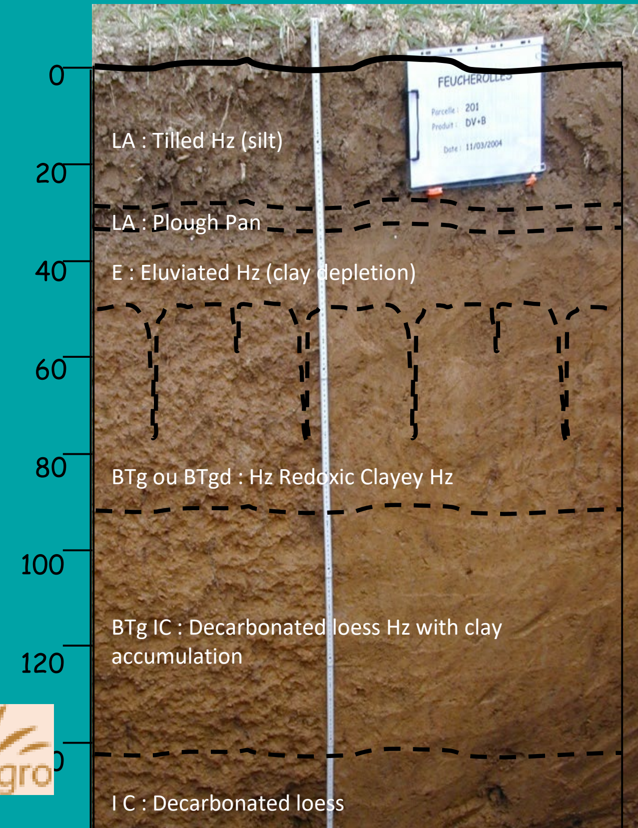
- For **polar compounds** : Accelerated transport in presence of DOM due to **competition** for sorption – Additional processs : **increased degradation** (μ)

  - **Not shown** : Differences between IPU/SMX transport could be explained by different sorption reactivity with the soil solid phase

- For **hydrophobic compounds** such as epoxiconazole : Increased and accelerated transport - in presence of DOM due to co-transport (following association with DOM) but also increased sorption (cumulative sorption)

  - Increased leaching of EPX in presence of DOM_{SURF} required the activation of **co-transport with DOM_{SURF}**





Thank you for your attention !!

The Pol DOC Model

Sink/Sources Processes

$$\Gamma_{i,R,j} = -k_{a,i,DOCj}\theta_i C_{i,DOCj} + k_{d,i,DOCj}\rho_b S_{i,DOCj}$$

→ Sorption of native Bt DOM (DOC_1) and topsoil DOM (DOC_2)

$$\Gamma_{i,T,j} = -\mu_{i,DOCj}\theta_i C_{i,DOCj}$$

→ Degradation of native Bt DOM and topsoil DOM

$$\Gamma_{i,H,1} = -k_h \rho_b SOC$$

→ Hydrolysis of native Bt DOM

$$\Gamma_{i,R,POL} = -k_{a,POL}\theta_i C_{POL} + k_{d,POL}\rho_b S_{POL}$$

→ Sorption of free contaminant (POL)

$$\Gamma_{i,R,POL-DOC2} = -k_{a,DOC2}\theta_i C_{POL-DOC2} + k_{d,DOC2}\rho_b S_{POL-DOC2}$$

→ Sorption of contaminant -topsoil DOM association ($POL\text{-}DOC_2$)

$$\Gamma_{i,T,POL} = -\mu_{POL}\theta_i C_{i,POL}$$

→ Degradation of free contaminant

$$\Gamma_{i,T,POL-DOC2} = -\mu_{POL}\theta_i C_{POL-DOC2}$$

→ Degradation of contaminant-topsoil DOM association

$$\Gamma_{i,A} = -k_{ass}\kappa\theta_i C_{i,COD2} C_{i,POL} + k_{diss}\theta_i C_{i,POL-COD2}$$

→ Association/dissociation of contaminant-topsoil DOM association

i is the index for mobile or immobile waters, j is the index for the type of solute

French ACROSS 2022 campaign: First results from CO_2/H_2O, energy and VOC fluxes measurements at the Rambouillet tower supersite

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Univ. Paris Cité and Univ. Paris Est Créteil, CNRS, LISA, France

EGU, Vienna, 26/04/2023

Introduction and objectives

- VOCs: Importance for atmospheric chemistry
- Forests: large emitters of BVOCs (55%; Karl et al, 2009)

This work is part of the ACROSS Rambouillet campaign (2022)

<u>Objectives:</u>
Fluxes of CO_2, energy, heat
Emissions (and deposition) of VOCs
Response to heat and drought stresses

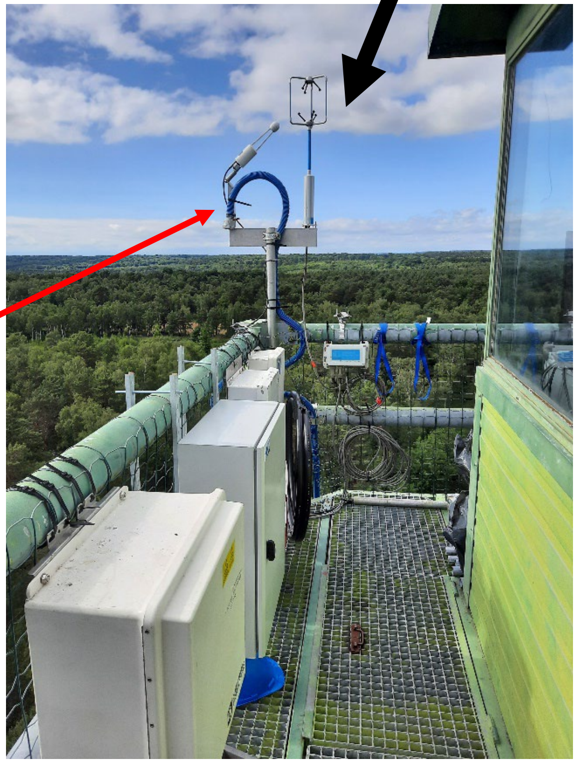
Site set-up

- **Site description:**
  - The Rambouillet mixed forest dominated by oaks and pines
  - Located South-West of Paris

- **Measurements set up**
  - Campaign duration: 23 June – 25 July 2022
  - PTR-Qi-TOF-MS with E/N: 120 Td
  - 10 Hz on-line peak integration and data storage
  - Eddy covariance and profiles* of VOCs
  - Turbulence
  - CO_2 and H_2O fluxes and profiles*

Flux @ 40m

View of the EC set-up



40m-long inlet line

Rambouillet super-site tower

Essences	% area
Oak	68%
Pines	19%
Open spaces	6%
other deciduous	3%
Beech	2%
Chesnut	2%

**Profile results will not be presented here*

Methods, Data treatment

Raw data acquistion @ 10 Hz using the **eddy-covariance method**
(sonic anemometer + PTR-Qi-ToF-MS, 40m-long heated line)

EddyFlux calculation using home-made LabView program

Filtering data:

-Removing calibration periods

-Removing disturbance periods (namely top of tower)

-Selecting significant compounds (Mean flux > 3*Flux uncertainty) ➔ About 400 masses

⚠ **Caution: PRELIMINARY DATA** ⚠

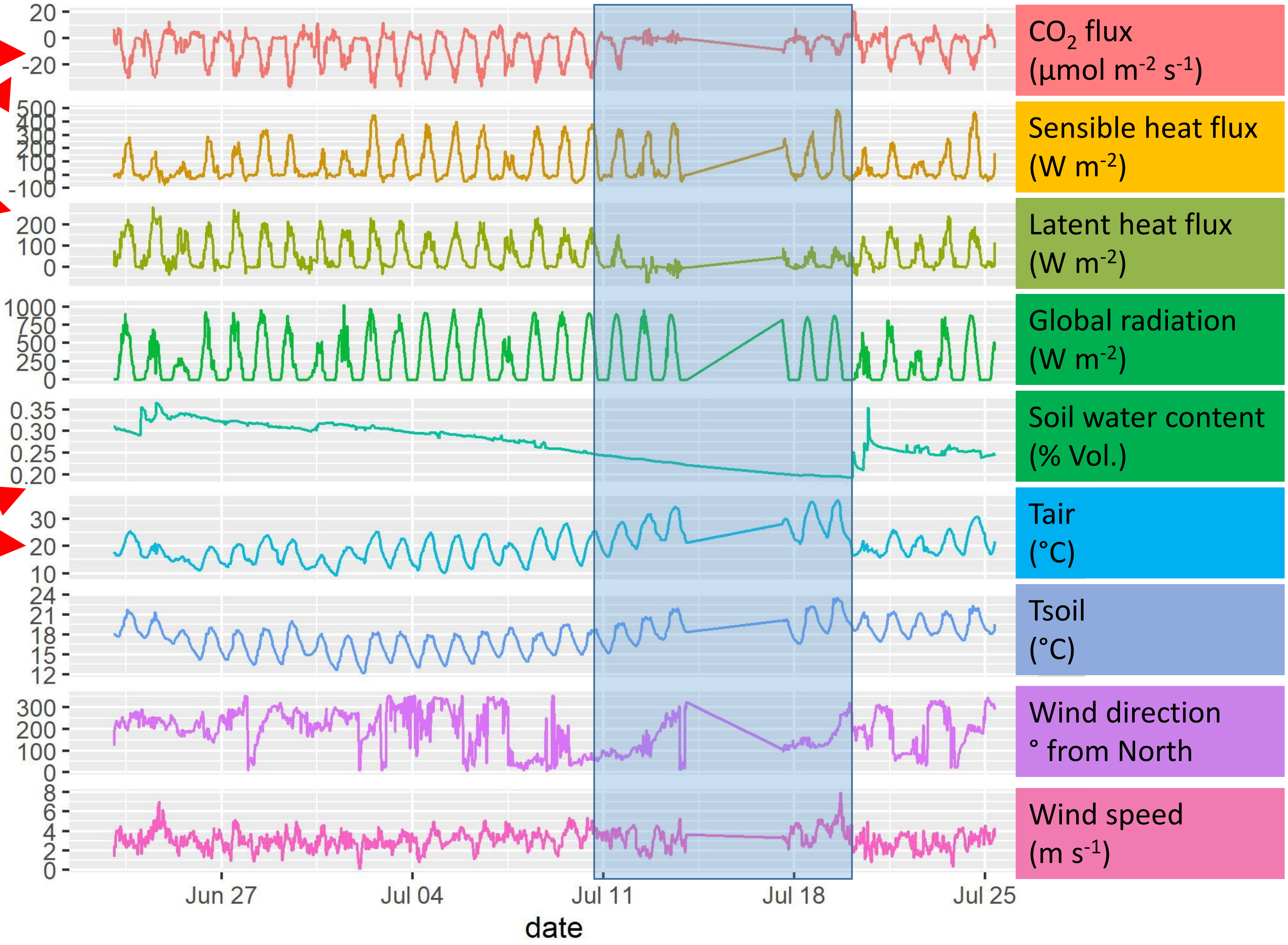
This talk ➔ m/z < 220

Results: Meteo and Micrometeorology

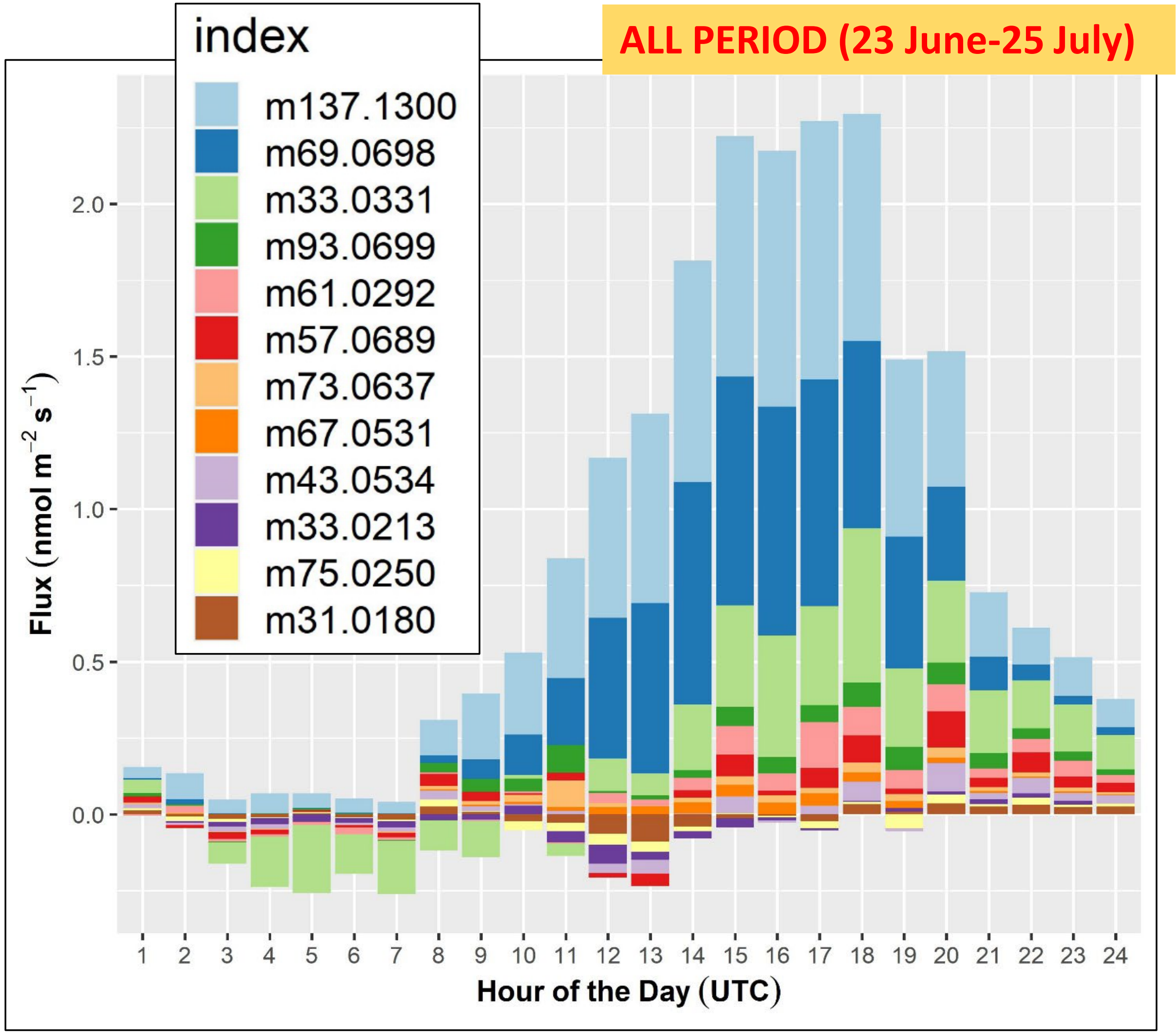
Forest was photosynthesizing actively

Signs of water shortage and heat stress between 11 and 20 July

Rather hot and dry period



Results: most emitted (9) and deposited (3) VOCs



Main emitted compounds:

- Monoterpenes (m/z 137.130)
- Isoprene (m/z 69.070)
- Methanol (m/z 33.033)

➔ Diurnal emission pattern

➔ Response to Tair and radiation

Deposited compounds:

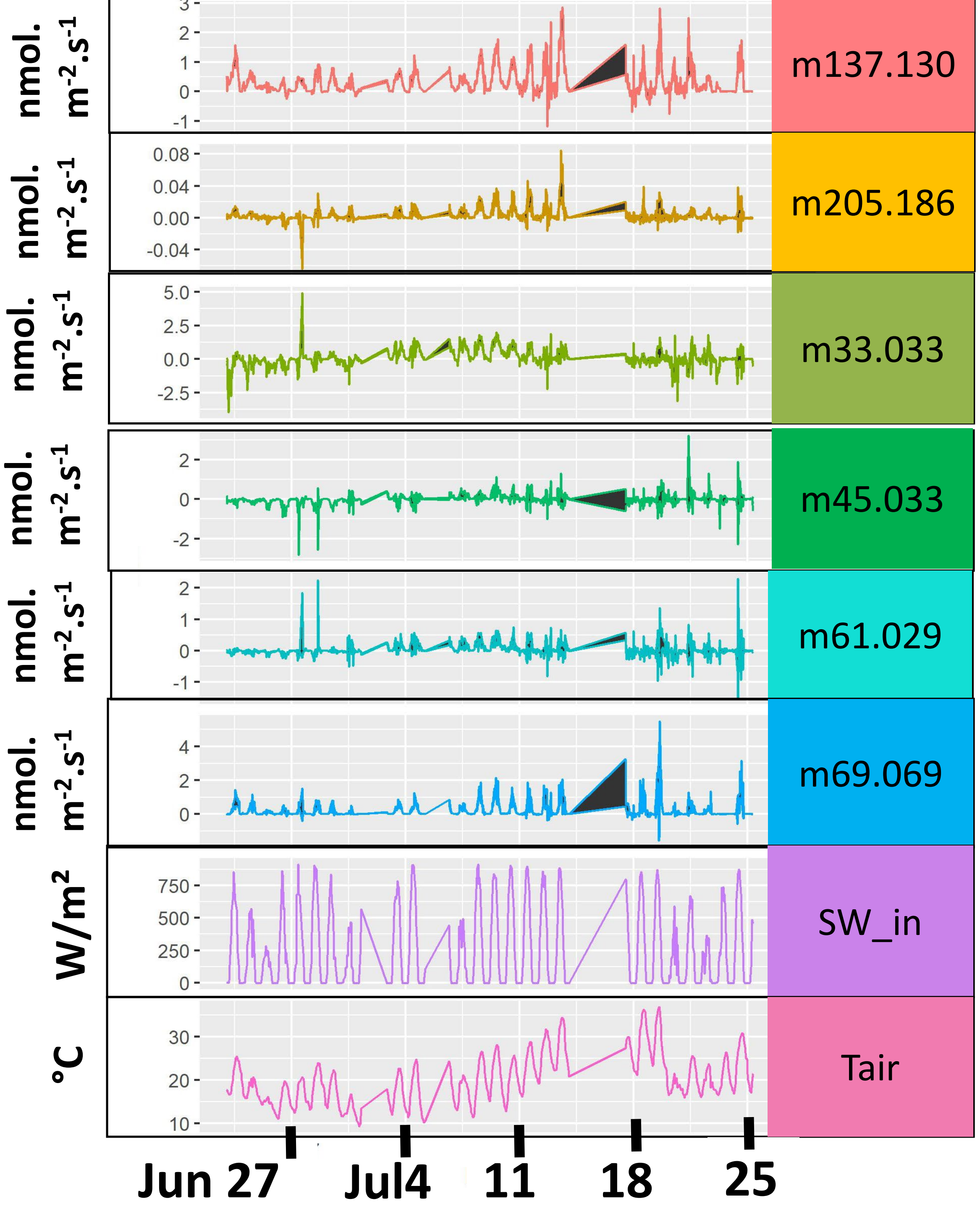
- First part of the campaign mostly
- Few compounds
- Heavy compounds during some specific periods (see further)

Results

VOC flux dynamics:
1/ over full period
(LEFT PANEL)

Main fluxes:

- **Monoterpenes**
- **Methanol**
- **Isoprene**

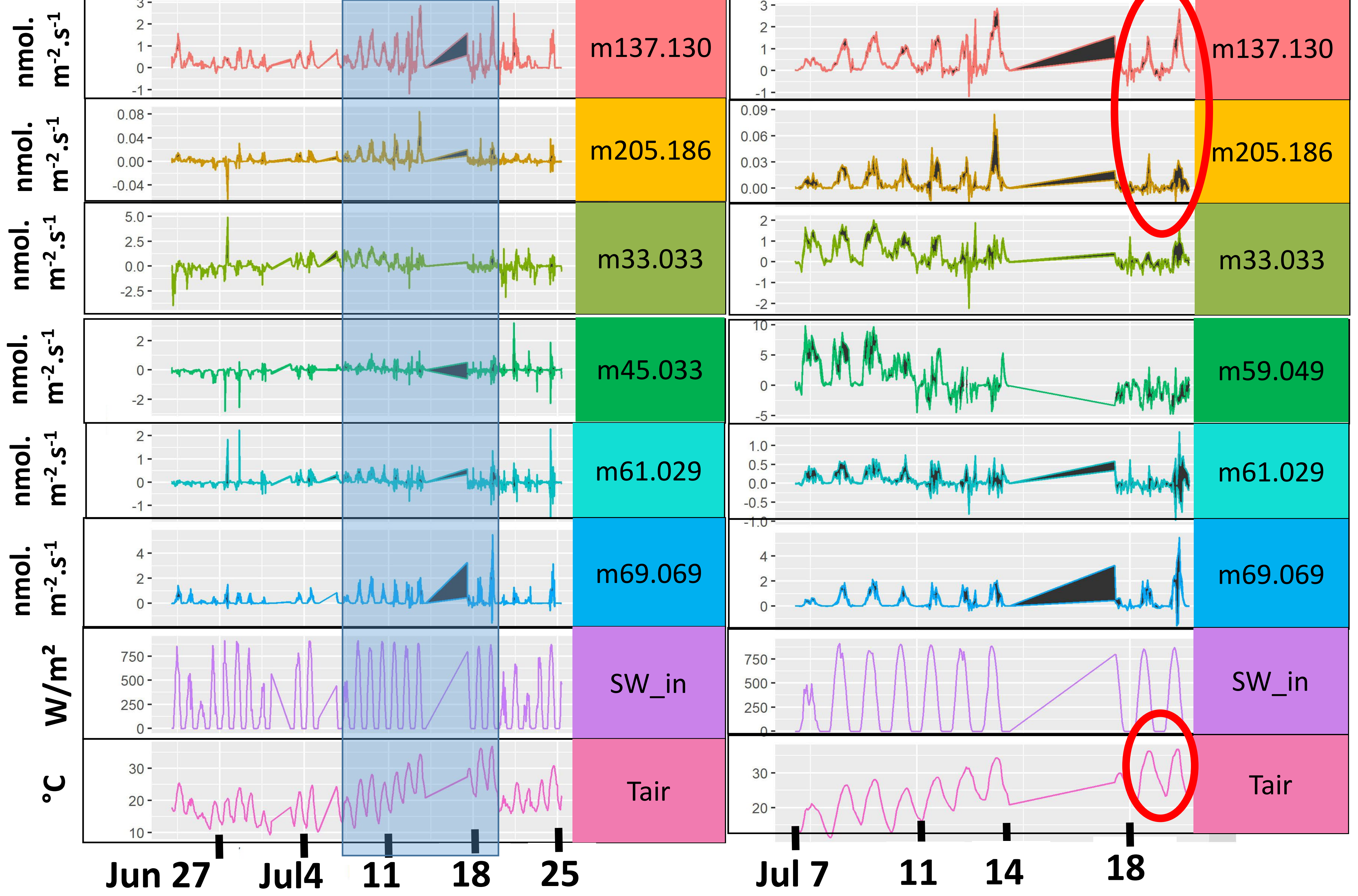


Results

VOC flux dynamics
1/ over full period
(LEFT PANEL)
2/over 7-19 July period
(RIGHT PANEL)

Main fluxes:
- Monoterpenes
- Methanol
- Isoprene

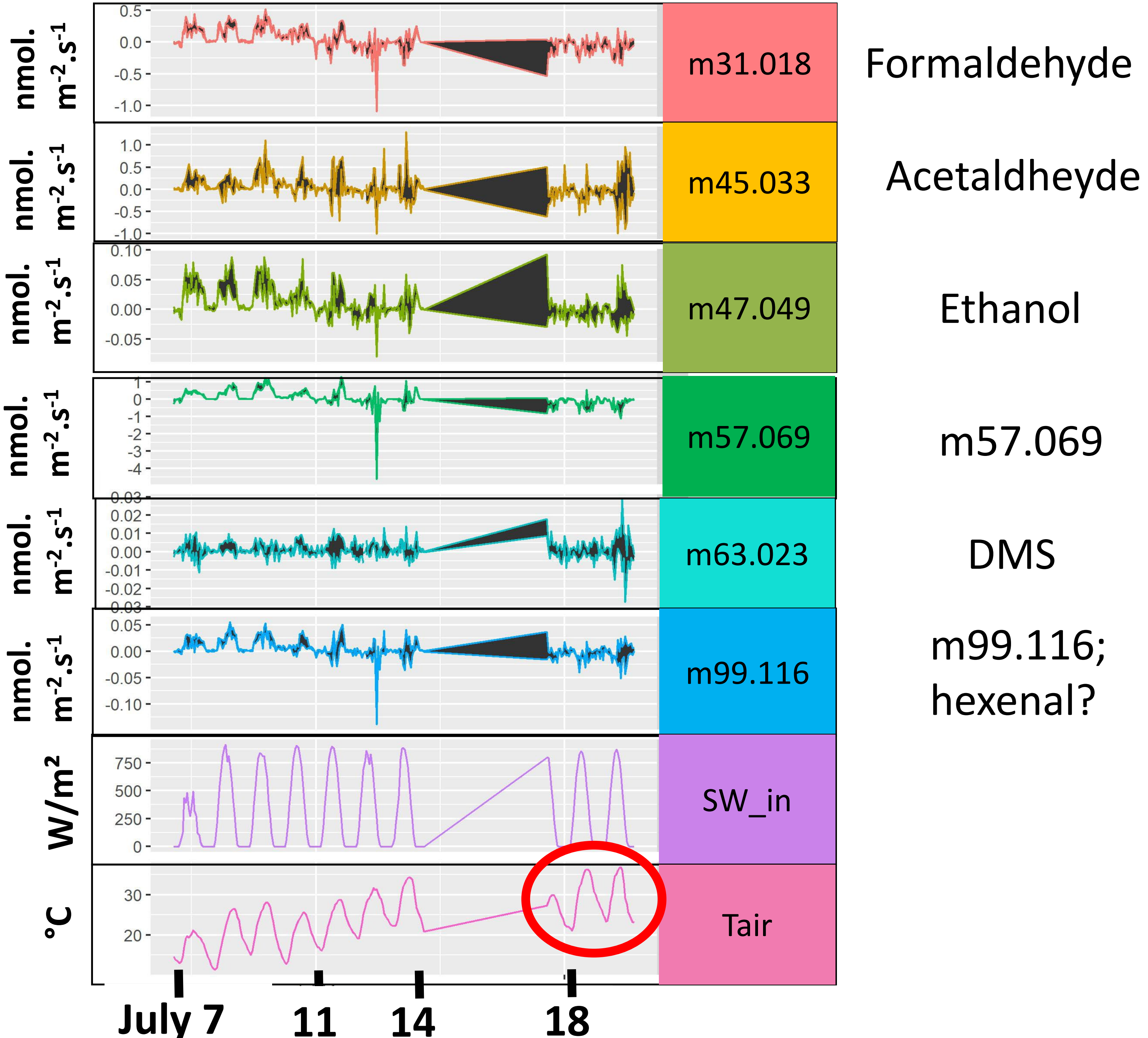
Monoterpenes, Sesquiterpenes: Possible effects of T° during a heat wave?



Results

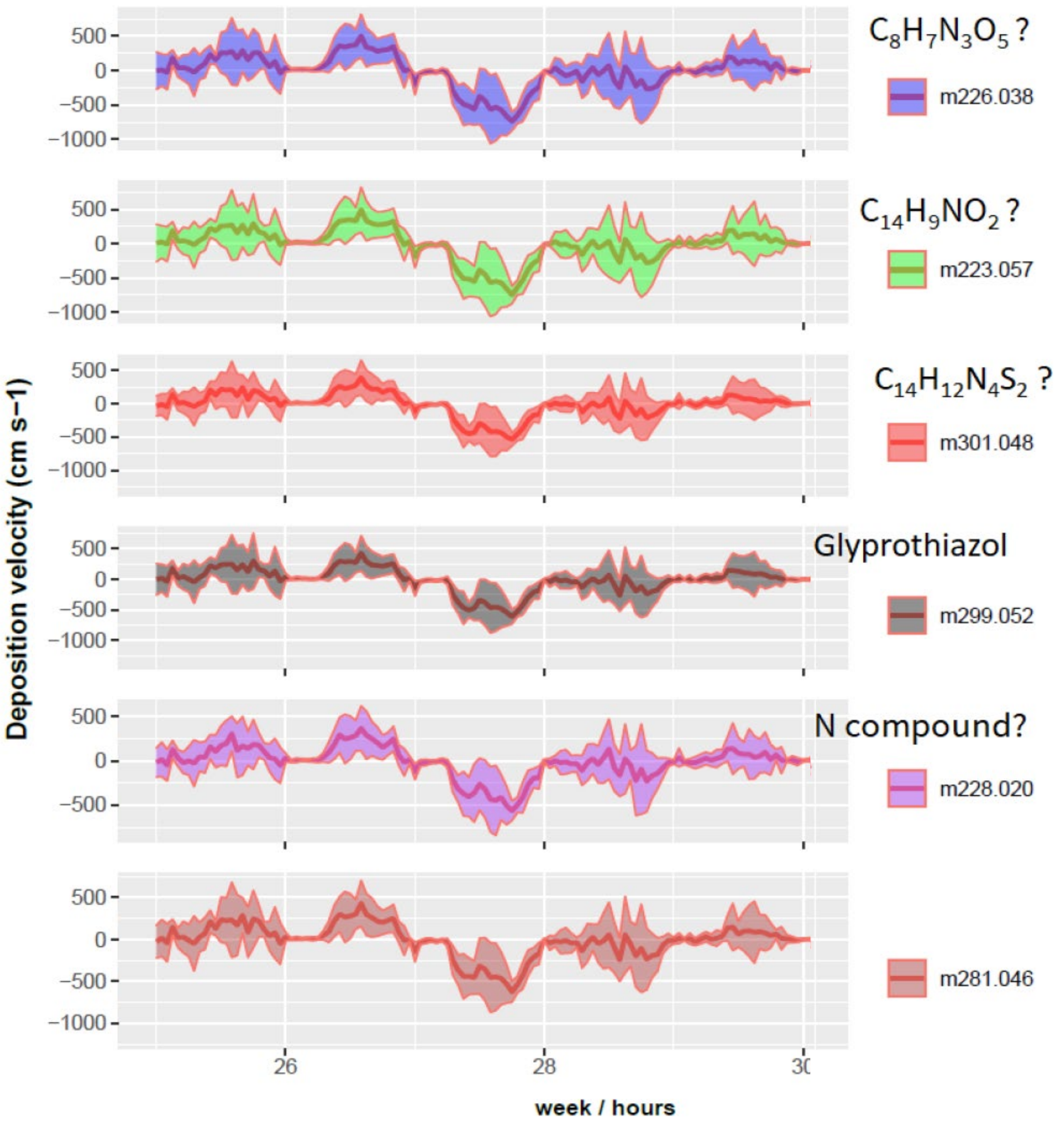
VOC flux dynamics
over warm and dry period
for some other compounds

➔ Likely reduced emissions as of 10 July for most of these compounds
➔ More analyses to be done



Depositing compounds

- Some heavy compounds showed a high deposition flux on weeks 25 (20 June) and 26 (27 June), followed by an emission on week 27 (4 July)
- Nitrogen and sulphur compounds
- Needs more analysis



Conclusion and perspectives

- Reminder: these first results are based on preliminary data.
- Main compounds emitted above the canopy were
  - monoterpenes (m/z 137.130),
  - isoprene (m/z 69.070),
  - methanol (m/z 33.033),
  - as well as a few compounds over short periods: sesquiterpenes (m/z 205.186), acetic acid (m/z 61.029), acetone, possibly GLV,…
- Possible increase of monoterpenes and sesquiterpenes with temperature. Isoprene, methanol seemed to remain unaffected. Needs further investigation.
- **Perspectives:**

  * Peak integration and mass calibration will be reprocessed
  * Data filtering will be further refined based on PTR pressure and source parameters
  * Disturbances due to other teams working on top of the tower will be also filtered
  * Looking into high m/z compounds (m/z > 220)

Thank you to all the team!
And thank you for your attention