Modelling **Nitrous Oxide (N_2O) emissions** and its **isotopic composition** with explicit representation of biochemical processes and fluid transfers in soil at fine scale

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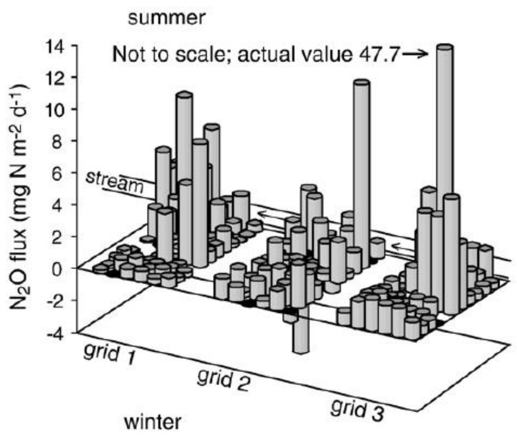
Journées Vsoil, 26-27/03/2026

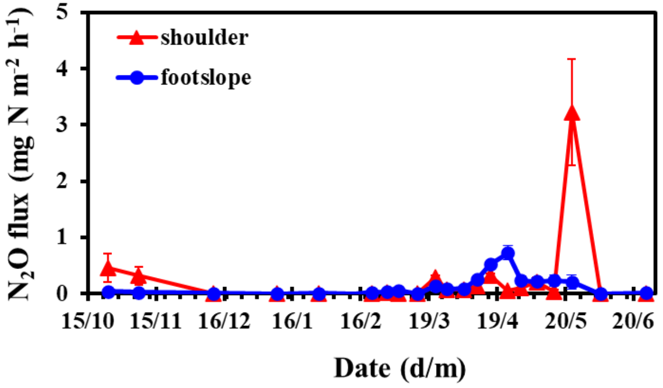
Introduction : Challenges in predicting N_2O emissions

- Large spatial variability of N_2O emissions



\+ Large temporal variability = intense emission during specific events

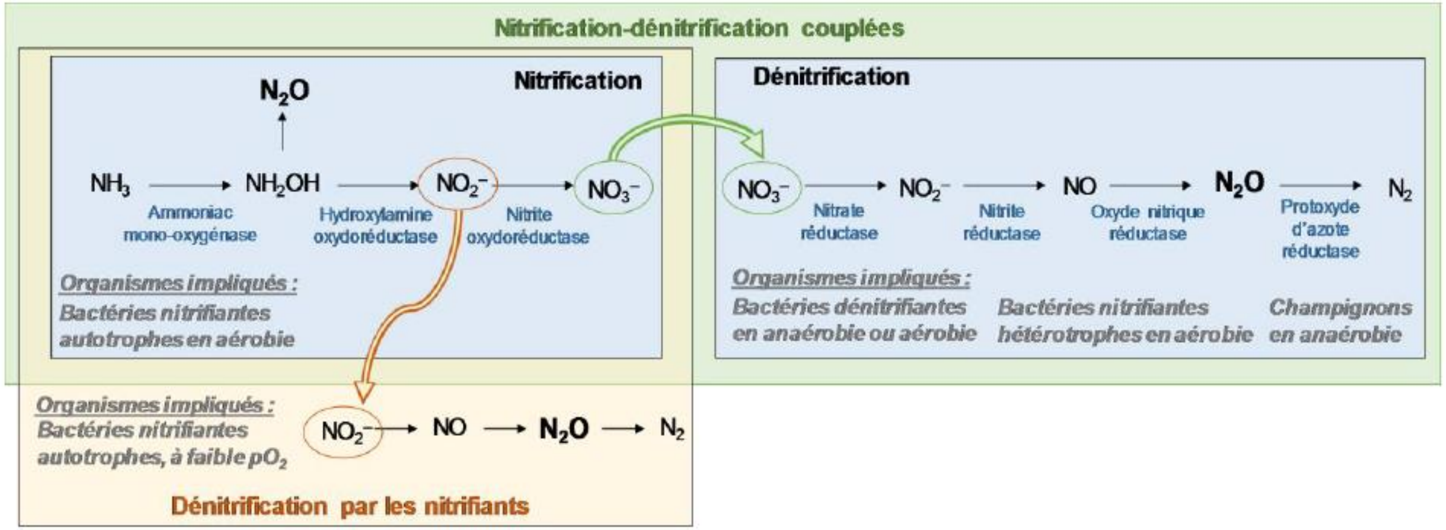
- Magnitude and timing of events is difficult to predict



Introduction : Challenges in predicting N_2O emissions

- several microbial processes of production in soil, in relation with soil anoxia

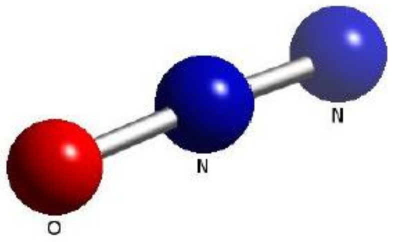
- Emission magnitude controlled both by production / consumption of N_2O



- Reduction also influenced by
  - soil properties (pH, clay, T°, O_2)

  - transfer time in soil.

Introduction : Challenges in predicting N_2O emissions

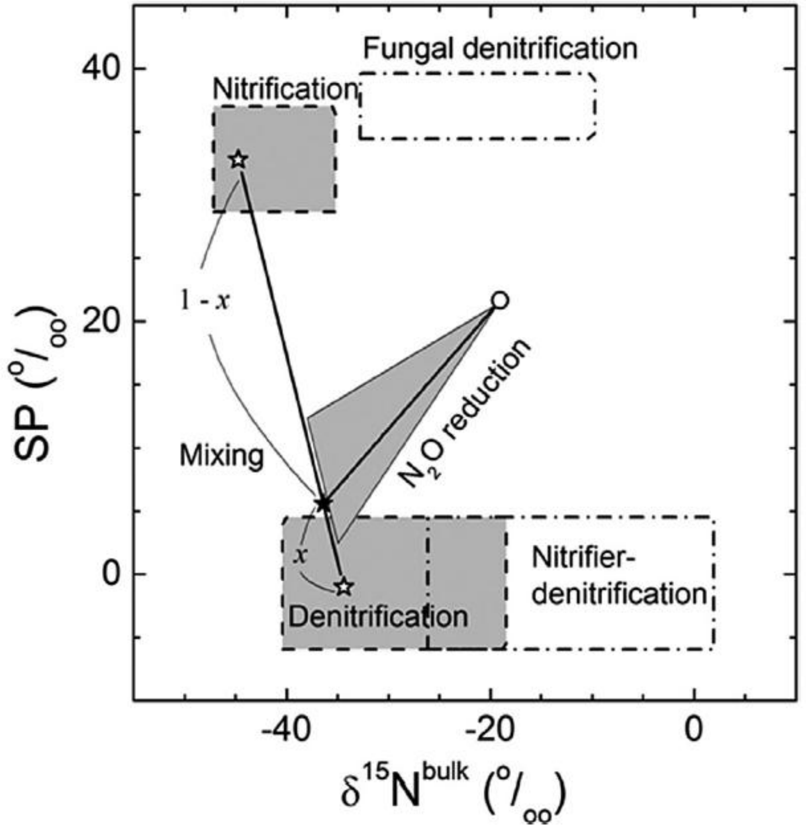


^{14}N-^{14}N-^{16}O

^{15}N-^{14}N-^{16}O : α form

^{14}N-^{15}N-^{16}O : β form

^{14}N-^{14}N-^{18}O



$\delta^{15}N$ = mean($\delta^{15}N^{\alpha}$ et $\delta^{15}N^{\beta}$)

Site preference SP = $\delta^{15}N^{\alpha}$ - $\delta^{15}N^{\beta}$

$\delta^{18}O$

$\Rightarrow$Isotopic fractionation occurs during reactions

$\Rightarrow$Isotopic N_2O signature could be used as a tracer of microbial pathways; site preference evolves during N_2O reduction.

$\Rightarrow$SP versus $\delta^{15}N$ or $\delta^{18}O$ is used to give qualitative information about processes. Could modelling give tools to provide quantitative information?

New model developments

<u>Objective :</u> Developping a **generic** model for N_2O emissions in **transient conditions**, taking into account **soil structure**

N_2O emissions : how to characterize the (transient) effect of:

- ✓ *Soil structure?* — Volumetric mass profile, 3D soil imaging
- ✓ *Water transfer?* — Water retention curves, water measurements
- ✓ *Gas transfer?* — Gas diffusivity measurements
- ✓ *Particulate organic matter?* — Total POM mass, 3D soil imaging
- ✓ *Microbial production processes?* — Enzymatic activities
- ✓ *N_2O Reduction ?* — Isotopic N_2O composition

Not all variables can be measured together with N_2O fluxes, at a sufficient frequency and with a sufficient replicate numbers…

The $NOE_{PREDiHR}$ model : development

Model first developped during PhD work : Flavien Poinçot, 2019:

Control of N_2O emissions by soil structural state

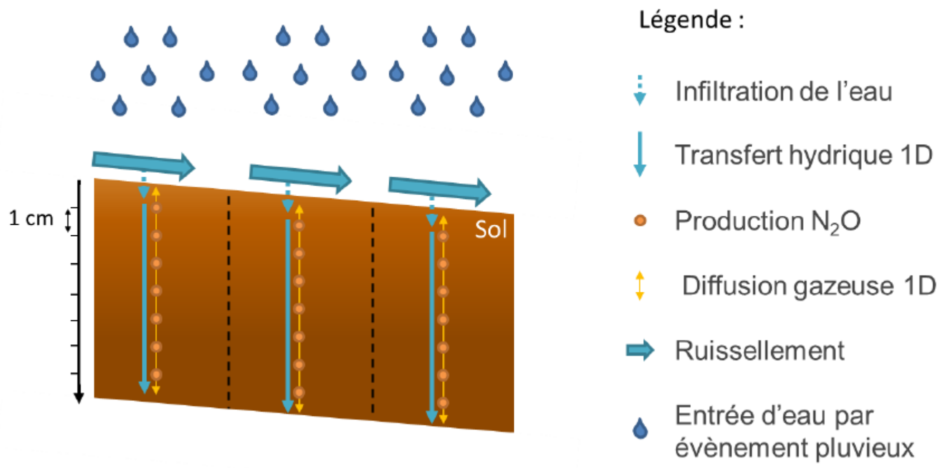


Figure 4-1: Représentation schématique du fonctionnement du modèle

$NOE_{PREDiHR}$

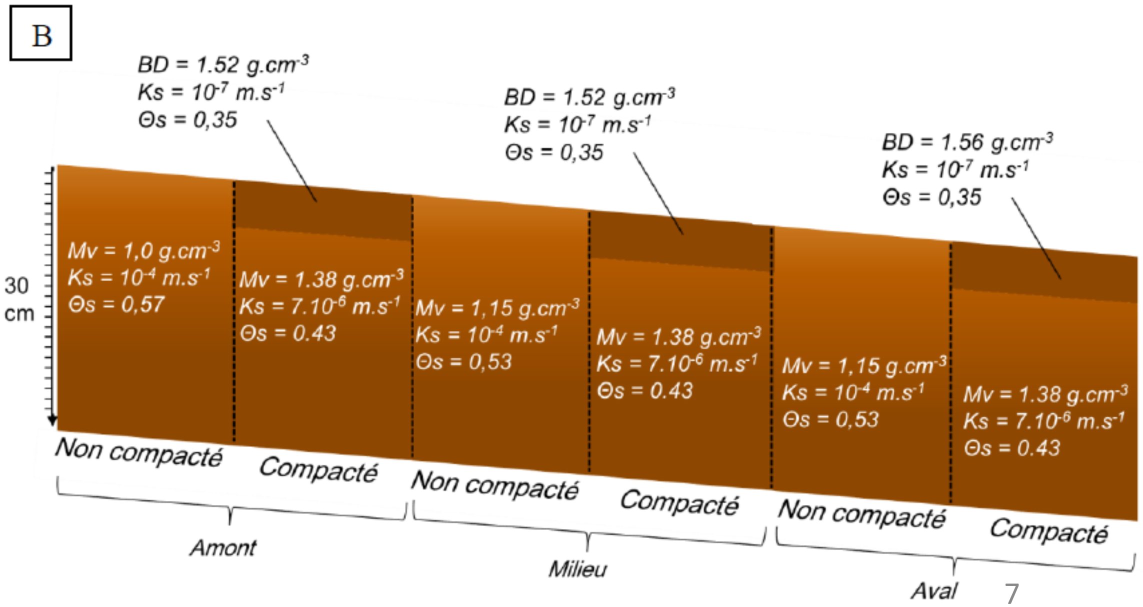
- 1D-model
- Water transfer following PASTIS (*Mualem-VG retention curve, rain imposed flux in surface, free drainage)*
- Solute transfer (local equilibrium assumption)
- Gas diffusion (PASTIS formalism)
- Gas-liquid equilibrium
- Nitrification and denitrification based on NOE module (*Hénault et al., 2005; Bessou et al., 2010*).
- O_2 is not simulated, but WFPS is used as proxy of anoxia by NOE

The NOE$_{PREDiHR}$ model : linked experiment

Application : What is the effect of rain on N_2O emissions from differently compacted soil profiles?

- Experimental set-up: rain simulation on a 5 x 2 m soil model,

differently compacted areas

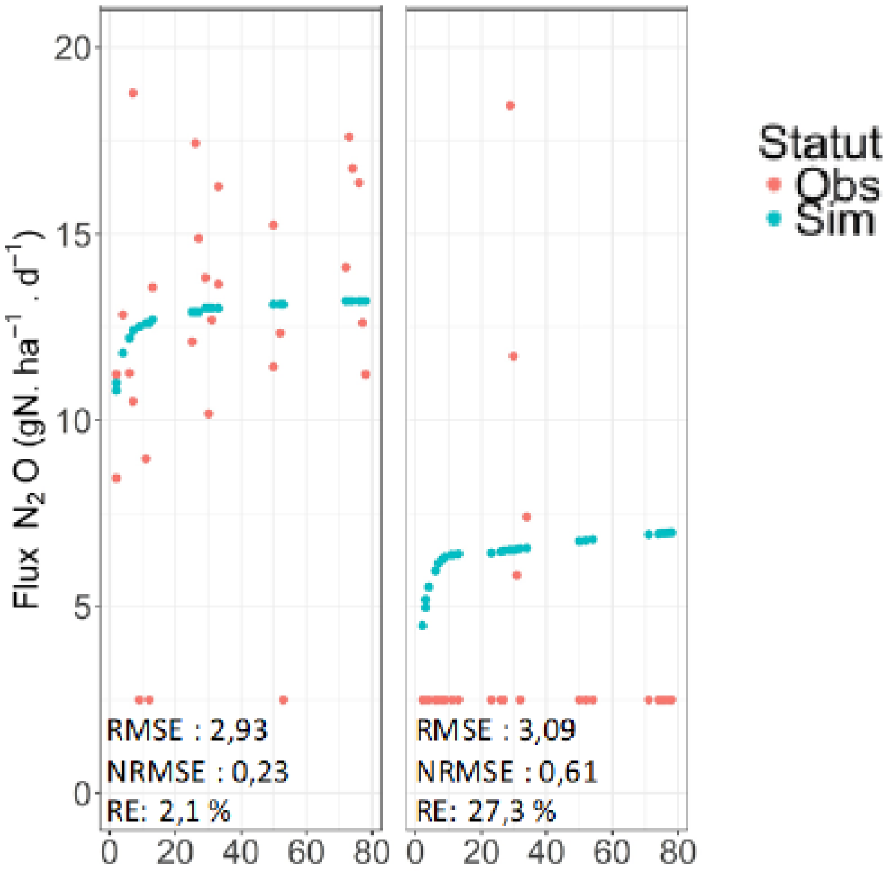


Specific conditions:
- Constant mineralization (only few days)
- Constant evaporation
- Hydrodynamic parameters fitted in Vsoil platform

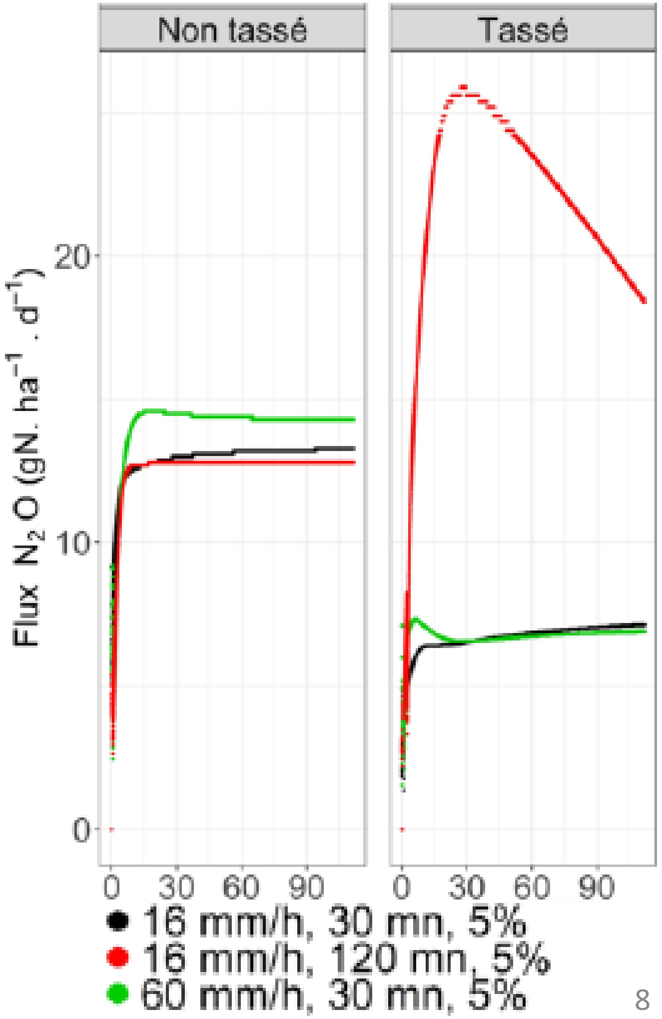
The $NOE_{PREDiHR}$ model : simulation results

Evaluation of model with observations :

N_2O fluxes, matric potential and water content measurements



Simulation of different rain scenarii



Poinçot 2019

New model developments : experiments

- **Experiment 1**

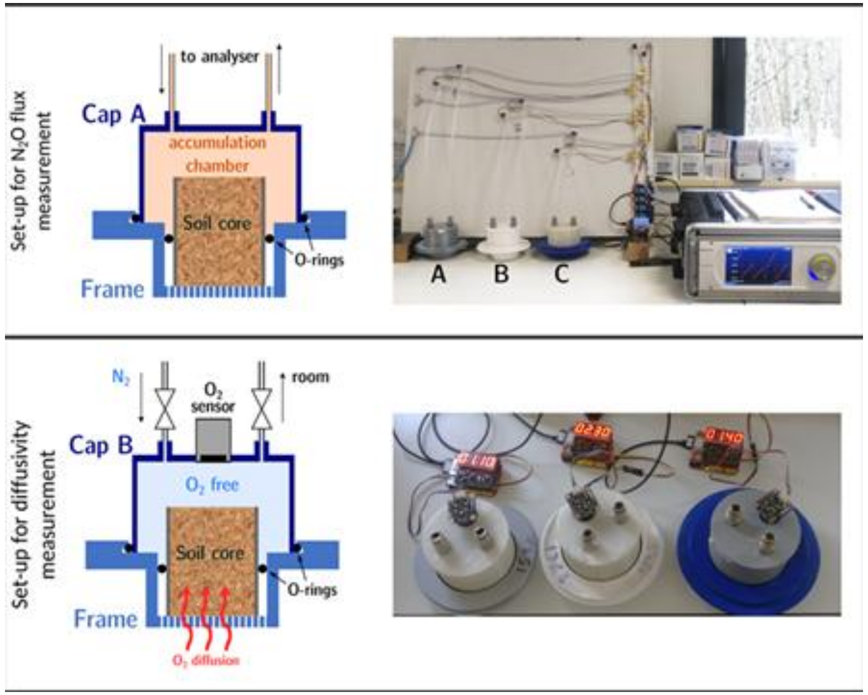
84 intact cores (compacted, uncompacted), 2 days equilibrium at -5cm, then 5 days desiccation, gas diffusivity and N_2O emissions

Experiment 2

24 intact cores (C/UNC, strip-till/till), simulated rain + X-ray tomography at 290 µm resolution and N_2O emissions after rain

- **Experiment 3**

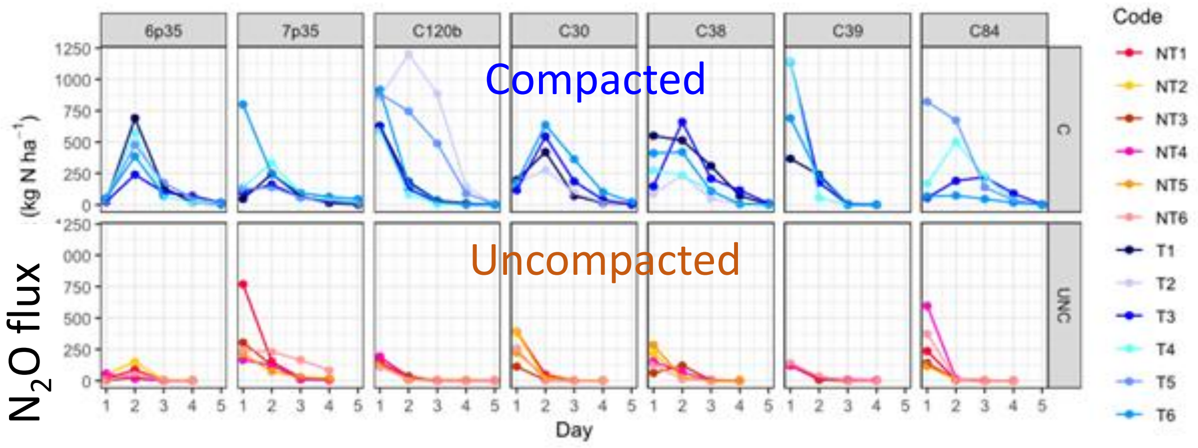
30 intact cores (C/UNC), simulated rain, 1 night free drainage, N_2O and isotopic N2O emissions

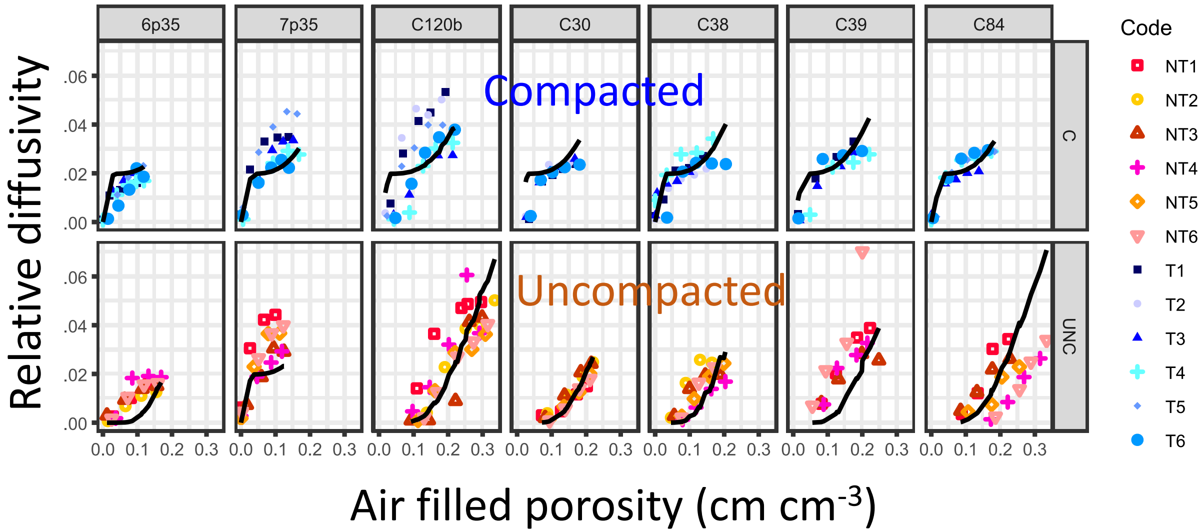


New model developments

- **Experiment 1 :** *Soil compaction, diffusivity & N_2O emissions under desiccation*

Results





✓ ***Larger N_2O emissions in compacted cores***

✓ ***But larger diffusivity in compacted cores !***

likely linked to soil cracking

⇒Application of a diffusivity model developped for cracks

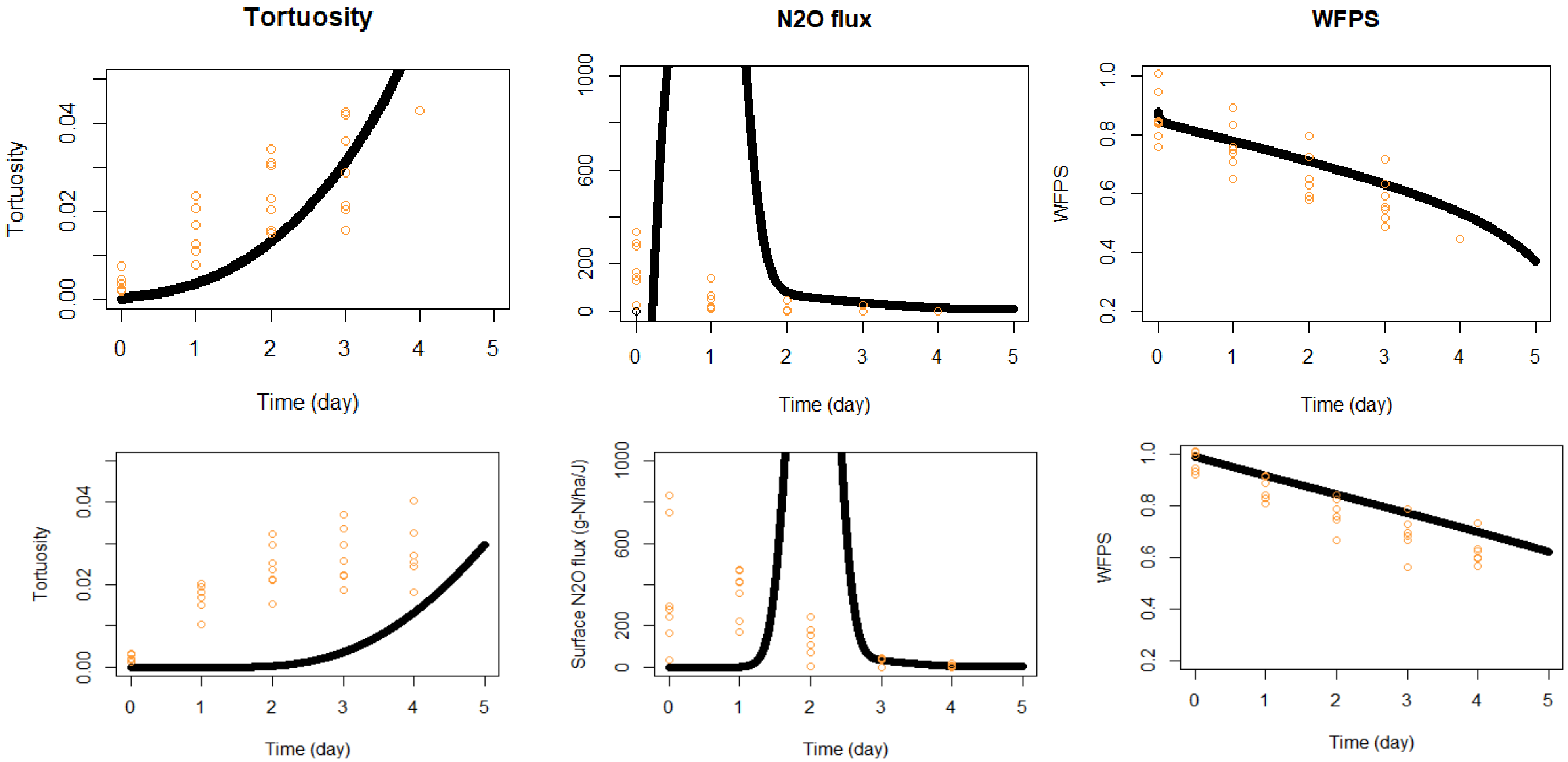
Kristensen et al, 2010, Gas-phase diffusivity and tortuosity of structured soils. Journal of contaminant hydrology

New model developments

- Simulation: first results

Conditions of simulation : *First equilibrium during 2 days: N_2O profile*

Constant mineralisation + Constant evaporation from measured mass variation



Uncompacted

Lakshani diffusivity model

Compacted

New model developments

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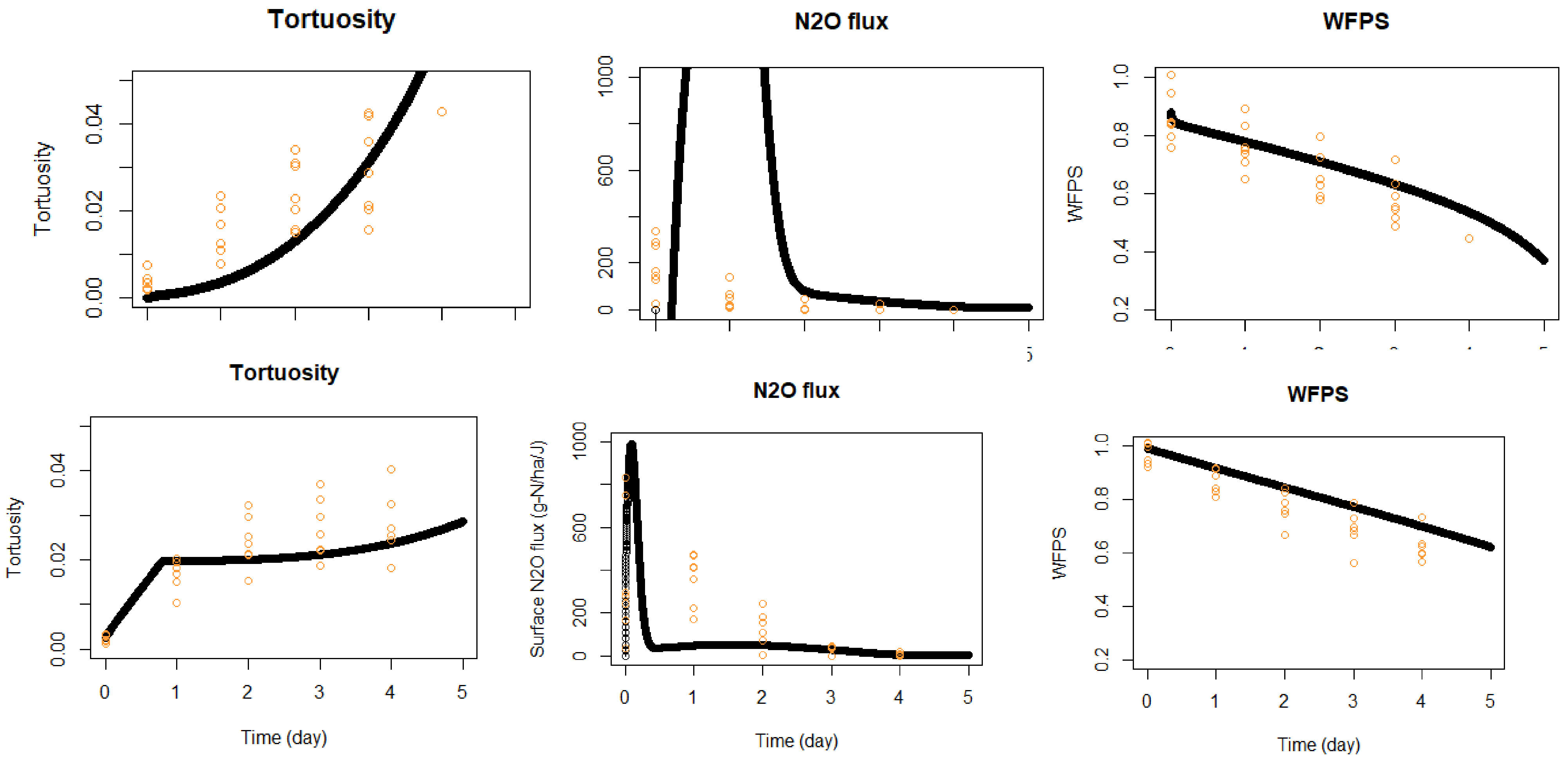


Uncompacted

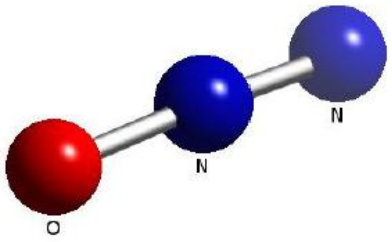
Lakshani diffusivity model

Compacted,
Kristensen model

Pesrpectives

Simulating isotopic N_2O

- **Experiment 3 :** *Soil compaction, N_2O emissions and isotopic N_2O after rain*



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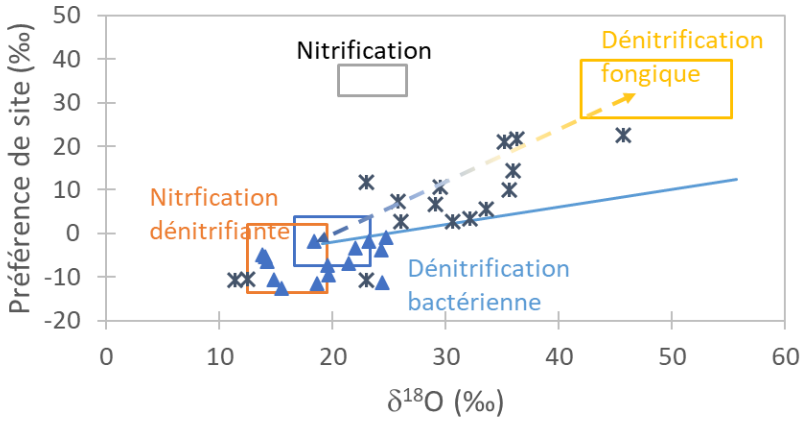
$\delta^{18}O$

- ✓ Compacted cores emitted 25 times more N_2O than uncompacted cores
- ✓ Isotopic signature : Compacted cores produced N_2O by bacterial denitrification / nitrifier denitrification



Perspectives

- **ongoing: Simulating isotopic N_2O : new module**

❑ Differential form of Rayleigh equation (Mariotti 1981)

$\alpha_{P/S}$ fractionation factor = constant

$$\frac{d^{15}N}{^{15}N} = \alpha_{P/S} \times \frac{d^{14}N}{^{14}N}$$

And

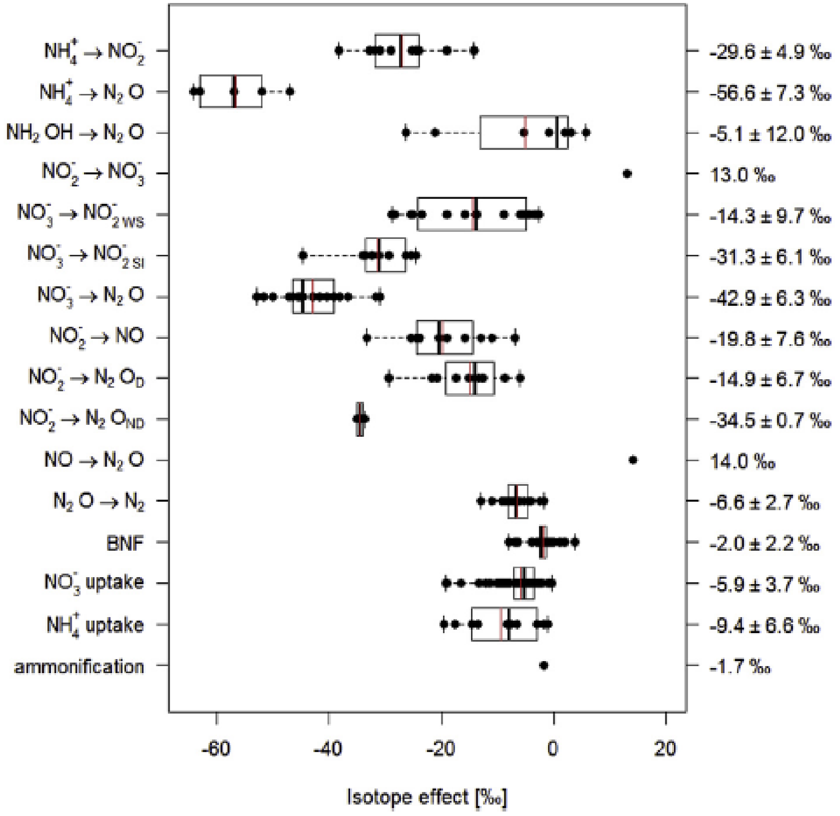
$$d^{14}N + d^{15}N = D_p \times dt$$

Where D_p production rate for process

❑ Integrated form of Rayleigh equation, closed system

$$R_s = R_{s,0} \times f^{\alpha_{p/s-1}} = R_{s,0} \times f^{\varepsilon}$$

ε isotope effect $= \alpha_{P/S} - 1$



Denk, T. R., Mohn, J., Decock, C., Lewicka-Szczebak, D., Harris, E., Butterbach-Bahl, K., ... & Wolf, B. (2017). The nitrogen cycle: A review of isotope effects and isotope modeling approaches. Soil Biology and Biochemistry,

Conclusion

Objective : Developping a **generic** model for N_2O emissions in **transient conditions**, taking into account **soil structure**

- Preliminary results…
- Specific objectives:
    - Improving gas diffusion simulation
    - Taking into account particulate organic matter
    - Simulating isotopic fractionation