Spatial controls of microbial pesticide degradation in soil: A model-based scenario analysis

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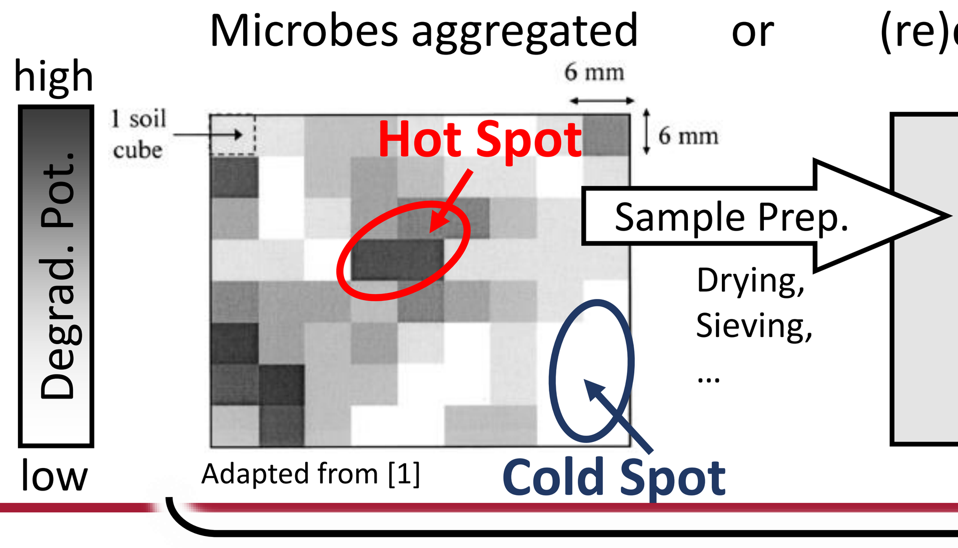
BACKGROUND

Pesticides are omnipresent diffuse environmental pollutants. Their biodegradation in complex natural environments is often more limited than expected from laboratory testing. Idealised experiments might neglect natural complexities such as the heterogeneous distribution of microbes and standard kinetic degradation models might be oversimplified.

Natural soils vs. Ideal lab conditions

Microbes aggregated or (re)distributed evenly



Standard models vs. Gene-informed models

Biomass action kinetics

- Simple rate laws
- No process insights
- Microbial biomass unspecific activity proxy

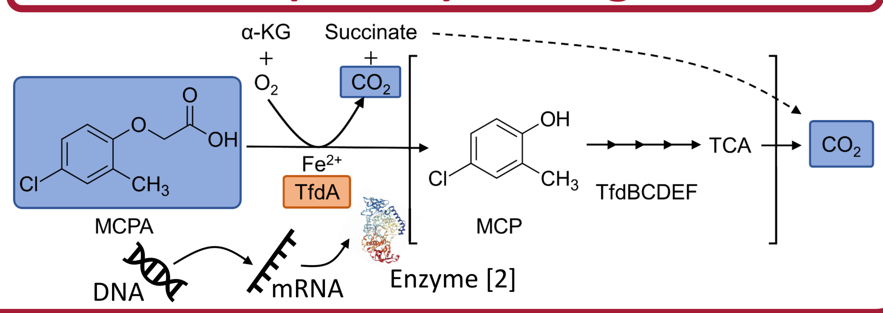
Process based description

- Complex interactions & feedbacks
- Insights into metabolic networks
- DNA, mRNA & enzyme concentrations as relevant activity proxies

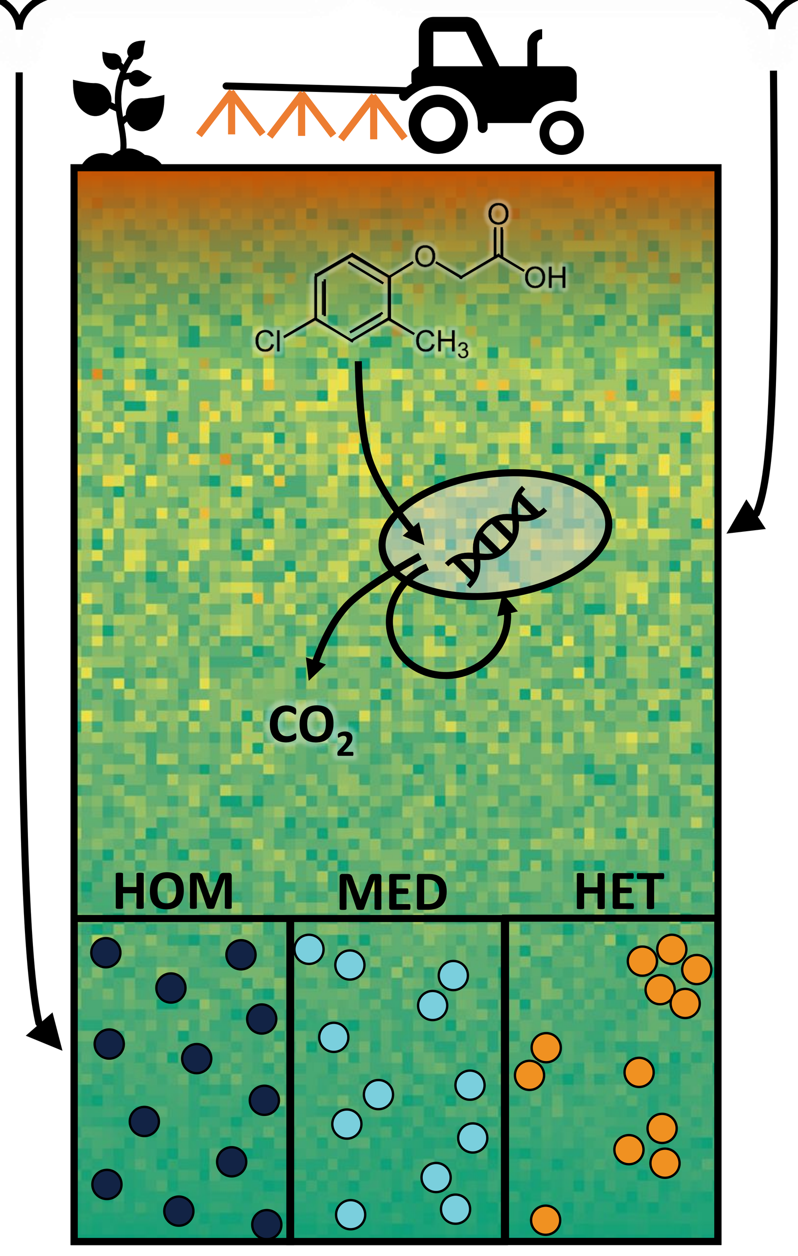
OBJECTIVES

- Upscaled relevance of microbial small-scale **spatial heterogeneity**?
- Possible **bio-kinetic constraints** of pesticide degradation?

Pesticide (MCPA) biodegradation



MATERIALS & METHODS

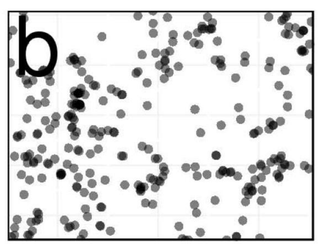


Microbial distribution scenarios

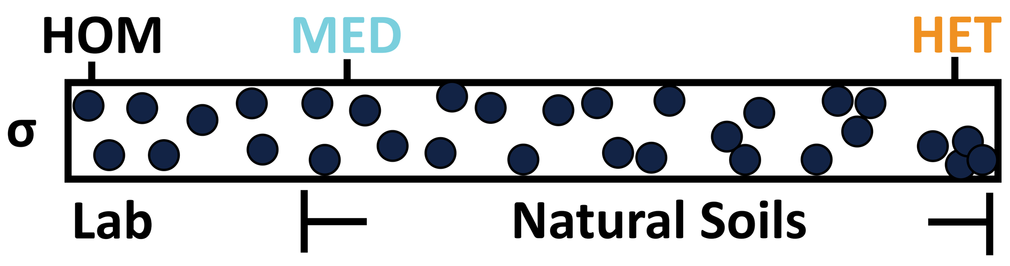
Log Gaussian Cox Process (Raynaud & Nunan[3])

- Creates stochastic aggregated point patterns
- Parametrised for natural microbial distributions

LGCP(λ,β,σ) →



Fixed: Microbial abundance (λ) and spatial scale (β)
Altered for scenario definition: Variance (σ)



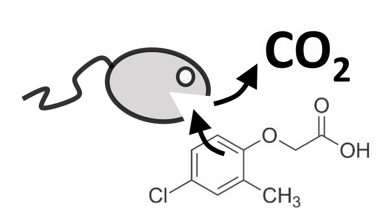
3 scenarios represent: i) ideal laboratory conditions, ii) lower and iii) upper end of natural heterogeneity

Compared microbial pesticide degradation models

Growth rate:

Standard Monod-type model (BM)

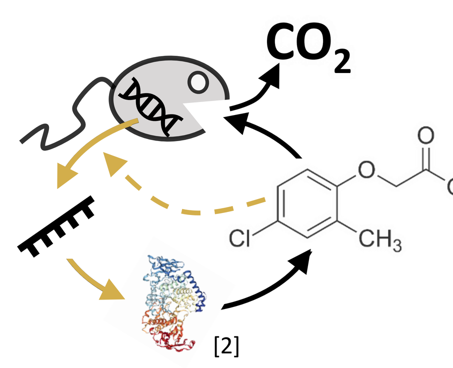
- Biomass as activity proxy
- Empirical Monod kinetics



$$r_{gr}^{BM} = \mu_{max} \left(\frac{C_L}{K_M + C_L} \right) \cdot B$$

Gene-informed model (GB)
(of Chavez Rodriguez et al.[4])

- Quantitative functional gene data as activity proxy
- Mechanistic transcription & translation dynamics
- Microbial dormancy considered (data not shown)



$$r_{gr}^{GB} = \mu_{max} \left(\frac{C_L}{K_M + C_L} \right) \cdot \left(\frac{C_L^{n_H}}{K_H^{n_H} + C_L^{n_H}} \right) \cdot DNA$$

Hill function describes quasi steady-state substrate dependent gene expression.

Models were calibrated by [4] with data provided by Bælum et al.[5].

Modelling tool for coupled reactive transport

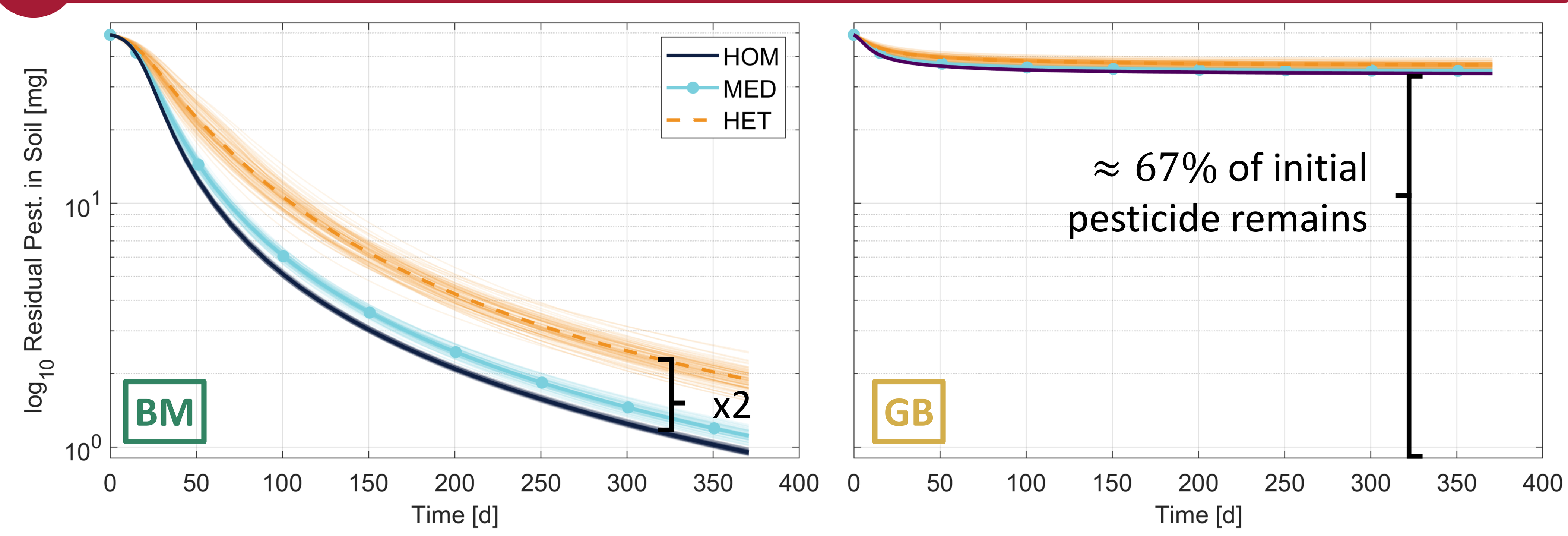
GeoSysBRNS (Centler et al.[6]) { Geohydrology: OpenGeoSys 5; Biogeochemistry: BRNS }

RESULTS

Residual pesticide amount in soil column

- Model type (BM vs. GB) most influential, heterogeneity as co-factor
- In GB model: degradation vastly constrained & thus reduced difference between heterogeneity scenarios
- HET constantly double residual pesticide amounts as HOM (for BM)

1 Pesticide degradation time series



References:

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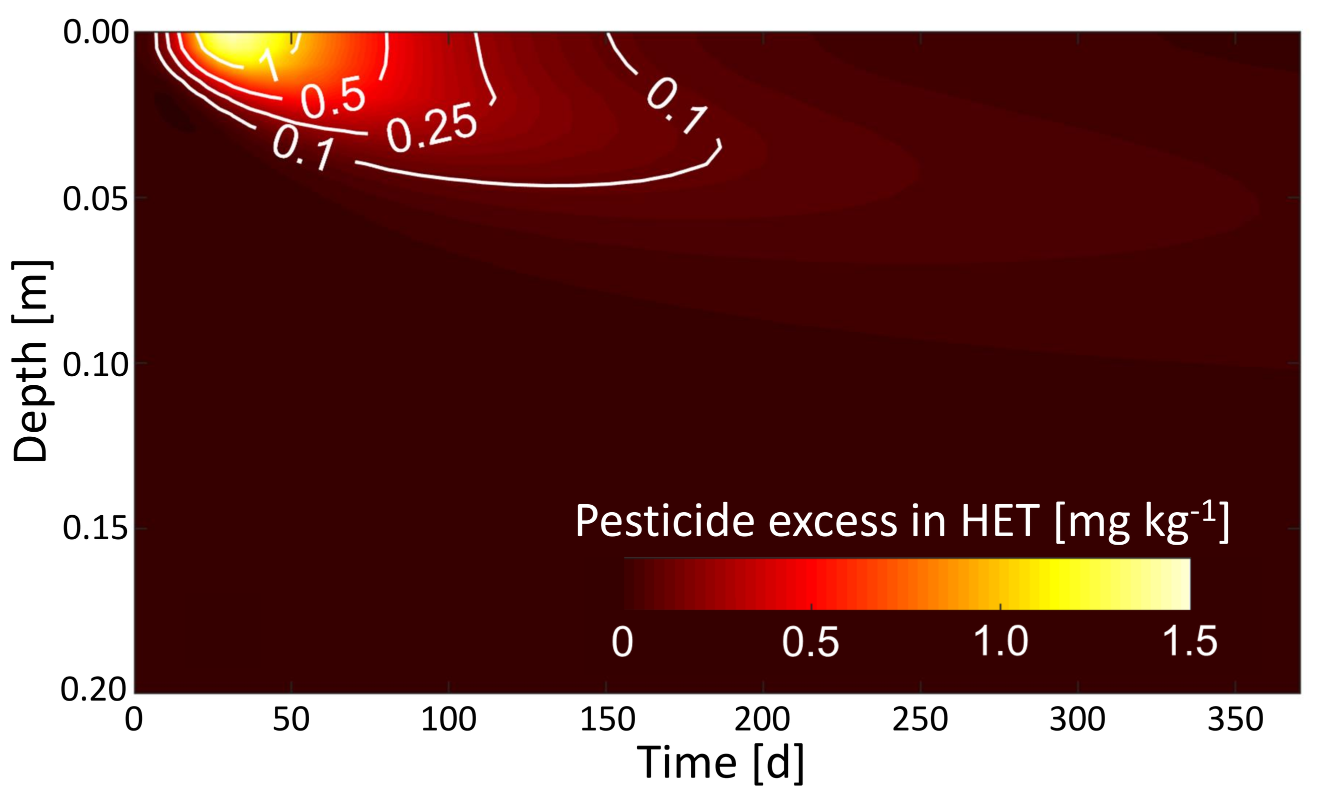
[2] https://www.rcsb.org/3d-view/3AML/1
[3] Raynaud, X., & Nunan, N. (2014). Spatial ecology of bacteria at the microscale in soil. *PloS one*, *9*(1), e87217.
[4] Chavez Rodriguez, L., Ingalls, B., Streck, T., Schwarz, E., Uksa, M., Wirsching, J., Poll, C., Kandeler, E., & Pagel, H. (in preparation). A biogeochemical model informed by genetic data for accurate prediction of pesticide degradation in soils: example case for 2,4-D and MCPA.
[5] Bælum, J., Nicolaisen, M. H., Holben, W. E., Strobel, B. W., Sørensen, J., & Jacobsen, C. S. (2008). Direct analysis of *tfdA* gene expression by indigenous bacteria in phenoxy acid amended agricultural soil. *The ISME journal*, *2*(6), 677-687.
[6] Centler, F., Shao, H., De Biase, C., Park, C. H., Regnier, P., Kolditz, O., & Thullner, M. (2010). GeoSysBRNS—A flexible multidimensional reactive transport model for simulating biogeochemical subsurface processes. *Computers & Geosciences*, *36*(3), 397-405.

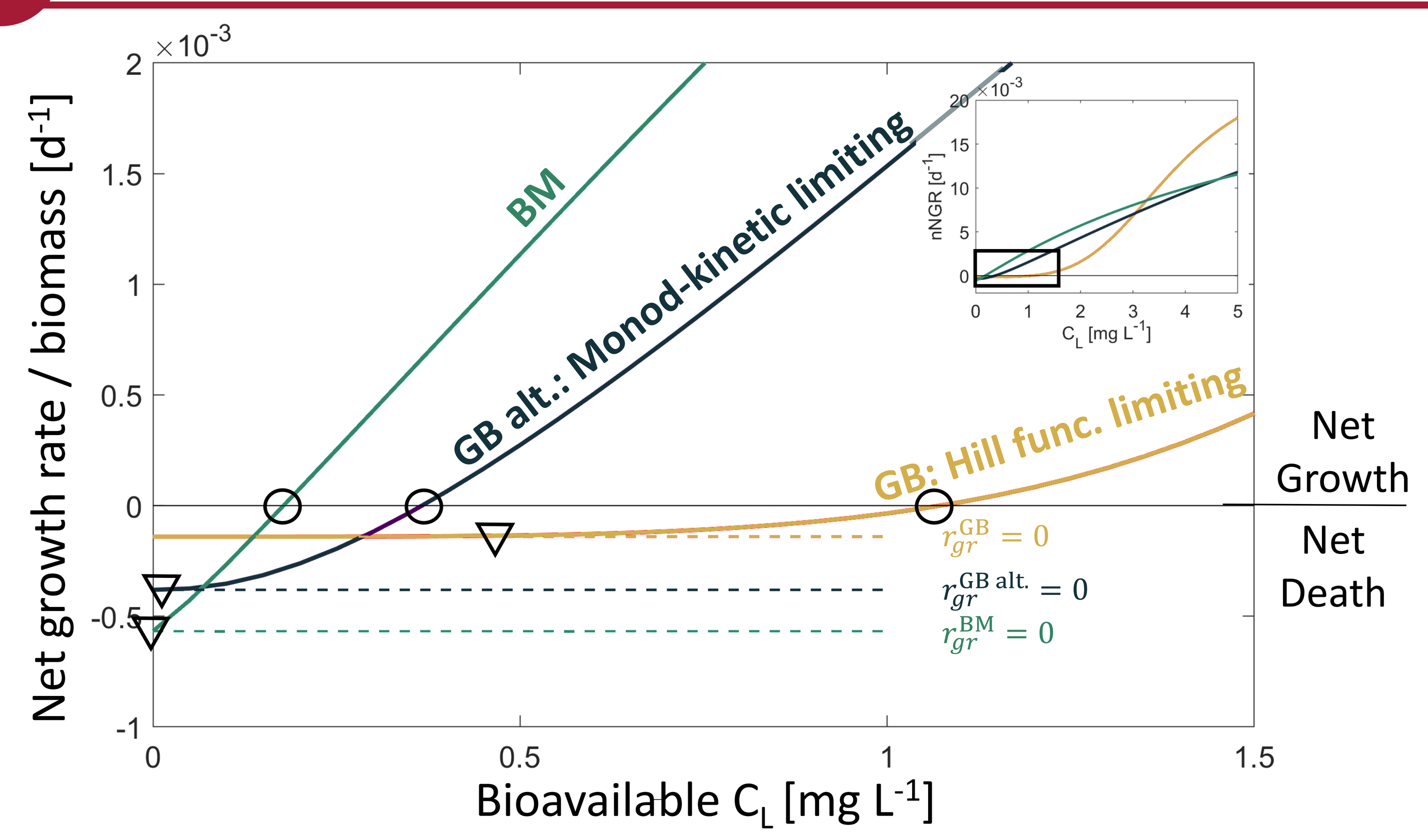
2.1 Spatial heterogeneity effects



Concentration difference (HET-HOM) in vertical profile

- Increased conc. in HET for continued time
- Prolonged detectability of pesticide in HET

2.2 Bio-kinetic constraints



Biomass-normed net growth rate (nNGR) as function of bioavailable C_L

○ nNGR < 0 — no net micobial growth
▽ $r_{gr}^{i} \to 0$ — no gene expression, no degradation
} at higher bioavailable C_L if Hill func. limiting

CONCLUSION

With increasing spatial heterogeneity:

- Decreased upscaled pesticide degradation rate
- Higher residual pesticide concentrations
- Prolonged detectability

Compared to ideal conditions, in natural soils the spatial heterogeneity of microbes can diminish pesticide biodegradation.

Bio-kinetic constraints:

- Gene expression dynamics can control degree of persistence

Integration of genetic data is a powerful tool but requires carefull calibration & evaluation.

CRC 1253 CAMPOS — Catchments as Reactors

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