



Modeling coupled pesticide degradation and organic matter turnover: From gene abundance to process rates



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ABSTRACT

The mechanistic integration of microbial behavior remains a major challenge in biogeochemical modeling of organic matter turnover in soil. We recently introduced dynamic feedbacks between specific microbial groups and their micro-environment in a biogeochemical model (Pagel et al., 2014). Here, the model was applied in a case study to simulate pesticide degradation coupled to carbon (C) turnover in the detritusphere. We aimed at unravelling the effects of litter-derived substrate supply on the spatio-temporal dynamics of the microbial community and the resulting biogeochemical processes at the mm-scale in soil. We linked genetic information on abundances of bacteria, fungi and specific pesticide degraders to the biogeochemical dynamics of C and a generic model compound (MCPA, 4-chloro-2-methylphenoxyacetic acid) in soil by multiobjective calibration. We observed and simulated increased dissolved organic and microbial C as well as accelerated MCPA degradation in soil up to a 6 mm distance to litter. We found that, whereas transport and sorption processes act as extrinsic control on the encounter of microorganisms and substrates, microbial traits such as substrate preference or metabolic capabilities intrinsically determine turnover rates triggering feedback effects on physicochemical processes such as diffusion. A process analysis revealed that C cycling and pesticide degradation in the detritusphere were strongly controlled by fungal dynamics. Our study demonstrates that integrating mathematical modeling with experiments provides comprehensive insight into the microbial regulation of matter cycling in soil.

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1. Introduction

Soil microorganisms control pivotal ecosystem services (Dominati et al., 2010; Paul, 2007). Yet, the mechanistic understanding how microbial dynamics and interactions in soil control biochemical processes in response to environmental change is still one of the most challenging questions in microbial ecology (Graham et al., 2016; Prosser, 2012). Since biogeochemical models are effective quantitative tools to combine microbial dynamics with physicochemical processes for investigating and predicting ecological interactions (Vereecken et al., 2016), there have been several calls to explicitly consider microorganisms in soil organic matter models (McGuire and Treseder, 2010; Schmidt et al., 2011;

Treseder and Lennon, 2015; Wallenstein and Hall, 2012).

A promising approach to gain further progress in ecological theory and models is to link functional trait distributions in microbial communities to key controls of decomposition and degradation processes (Boon et al., 2014; Green et al., 2008; Krause et al., 2014; Webb et al., 2010). Consequently, a few models successfully adopted trait-based theory for improved prediction and understanding of, e.g., litter decomposition (Allison, 2012; Kaiser et al., 2014), nitrification in soil (Bouskill et al., 2012; Le Roux et al., 2016), and soil C dynamics responses to warming via microbial adaption of C use efficiency (Allison, 2014). Alternative “new generation” models consider metabolic and physiological traits, such as enzyme production, life-history characteristics (e.g., r-/K-selection) or microbial dormancy, to account explicitly for microbial feedbacks to substrate availability (Blagodatsky and Richter, 1998; Falconer et al., 2015; Gras et al., 2011; Manzoni and Porporato, 2009; Moore et al., 2014; Neill and Guenet, 2010; Perveen et al., 2014; Sistla et al., 2014; Wieder et al., 2015).

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Based on these approaches, the recently developed PECCAD (PEsticide degradation Coupled to Carbon turnover in the Detritusphere) model (Pagel et al., 2014) links carbon cycling with pesticide degradation in soil. It explicitly considers growth and activity of specific microbial groups and accounts for substrate use preferences and dormancy. While PECCAD provides enough flexibility to reflect metabolic and physiological traits of microbial communities in soil, it also considers for depth distributions of organic carbon, pesticides and microbes as well as sorption and one-dimensional transport of solutes. Only few other models (Chalhoub et al., 2013; Ebrahimi and Or, 2015; Rosenbom et al., 2014; Vogel et al., 2015) similarly account directly for interactions between microbial dynamics and physicochemical processes.

PECCAD was specifically designed to elucidate regulation mechanisms of accelerated pesticide degradation in the detritusphere, i.e. the soil-litter interface and the adjacent soil influenced by litter (Poll et al., 2006). This microhabitat is a microbial hot spot characterized by high C turnover rates (Gaillard et al., 2003; Kuzyakov and Blagodatskaya, 2015; Marschner et al., 2012; Poll et al., 2008). Here, interactions between transport processes and microbial dynamics strongly control organic matter turnover (Poll et al., 2006). In particular, litter-derived C stimulates the degradation of herbicides such as 4-chloro-2-methylphenoxyacetic acid (MCPA) (Duah-Yentumi and Kuwatsuka, 1980; Ghani and Wardle, 2001; Poll et al., 2010b). Poll et al. (2010b) identified three possible regulation mechanisms of accelerated MCPA degradation in the detritusphere: increased growth of specific degraders by additional energy supply from litter-derived substances, increased production of specific enzymes by alleviating resource limitation of specific degrader organisms or enhanced co-metabolic MCPA degradation via litter-stimulated fungal growth. However, direct evidence on the microbial regulation of accelerated MCPA degradation is missing and our understanding of underlying mechanism of such priming effects is in general still very limited (Kuzyakov, 2010).

In the present work, MCPA degradation in the detritusphere was utilized as an example process to gain insight into the microbial regulation of matter fluxes and priming phenomena in soil. We aimed at unravelling the effects of litter-derived substrate supply on the spatiotemporal dynamics of the microbial community and the resulting biogeochemical processes at the mm-scale in soil. Our specific objectives were: i) to quantify litter, MCPA-, and soil-derived carbon utilization of microorganisms in the detritusphere, and ii) to estimate the relative contribution of fungal co-metabolisms on litter-stimulated MCPA degradation.

We integrated an experimental microcosm study with biogeochemical modeling. Since development and parameterization of biogeochemical models can strongly benefit from using genetic and 'omic' data on functional traits (Ponomarova and Patil, 2015; Treseder and Lennon, 2015; Trivedi et al., 2013), first approaches have already integrated functional genes with biochemical models (Bouskill et al., 2012; Reed et al., 2014). In extension of much simpler approaches (Batoglu-Pazarbasi et al., 2013), we integrated genetic data on abundances of bacteria, fungi and MCPA degraders with PECCAD. It has been demonstrated, albeit primarily in hydrological applications, that multiobjective calibration can improve the understanding of a model's structural limitations (Efstratiadis and Koutsoyiannis, 2010; Moore et al., 2011; Price et al., 2012; Wöhling et al., 2013). Therefore, we adopted a multiobjective calibration approach to verify the representation of microbial dynamics in PECCAD based on empirical evidence in the form of multimodal physicochemical and genetic data.

2. Material and methods

2.1. Microcosm experiment

2.1.1. Experimental design

We used topsoil from a loamy Luvisol (WRB 2006) from an agricultural field at the research station Scheyern (Germany; 48°30'N, 11°21'E). The soil was sampled, sieved (<2 mm) and stored in the dark at –20 °C in July 2008. Before use the soil was thawed and its initial gravimetric water content (θ_g) of 27% was reduced to 22% by air drying at 20 °C during an acclimatization period of 10 days in the dark. Then the soil was mixed with unlabeled MCPA (Sigma-Aldrich, PESTANAL®) dissolved in distilled water to give a final concentration of 20 µg/g and incubated at 20 °C in the dark for 29 days. This pre-incubation was carried out to increase the abundance of MCPA-degrading bacteria. The pre-incubated soil ($\theta_g = 22\%$) was then immediately used in the microcosm experiment. It contained some residual MCPA ($0.18 \pm 0.03 \mu\text{g g}^{-1}$), which was considered negligible in relation to the subsequent MCPA amendment. To induce the formation of a detritusphere, we employed a one-to-one mixture of shredded (2–10 mm) maize leaves and stems. See [supplementary Table S1](#) (Supplement 1) for basic soil and litter properties.

We set up three experimental treatments: A) addition of litter (L), B) addition of MCPA (M), and C) combined addition of MCPA and litter (ML). All treatments were performed with four replicates. We prepared a mixture of unlabeled and ^{14}C -labeled MCPA (ring- ^{14}C , >95% radiochemical and chemical purity, Izotop, Hungary) dissolved in distilled water and adjusted to pH 5.3 with NaOH. The pre-incubated soil was then homogeneously spiked with this stock solution. On average we obtained a final MCPA concentration of $53.6 \mu\text{g g}^{-1}$ and a specific ^{14}C activity of 341 Bq g^{-1} (see Online Resource 1 of Pagel et al., 2014). In the litter treatment we only added distilled water to the soil.

The soil was filled to a height of 30 mm into stainless steel cylinders (diameter 56 mm, height 40 mm) and compacted to a bulk density of 1.2 g cm^{-3} . The soil had a volumetric water content of 35%, corresponding to a matric potential of –63 hPa. In L and ML treatments we placed 0.5 g of maize residues (rewetted with 2 ml 0.01 M CaCl_2) as a thin layer on top of the soil cores. Soil cores were placed in airtight microcosms on ceramic plates, which were kept at a defined suction of –63 hPa (Poll et al., 2010b). We incubated the microcosms at 20 °C in the dark. The soil was irrigated with 0.01 M CaCl_2 solution at a rate of 0.2 ml min^{-1} on four events (1.97, 8.92, 14.76 and 21.95 days). In total we applied 13 ml solution, 4 ml at the first irrigation event and 3 ml at each of the remaining three events. Based on a transient simulation of water movement using the Richards equation, we calculated an average water flow rate of 0.191 mm d^{-1} , which was then used to model the steady state water flow with PECCAD.

2.1.2. Analysis of litter and soil pools

We destructively sampled four microcosms of each treatment after 4.9, 7.8, 10.0, 13.9 and 22.8 days. After removing the litter layer the soil cores were immediately frozen at –20 °C. They were then sliced using a cryostat microtome (HM 500 M, MICROM International GmbH, Walldorf, Germany) in 0–1, 1–2, 2–3, 3–4, 4–6, 6–10 and 10–20 mm layers. To obtain sufficient material for analyses, we combined and homogeneously mixed the soil from the associated layers of two soil cores. This procedure yielded two replicate samples per treatment, layer and sampling date derived from four replicate soil cores.

Residual MCPA in soil was extracted by agitation of 1.5 g soil with a 7.5 mL methanol/ H_2O (1:1 by volume) solution in 15 mL centrifuge tubes (polyethylene) on a horizontal shaker at 200 rpm

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