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Modelling the fate of PAH added with composts in amended soil according to the origin of the exogenous organic matter

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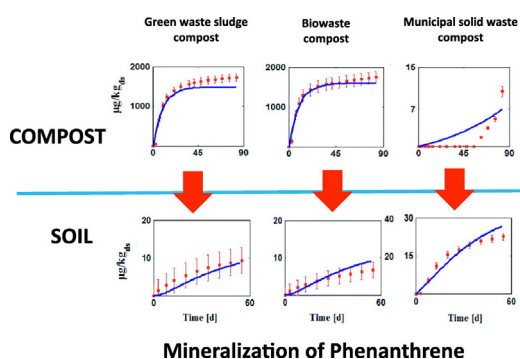
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HIGHLIGHTS

- The model simulates the release of PAH from compost in soil according to organic carbon degradation.
- Processes that occur before compost application to the soil influenced the fate of PAHs in the soil.
- The PAH dissipation was higher in incubations of mature composts.
- The PAH dissipation was higher in incubations of soil amended with non-mature composts.
- The model calculates the proportion of biogenic and physically bound residues of PAHs.

GRAPHICAL ABSTRACT



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ABSTRACT

A new model that was able to simulate the behaviours of polycyclic aromatic hydrocarbons (PAH) during composting and after the addition of the composts to agricultural soil is presented here. This model associates modules that describe the physical, biological and biochemical processes involved in PAH dynamics in soils, along with a module describing the compost degradation resulting in PAH release. The model was calibrated from laboratory incubations using three ¹⁴C-PAHs, phenanthrene, fluoranthene and benzo(a)pyrene, and three different composts consisting of two mature and one non-mature composts. First, the labelled PAHs were added to the compost over 28 days, and spiked composts were then added to the soil over 55 days. The model calculates the proportion of biogenic and physically bound residues in the non-extractable compartment of PAHs at the end of the compost incubation to feed the initial conditions of the model for soil amended with composts. For most of the treatments, a single parameter set enabled to simulate the observed dynamics of PAHs adequately for all the amended soil treatments using a Bayesian approach. However, for fluoranthene, different parameters that were able to simulate the growth of a specific microbial biomass had to be considered for mature compost. Processes that occurred before the compost application to the soil strongly influenced the fate of PAHs in the soil. Our results showed that the PAH dissipation during compost incubation was higher in mature composts because of the higher specific microbial activity, while the PAH dissipation in amended soil was higher in the non-mature compost because of the higher availability of PAHs and the higher co-metabolic microbial activity.

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1. Introduction

The recycling of composted organic residues in soils is a practice that is increasingly used in agriculture. It helps to prevent the loss of soil fertility by restoring soil organic matter contents as well as improving soil physical properties (Annabi et al., 2011; Goss et al., 2013; Mohammed et al., 2016; Tejada et al., 2009). However, certain organic pollutants, among them polycyclic aromatic hydrocarbons (PAH), may be present in the feedstock materials of these composts, leading to a soil contamination risk when they are recycled in agricultural areas (Brändli et al., 2005; Wilcke, 2000; Wild et al., 1991). It is of special importance to understand the dissipation of PAH that is added to soils with composted organic residues.

A number of studies have addressed the impact of compost applications on PAH-contaminated soils (as Puglisi et al., 2007; Zhang et al., 2012). They reported that compost application promotes both the formation of sequestered fractions of PAHs and its biodegradation, leading to the reduction of its concentration in contaminated soils. However only a few studies have addressed the fate of PAH when added to agricultural soils in composts (Haudin et al., 2013; Kästner et al., 1999). Haudin et al. (2013) studied the application of green waste and sludge compost containing different spiked ^{14}C -organic pollutants (and among them one PAH molecule, fluoranthene) on their fates in soil. They found that their dynamic in soil depended on the pollutant properties but also on its distribution between the available and non-available fractions in the composts that enter the soil. Little is known about the impact of the composting process and the final quality of composts on the fate of PAHs in soil according to their physico-chemical properties.

A number of models have been developed to explore the fates of organic pollutants in amended soils (e.g., Morais et al., 2013; Wu et al., 2013; Zarfl et al., 2009), but models that consider the impacts of organic matter decomposition on the sorption and degradation of the pollutants explicitly are very scarce. Lashermes et al. (2013) simulated the mineralization of four organic pollutants during the composting of green waste and sludge. Geng et al. (2015) simulated the mineralization of these four organic pollutants after their incorporation with compost into the soil. Both studies show the broad interest in simulating the explicit interactions between pollutants and organic matter in models. The impact of the composting process and the type of composted organic matter on the organic pollutant's fate after its addition to the soil has never been simulated.

The aims of the present work were threefold: (i) use an experimental approach to study the impact of the compost quality (for three composts consisting of green waste and sludge compost, biowaste compost, and municipal solid waste compost) on the fate of PAHs in composts and after compost applications to soil for three different ^{14}C -labeled PAHs (phenanthrene, PHE, fluoranthene, FLT and benzo(a)pyrene, BAP), (ii) propose a new coupled model to study the dynamics of PAHs in soil-compost mixture systems that explicitly accounts for the type of organic amendments on the fate of the PAHs during the decomposition of compost in the soil and (iii) calibrate the model with the experimental data and compare the kinetics of mineralization and dissipation for each PAH according to the compost quality.

2. Modelling

2.1. Model description

2.1.1. General structure

The PAH model is made of the following 3 modules: a PAH biodegradation/adsorption module, an OC (organic carbon) module and a PAH release module (Fig. 1 and Table A1). The structure of the PAH biodegradation/adsorption module is based on the model described by Brimo et al. (2016). The specific module of the OC dynamic and its interaction with the PAH module were added according to the models developed in

Lashermes et al. (2013) and Geng et al. (2015) that simulate the interactions between organic matter and organic pollutant (such as PAHs) dynamics during composting and after compost application to the soil. The novelty of our model here is that we add a PAH release module to simulate the release of PAHs from compost into soil during the decomposition of the compost.

The PAH biodegradation/adsorption module associated with the OC module is able to simulate the fate of PAH dynamics during compost incubation. The PAH biodegradation/adsorption module alone is able to simulate the PAH dynamic in soil without compost, and the 3 modules together are built to simulate the PAH dynamic in soils amended with compost.

In our previous model described in Brimo et al. (2016) the biological and chemical mechanisms controlling PAH behaviours in soil are modelled using two sub-modules as shown in Fig. 1: the adsorption module and the biodegradation module. The adsorption module is based on a bi-phasic first-order kinetic model with an initial fast kinetics characterized by weak sorption (PAH_{WS} , where “ws” refers to weakly sorbed), and a slower kinetics with strong sorption (PAH_{SS} , where “ss” refers to strongly sorbed). The biodegradation module assumes that biodegradation uses only the soluble PAH (PAH_{AV} , where “av” refers to available) with specific degradation pathways from a specific microbial biomass (B_{SPE}) whose growth and maintenance is described by the Monod equation (as indicated by dotted lines in Fig. 1) and co-metabolic degradation pathways modelled using second-order kinetics from the microbial biomass that degraded the compost (X_{CP}) (dashed lines in Fig. 1). The degradation of PAH produces CO_2 emissions (PAH_{CO_2}), metabolites (PAH_{MET}), and biogenic non-extractable residues (PAH_{BS}). The influences of the temperature and the water content on the biological processes are taken into account using the correction factors f_T and f_W for the temperature and the water content, respectively (see Table A1 in SI).

The OC dynamic module was based on the modules proposed by Lashermes et al. (2013) and Geng et al. (2015), which describe organic matter transformations during composting and during compost decomposition in soil, respectively. The organic carbon in the compost was divided into several pools that were measured using the Van Soest fractionation method and characterized by their specific degradability. All the organic pools are hydrolysed into available substrates (DOC) for the growth of the compost-degrading microbial biomass (X_{CP}) according to their specific hydrolysis constants. The microorganisms die at a specific death rate and the dead cells are recycled into either the compost organic compartment SND_{slow} (with slow degradation rate) or directly into the DOC compartment. Humified organic C (HOC) was assumed to be derived from dead microbial biomass to simulate the “Soil” condition, while for the “compost” condition, this part of the model is not activated and all the dead biomass is recycled. The PAHs available in the PAH_{AV} solution (as calculated in the PAH module) can be degraded through co-metabolism by microorganisms X_{CP} that use the compost organic matter as their primary energy source (as calculated in the OC module). We assumed that the contribution of PAH_{AV} to X_{CP} growth and maintenance can be neglected because PAH_{AV} has low concentrations of PAH compared to the total quantity of organic carbon substrates in the compost. The evolution of the microbial biomass in a soil-compost mixture system is essentially driven by the decomposition of the fresh organic matter that is added with the compost (see explanations in SI 1).

A new PAH Release module was developed in this study to describe the release of the PAHs contained in compost during the decomposition of the compost that was applied to the soil. This module is used only for amended soil incubations and not for composting incubations. The PAH_{CPWS} (where “cpws” refers to PAHs that are weakly sorbed onto organic carbon pools of compost) is subject to dual processes (Fig. 1). We assumed that the PAH is distributed among the OC fractions proportionally to the relative mass of each fraction. One fraction of PAH moves into the soil solution (PAH_{AV}), with the hydrolysis of organic pools of

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