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ENVIRONMENTAL MODELS, MODULES, AND DATASETS

Simulation of Organic Matter and Pollutant Evolution during Composting: The COP-Compost Model

G. Lashermes, Y. Zhang, S. Houot, J. P. Steyer, D. Patureau, E. Barriuso, and P. Garnier*

Organic pollutants (OPs) are potentially present in composts and the assessment of their content and bioaccessibility in these composts is of paramount importance. In this work, we proposed a model to simulate the behavior of OPs and the dynamic of organic C during composting. This model, named COP-Compost, includes two modules. An existing organic C module is based on the biochemical composition of the initial waste mixture and simulates the organic matter transformation during composting. An additional OP module simulates OP mineralization and the evolution of its bioaccessibility. Coupling hypotheses were proposed to describe the interactions between organic C and OP modules. The organic C module, evaluated using experimental data obtained from 4-L composting pilots, was independently tested. The COP-Compost model was evaluated during composting experiments containing four OPs representative of the major pollutants detected in compost and targeted by current and future regulations. These OPs included a polycyclic aromatic hydrocarbon (fluoranthene), two surfactants (4-*n*-nonylphenol and a linear alkylbenzene sulfonate), and an herbicide (glyphosate). Residues of ^{14}C-labeled OP with different bioaccessibility were characterized by sequential extraction and quantified as soluble, sorbed, and nonextractable fractions. The model was calibrated and coupling the organic C and OP modules improved the simulation of the OP behavior and bioaccessibility during composting.

Across Europe in recent years, there has been a huge growth in organic waste treatment by composting (European Communities, 2005), which produces organic amendments useful to improve soil fertility. However, composts may contain organic pollutants (OPs) caused by their presence in the initial feedstock materials (Brändli et al., 2005). The assessment of OP content and bioaccessibility in the final composts is of paramount importance to estimate the environmental impacts after their application to agricultural soils (Bright and Healey, 2003; Semple et al., 2004). Several countries have established a legal framework for OP levels in composts; these pollutants include polycyclic aromatic hydrocarbons, polychlorinated biphenyls and polychlorinated dibenzo-p-dioxins/furans (Hogg et al., 2002). New regulations including the limitation of other emergent OPs, such as linear alkylbenzene sulphonates (LAS) or nonylphenol, are under discussion (European Commission, 2000, 2001).

Composting is a complex process during which organic matter is transformed and intense microbial activity strongly influences OP behavior. Organic pollutants can be degraded by microorganisms, depending on the intrinsic recalcitrance of the molecule and the degrading ability of microbial communities (Haderlein et al., 2006). In parallel, OPs can be stabilized through sorption on organic matter, culminating in the formation of nonextractable residues (NER) that remain in the compost after classic analytical extractions procedures (Barriuso et al., 2008). The formation of NER has been found to be influenced by both the extent of sorption (Kästner et al., 1999) and the total microbial activity (Benoit and Barriuso, 1997). Sorption interactions are influenced by the physicochemical nature of OP (Sabljić et al., 1995) and organic matter, such as polarity (Xing et al., 1994), aromaticity, and aliphaticity (Chefetz and Xing, 2009). Sorption is thought to limit the biodegradation of OPs by decreasing their aqueous concentration and reduce

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Abbreviations: CEL, cellulose-like fraction; HEM, hemicellulose-like fraction; LAS, linear alkylbenzene sulfonate; LIG, lignin-like fraction; NER, nonextractable residues; NP, 4-*n*-nonylphenol; OP, organic pollutant; SND, soluble in pH-neutral detergent; TOC, total organic carbon.

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their accessibility to enzymes, microorganisms, and plants (Wauchope et al., 2002). The bioaccessibility of OP residues varies depending on conditions. Organic pollutants, that are extractable with water or another solvent, are considered easily and potentially bioaccessible, respectively (Benoit and Barriuso, 1997). Nonextractable residues are considered inaccessible (Gevao et al., 2000; Reichenberg and Mayer, 2006).

Mathematical models are a helpful tool to conceptualize our understanding of complex processes and to formalize hypotheses on the determining interactions between organic matter, microbial biomass and OPs (Zarfl et al., 2009). Future challenges lie in developing predictive tools to use on composting plants to define composting conditions that optimize OP elimination in the final compost to reach OP levels recommended in regulations and quality labels.

To our knowledge, no model describing OP behavior during composting has been reported in the literature. Nevertheless, mechanisms of sorption–desorption and biodegradation of OPs in soil described in proposed models are likely transposable to composting (Shelton and Doherty, 1997; Saffih-Hdadi et al., 2003). Moreover, models simulating the transformation of organic matter quality and microbial biomass dynamics during composting have been proposed (Kaiser, 1996; Sole-Mauri et al., 2007; Zhang et al., 2012) and can be coupled to OP behavior.

The aim of this work was to propose a model that simulated OP behavior during composting and test whether the representation of organic matter transformation and microbial biomass dynamics improved simulations. This model included a module describing OP behavior that could be coupled to a module describing organic C evolution during composting, as proposed by Zhang et al. (2012). The second objective of this study was to calibrate this new model, named COP-Compost (simulation of Carbon and Organic Pollutant evolutions during Composting), to simulate the behavior of four OPs that are representative of some of the major groups detected in compost and targeted by current and future regulations. These OPs include polycyclic aromatic hydrocarbon (fluoranthene), two surfactants [4-*n*-nonylphenol (NP) and a linear alkylbenzene sulfonate (LAS)], and an herbicide (glyphosate). The calibration was performed using data of composting experiments that incorporated ^{14}C-labeled OP (Lashermes et al., 2010; Lashermes et al., 2012b). This radioisotope was required to differentiate OP behavior pathways (mineralization compared with NER formation).

Description of the COP-Compost Model

The COP-Compost model was programmed in MATLAB (Mathworks, Natick, MA) (Fig. 1, Table 1).

Organic Carbon Module

The module describing organic C evolution during composting and the original set of parameters proposed by Zhang et al. (2012) were included in the COP-Compost model. Briefly, organic C was divided into five pools (C_i, i = 1–5) with decreasing degradability. Following first order kinetics with specific hydrolysis constants, these organic pools were hydrolyzed into one organic pool. This pool was the hot water soluble fraction of total organic C (S_W) and predicted to be the substrate available for microbial growth. The organic C pools [organic C soluble in neutral detergent (SND) and hemicellulose-like (HEM), cellulose-like (CEL), and lignin-like (LIG) fractions] were determined using the Van Soest fractionation method (French standard XPU44–162, AFNOR, 2005). The SND fraction was further divided into two pools with fast (SND-fast) and slow (SND-slow) degradability rates, which represented the heterogeneity of the SND fraction observed during composting that contained easily degradable and recalcitrant substrates (Francou et al., 2008; Peltre et al., 2010). The

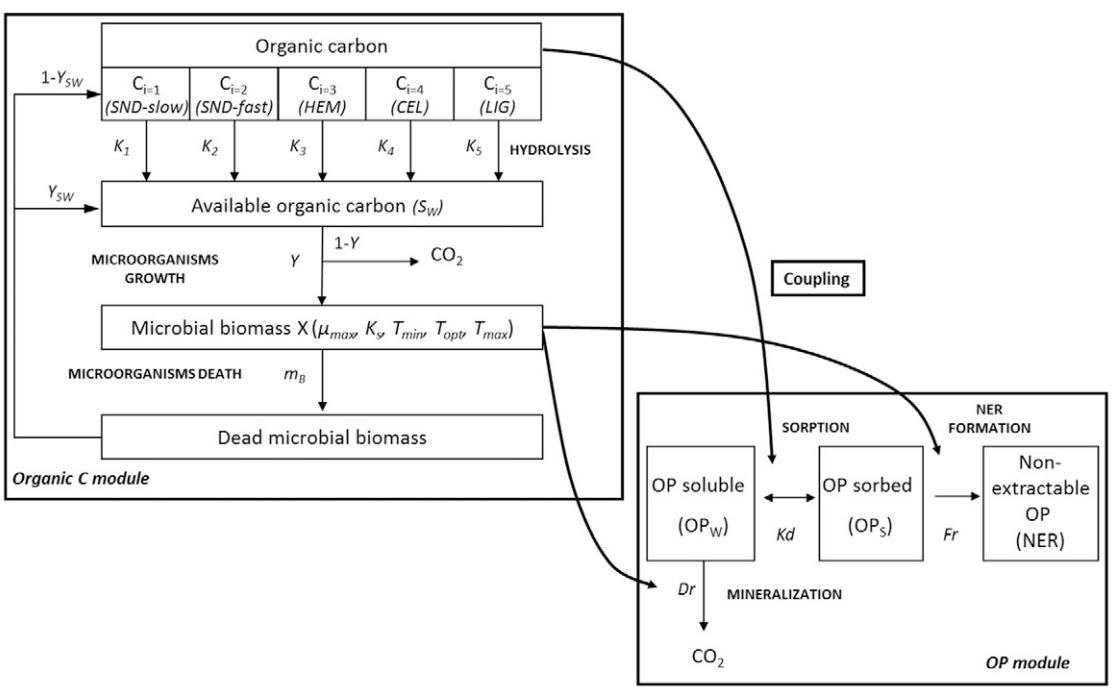

Fig. 1. Carbon flow diagram for the COP-Compost model (simulation of Carbon and Organic Pollutant evolutions during composting). The model includes two modules: one describing organic pollutant (OP) behavior that could be coupled to the module describing organic C evolution during composting proposed by Zhang et al. (2012). Parameters and variables are described in Table 1.

growth of microbial biomass (X) from the available substrate (S_W fraction) was modeled using Monod kinetics using physiological and metabolical parameters. A temperature growth-limiting function was used to modulate microbial growth depending on the minimum, maximum, and optimum temperatures of microbial development (Rosso et al., 1993). A single microbial population was considered because of the lack of experimental data but several microbial biomasses could be represented with varying physiological and metabolical parameters and temperature function. The microbial biomass gradually died off, and the dead cells were recycled into either the SND-slow pool (characterized by a slow hydrolysis rate) or the available substrate (S_W). The original set of parameters was calibrated and validated by Zhang et al. (2012) using composting experiments performed in 170 L pilot that included mixtures of biowaste (Francou et al., 2008) and sewage sludge (Doublet et al., 2011).

Organic Pollutant Module

The model proposed by Saffih-Hdadi et al. (2003) to describe pesticide behavior in soil was simplified and adapted to compost conditions. The composting OP module considered three pools of OPs of decreasing bioaccessibility: soluble, sorbed, and bound to organic matter. The model also considered a compartment of CO_2 arising from OP mineralization. The OP compartments were characterized by successive extractions with water (soluble fraction) followed by another solvent adapted to the properties of the OP (sorbed fraction). Finally, NER were measured after the extractions and represented OP bound to organic matter. The model assumed that NER were produced from sorbed OPs, and OP biodegradation only occurred in the soluble phase, similarly to Saffih-Hdadi et al. (2003). In the model, the remobilization of NER was assumed to be neglected at the timescale of composting. The NER formation and OP biodegradation rates were

Table 1. Variables and parameters in the COP-Compost (simulation of Carbon and Organic Pollutant evolutions during composting) model.

	Symbol	Description	Parameter values†	Unit
		Variables of the model		
Organic C module	$C_{i=1}$ (SND-slow)	Proportion of organic C in the soluble fraction of pH-neutral detergent with slow degradation		% of initial total organic carbon (TOC)
	$C_{i=2}$ (SND-fast)	Proportion of organic C in the soluble fraction of pH-neutral detergent with fast degradation		% of initial TOC
	$C_{i=3}$ (HEM)	Hemicellulose-like fraction		% of initial TOC
	$C_{i=4}$ (CEL)	Cellulose-like fraction		% of initial TOC
	$C_{i=5}$ (LIG)	Lignin-like fraction		% of initial TOC
	C_s (S_W)	Organic C soluble in hot water		% of initial TOC
	X	Microbial biomass		% of initial TOC
	CO_2	Carbon dioxide gas		% of initial TOC
Organic pollutant (OP) module	OP_W (water extract)	Soluble OP in water		% of initial ^{14}C
	OP_S (solvent extract)	Sorbed OP extracted with solvent		% of initial ^{14}C
	NER (nonextractable)	Nonextractable residues OP		% of initial ^{14}C
	C-CO_2	Carbon dioxide gas from OP mineralization		% of initial ^{14}C
		Parameters of the model		
Organic C module	K_1	Hydrolysis constant of $C_{i=1}$ (SND-slow)	0.0179	d^{-1}
	K_2	Hydrolysis constant of $C_{i=2}$ (SND-fast)	0.0612	d^{-1}
	K_3	Hydrolysis constant of $C_{i=3}$ (HEM)	0.0190	d^{-1}
	K_4	Hydrolysis constant of $C_{i=4}$ (CEL)	0.0090	d^{-1}
	K_5	Hydrolysis constant of $C_{i=5}$ (LIG)	0.0001	d^{-1}
	Y	Assimilation yield of organic C available to microbial biomass	0.5	
	μ_{max}	Maximum specific growth rate for microbial biomass	5.9958	d^{-1}
	K_s	Saturation constant for Monod kinetic	101.10	% of initial TOC
	T_{min}	Minimum temperature for microbial growth	0	°C
	T_{opt}	Optimum temperature for microbial growth	49	°C
	T_{max}	Maximum temperature for microbial growth	83	°C
	m_B	Death constant for microbial biomass	0.2290	d^{-1}
	Y_{SW}	Availability yield for dead microbial biomass	0.4	
Organic pollutant (OP) module	K_d	Sorption coefficient of organic C		g sorbed C g^{-1} soluble C
	K_{d1}	Sorption coefficient of $C_{i=1}$		g sorbed C g^{-1} soluble C
	K_{d2}	Sorption coefficient of $C_{i=2}$		g sorbed C g^{-1} soluble C
	K_{d3}	Sorption coefficient of $C_{i=3}$		g sorbed C g^{-1} soluble C
	K_{d4}	Sorption coefficient of $C_{i=4}$		g sorbed C g^{-1} soluble C
	K_{d5}	Sorption coefficient of $C_{i=5}$		g sorbed C g^{-1} soluble C
	Fr	Nonextractable residue formation rate		d^{-1}
	Dr	OP degradation rate		d^{-1}
	NER_0	Nonextractable residues in the initial mixture		% of initial ^{14}C

† The parameter values used for the organic C module were taken from Zhang et al. (2012).

represented by Fr and Dr, respectively. Because the early formation of NER on initial waste mixture has frequently been observed (Michel et al., 1995; Benoit and Barriuso, 1997) a parameter, NER_0, representing initial NER content was included in the model. Moreover, the distribution of OP between the soluble and sorbed pools was an instantaneous equilibrium described using a sorption coefficient (K_d). The OPs were considered a unique pool that included the parent nondegraded molecule and metabolites. When experimental data are available, distinct pools for the main metabolites could be represented in the same way as the parent OPs (Saffih-Hdadi et al., 2003; Zarfl et al., 2009).

Model Coupling Organic Carbon and Organic Pollutant Modules

The two modules could be used separately or coupled. In this case, we assumed and tested three interactions between organic C and OP modules:

- **Interaction 1**: The biochemical nature of an organic substrate influences its degradability as well as the degree of OP sorption (Benoit et al., 1996). The OP sorption capacities of lignin were found to be markedly higher than those of cellulose (Xing et al., 1994). We assumed the overall OP sorption coefficient, K_d, was the weighted mean of the sorption coefficients (K_{di}) in the different organic C pools (C_i, i = 1–5) relative to the proportion of organic C in the pools. This hypothesis was used successfully to evaluate herbicide sorption by plant residues based on their biochemical fractions, such as water soluble, cellulose and lipid compounds fractions (Gaillardon et al., 1983). The change in sorption properties observed during composting because of organic matter transformations and humification was thus simulated with the change in the proportion of organic C fractions.

- **Interaction 2**: OPs can be degraded through classical metabolism by specific biomass modeling with a Monod kinetic. Nevertheless, the biodegradation of OPs in trace concentrations (ng L^{-1}, μg L^{-1}) did not result in any significant biomass growth (Clara et al., 2005). Thus, we assumed that during composting, most OPs were degraded through co-metabolism by microorganisms that used compost organic matter as a primary energy source (Barker and Bryson, 2002; Kocamemi and Çeçen, 2005). The level of OP degradation was predicted to depend on the potential degradability of the chemicals and on the microbial activity driven by organic matter decomposition (Laine et al., 1997).

- **Interaction 3**: The model assumed that the NER were formed through physical and chemical stabilization of OPs in the sorbed phase (Kästner et al., 1999), which brings the OP molecules in contact with the sorption surfaces of organic matter. The formation of NER was assumed to depend on the chemical reactivity of the OPs and microbial activity whose influence has long been reported (Benoit and Barriuso, 1997). The parent chemicals, and the metabolites formed from their degradation, may be stabilized with the establishment of crosslinking reactions with organic matter (Kästner et al., 1999; Barriuso et al., 2008), possibly enhanced by extracellular enzymes secreted by microbial biomass (Gevao et al., 2000).

Equations of the COP-Compost Model

Organic Carbon Module

The organic C dynamic during composting was described using equations based on mass balance and includes a daily time step (Zhang et al., 2012). The unit used was the percentage of initial total organic carbon (TOC) (Table 1). Briefly, the $C_{i=1\text{-}5}$ (SND-slow, SND-fast, HEM, CEL, LIG) organic pools were hydrolyzed to produce available substrate (S_W) with a corresponding rate coefficient of K_i (i = 1–5) according to a first order equation. The equations relating the dynamic of microbial biomass (X) were:

$$\frac{dX}{dt} = \mu X - m_B X \quad [1]$$

where X is the content of microbial biomass, with a microbial growth rate μ and a death rate m_B. The microbial growth rate μ followed Monod kinetics:

$$\mu = \mu_{max} \frac{S_W}{K_S + S_W} f_T \quad [2]$$

where μ_{max} is the specific maximum growth rate, S_W is the content of available substrate, K_S is a saturation constant of the available substrate for microbial biomass and f_T is the growth-rate correcting function that was dependent on the temperature measured in the compost (Rosso et al., 1993). Thirteen parameters and eight variables were needed to run the organic C module (Table 1).

Organic Pollutant Module

The behavior of OPs during composting was described through equations based on OP mass balance using a daily time step. The unit used was the percentage of initial OP applied (^{14}C-labeled OP) (Table 1). In the OP module, the instantaneous equilibrium between soluble (OP_W) and sorbed (OP_S) OPs was described with the following equation:

$$OP_S = K_d \times OP_W \quad [3]$$

where K_d is the sorption coefficient of OPs on the compost organic matter. We assumed that there was no sorption interaction between OPs and soluble organic C.

The OP mineralization ($^{14}C\text{-}CO_2$) depended on the amount of soluble OPs and the biodegradation rate (Dr):

$$\frac{d(^{14}C\text{-}CO_2)}{dt} = Dr \times OP_W \quad [4]$$

In the OP module, the NER formation followed the equation:

$$\frac{dNER}{dt} = NER_0 + Fr \times OP_S \quad [5]$$

where NER_0 is the initial amount of NER and Fr is the NER formation rate. A total of four parameters and four variables were needed to run the OP module (Table 1).

Model Coupling the Organic Carbon and Organic Pollutant Modules

The three interactions were derived into equations. For the OP module considered alone, Eq. [3] represented the instantaneous

equilibrium between soluble and sorbed OPs. However, in the case of model coupling, the sorption coefficient was expressed as:

$$K_{\mathrm{d}} = \sum_{i=1}^{5} K_{\mathrm{d}i} \times \frac{C_i}{\sum_{i=1}^{5} C_i} \quad [6]$$

where K_{d} is the sorption coefficient of OPs by total compost organic C and $K_{\mathrm{d}i}$ is the sorption coefficient of OPs in the pools C_i.

The influence of microbial activity on the ^{14}C-OP mineralization was described by:

$$\frac{\mathrm{d}(^{14}\mathrm{C\text{-}CO_2})}{\mathrm{d}t} = \mathrm{Dr} \times X \times \mathrm{OP_W} \quad [7]$$

where X is the microbial biomass growing on the organic C decomposition and Dr is the biodegradation rate of the OP.

The following equation of NER formation was first tested:

$$\frac{\mathrm{dNER}}{\mathrm{d}t} = \mathrm{NER_0} + (\mathrm{Fr_B} \times X + \mathrm{Fr_C}) \times \mathrm{OP_S} \quad [8]$$

where $\mathrm{Fr_B}$ and $\mathrm{Fr_C}$ are parameters for the NER formation related to biological activity and chemical reactivity of organic matter, respectively. Because the $\mathrm{Fr_C}$ parameter was close to zero in all simulations, the equation of NER formation was simplified:

$$\frac{\mathrm{dNER}}{\mathrm{d}t} = \mathrm{NER_0} + \mathrm{Fr} \times X \times \mathrm{OP_S} \quad [9]$$

where Fr is the rate of NER formation and included both chemical and biological origins. The microbial biomass (X) drove the intensity of the degradation and NER formation (interactions 2 and 3) and consequently appeared as a multiplicative factor of the constant rates in Eq. [8] and [9].

To run the COP-Compost model, a maximum of 21 parameters and 12 variables were needed (Table 1).

Data Used for Model Calibration and Evaluation

The data collected by Lashermes et al. (2010, 2012a, 2012b) were used (i) to test the organic C module with data acquired at a smaller composting scale than originally calibrated and (ii) to propose a calibration of the OP module for each OP. The selected OPs showed contrasted chemical structures, water solubilities with 25×10^4, 1×10^4, 7 and 0.36 mg L^{-1} for LAS, glyphosate, NP, and fluoranthene, respectively (PHYSPROP database, Syracuse Research Corporation). All data were acquired from composting experiments using the same reactor system, initial mixture and procedure.

Composting Setup

The initial waste mixture contained aerobic digested sewage sludge, branches, grass clippings, hedge trimmings, and roughly ground leaves. The branches were hand-cut into 4-cm pieces, and the leaves and privet trimmings were roughly ground to centimetric size. The composting system comprised 4-L glass reactors surrounded by an external heating system. During the first 6 d, the temperature increased by self-heating, then the temperature was modulated to mimic a typical composting temperature profile. The composting mixtures were sampled at the end of the thermophilic phase (day 13), at the end of the cooling phase (day 41) and at the end of the maturation phase (day 83).

Data Used for Organic Carbon Module Evaluation

Data used to evaluate the organic C module were acquired during a set of six replicated composting experiments performed without the addition of ^{14}C-OP at the beginning of composting (Lashermes et al., 2012a). The data contained the Van Soest biochemical fractionation performed on the initial mixture and on the compost sampled during composting on 3 dates (13, 41, and 83 d): the S_{W} fraction (water, 100°C, 30 min), the SND fraction (neutral detergent, 1 h), and the HEM, CEL, and LIG fractions obtained according to French standard XPU 44–162 (AFNOR, 2005). All fractions were expressed as a percent of initial total organic C. The amount of mineralized organic C was calculated as the difference between the TOC in the initial mixture and the TOC remaining in the reactor at the sampling date. Because a standardization of a method for microbial biomass determination in compost has not been yet established (Fourti et al., 2011), the microbial biomass was indirectly characterized measuring the microbial activity through the O_2 consumption and CO_2 respiration and its efficiency assessing substrate transformation (Lashermes et al., 2012a).

Data Used for Organic Pollutant Module Calibration

The same composting experiment was first used to determine the sorption coefficient (K_{d}) (g sorbed C/g soluble C) on fresh compost (Lashermes et al., 2010). Compost samples were shaken for 24 h in a ^{14}C-OP solution. Then, water extracts were recovered by centrifugation and the ^{14}C-activity in the supernatant was measured by liquid scintillation counting. The K_{d} was determined as the ratio between the proportion of sorbed ^{14}C-OP and the proportion of initial ^{14}C-OP in solution after equilibration. K_{d} determined on samples of mature compost rather than on initial waste mixture were chosen for model calibration because this analysis is the easiest realizable for further OPs.

Other set of composting experiments with initial artificial contaminations of ^{14}C-OP were used to characterize the OP behavior or distribution during composting (Lashermes et al., 2012b). These experiments were performed in triplicate for each ^{14}C-OP. The mineralized ^{14}C-CO_2, the volatile organic compounds and the produced leachates were analyzed. Sequential extractions were performed on fresh samples of initial waste mixture and compost. Two fractions were extracted with (i) MilliQ water (24-h shake extraction) and (ii) methanol (or ammonium hydroxide solution to measure glyphosate) (22-h, 20-h, 6-h successive shake extractions). Each extracts were recovered by centrifugation and their ^{14}C-OP content was measured by liquid scintillation counting. Finally the remaining nonextracted radioactivity (corresponding to the NER) was determined by scintillation counting of the ^{14}C-CO_2 evolved after combustion of the extracted compost residues. At each sampling date, the percentages of ^{14}C-activity in the different fractions were calculated based on the total recovered ^{14}C-activity at the sampling date (sum of ^{14}C in the different fractions).

Model Evaluation and Calibration

Evaluation of the Organic Carbon Module

The total root mean square error was first used to evaluate the simulations of the organic C module (RMSE-$\mathrm{OC_{tot}}$). The

RMSE-OC_{tot} is defined as the sum of all the RMSE-OC(j) values calculated between the experimental and simulated values of the j variables of the organic C module (j = 1–6 for the SND, HEM, CEL, LIG, S_W fractions, and for CO_2 production) (Smith et al., 1997), as follows:

$$\text{RMSE-OC}(j) = \frac{100}{\overline{E(j)}} \times \sqrt{\sum_{i=1}^{n} \frac{(S(j)_i - E(j)_i)^2}{n}} \quad [10]$$

where n is the number of measurement dates, $S(j)_i$, and $E(j)_i$ are the simulated and experimental values of variable j, respectively. $\bar{E}(j)$ is the average of n experimental values. The best simulation produced the lowest RMSE-OC_{tot}.

Calibration of the Organic Pollutant Module

The parameters of the OP module were optimized for each composting experiment to minimize the difference between simulated and experimental values of OP behavior. The optimization was performed using the *fmincon* function of the MATLAB Optimization Toolbox (Mathworks, Natick, MA), which applies a sequential quadratic programming algorithm. The objective function was the total root mean square error (RMSE-OP_{tot}) defined as the sum of all the RMSE-OP(j) calculated between the experimental and simulated values of the j variables (j = 1,4 for the soluble and sorbed fractions, NER and CO_2) (Eq. [10]). Two statistical criteria were used in complement to evaluate the simulations (Smith et al., 1997). The efficiency coefficient, E_f, compared the efficiency of the model with the efficiency of describing the data as the mean of the observations. E_f can be negative or positive with a maximum value of 1, a positive value indicating that the model is better than the mean of the observations. The mean difference, $\overline{D}$, was the sum of the differences between simulated and measured values giving an indication of the bias in the simulations.

Four sets of simulations (A, B, C, D) were conducted. The first (Set A) was performed with the OP module only; organic C evolution had no influence on the parameters. Sets B, C, and D coupled the OP and organic C modules. In all sets of simulations, the NER formation rate (Fr) and the OP degradation rate (Dr) were optimized; the sorption coefficient (K_d) was treated differently:

- In Set A (without coupling) and Set B (with coupling), experimental K_d values determined on mature compost samples were used as fixed values for the K_d parameter.
- In Set C, the same K_d parameter was considered for all pool C_i (i.e., $K_d = K_{d1} = K_{d2} = \ldots = K_{dS}$) and was optimized for each OP.
- In Set D, the values of the sorption coefficients K_{di} on the organic C pool C_i were optimized for each OP (with $K_{d1} = K_{d2}$ for the neutral detergent soluble pools SND-slow and SND-fast).

The sum of RMSE-OP_{tot} obtained in a set of simulations was multiplied by the number of parameters requiring optimization to assess the overall performance of the simulations. The objective was to limit the number of parameters requiring optimization to not complicate the modeling effort. The best set of simulation, producing the lowest weighted sum of RMSE-OP_{tot}, was selected, and median values of the parameters obtained for the three replicated composting experiments for each OP were used for model calibration.

Relationships between parameters of the OP module (Dr and Fr) and experimental data were examined to assess the parameters values for further OPs.

Sensitivity Analysis

A sensitivity analysis was conducted to test the behavior of the COP-Compost model. The model sensitivity was explored using the original set of parameters of the organic C module and the set of parameters proposed in this study for the OP module as baseline. The effect of the individual changes of these 14 parameters was investigated on the simulated value of (i) the OP fraction potentially bioaccessible (soluble + sorbed), (ii) the cumulative ^{14}C-CO_2 mineralized, and (iii) the NER fraction. The sensitivity coefficient, σ_P, for the parameter, P, as previously defined (Myint et al., 2007), was calculated to quantify the average spread of each of the parameters:

$$\sigma_P = \frac{1}{t_f} \times \int_0^{t_f} \frac{S_{P+\Delta P} - S_P}{S_P} \times \mathrm{d}t \quad [11]$$

where t_f is the test duration, $S_{P+\Delta P}$ is the simulated value predicted by the model when the value of the P parameter changed from the reference value by an amount ΔP and S_p is the simulated value predicted by the model with a reference value for the P parameter. Duration of 83 d and variation of 20% in the value of the P parameter were tested. The average spread of each parameter was calculated considering the three replicates of composting ± standard deviation.

Results and Discussion

Evaluation of the Organic Carbon Module

The original set of parameters for the organic C module was calibrated using eight composting experiments and validated using four independent experiments conducted in 170 L pilots (Zhang et al., 2012). In this study, this calibration was used to simulate the composting experiment performed in 4 L pilots. The average RMSE-OC_{tot} value of 114, calculated from the six composting replicates, was lower than the initial calibration (184) and validation datasets (165) showing an improvement in the simulations for validation at the two composting scales (170 or 4 L). The simulations of organic matter dynamics obtained in this study were within the range of variation of the experimental measurements of the six replicates (Fig. 2). The best simulated pools were LIG, CEL, then SND, attesting to the relevance of the proposed hydrolysis constants for these pools. Mean differences $\overline{D}$ were within the range (−1; 1) (not shown) and showed no important bias in the simulations, except for the S_W pool, which was underestimated, especially at the beginning of composting. Although no data were available to validate the evolution of the microbial pool, the results suggested that the simulated microbial growth on the available substrate was probably too high. If a lower maximum growth rate for microbial biomass (μ_{max}) and a higher saturation constant for the Monod kinetic (K_S) had been used, the available organic C evolution would have better matched the experimental data. Moreover, the simulated amount of microbial biomass reached a peak of 11% of initial TOC after

8 d of composting before declining exponentially. This value could be slightly overestimated in comparison with the peak values reported in the literature of 1 to 7.5% (Hellmann et al., 1997; Ntougias et al., 2006). Nevertheless, the parameterization proposed by Zhang et al. (2012) gave satisfactorily simulations of organic matter transformation and could be validated at the scale of composting (4 L), which was different from that initially used for model calibration (170 L).

Calibration of the Organic Pollutant Module

Comparison of the Different Simulation Sets

Simulations generally improved from Set A to Set D, as shown by the decrease in the sum of RMSE-OP_{tot} (Table 2). One example of the different sets of simulations with a median goodness of fit is presented in Fig. 3 for LAS.

Coupling with the organic C module enabled the best improvement in simulat_ion. Indeed, the most marked decrease in the sum of RMSE-OP_{tot} was found between Sets A (without coupling) and B (with coupling); both sets used an experimental K_d as fixed values for the K_d parameter while Fr and Dr were optimized. For Sets A and B, the evolution of fluoranthene distribution was the best simulated (average RMSE-OP_{tot} of 78 and 61, respectively) and NP gave the poorest fits (average RMSE-OP_{tot} of 117 and 87, respectively). This poor result probably resulted from an experimental K_d value too high.

When optimizing a single K_d parameter for all C_i pools (Set C), the optimized K_d values were twice as low as the experimental values for NP, and the simulated amount of soluble NP matched the experimental observations, as was also the case for LAS. For fluoranthene and glyphosate, a small difference was observed between the experimental K_d (used in Sets A and B) and the optimized K_d (Set C). For the two surfactants (LAS and NP), the experimental K_d measured on mature compost were higher than the optimized value required by the model, the experimental K_d measured on initial mixture being even higher than on mature compost (Lashermes et al., 2010).

The optimization of four K_{di} parameters for the C_i pools (Set D) further improved the simulation when compared with Set C. Nevertheless, the benefits were not so important when considering the number of parameters (six) optimized in Set D compared with Set C (only three optimized parameters). Moreover, the K_{di} parameters were correlated and several different combinations produced simulations of similar quality, which made it difficult to interpret the effect of the sorption coefficient K_{di} for each C_i pool. Data of sorption coefficients measured independently on initial organic mixtures with different biochemical nature would have more constrained the model.

Selection of the Best Set of Parameters to Calibrate the Model

Set B appeared to produce the most efficient simulations. Indeed, when optimizing only two parameters (Dr and Fr), it produced the lowest weighted sum of RMSE-OP_{tot} (Table 2). The simulated amounts of soluble and sorbed fractions, NER and mineralized OP in Set B accounted for more than 86% of the variability of the corresponding experimental values (Fig. 4). This result confirmed that the COP-Compost model was able to satisfactorily simulate the experimental behavior of each OP studied. The best simulated pools were the NER and mineralized ^{14}C-CO_2 with average E_f values of 0.99 ± 0.01 and 0.93 ± 0.07, respectively (Table 3). In addition, both the low average $\overline{D}$ ($\overline{D}$ ± standard errors) of 0.7 ± 1.3% of the initial ^{14}C for NER and 0.9 ± 1.1% for mineralized ^{14}C-CO_2 simulations indicated no bias in the simulations of these pools using the model. The simulations also agreed with the experimental evolution of sorbed OPs, with an average E_f of 0.85 ± 0.19. However, $\overline{D}$ values indicated that the model overestimated the sorbed amount of LAS when compared with experimental data. The quality of the fit of the soluble pool was satisfactory for glyphosate (average E_f = 0.89), intermediate for fluoranthene (average E_f = 0.20) (mainly because of heterogeneous experimental data), and poor for the two surfactants (average E_f = −1.03 for LAS and E_f = −6.04 for NP), because of the high K_d values used for simulation which corresponded to experimental

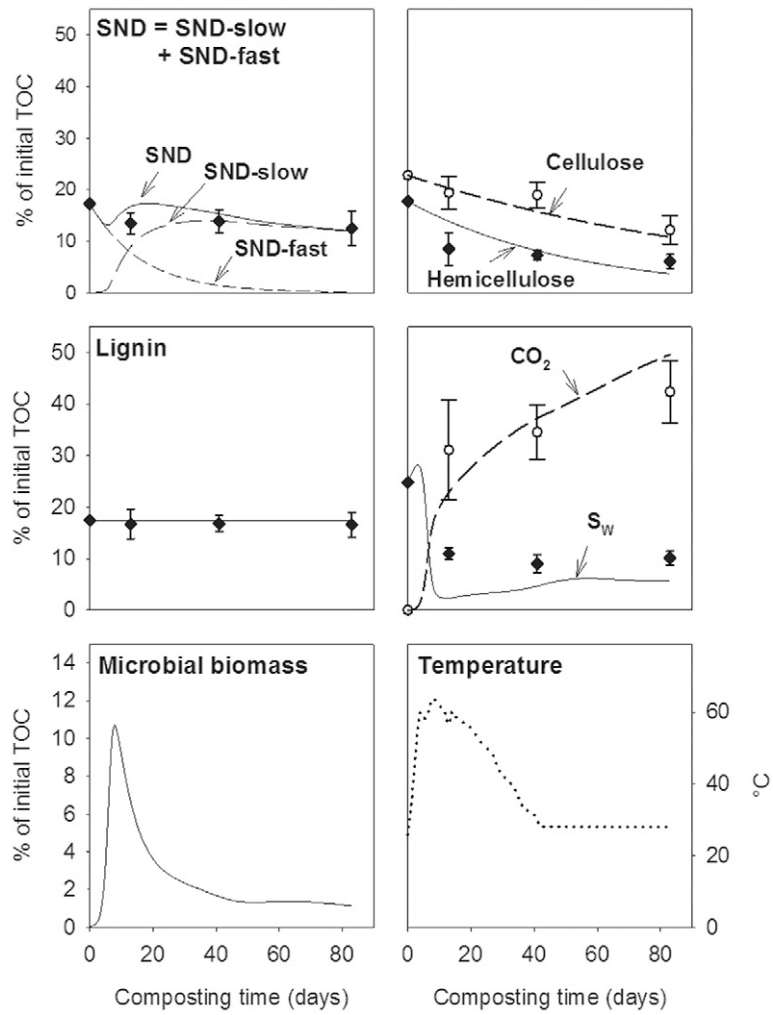

Fig. 2. Experimental (symbols) and simulated (solid and dashed lines) data on biochemical fractions, carbon dioxide, simulated microbial biomass, and experimental temperature (dotted line) during composting. The simulations were obtained using the organic C module parameterized by Zhang et al. (2012). The symbols represent the mean ± standard errors of experimental values of the six composting replicates. SND is pH-neutral detergent soluble fraction; SND-slow and SND-fast are the proportions of pH-neutral detergent soluble fraction with respectively slow and fast degradation; S_W is hot water-soluble fraction.

Table 2. Parameter values and statistics of the organic pollutant (OP) module for the four sets of simulations A, B, C, and D (units are given in Table 1). Data are for three independent 83-d replicated composting experiments 1, 2, 3 for each OP.

Set of Simulations†	Model Coupling		Glyphosate			LAS			Fluoranthene			4-*n*-Nonylphenol			Sum	Weighted Sum‡
			GLY-1	GLY-2	GLY-3	LAS-1	LAS-2	LAS-3	FLT-1	FLT-2	FLT-3	NP-1	NP-2	NP-3		
A, B, C, D		NER_0		3.9			4.6			5.4			27.4			
A	no	K_d		0.9			4.8			21.9			6.4			
Experimental K_d§		Fr	0.020	0.028	0.060	0.004	0.006	0.004	0.002	0.005	0.004	0.030	0.030	0.023		
		Dr	0.009	0.019	0.032	0.103	0.208	0.185	0.001	0.002	0.001	0.255	0.380	0.326		
		$RMSE\text{-}OP_{tot}$¶	103	101	113	86	105	109	70	49	116	105	112	134	1203	2406
B	yes	K_d		**0.9**#			**4.8**			**21.9**			**6.4**			
Experimental K_d		Fr	**0.0066**	0.0065	0.0127	**0.0011**	0.0014	0.0009	0.0007	0.0016	**0.0013**	0.0061	0.0043	**0.0044**		
		Dr	0.0027	**0.0044**	0.0069	0.0263	**0.0335**	0.0360	0.0002	0.0005	**0.0004**	0.0483	**0.0500**	0.0550		
		$RMSE\text{-}OP_{tot}$	81	51	84	115	68	75	58	45	80	81	75	103	915	1831
C	yes	K_d	1.0	1.0	1.5	2.9	2.5	2.7	23.2	21.5	15.0	3.1	3.2	2.5		
Optimization of K_d (single value)		Fr	0.0062	0.0061	0.0090	0.0012	0.0017	0.0011	0.0007	0.0016	0.0014	0.0062	0.0056	0.0047		
		Dr	0.0028	0.0043	0.0087	0.0175	0.0210	0.0249	0.0002	0.0005	0.0003	0.0252	0.0328	0.0239		
		$RMSE\text{-}OP_{tot}$	79	49	70	82	50	59	57	45	63	63	59	67	743	2228
D	yes	$K_{d1} = K_{d2}$ (SND)	0.0	1.4	0.1	0.0	2.7	10.0	68.4	38.5	42.2	3.0	9.1	8.5		
Optimization of the K_{di} (i = 1–5)		K_{d3} (HEM)	0.3	0.0	0.0	0.0	8.9	6.8	14.3	28.4	15.0	12.2	0.0	0.0		
		K_{d4} (CEL)	0.0	0.0	4.5	8.7	0.0	0.0	26.7	29.0	15.4	0.0	1.0	4.0		
		K_{d5} (LIG)	3.0	2.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	6.7	0.0		
		Fr	0.0062	0.0061	0.0090	0.0012	0.0017	0.0011	0.0007	0.0016	0.0014	0.0062	0.0056	0.0047		
		Dr	0.0028	0.0043	0.0087	0.0175	0.0210	0.0249	0.0002	0.0005	0.0003	0.0252	0.0328	0.0239		
		$RMSE\text{-}OP_{tot}$§	75	48	68	79	43	57	57	44	60	56	58	66	711	4268

† In all sets of simulations, Fr and Dr were optimized.

‡ Sum of $RMSE\text{-}OP_{tot}$ multiplied by the number of parameters requiring optimization.

§ Values of experimental K_d were determined on mature compost samples, from Lashermes et al. (2010).

¶ Total root mean square error of the OP module, $RMSE\text{-}OP_{tot}$.

Parameter values highlighted in bold are the value proposed for the model calibration for each OP.

measurements on mature composts. This experimental K_d value was used because it is an easily accessible characteristic. Nonetheless, in the case of surfactants, analyses must be performed with particular care.

Median values of Fr and Dr parameters obtained during Set B were used to calibrate the COP-Compost model for the four studied OPs (see bold letters in Table 2). The simulated evolution of OP distribution during composting obtained with this calibration agreed with experimental data (Fig. 5). In some cases, the sum of the measured fractions was lower than 100%, where volatilization and leaching were observed experimentally. These values were not taken into account by the model, which explains the differences between simulated and experimental pools in these cases. The NER formation from glyphosate was slightly overestimated by the model at the beginning of composting, but the simulated amount of NER in mature compost (39% of initial ^{14}C) remained in agreement, as did the sorbed amount of ^{14}C-residues (14%) and the mineralized ^{14}C-CO_2 (30%). However, soluble ^{14}C-residues of glyphosate in mature compost were overestimated by the model (17% of initial ^{14}C) compared with experimental data (median of 9% of recovered ^{14}C). For LAS, the simulated amount of sorbed ^{14}C-residues in mature compost was overestimated (18% of initial ^{14}C) and the corresponding experimental median value was 5% of recovered ^{14}C. The simulated amounts of soluble ^{14}C-residues in mature compost (4% of initial ^{14}C), the NER (13%) and the mineralized ^{14}C-CO_2 (65%) all matched experimental observations. The evolution of fluoranthene distribution was well simulated; no mineralization was simulated and soluble ^{14}C-residues accounted for 3% of initial ^{14}C, the sorbed fraction for 68% and NER for 29%. For NP, NER were slightly overestimated in mature compost (54% of initial ^{14}C), while only 45% of recovered ^{14}C was observed forming NER under experimental conditions. However, the amounts of soluble ^{14}C-residues

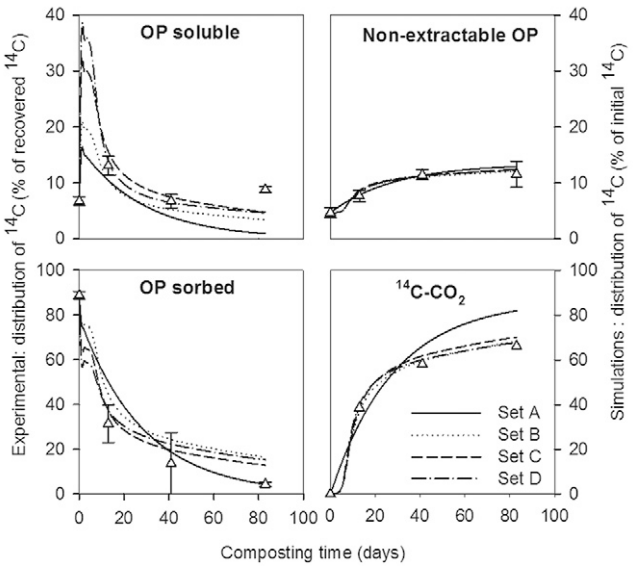

Fig. 3. Experimental (symbols) and simulated (lines) data on soluble, sorbed, nonextractable, and mineralized linear alkylbenzene sulfonate (LAS) during composting. The simulations were obtained successively with sets A, B, C, and D for replicate number 2 of the LAS experiment that presented a median quality of fitting. Symbols represent experimental values ± standard errors.

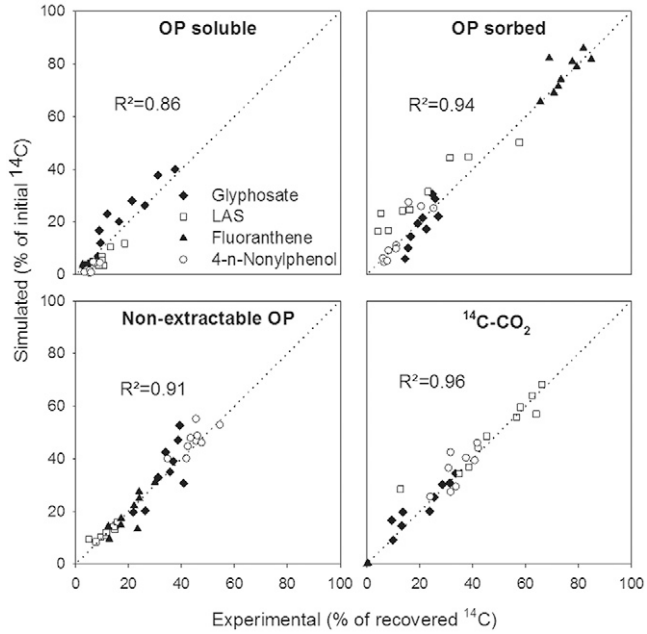

Fig. 4. Relationships between experimental and simulated values for soluble, sorbed, nonextractable and mineralized organic pollutants obtained during set B of simulations with the best efficiency. The dotted line is the 1:1 line.

in mature compost (1% of initial ^{14}C), sorbed fraction (5%), and mineralized $^{14}C\text{-}CO_2$ (39%) were satisfactorily simulated.

The parameters estimated from the four OPs were linked to their chemical properties. The LAS, whose structure presents a single aromatic ring and low reactivity, had a high mineralization rate Dr and the lowest rate of NER formation Fr. The glyphosate and NP, which have also a simple structure but a high chemical reactivity with functional groups such as carboxylic, amino, phosphate and phenolic groups had the highest Fr parameter (Gevao et al., 2000; Kästner et al., 1999). The NP showing a higher Dr parameter than the glyphosate. In contrast, the fused aromatic ring structure of fluoranthene without any reactive functional groups had a low Fr and the lowest Dr. The fluoranthene showed the highest sorption coefficient K_d and remained potentially bioaccessible in the sorbed phase rather than in the soluble phase. The amount of water soluble residues considered directly bioaccessible were generally small, suggesting a low risk linked with direct OP assimilation by plants or leaching in soils.

Evaluation of Organic Carbon and Organic Pollutant Coupling Hypotheses

The hypothesis of the overall sorption coefficient K_d as the sum of K_{di} sorption coefficients in different organic C pools (interaction 1) could not be supported by the results of this study. However, the sorption properties of organic substrates do undergo change during composting because of organic

Table 3. Statistics to evaluate the simulations obtained using the coupled model during the most efficient set of simulations (set B). The parameter values used for simulations in set B are reported in Table 2.

Statistics	Organic pollutant fraction	Glyphosate			LAS			Fluoranthene			4-*n*-Nonylphenol		
		GLY-1	GLY-2	GLY-3	LAS-1	LAS-2	LAS-3	FLT-1	FLT-2	FLT-3	NP-1	NP-2	NP-3
RMSE-OP†	OP‡ soluble	7	30	17	38	44	35	20	12	31	53	38	59
	OP sorbed	15	7	20	24	18	30	3	2	9	4	24	12
	NER‡	21	7	31	25	4	6	16	7	28	12	4	9
	$^{14}C\text{-}CO_2$	38	6	16	29	2	4	19	24	11	13	10	23
	$RMSE\text{-}OP_{tot}$	81	51	84	115	68	75	58	45	80	81	75	103
$\bar{D}$ §	OP soluble	1.6	6.4	2.0	−3.3	−3.6	−2.4	0.2	−0.1	−1.1	−2.6	−1.6	−3.3
	OP sorbed	−1.0	0.2	−3.4	4.7	5.9	9.0	0.2	0.6	3.1	−0.2	3.0	0.4
	NER	0.5	0.4	2.9	0.7	0.2	0.2	−0.3	−0.1	−1.6	2.7	0.6	2.1
	$^{14}C\text{-}CO_2$	0.7	0.7	1.6	3.0	0.1	0.4	0.0	0.0	0.0	1.5	0.2	2.7
E_f¶	OP soluble	0.96	0.76	0.94	0.22	−2.89	−0.42	0.48	0.69	−0.57	−11.63	−0.94	−5.56
	OP sorbed	0.82	0.98	0.87	0.89	0.95	0.90	0.58	0.96	0.36	1.00	0.94	0.98
	NER	0.99	1.00	0.98	0.99	1.00	1.00	0.99	1.00	0.98	1.00	1.00	1.00
	$^{14}C\text{-}CO_2$	0.77	0.99	0.95	0.88	1.00	1.00	0.93	0.92	0.97	0.96	0.97	0.85

† Root mean square error of the organic pollutant fractions.

‡ OP, organic pollutant; NER, nonextractible residues.

§ Mean difference (as a percent of initial ^{14}C).

¶ Efficiency coefficient.

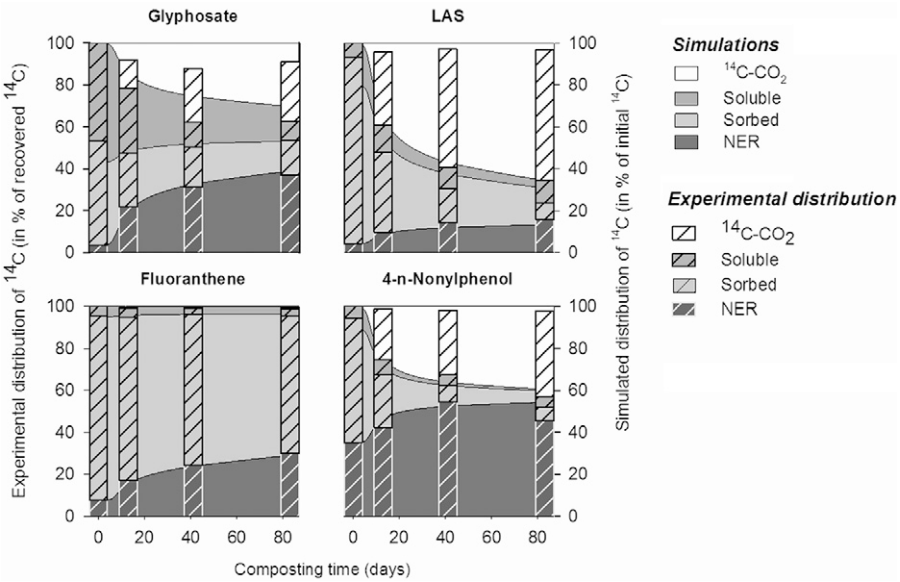

Fig. 5. Experimental and simulated distribution kinetics during the composting of ^{14}C between mineralized, soluble, sorbed and nonextractable residues (NER) fractions from ^{14}C-labeled glyphosate, linear alkylbenzene sulfonate (LAS), fluoranthene, and 4-*n*-nonylphenol (NP) applied at the beginning of composting experiments. Simulations were performed using parameters proposed for the COP-Compost (simulation of Carbon and Organic Pollutant evolutions during composting) model calibration (see parameters in Table 2, in bold letters) and were obtained for replicates that presented a median quality of simulations. Area plots represent simulations. Hatched histograms represent experimental values.

matter transformation and humification but contradictory results were found. Both an increase (Benoit et al., 1996) and decrease (Oleszczuk, 2009; Lashermes et al., 2010) in sorption properties were observed. Thus, taking into account in the model the variations in the sorption properties of the organic matter undergoing composting would certainly improve the simulations of the soluble and sorbed pools. Further research on the influence of different initial waste mixtures with contrasted biochemical properties on the OP behavior during composting should help evaluate this hypothesis.

On the other hand, it was possible to accept the second hypothesis of microbial biomass being active in OP degradation. The description of the composting process, as initially proposed by Kaiser (1996), was shown to be relevant to the simulation of OP behavior. When the influence of total microbial biomass size was considered, the mineralization of the four studied OPs was satisfactorily simulated by the coupled model. The limitation of considering a single microbial biomass was previously reported (Sole-Mauri et al., 2007), especially if one considers that the different microbial populations that occur during the process have contrasted capacities for OP mineralization (Haderlein et al., 2006). The model could be improved by the addition of microbial populations with different growing conditions and contrasted abilities to degrade OPs.

The third hypothesis specifying that NER formation was dependent of the chemical reactivity of the OP and microbial activity could satisfactorily simulate the NER dynamics in the coupled model. Nevertheless, in the COP-Compost model the simulated NER pool implicitly included different types of binding between the organic matrix and the OP from the sorbed phase. The NER formation directly from the soluble phase could also be tested in the future, as proposed by Zarfl et al. (2009). Additional mechanisms of NER formation, including the fixation of ^{14}C-CO_2 mineralized from ^{14}C-OP (Kästner et al., 1999) and ^{14}C-activity incorporation in the growing biomass (Barriuso et al., 2008), were not represented. These mechanisms, as well as the chemical stabilization, are likely to be irreversible and involve OP whose highly transformed structure could probably not be identified anymore (Kästner et al., 1999). In contrast, the NER formation could also result from strong sorption interactions and be more reversible (Zarfl et al., 2009). The mild extraction procedure employed in this work could have led to measure a proportion of potentially reversible NER. At the timescale of composting, the remobilization of NER could not be clearly demonstrated (Hartlieb et al., 2003; Lashermes et al., 2012b) but if the COP-Compost model was expanded to model the evolution of OP availability in soil after compost spreading, remobilization should be represented. Moreover the model took into account NER_0, the content of NER in the initial mixture rapidly formed. This parameter represented the abiotic sorption or sequestration that occurred during the extraction procedure (48 h in this study) (Benoit and Barriuso, 1997) whereas the NER formed from the sorbed phase during composting was dependent of the biochemical transformation of the organic matter and the biological activity.

Assessment of the Fr and Dr Parameters from Incubation Experiments

Incubations in compost are more accessible than full composting experiments and offered an interesting way to assess values of Fr and Dr parameters for further OPs, even if they also require the use of ^{14}C-labeled OPs. Additional data of potential mineralization of OPs measured during incubation in mature compost samples at 28°C were used (Lashermes et al., 2010). ^{14}C-OPs were added at the beginning of the incubation, the ^{14}C-CO_2 produced was trapped in NaOH plugs and the ^{14}C-activity in NaOH was measured. The mineralization kinetics were described using the following equation (Benoit et al., 1999):

$$M(t) = M_1 \times (1 - e^{-k_1 t}) + k_2 \times t \qquad [12]$$

where $M(t)$ is the total mineralized ^{14}C-CO_2 at time t (expressed in % of initial ^{14}C), M_1 represented a degradable pool that rapidly mineralizes with a mineralization rate of k_1 and the linear mineralization rate of a second less degradable pool k_2. Among the four OPs, a significant and positive correlation was found between the ^{14}C-CO_2 mineralized after 7 d in incubation and Dr parameters (r^2 = 1.00, p > 0.001). Moreover, a significant and positive correlation was found between k_2 parameters (Eq. [12]) and Fr parameters (r^2 = 0.78, p > 0.05). The k_2 parameters represented the degradation rate of a second less degradable pool with lower accessibility for mineralization that has been attributed

to rate-limiting processes such as desorption or diffusion (Benoit et al., 1999). The positive relation between k_2 and Fr would indicate that the more an OP is susceptible to form NER, the more it is susceptible to undergo slow mineralization, suggesting a competition between the two phenomena in the sorbed phase.

Sensitivity Analysis

Sensitivity analysis was performed on the input parameters proposed for the calibration of the COP-Compost model and tested against the simulated pools. The effect on the soluble and sorbed fractions potentially bioaccessible are displayed in Fig. 6. Parameters linked to microbial functioning, such as assimilation yield of available C (Y) and the death constant for microbial biomass (m_B) were the most sensitive parameters for all studied OP. This finding was consistent with the NER formation hypothesis, where the microbial activity stimulates NER formation and suggested that the co-metabolism hypothesis, where the degradation of OP was associated with microbial activity on an organic substrate, might be important. In fact, Y and m_B parameters strongly influenced the microbial biomass pool size (X) that was implicated in OP degradation and NER formation equations; these equations regulate the outflows of the soluble and sorbed pools. The OP degradation rate (Dr) and sorption coefficient (K_d) parameters also influenced the potentially bioaccessible fraction of LAS, NP, and glyphosate. For NP and glyphosate, the NER formation rate (Fr) was also a sensitive parameter. The Dr and Fr parameters are representative of OP dissipation pathways directly controlling the outflows from the soluble and sorbed pools. The K_d parameters controlled the balance between these two pools, favoring one dissipation pathways to the detriment of the other. The mineralized fraction was most sensitive to Dr and Y, then to the K_d and m_B parameters (not shown), and the NER fraction to Y, Fr, the NER_0 in the initial mixture and m_B parameters (not shown). Moreover, hydrolysis of organic matter (K_i, $i = 1–5$) had a lower influence on OP behavior, though this step is considered limiting during composting. The use of a unique K_d parameter for all organic C pools in the final version of the model, instead of specific K_{di} for each organic C pool C_i ($i = 1–5$), could explain this loss of sensitivity.

Conclusions

Using an innovative approach, the COP-Compost model simulates the behavior of OPs during composting and bioaccessibility in final compost combined with the dynamic of waste organic C. The organic C module proposed by Zhang et al. (2012) reasonably simulated the transformation of organic matter, even with a change in the study scale. The calibration of the OP module led to satisfactory simulations. The parameters obtained to simulate the behavior of the four OPs differed, in relation to their chemical properties. We obtained the lowest degradation rate, the highest sorption coefficient and low rate of NER formation for the polycyclic aromatic hydrocarbon (fluoranthene). The glyphosate gave the lowest sorption coefficient with the highest rate of NER formation that could be explained by its high chemical reactivity. We estimated the lowest rate of NER formation rate from LAS but, as for NP, a high degradation rate in relation to the simple chemical structure of the two surfactants.

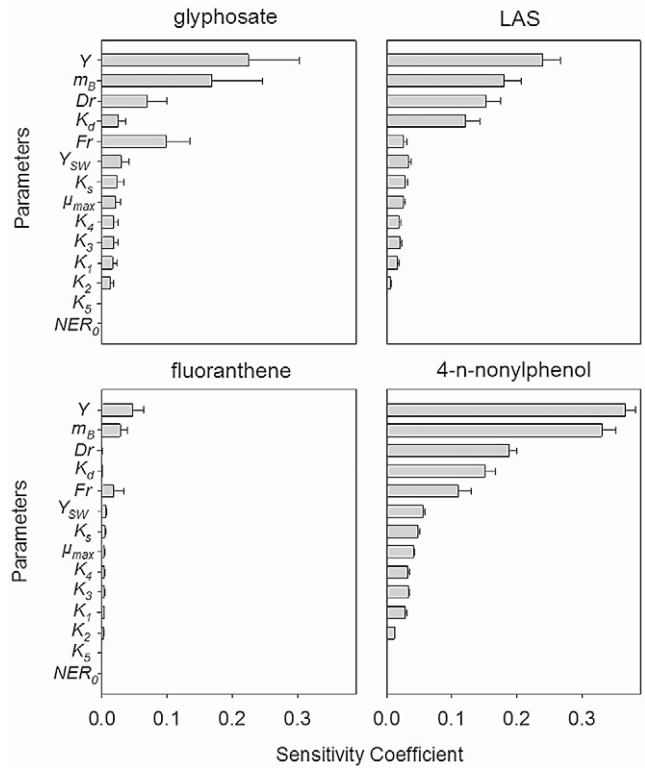

Fig. 6. Sensitivity coefficients, σ_p, for the COP-Compost (simulation of Carbon and Organic Pollutant evolutions during composting) model parameters on the potentially available simulated organic pollutant (OP) fraction (soluble + sorbed). Histograms represent mean ± standard errors of sensitivity coefficient obtained on the three composting replicates.

The sensitivity analysis and the calibration procedure of the model show also the strong impact of organic C dynamic on the simulated behavior of OP. Future composting experiments with different initial organic mixtures would contribute to evaluating the impact of organic C on OP. Our model needs to be integrated into a more complete model of composting where temperature, gas production and their influence on decomposition could be represented. The model has been calibrated for three OPs poised for future regulations and a widely used pesticide. This model could be useful in composting plants and optimizing the process for some targeted OP. In the future, the model should be coupled with a typology of OPs, relating their structural or physic-chemical descriptors to their reactivity toward organic matter or potential degradability, which could be used as a potential assessment for many types of OPs.

Acknowledgments

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