

Generalized models for prediction of pentachlorophenol dissipation dynamics in soils

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The empirical models were obtained for predicting PCP dissipation in soil.

Abstract

Dissipation of pentachlorophenol (PCP) in soil was investigated and the chemical relationships with soil properties were addressed. The results indicate that the dissipation of extractable PCP residues can be described using first-order kinetics equations, with a half-dissipation time ($T_{1/2}$) ranging from 6.5 to 173.3 d. The sharply different patterns of PCP dissipation in different soils were closely related to soil properties. Correlations of stepwise regression equations obtained were significant at 0.01 probability level between soil parameters and extractable PCP residues ($R^2 = 0.974^{**}$) as well as $T_{1/2}$ values ($R^2 = 0.882^{**}$). Using pH together with organic carbon content (OC) and soil particle size distribution, the dissipation dynamics of PCP in soil could be accurately predicted.

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1. Introduction

Pentachlorophenol (PCP, C_6Cl_5OH) is a highly chlorinated organic compound and a weak acid with a molecular weight of 266.5 g mol^{-1} , solubility of $3.0 \text{ } \mu\text{g ml}^{-1}$ at 25°C , pK_a of 4.75, and $\log K_{ow}$ of 5.01 (Ferro et al., 1994; Joel and Jerald, 1998). As a pesticide, herbicide, and antiseptic, it was once used worldwide, but has since been designated as a priority pollutant and is a probable human carcinogen (U.S. Environmental Protection Agency, 1980). In the 1970s PCP was used in China in the fight against snail fever and as a herbicide. Due to slow biodegradation, PCP may present a toxicity risk in contaminated soils for prolonged periods of time. Hence it is not surprising that it still causes environmental problems at many locations (Sanjoy et al., 1996). The highest concentrations of PCP are usually found in soil and aquatic sediments

(Abrahamsson and Klick, 1991; Maatela et al., 1990; Sung-Kil and Angela, 2003).

Applications of microbial processes have been used successfully for the remediation of PCP-contaminated soil in laboratory studies (Chang et al., 1996; Chaudri et al., 2000; Combrisson and Jocteur, 1999; Yu and Ward, 1996). Even in these small-scale laboratory settings, transport and transformation phenomena have been identified as critical factors governing PCP's bioavailability. The impact of mass transfer limitations on contaminant bioavailability can be underestimated if all of the key substrate properties are not considered. To date, adsorption and desorption have been the principal mechanisms in the majority of studies of environmental transport and transformation of PCP (Divincenzo and Sparks, 1997; Park and Bielefeldt, 2003; Tse and Lo, 2002). Few reports are related to the real-time dissipation dynamics of PCP and the mechanisms are less direct and have not been forthcoming especially in soils with contrasting physico-chemical properties. Neglect of the contribution of soil properties might result in unsuccessful attempts to clarify dissipation mechanisms.

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Therefore, the influence of soil properties on dissipation dynamics of PCP should be reevaluated for soils with different physico-chemical properties. If soil properties are well correlated with the dissipation results, the fate and transport of PCP and its subsequent remediation may eventually be predicted using soil properties.

The aim of the present work was thus to study the dissipation dynamics of PCP in different types of soil. We hypothesized that the dissipation characteristics of PCP would be influenced by the various properties of the soil matrix.

2. Materials and methods

2.1. Soils

Thirteen soil samples, from Zhejiang Province in southeastern China, with different properties were used for laboratory experiments in this study. Soils were chosen based on contrasting physico-chemical properties. All soils were taken from the surface layer (0–20 cm) of cultivated lands. They were air-dried, ground, and sieved to pass through a 2-mm plastic mesh before use. Precautions were taken to avoid contamination during sampling, drying, grinding, and storage. Selected properties of the test soils are listed in Table 1.

2.2. Incubation experiments

PCP, with a purity of more than 98% and purchased from Aldrich Chemical Co., was used as the model compound. A spiking solution was prepared by dissolving PCP in methanol to give a concentration of 10 g L^{-1} . The fresh soil samples (100 g oven-dried weight equivalent) were placed into 250 ml Erlenmeyer flasks and soil moisture was adjusted to 50% of the soil maximum water-holding capacity by addition of distilled water. The soil sample in each flask was spiked with 1 ml of the spiking solution. The spiked soil was then vented for 24 h to remove methanol and then mixed thoroughly, giving an initial soil concentration of $100 \text{ mg PCP kg}^{-1}$ soil. Our preliminary experiments indicated that the percentage recovery of PCP in any 5 g of the evenly mixed samples was $99.4 \pm 0.6\%$, and that the residual methanol in the treated soil was less than 0.05 mg kg^{-1} , which was not expected to influence the microbial activity (EL-Ghamry et al., 2002; Xu et al., 2002). After complete mixing of soil and PCP, the flasks were sealed with a sponge ball, incubated at $25 \pm 1^\circ \text{C}$ in the incubator (14D-78532, Binder, Germany), and aerated weekly, at which time water loss was supplemented by addition of distilled water to keep the moisture content constant. Flasks were kept in the dark until they were removed for sampling or watering. In no cases did obvious soil humidity and

temperature variation occur in the experimental systems. Photolysis was minimized by the absence of direct light. Aliquots of soil (5 g, oven-dried weight equivalent) were removed from the sample flasks at 3, 7, 14, 28, 56, and 112 days after application of PCP and subjected to the following extraction and analysis. Three replicate samples were used for each soil type.

2.3. PCP analysis

PCP extractable residues in soil were determined by ultrasonic extraction, subsequent solid phase enrichment and followed by HPLC analysis. Each 5 g soil sample was extracted by ultrasonic agitation (60 KHz, 25°C) in 30 ml methanol for 15 min. After centrifugation at $1932 \times g$ for 15 min, the supernatant was then decanted and collected. The soil residue was extracted two additional times with 20 ml methanol followed by centrifugation. The supernatant extracts were combined and concentrated to approximately 1 ml in a rotary evaporator, transferred through SPE C_{18} cartridge (10 ml, 500 mg) with 10 ml Milli-Q ultrapure water, eluted with methanol to volumetric flasks and made up to a final volume of 5 ml. Samples were then filtered through a syringe of $0.22 \mu\text{m}$ Millipore membrane (ANPEL, $\phi 13 \text{ mm}$) prior to analysis.

HPLC analysis was carried out on a Waters Alliance 2695-2487 HPLC system fitted with a Symmetry C_{18} column ($5 \mu\text{m}$, $3.9 \times 150 \text{ mm}$, Waters, USA). Chromatography was performed at 30°C . The flow rate was maintained at 1 ml min^{-1} by a gradient controller and solvent delivery system. The mobile phase was made from 1% acetic acid (10%) and methanol (90%), and the injection volume was $20 \mu\text{l}$. PCP was detected at 220 nm, and readings were integrated by the Millennium³² software system (Waters, USA). The PCP concentration was quantified with an external standard method.

2.4. Statistical analysis

First-order dissipation kinetics ($C = C_0 e^{-Kt}$, where C = concentration after time t , C_0 = apparent initial concentration, and K = rate constant) were used to interpret the PCP extractable residues data. Respective equation correlation coefficients and the fitting levels were calculated. From the data obtained, the $T_{1/2}$ (half-dissipation time) was calculated. Simple correlation and a stepwise regression procedure were used to study the relationship between the extractable amount, $T_{1/2}$, and the soil properties. Also, path analysis was conducted to determine the relative importance of direct and indirect effects of soil properties on PCP dissipation.

Path analysis is a prediction tool based on the regression analysis. The goal of path analysis is to determine the causal relationships by constructing the path diagram and assessing the incorporation effects of independent variables (in this case, soil properties) on the dependent variable (in this case, PCP dissipation extent). Usually only a few independent variables can be selected to

Table 1
Selected properties of soils used in the present study

Soil	pH	TN ^a (g kg ⁻¹)	HN (mg kg ⁻¹)	CEC (cmol (+) kg ⁻¹)	OC (g kg ⁻¹)	C _{mic} (mg kg ⁻¹)	Particle size (%)		
							Clay	Silt	Sand
1	5.61	1.3	162.5	12.3	6.6	257.8	17.2	7.4	75.4
2	5.82	2.5	218.3	15.9	11.8	728.9	22.1	50.3	27.6
3	6.50	4.2	333.0	27.6	24.3	782.2	44.3	46.4	9.3
4	5.78	3.5	252.0	22.0	17.9	524.4	40.4	48.0	11.6
5	5.25	1.4	134.6	14.9	11.0	115.6	34.5	31.0	34.5
6	8.40	4.2	410.6	9.7	28.7	886.7	15.4	74.2	10.4
7	7.06	2.9	287.3	16.3	19.5	302.2	8.0	71.3	20.8
8	9.04	1.8	88.1	7.1	5.5	160.0	24.3	71.1	4.6
9	5.42	2.1	172.6	11.8	12.8	437.8	30.5	39.6	30.0
10	7.26	6.1	540.0	24.5	22.6	731.1	37.2	51.2	11.7
11	6.20	3.9	256.5	25.1	23.6	928.9	35.3	60.6	4.2
12	6.22	3.7	292.6	28.5	18.3	995.6	40.0	57.0	3.0
13	6.32	3.7	312.0	22.3	22.9	973.3	45.6	43.9	10.5

^a TN: Total nitrogen; HN: Hydrolysis nitrogen; CEC: Cation exchange capacity; OC: Organic carbon; C_{mic}: Microbial biomass carbon.

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