

SUPPORTING MATERIALS

Adsorption of flupyradifurone onto five different soils: Kinetics, isotherms, and influences of soil properties

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Chemicals and reagents

FPO (purity>99.5%) was purchased from Chem Service (West Chester, PA, USA). Chromatographic grade acetonitrile (ACN) was purchased from Thermo Fisher Scientific (Waltham, MA, USA). Ultrapure water was prepared using a Milli-Q system (Bedford, MA, USA). The primary-secondary amine (PSA) sorbent was purchased from Agilent (Santa Clara, CA, USA). All other chemicals, including formic acid, sodium chloride (NaCl), anhydrous magnesium sulfate (MgSO₄), and calcium chloride (CaCl₂) were of analytical-reagent and were obtained from Shanghai Aladdin Biochemical Technology (Shanghai, China).

Quantitation control (QC)

The QC of FPO in the adsorption samples was carried out simultaneously with the analysis of the adsorption samples. The external standard method was used for the quantification of FPO. The results are shown in Table S3. FPO recoveries in supernatant samples ranged from 87.3% to 94.4% (intraday) with the relative standard deviations (RSDs) ranging from 3.6% to 6.7%, and 91.5% to 94.9% (interday) with RSDs ranging from 1.9% to 8.7%. It indicated that the analysis method fulfilled the QA/QC required by the GB/T 31270.4-2014 guideline.

Table S1 Selected physicochemical properties of soils.

Soil	Location	pH	TOC ^a (%)	CEC ^b (cmol kg ⁻¹)	Soil texture (%)		
					Clay (<2 μm)	Silt (2-20 μm)	Sand (>20 μm)
S1	Changchun (125°41'34 E, 43°82'33 N)	6.20	0.49	20.38	21.18	44.86	33.96
S2	Harbin (126°28'36 E, 45°51'46 N)	5.76	1.62	16.52	44.67	49.37	5.96
S3	Hangzhou (120°12'19 E, 30°19'11 N)	7.36	2.65	24.98	68.45	22.39	9.16
S4	Langfang (116°36'52 E, 39°31'8 N)	4.14	0.62	22.94	36.12	38.67	25.21
S5	Jinan (117°21'65 E, 36°82'17 N)	8.31	1.45	48.34	30.49	40.84	28.67

^a TOC: Total organic carbon.

^b CEC: Cation exchange capacity.

Table S2 HPLC-MS/MS conditions for the determination of Flupyradifurone.

HPLC condition				
Instrumental	Agilent 1260 HPLC, Santa Clara, CA, USA.			
Column	Agilent C ₁₈ column, ZORBAX RRHD Eclipse Plus, 3.0 mm × 100 mm, 1.8 μm.			
Column oven	30 °C			
Injection volume	5 μL			
Flow rate	0.3 mL/min			
Mobile phase	A: 0.1% formic acid aqueous solution. B: acetonitrile.			
Gradient elution	0–4 min, linear gradient 80%–60% solvent A; 4–6 min, linear gradient 60%–20% solvent A, and held for 1 min; 7–10 min, linear gradient 80% solvent A.			
MS/MS condition				
	Positive mode	Negative mode		
Instrumental	Agilent 6470 triple quadrupole mass spectrometer, Santa Clara, CA, USA.			
Ion source	Electrospray ionization			
Nebulizer pressure (psi)	30	30		
Capillary voltage (kV)	4.0	4.0		
Nozzle voltage (kV)	0.5	0.5		
Desolvation flow rates (L/min)	7	7		
Sheath gas flow rates (L/min)	8	8		
Desolvation temperature (°C)	330	330		
Source temperature (°C)	300	300		
MRM ^a condition	Retention time (min)	Precursor ion (fragmentor, eV)	Qualitative ion (CE ^b , eV)	Quantitative ion (CE, eV)
Flupyradifurone	5.84	289.0 (140)	245.1 (15)	126.1 (25)

^a MRM: multiple reaction monitoring.^b CE: collision energy.

Table S3 Mean recoveries and RSD for Flupyradifurone from supernatant samples at three spiked levels.

Spiked level (mg L ⁻¹)	Intraday (n=5) %Recovery (RSD _r ^a)	Inter-day (n=15) %Recovery (RSD _R ^b)
0.01	94.1 (6.7)	94.9 (6.1)
1	90.5 (4.6)	91.5 (8.7)
30	87.3 (3.6)	92.2 (1.9)

^a the intraday relative standard deviation for repeatability (n=5)

^b the inter-day relative standard deviation for repeatability (n=15)

Table S4 The K_{oc} of flupyradifurone in different soil samples under different temperature condition.

Soils	TOC (%)	Temperature (K)	K _d	K _{oc}
S1	0.49	298	0.8433	1.7211
		308	0.5742	1.1718
		318	0.5160	1.0532
S2	1.62	298	1.8725	1.1558
		308	3.5800	2.2099
		318	2.9704	1.8336
S3	2.65	298	3.4252	1.2925
		308	6.4892	2.4488
		318	4.9004	1.8492
S4	0.62	298	1.7539	2.8289
		308	3.5048	5.6529
		318	2.7967	4.5108
S5	1.45	298	2.1444	1.4789
		308	3.5029	2.4158
		318	3.0295	2.0893