# Ground Water Leaching Potential of Flupyradifurone

Introduction:

Flupyradifurone, 4-((6-chloro-3-pyridylmethyl)(2,2-difluoroethyl)amino)furan-2(5H)-one, is a systemic insecticide that is newly proposed to protect various crops (e.g., vegetables, fruits, and grapes) from piercing and sucking insects (e.g., aphids, whiteflies, and thrips). The compound belongs to the chemical class of butenolide, and its putative mode of insecticidal action is to inhibit the nicotinic acetylcholine receptor that results in a disorder of the nervous system of insects, followed by death. It is labeled for agricultural applications of foliar spray, chemigation, and soil drench to many crops including a seed treatment for soybeans, but not for residential uses. The compound was found to be less toxic to humans and non-target organisms, when compared to other insecticides such as pyrethroids, neonicotinoids, and organophosphates. The trade name of this compound is Sivanto (developed by Bayer CropScience) and is currently under registration process by the US EPA (CAS number: 951659-40-8).

Selected Physical/Chemical Properties of Flupyradifurone:

Chemical structure:
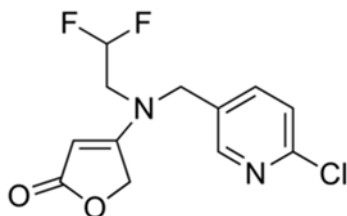
Literature data

Chemical formula:	$C_{12}H_{11}ClF_2N_2O_2$
Molecular mass:	288.68 g/mole
Physical state:	Solid powder (white to beige colors)
Water solubility (at 20°C):	3,200 mg/L
Log P_{ow} (at pH 7, 20°C):	1.2
(at pH 4, 7, and 9, 25°C):	1.2 (registrant)
Vapor pressure (at 25°C):	9.1×10^{-04} mPa
Henry law constant (at 25°C):	8.2×10^{-08} Pa·m^3/mol
(at 20°C):	3.37×10^{-11} dimensionless
K_{oc}:	85.2–333 (typical 162.2) mL/g
	74.9–132.2 (registrant) mL/g
Soil degradation half-life (lab & field):	8.3–371 (typical 138.4) days
	10.1–228 (registrant) days
Freundlich coefficients (K_f):	0.60–3.82 (typical 2.26) mL/g
Freundlich coefficient (1/n):	0.845–0.902 (typical 0.866)
GUS index:	3.53 (high leachability)
SCI-GROW index (ppb) for 1 kg/ha dose:	6.15×10^{-01} µg/L
Potential for particle bound transport index:	Medium

Environmental Fate Data:

Hydrolysis

Sterile aqueous buffer solutions of different pH values were treated with 1.0 mg a.i./L [Furanone-4-^{14}C] BYI 02960 to investigate its hydrolytic stability. The test matrices included acetate (for pH 4), tris (for pH 7), and borate buffers (for pH 9). Samples were incubated in the dark at 50°C and analyzed at selected time intervals for 5 days. From the experiments, the registrant confirmed that the compound was stable in sterile aqueous solutions because none accounted for more than 5% of applied radioactivity at all pH values. Thus, the half-life of the compound could not be estimated in this study. Also, no significant volatiles were detected during hydrolysis.

Photodegradation in Sterile Buffer and Natural Water

The photodegradation of [^{14}C]-labeled compound (BYI 02960) was studied by the registrant in sterile potassium phosphate buffer (10 mM, pH 7) under artificial sunlight. Duplicate samples were continuously irradiated at 25°C for 35 hours using a xenon lamp with a UV cutoff filter (λ < 290 nm). Dark controls were also included in the experiment. The concentration of the compound was 1.0 mg a.i./L. Two major degrades (i.e., BYI 02960-succinamide and BYI 02960-azabicyclosuccinamide) that explained more than 10% of applied radioactivity were identified from the irradiated samples. However, one minor metabolite (i.e., BYI 02960-deschlorohydroxy-succinamide) and polar mixture accounted for less than 5% of applied radioactivity during the experimental period. The experimental half-life value estimated was 13.8 hours and its corresponding value under field condition (at Phoenix, AZ, USA) was expected to be 1.75 days. The compound was found to be stable in the dark control samples.

The same applies to the experiments using sterile natural water at pH 8. The only difference was that the samples were irradiated and analyzed for 28 hours which corresponded to 7.5 environmental days at Tokyo, Japan. Identical metabolites such as major and minor transformation products as described above were also detected from the experiments. The estimated half-life values under laboratory and field conditions were 14.0 hours and 3.8 days, respectively, with a half-life of over 45 days for dark controls. All these results indicated that the compound was rapidly degraded through aqueous photolysis.

Photodegradation in Soil

The registrant investigated a photodegradation of [pyridinylmethyl-^{14}C]- and [furanone-4-^{14}C]-labeled compounds on a loam soil (with a pH of 6.5 and a carbon content of 0.6%) under artificial sunlight, as described above. Stock solutions were applied to the soil surface at the single maximum field use rate of 400 g a.i./ha (or at a concentration of 40.8 μg/3g soil). The soil moisture content was adjusted at 75% of field capacity (at 1/3 bar) during the experiment. Duplicate samples were continuously irradiated at 20°C for 8 days. Dark controls as well as air dried samples were prepared in parallel. The soil samples taken at selected time intervals were extracted in two steps, first with ambient organic extracts (i.e., 8 mL acetonitrile/water (1/1, v/v), 5 mL acetonitrile/water (1/1, v/v), 5 mL acetonitrile/water (8/2, v/v), and 5 mL acetontrile in series) and second with aggressive organic extracts (i.e., 8 mL of acetonitrile/water (8/2, v/v) at 70°C). CO$_2$ and organic volatiles were collected through traps connected to test vessels. Results showed that phototransformation in soil had a minimal impact on the degradation of the parent compounds. The parent compound treated with two labels accounted for around 94% of

applied activity at test termination in the irradiated samples, whereas over 97% of applied activity was observed at the end of the study for both labels in the dark samples. Some minor degradates were also detected for both labels in the irradiated samples, but did not explain more than 2% of applied activity during the study period. Negligible amounts of CO_2 and organic volatiles were detected for two labels in both irradiated and dark samples. There was no significant difference in the degradation of the parent compound (treated with both labels) between humid and dry soil samples. The experimental half-life values estimated using a simple first order kinetic were 99.6 (for label P) and 109.3 days (for label F). Their corresponding values under environmental conditions were expected to be 358 and 405 days (at Los Angeles, CA, USA), 466 and 527 days (at Athens, Greece), and 638 and 722 days (at Tokyo, Japan).

Photodegradation in Air
The photodegradation of the parent compound BYI02960 in air was estimated using the Atmospheric Oxidation Program (i.e., AOPWIN™), one of models provided by the software Estimation Programs Interface (EPI Suite™ version 1.92) released by the US EPA. The EPI Suite™ indicates a screening-level tool to estimate characteristics and environmental fate of the chemical when measured values are not available. The AOPWIN™ refers to a model that calculates rate constants for the gas-phase reactions between a chemical of interest and photochemically generated active species such as hydroxyl radical and ozone concentrations, as examined in this study. The half-life values of the parent compound were estimated to be 4.37 (for short-term scenario) and 13.12 hours (for long-term scenario), when default values for hydroxyl radical concentrations averaged over 12 (during daylight) and 24 hours (during day and night-time) were used, respectively. Here, hydroxyl radical was selected as the main reaction partner, which was responsible for degradation of the parent compound. In contrast, the compound was considered to react with ozone more slowly by a factor 2 to 10. The compound was neither accumulated nor likely to enter in the atmosphere due to its short half-life and low vapor pressure.

Aerobic Degradation Studies in Water
Two aerobic aquatic metabolism studies were carried out separately using natural water/sediment systems at two locations in Germany, one for [Pyridine-2,6-^{14}C]- labeled compound and the other with [Furanone-4-^{14}C]-, and [Ehtyl-1-^{14}C]-labeled compounds. The two water/sediment systems used for each parent compound treated with different labels were characterized differently in terms of pH and organic carbon values in waters and sediments as well as sediment textures. Their major characteristics treated with [Pyridine-2,6-^{14}C]- labeled compound were explained as follows: natural waters with pH values of 7.4 and 7.7 and total organic carbons of < 2 mg/L and < 2 mg/L as well as sediments with textual classes of sandy loam and loamy sand, pH values of 5.2 and 6.7 in calcium chloride, and carbon contents of 3.6% and 1.2%. Also, those with [Furanone-4-^{14}C]-, and [Ehtyl-1-^{14}C]-labeled compounds were explained as follows: natural waters with pH values of 6.5 and 6.9 and total organic carbons of 5 mg/L and < 2 mg/L as well as sediments with textual classes of loam and sand, pH values of 4.8 and 6.8 in calcium chloride, and carbon contents of 5.1% and 0.4%. Based on the maximum field application rate of 400 g a.i./ha, each compound was applied to the water/sediment systems and then incubated at 20°C in the dark on a horizontal shaker at 65 rounds per minute. Duplicate test systems were analyzed at selected time intervals for 119-120 days for all radiolabeled compounds. The water samples were centrifuged with or without filtration to measure radioactivity, whereas the sediment samples were extracted in two steps, first with ambient organic extracts (i.e., 3 × acetonitrile/water (8/2,

3

v/v), followed by 1 × acetonitrile at room temperature) and second with aggressive organic extract (i.e., 1 × acetonitrile/water (8/2, v/v) at 70°C) for all radiolabeled compounds. CO_2 and organic volatiles were collected through traps connected to test vessels. Note that supplemental tests sterilized by gamma radiation or steam pressure were performed only for the systems treated with [Pyridine-2,6-^{14}C]-labeled compound.

From the experiments, the registrant confirmed that the compounds treated with different labels were degraded slowly under aerobic aquatic conditions. While the parent compounds treated with different labels showed large decreases in applied radioactivity in the water phases, the amounts of the parent compounds increased considerably in the sediment phases during the study period. In fact, [Pyridine-2,6-^{14}C]-labeled compound accounted for less than 23 % of applied radioactivity in the water phases of the two systems at study termination, whereas [Furanone-4-^{14}C]-, and [Ehtyl-1-^{14}C]-labeled compounds exhibited less than 15 and 37% of applied radioactivity, respectively. In contrast, [Pyridine-2,6-^{14}C]-labeled compound explained around 50% of applied radioactivity in the sediment phases of the two systems at study termination, whereas [Furanone-4-^{14}C]-, and [Ehtyl-1-^{14}C]-labeled compounds showed more than 50 and 37% of applied radioactivity, respectively. Up to three minor metabolites were indentified for the water phases in the systems treated with [Pyridine-2,6-^{14}C]-labeled compound, but not for the sediment phases. However, various minor degradation products were detected for both water and sediment phases in the systems treated with [Furanone-4-^{14}C]-, and [Ehtyl-1-^{14}C]-labeled compounds, including one major or minor metabolite difluoroacetic acid in the systems of [Ehtyl-1-^{14}C]-labeled compound. CO_2 accounted for less than 10% applied radioactivity during the entire study period for all radiolabeled compounds, and no significant amounts of volatile organics were detected. Non-extractable residues explained 13.6-26.6% of applied radioactivity during the study period depending on each compound, which were partially attributed to microbial processes (from the supplemental test results). The half-life values estimated using a simple first-order kinetic were 193.1 and 246.9 days for [Pyridine-2,6-^{14}C]-labeled compound, 208.2 and 246.1 days for [Furanone-4-^{14}C]-labeled compound, and 202.4 and 285.0 days for [Ehtyl-1-^{14}C]-labeled compounds.

Aerobic Degradation Studies in Soil

The registrant reported six aerobic soil metabolism studies of the parent compound treated with different labels using various soils in Europe and the USA (see Tables 1 and 2). Table 1 presents the characteristics of test soils examined for each compound. Table 2 also shows the main experimental conditions and their corresponding outcomes of individual studies. Soils used in the studies differed in terms of pH and the percentage of organic matter (see Table 1). In duplicate samples, each compound except for [Pyridinylmethyl-^{14}C] BYI02960 was applied at similar rates, which corresponded to the maximum single field usage rate of 400-410 g a.i./ha (see Table 2). Soil samples maintained at different moisture conditions were incubated at 20°C in the dark condition and analyzed at selected time intervals for each period of the study. The soil samples were extracted using two different sequential extraction procedures (see Table 2). Ethylene glycol and potassium hydroxide solutions were used to collect organic volatiles and CO_2 passed through traps for all studies, respectively. Note that non-sterile experiments were only performed at the soils collected in the USA (see Table 1).

It was found that all parent compounds treated with different labels underwent extensive mineralization to CO_2 under aerobic soil conditions (see Table 2). Depending on test soils and compounds, some major degradates such as 6-chloronicotinic acid (17.1 % of applied

radioactivity for A soil using [Pyridine-2,6-^{14}C] BYI02960) and difluoroacetic acid (30.2, 22.0, and 33.8% of applied radioactivity for A, B, and C soils using [Ehtyl-1-^{14}C] BYI02960, respectively) were found during the study period (see Tables 1 and 2). Non-extractable (bound) residues which accounted for more than 10% of applied radioactivity increased considerably at the end of all non-sterile studies, whereas very negligible amounts of volatile organics were detected. Biologically-mediate processes were found to be responsible for dissipation of the parent compound, to a lesser extent, when sterile and non-sterile soils were compared to each other. 6-chloronicotinic acid, BYI 02960-chloro, and BYI 02960-des-difluoroethyl were indentified as minor transformation products in some studies (see Table 2). The two kinetic models, i.e., simple first-order and double first order in parallel, were found to provide the best fit to the observed data in different studies. The half-life values estimated based on these two models ranged 33.0 to 228 days for all tested soils (see Table 2). Note that a rigorous evaluation of degradation rates was additionally done for the parent compounds treated with different labels and their metabolites (see Table 3), which slightly showed different values compared to those of the original studies (compare the half life values of the parent compounds in Tables 2 and 3). The metabolite 6-chloronicotinic acid had very short half life (less than 6 days), whereas difluoroacetic acid exhibited a relatively long half-life (ranging from 44.9 to 73.6 days) than 6-chloronicotinic acid.

Table 1. The test soils used for each substance in aerobic soil metabolism studies.

Test items	Test soils	Geographic locations
[Furanone-4-^{14}C] BYI02960	A. Silt loam (pH[1] 6.5; OC[2] 2.3%) B. Sandy loam (pH 7.0; OC 0.6%)	A. Springfield, NE, USA B. Sanger, CA, USA
[Pyridine-2,6-^{14}C] BYI02960	A. Silt loam (pH 6.5; OC 2.3 %) B. Sandy loam (pH 7.0; OC 0.6%)	A. Springfield, NE, USA B. Sanger, CA, USA
[Ehtyl-1-^{14}C] BYI02960	A. Clay loam (pH 7.1; OC 5.1%) B. Loamy sand (pH 6.2; OC 1.9%) C. Silt loam (pH 6.5; OC 2.4%)	A. Blankenheim, Germany B. Monoheim, Germany C. Burscheid, Germany
[Pyridine-2,6-^{14}C] BYI02960	A. Silt loam (pH 6.5; OC 2.4%)	A. Burscheid, Germany
[Furanone-4-^{14}C] BYI02960	A. Sandy loam (pH 6.1; OC 2%) B. Silt loam (pH 6.5; OC 2.5%) C. Silt loam (pH 4.8; OC 3.3%) D. Silt clay (pH 7.1; OC 4.1%)	A. Monoheim, Germany B. Burscheid, Germany C. Burscheid, Germany D. Blankenheim, Germany
[Pyridinylmethyl-^{14}C] BYI02960	A. Sandy loam (pH 6.4; OC 1.2%) B. Silt loam (pH 6.5; OC 1.8%) C. Loam (pH 5.4; OC 2.3%) D. Clay loam (pH 7.4; OC 4.6%)	A. Monoheim, Germany B. Burscheid, Germany C. Burscheid, Germany D. Blankenheim, Germany

[1] Soil pH presents a value measured in calcium chloride (CaCl$_2$).
[2] OC indicates the percentage of organic matter.

Anaerobic Degradation Studies in Water
The registrant studied anaerobic aquatic metabolism of the parent compound treated with [Pyridine-2,6-^{14}C]-label using two natural water/sediment systems of Lawrence, KS and Pikeville, NC in USA. Their major characteristics in the KS and NC systems were explained as

Table 2. Summary of six different aerobic soil metabolism studies.

Test items	[Furanone-4-^{14}C] BYI02960	[Pyridine-2,6-^{14}C] BYI02960	[Ehtyl-1-^{14}C] BYI02960	[Pyridine-2,6-^{14}C] BYI02960	[Furanone-4-^{14}C] BYI02960	[Pyridinylmethyl-^{14}C] BYI02960
Test concentrations	1.1 µg a.i./g soil (410 g a.i./ha)	1.1 µg a.i./g soil (410 g a.i./ha)	106.7 µg a.i./100 g soil (400 g a.i./ha)	106.7 µg a.i./100 g soil (400 g a.i./ha)	106.7 µg a.i./100 g soil (410 g a.i./ha)	0.53 mg/kg a.i. soil (200 g a.i./ha)
Duration of study	120 days	120 days	118 (for A soil) and 117 days (for B and C soils)	117 days	120 days	120 days
Soil moisture contents	pF 2.0 to 2.5	pF 2.0 to 2.5	55% of max water holding capacity	55% of max water holding capacity	55% of max water holding capacity	55% of max water holding capacity
Extraction of soil samples[1]	1. 3 × ACN: water (70: 30) 2. ACN (100%) 3. ACN: water (70: 30) at 70°C	1. 3 × ACN: water (70: 30) 2. ACN (100%) 3. ACN: water (70: 30) at 70°C	1. 2 × ACN: water (50:50) 2. ACN: water (80:20) 3. ACN (100%) 4. ACN: water (80:20) at 70°C	1. 2 × ACN: water (50:50) 2. ACN: water (80:20) 3. ACN (100%) 4. ACN: water (80:20) at 70°C	1. 2 × ACN: water (50:50) 2. ACN: water (80:20) 3. ACN (100%) 4. ACN: water (80:20) at 70°C	1. 2 × ACN: water (50:50) 2. ACN: water (80:20) 3. ACN (100%) 4. ACN: water (80:20) at 70°C
The estimated $T_{1/2}$ values[2]	A. 228 days B. 65.7 days	A. 211 days B. 62.1 days	A. 33.9 days B. 62.0 days C. 34.1 days	A. 33.0 days	A. 62.2 days B. 33.2 days C. 98.3 days D. 49.3 days	A. 63.4 days B. 52.4 days C. 120.0 days D. 56.4 days
Kinetic models[3]	SFO	SFO	DFOP	DFOP	DFOP	DFOP
Major degradates	CO_2	CO_2 and 6-chloronicotinic acid (for A soil)	CO_2 and Difluoroacetic acid	CO_2	CO_2	CO_2
Minor degradates[4]	-	-	1	3 (6-chloronicotinic acid)	5 (BYI 02960-chloro and BYI 02960-des-difluoroethyl)	3
Report numbers[5]	MERVP037-2	MERVP038-1	MEF-10/858	MEF-10/880	MEF-10/804	MEF-07/334

[1] ACN indicates acetonitrile; no temperature is shown for the experiments conducted at ambient temperature.

[2] The upper-case letters signify the test soils examined with each parent compound (see Table 1).

[3] SFO and DFOP represent the simple first-order and double first order in parallel, respectively

[4] The compounds in parenthesis indicate the identified metabolites among them.

[5] Refer to the reports submitted by the registrant directly below the reference list.

Table 3. In-depth kinetic evaluation of the parent compounds treated with different labels and their metabolites for modeling (endpoint).

Test items	[Ehtyl-1-^{14}C] BYI02960	[Pyridine-2,6-^{14}C] BYI02960	[Furanone-4-^{14}C] BYI02960	[Pyridinylmethyl-^{14}C] BYI02960
The estimated T$_{1/2}$ values[1]	A. 34.0 days B. 62.0 days C. 34.1 days a. 44.9 days b. 73.6 days c. 67.4 days	A. 33.1 days a. 3.1 days	A. 141.5 days B. 40.5 days C. 157.5 days D. 55.1 days	A. 169.1 days B. 54.4 days C. 157.5 days D. 60.1 days
Kinetic models[2]	A. DFOP B. DFOP C. FOMC a. SFO b. SFO c. SFO	A. FOMC a. SFO	A. DFOP B. SFO C. DFOP D. SFO	A. DFOP B. SFO C. DFOP D. SFO
Major degradates	CO_2 and Difluoroacetic acid	CO_2	CO_2	CO_2
Minor degradates	1	3 (6-chloronicotinic acid[3])	5 (BYI 02960-chloro and BYI 02960-des-difluoroethyl)	3
Report numbers[4]	MEF-11/855	MEF-11/838	MEF-11/620	MEF-11/619
Supplements	MEF-10/858	MEF-10/880	MEF-10/804	MEF-07/334

[1] The upper-case letters signify the half-life values for each parent compound tested in different soils (see Table 1), whereas the lower-case letters indicate those with their degradates.
[2] SFO, FOMC, and DFOP represent the simple first-order, first-order multiple-compartment, and double first order in parallel, respectively.
[3] The half-life values estimated from the degradation study of 6-chloronicotinic acid only using SFO model were 2.2, 2.9, and 5.3 days in three European soils (see the report MEF-11/837).
[4] Refer to the reports submitted by the registrant directly below the reference list.

follows: natural waters with pH values of 8.3 and 7.4 and total organic carbons of 7.8 mg/L and 11.9 mg/L as well as sediments with textual classes of silty clay and loamy sand, pH values of 7.6 and 4.7 in calcium chloride, and carbon contents of 1.1% and 1.5%. All experimental conditions were identical to those described above in the section of "Aerobic Degradation Studies in Water", except for the duration of study, extraction solutions and procedures, and attached traps used for the volatile and CO_2 analysis. The experiments treated with the maximum field application rate of 410 g a.i./ha were conducted for 102 days. Acetonitrile/water (8/2, v/v) used in the European soil as the ambient and aggressive organic solvent extracts was replaced with acetonitrile/water (7/3, v/v) for ambient temperature and acetonitrile/water (7/3, v/v) with 1:1 methanol: water for high temperature (at 70°C), respectively. Also, a series of volatile traps that contained ethylene glycol, potassium hydroxide, and sulfuric acid solutions were used in the anaerobic phase for both soils.

From the results, it was found that the parent compound in the water phases was rapidly translocated into sediments and then remained stable under anaerobic conditions. The compound accounted for 25.1 and 18.5 % of applied radioactivity in the water phases of the two systems at study termination, whereas 68.9 and 64.8% of applied radioactivity were observed in the sediment phases. CO_2 and volatile organics remained very low during the study period and bound residues explained 4.9-12.0% of applied radioactivity. The half-life values estimated using double first-order in parallel were >1,000 for KS system and 415 days for NC system under anaerobic conditions.

Anaerobic Degradation Studies in Soil
Anaerobic soil metabolism study of [Furanone-4-^{14}C]-, [Ehtyl-1-^{14}C]-, and [Pyridine-2,6-^{14}C]-labeled compounds was conducted in one European soil, a silt loam (with a pH of 6.4 in calcium chloride and a carbon content of 2.7%). The parent compounds treated with different labels were applied to the soil at the field use rate of 400 g a.i./ha which corresponded to actual rates between 104.6 and 110.1µg/100 g soil depending on individual compounds. In the aerobic phase, the soil samples maintained at 55% max water holding capacity were incubated at 20°C in the dark and analyzed at selected time intervals for 30 days. Then, the experimental condition changed from aerobic to anaerobic by flooding the soil samples with oxygen-depleted deionized water (with a water layer of around 3 cm above soil level). The anaerobic soil samples were incubated at 20°C in the dark under a nitrogen gas atmosphere and analyzed at selected time intervals for additional 123 days. Duplicate soil samples were extracted in two steps, ambient and aggressive organic extract, as described above in the section of "Aerobic Degradation Studies in Water". CO_2 and organic volatiles were collected not only through air-permeable traps in the aerobic phase, but also by plastic gas sampling bags (that protected the system from the outer atmosphere) in the anaerobic phase.
It was shown that three radiolabeled compounds were degraded much more rapidly during the aerobic phase than under the anaerobic condition. The parent compounds showed 53.7 (for [Furanone-4-^{14}C]-labeled compound), 52.6 (for [Ehtyl-1-^{14}C] -labeled compound), and 54.7% of applied radioactivity (for [Pyridine-2,6-^{14}C]-labeled compound) at the end of the aerobic phase, which decreased further to 47.8, 47.2, and 47.7% of applied radioactivity under the anaerobic condition. Difluoroacetic acid (BYI 02960-DFA) was identified as the major degradate that exceeded 5% of applied radioactivity during the study period, which accounted for 25.1% of applied radioactivity in the aerobic phase and then almost remained stable in the anaerobic phase. Up to five, four, and one minor transformation products which were not identified due to their low amounts were observed for [Pyridine-2,6-^{14}C]-, [Furanone-4-^{14}C]-, and [Ehtyl-1-^{14}C]-labeled compounds, respectively. Very negligible amounts of CO_2 and organic volatiles were detected for all radiolabeled compounds in the anaerobic phase. Non-extractable residues increased slightly for the radiolabeled compounds in the anaerobic phase compared to those under the aerobic condition. Based on a simple first-order kinetic model, the estimated half-life values were 581.8, 693.2, and 693.2 days for [Pyridine-2,6-^{14}C]-, [Furanone-4-^{14}C]-, and [Ehtyl-1-^{14}C]-labeled compounds, respectively. A metabolic pathway for degradation of the parent compounds in one European soil during the entire study period suggested by the registrant is illustrated in Figure 1a.

Similar studies were also conducted by the registrant using [Pyridine-2,6-^{14}C]- labeled compound on two US soils, one from Springfield, NE and the other from Sanger, CA. Soils from

NE and CA were characterized by sandy clay loam (with a pH of 6.5 in calcium chloride and a carbon content of 1.9%) and loamy sand (with a pH of 6.7 in calcium chloride and a carbon content of 0.5%), respectively. All experimental conditions were identical to those described above, except for the duration of study, wet soil condition, extraction solutions and procedures, and attached traps used for the volatile and CO_2 analysis. The experiments were conducted for 29 (under the aerobic condition) and 60 days (under the anaerobic condition) in NE soil as well as 32 (under the aerobic condition) and 121 days (under the anaerobic condition) in CA soil. Both soil samples were flooded with a water layer of around 2 cm above soil level. The extraction solutions and procedures as well as attached traps are described in detail in the section of "Anaerobic Degradation Studies in Water".

Results showed that the parent compound was fairly stable during the anaerobic phase in NE soil. While three minor metabolites were indentified during the anaerobic phase of the study, no significant organic volatiles were detected. CO_2 and non-extractable residues reached a max of 18.4 and 14.8% of applied radioactivity during the entire study period, respectively. As a result, no half-life was estimated for the parent compound in NE soil. In contract, the parent compound was degraded further in CA soil, exhibiting 51.1 and 26.2% of applied radioactivity at the beginning and end of the anaerobic phase, respectively. However, any significant amounts of CO_2 and organic volatiles were not produced under the anaerobic condition. 6-chloronicotonic acid and chloro-BYI 02960 were designated as the major and minor metabolites, respectively, which remained, after reaching their maximum amounts in the aerobic phase, fairly stable under the anaerobic condition. The half-life values estimated using a simple first-order kinetic, first-order multiple-compartment, and double first-order in parallel were 152, 164, and 584 days, respectively. A proposed metabolic pathway for degradation of the parent compound in CA soil during the entire study period is illustrated in Figure 1b.


Adsorption and Desorption to Soil

The adsorption and desorption characteristics of [Pyridinylmethyl-^{14}C] BYI02960 were studied using batch equilibrium experiments. Experiments were conducted separately with soils from two different geographic areas, four soils in Europe and two soils in USA. Table 4 shows the key characteristics of six soils used in this study. As shown in the table, the test soils differed significantly in terms of the textural class, pH, bulk density (BD), moisture content (FC), organic carbon content (OC), and cation exchange capacity (CEC). 0.01 M $CaCl_2$ was used as background solution in the batch experiments, to which five different concentrations of the compound (i.e., 0.01, 0.03, 0.1, 0.3, and 1 mg/L) were applied at a soil to solution ratios of 1:4 for four European soils and 1:1 for two US soils. The soil samples were allowed to shake for 24 hours in the dark at 20°C during the adsorption/desorption cycle. In the desorption study, the supernatant liquid removed in the adsorption step was replaced by an equal volume of $CaCl_2$ solution without test item, and then agitated for 24 hours. The supernatant at each adsorption and desorption step was centrifuged at 8500 rpm for 15 min for European soils and at 3000 rpm for 10 min for US soils. Note that two additional desorption cycles were done only for the highest concentration in US soils.

The Freundlich isotherm model was used to fit the experimental data (see Table 5). In the adsorption study, the estimated K_d values varied between 0.60 and 3.82 mL/g for six different soils. Based on the organic carbon content for each soil, the K_{oc} values estimated varied between 74.9 and 132.2 mL/g. The Freundlich exponent ($1/n$) ranged from 0.84 to 0.90, indicating that the adsorption behavior was affected by the test soils in addition to the concentrations of the test
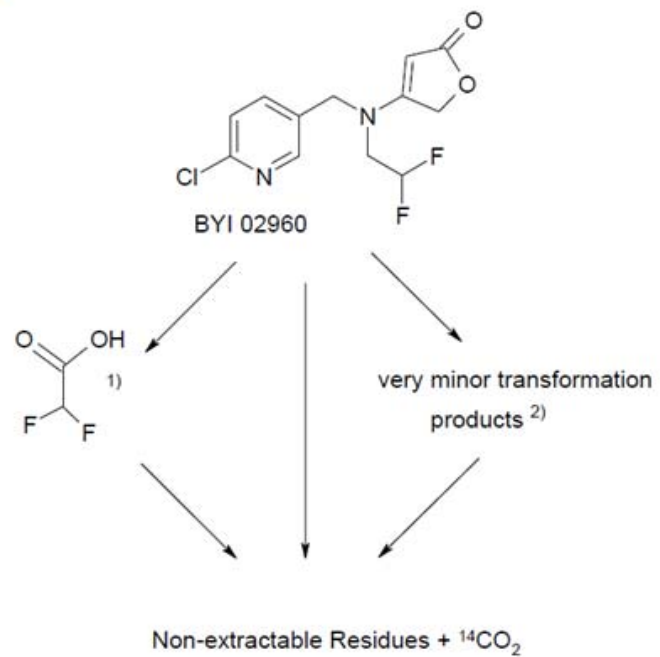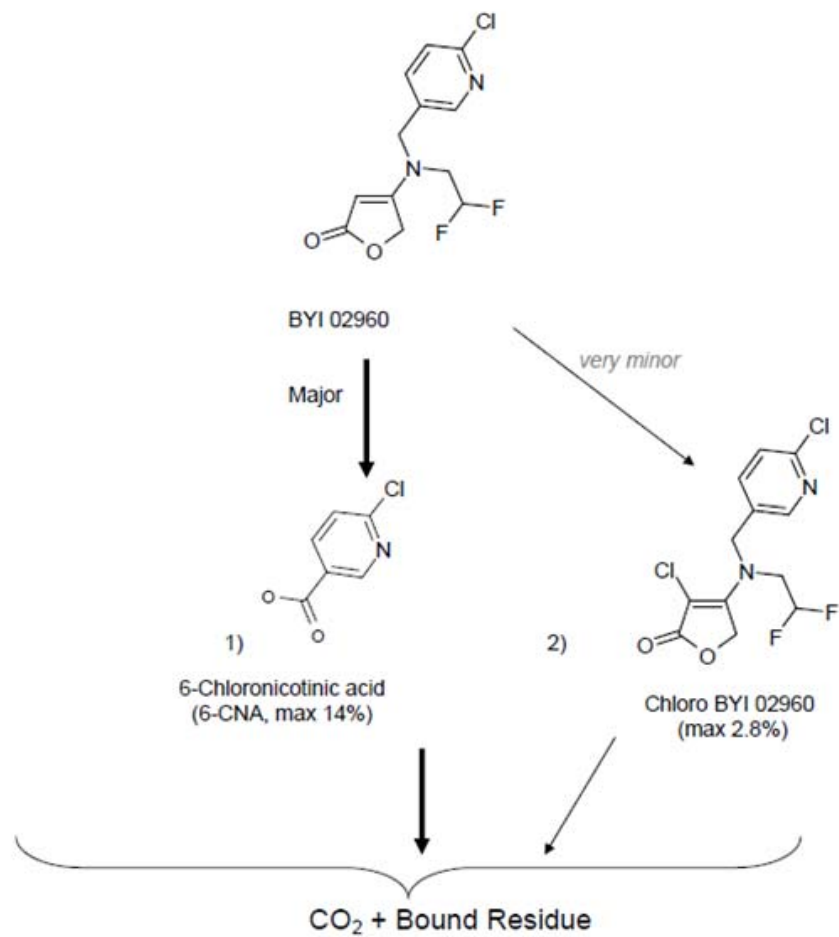
Figure 1. Proposed pathway for the parent compounds under aerobic and anaerobic conditions on (a) a silt loam soil in Europe and (b) a loamy sand soil (at CA) in USA.

compound. Similarly, in the desorption study, the estimated K_d values varied between 2.14 and 5.21 mL/g for six test soils, and their corresponding K_{oc} values ranged from 138.4 and 306.2 mL/g for six test soils. The estimated K_d and K_{oc} values in the desorption study were much higher than those of adsorption study, suggesting that the compound once adsorbed to the soils was not readily detached.

Table 4. The key characteristics of the six test soils in Europe and the USA[1].

Soil origin	Class[2]	pH[3]	BD	FC	OC	CEC
	–	–	g/cm^3	%	%	meq/100g
Laacher Hof AXXa, Germany	Sandy loam	6.2	1.22	12.5	2.1	9.4
Hoefchen am Hohenseh 4a, Germany	Loam	6.6	1.04	24.3	2.4	12.3
Hanscheiderhof, Germany	Loam	5.3	1.05	23.9	2.2	8.8
Dollendorf II, Germany	Loam	7.2	0.98	36.6	5.1	20.3
Sanger, California, USA	Sandy loam	6.8	1.30	11.5	0.7	6.7
Springfield, Nebraska, USA	Silt loam	6.5	0.96	25.0	1.9	19.0

[1] Abbreviation: BD = the bulk density, FC = the moisture content at 0.33 bar, OC = the organic carbon content, and CEC = the cation exchange capacity.
[2] Soil textural classes were determined according to the USDA classification.
[3] The pH was measured in calcium chloride ($CaCl_2$).

Table 5. The sorption and desorption parameters of the parent compound for the six test soils.

Soil type	Adsorption				Desorption			
	K_d	$1/n$	R^2	K_{oc}	K_d	$1/n$	R^2	K_{oc}
	mL/g	–	–	mL/g	mL/g	–	–	mL/g
Laacher Hof AXXa	2.077	0.8445	0.9988	98.9	4.115	0.8786	0.9994	196.0
Hoefchen am Hohenseh 4a	2.213	0.8682	0.9999	92.2	4.431	0.9086	0.9999	184.6
Hanscheiderhof	2.354	0.8643	0.9998	107.0	5.208	0.9099	0.9996	236.7
Dollendorf II	3.822	0.8648	0.9995	74.9	7.056	0.8923	0.9998	138.4
Sanger	0.597	0.9021	0.9993	85.2	2.143	0.9407	0.9992	306.2
Springfield	2.512	0.8505	0.9995	132.2	5.096	0.8603	0.9999	268.2
Mean	2.263	0.8657	0.9995	98.4	4.675	0.8984	0.9996	221.7

Field Dissipation Studies

The registrant examined terrestrial field dissipation of the parent compound BYI02960 at three geographic locations in USA, one soil in California (NAFTA Ecoregion 11.1), another soil in Florida (EPA Crop Region 3), and the other soil in Idaho (NAFTA Ecoregion 10.1). In each soil, the compound was applied to four replicate (bare ground) plots at one time through a broadcast application at a target rate of 600 g a.i./ha which exceeded the maximum single field usage rate (i.e., 410 g a.i./ha). One control plot was also tested in parallel. The total amount of water added to the plots during the study period corresponded to 582, 136, and 434% of the average of 30 years of rainfall data for the target crops in California, Florida, and Idaho soils, respectively. The test plots were divided into eight segments (at a soil depth 48 inches), six-inch length for each segment. Three soils were texturally classified from the top to the bottom as follows: 1) loam, loam, loam, loam, loam, loam, sandy loam, and loam for California soil, 2) loamy sand, loamy sand, sandy loam, sandy clay loam, sandy clay loam, sandy clay, sandy clay, and sandy clay for

Florida soil, and 3) loam, loam, loam, loam, loam, loam, sandy loam, and sandy loam for Idaho soil. The soil samples were analyzed for the parent compound (for BYI02960) and its metabolites (for 6-chloronicotinic acid and 2,2-difluoroacetic acid) using a mixture of acetonitrile/water (7/3, v/v) for 535 (in California soil), 363 (in Florida soil), and 364 days (in Idaho soil).

Results showed that the residues of the parent compound BYI02960 and its metabolites 6-chloronicotinic acid and 2,2-difluoroacetic acid were not detected below 12, 24, and 24 inch depths in California soil, respectively, with respect to the limit of quantification. However, all three residues, except for some samples, were not generally observed below 6 inch depths in Florida soil in terms of the method detection limit. In the case of Idaho soil, BYI02960, 6-chloronicotinic acid, and 2,2-difluoroacetic acid were not detected below 12, 24, and 36 inch depths, respectively, with respect to the method detection limit. The degrades 6-chloronicotinic acid and 2,2-difluoroacetic acid accounted for a maximum 6.3 and 21.9% of applied amount for California soil, 4.9 and 5.1% for Florida soil, and 5.9 and 7.8% for Idaho soil. The double first order in parallel kinetic model provided the best-fit to the observed data in terms of χ^2 and R^2. The half-life values estimated based on this model were 57.3, 10.1, and 49 days for California, Florida, and Idaho soils, respectively. Tables 6, 7, and 8 describe the degradation pathway of the parent compound in three US soils suggested by the registrant.

Table 6. Dissipation routes for BYI02960 in California soil.

Routes of dissipation	Percent of applied amount
Accumulation of BYI02960 in soil at 366 days	**27%** - Average soil residue of BYI02960
Max transformation products during the study	**6%** - 6-chloronicotinic acid **22%** - 2,2-difluoroacetic acid
Max mineralization to CO_2 at 120 days	**40.5%** - Radiolabeled soil metabolism studies[1]
Max non-extractable residue at 120 days	**26.4%** - Radiolabeled soil metabolism studies[1]
Leaching, if measured	0.0% - No leaching below the sampling zone.
Volatilization, if measured	0.0% - Non-volatile product
Run off, if measured	0.0% - Not expected

[1] Shepherd, J.J.; [Pyridine-2,6-14C]BYI 02960: Aerobic Soil Metabolism in Two US Soils; Bayer CropScience LP, Stilwell, KS, USA; Report No. MERVP038; September 6, 2011.

Table 7. Dissipation routes for BYI02960 in Florida soil.

Routes of dissipation	Percent of applied amount
Accumulation of BYI02960 in soil at 364 days	**18%** - Average soil residue of BYI02960
Max transformation products during the study	**4.9%** - 6-chloronicotinic acid **5.1%** - 2,2-difluoroacetic acid
Max mineralization to CO_2 at 120 days	**40.5%** - Radiolabeled soil metabolism studies[1]
Max non-extractable residue at 120 days	**26.4%** - Radiolabeled soil metabolism studies[1]
Leaching, if measured	0.0% - No leaching below the sampling zone.
Volatilization, if measured	0.0% - Non-volatile product
Run off, if measured	0.0% - Not expected

[1] Shepherd, J.J.; [Pyridine-2,6-14C]BYI 02960: Aerobic Soil Metabolism in Two US Soils; Bayer CropScience LP, Stilwell, KS, USA; Report No. MERVP038; September 6, 2011.

Table 8. Dissipation routes for BYI02960 in Idaho soil.

Routes of dissipation	Percent of applied amount
Accumulation of BYI02960 in soil at 364 days	**21.9%** - Average soil residue of BYI02960
Max transformation products during the study	**5.9%** - 6-chloronicotinic acid **7.8%** - 2,2-difluoroacetic acid
Max mineralization to CO_2 at 120 days	**40.5%** - Radiolabeled soil metabolism studies[1]
Max non-extractable residue at 120 days	**26.4%** - Radiolabeled soil metabolism studies[1]
Leaching, if measured	0.0% - No leaching below the sampling zone.
Volatilization, if measured	0.0% - Non-volatile product
Run off, if measured	0.0% - Not expected

[1] Shepherd, J.J.; [Pyridine-2,6-14C]BYI 02960: Aerobic Soil Metabolism in Two US Soils; Bayer CropScience LP, Stilwell, KS, USA; Report No. MERVP038; September 6, 2011.

Evaluation of Leaching Potential to Ground Water for Flupyradifurone

Leaching potential of the parent compound was examined in soils (n=2,789) on Oahu, Hawaii. Since there is difference between literature and registrant's recommended values for K_{oc} and half-life, we have run the CLERS model twice to assess leaching potential of the parent compound. The mean and standard deviation in literature were 0.162 and 0.116 m^3/kg for K_{oc} and 138.4 and 139.4 days for half-life. And those of registrant values were determined as 0.098 and 0.020 m^3/kg for K_{oc} and 76.8 and 55.7 days for half-life. Note that all available values in relevant laboratory and field studies were used to calculate the mean and standard deviation.
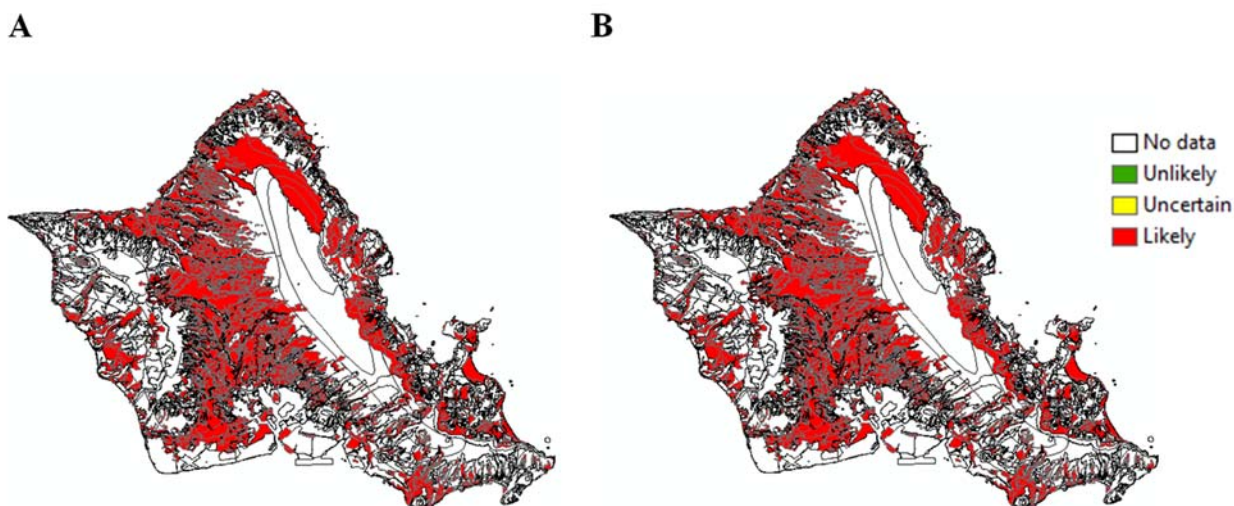

Figure 2. Leaching potential of the parent compound (on Oahu Island, Hawaii) using (a) literature and (b) registrant' recommended values in the CLERS model.

Figure 3 shows the leaching potential of the parent compound on Oahu Island, Hawaii, determined by literature and registrant' recommended values in the CLERS model. As shown in the figure, no difference is observed in the leaching potential of the parent compound using literature and registrant' recommended values, although they show some differences in K_{oc} and half-life values. Most areas are classified as likely according to classification scheme. Table 9

also shows a descriptive statistics of the main evaluation criteria in the CLERS model. From the table, it is determined that there is a slight difference in the revised attenuation factor (AFR) using both literature and registrant' recommended values in the CLERS model. As AFR decreases, the leaching potential of the chemical is high. The retardation factor (RF) using literature values is higher than that of registrant values, indicating that the parent compound may be bound onto the soils slightly more. Volatilization of the compound also does not likely occur in the soils due to its very low Henry's law constant. Based on these results, it can be suggested that the compound is considered as a potential leacher in Hawaii. Thus, the compound should be used carefully in appropriate plan.

Table 9. Summary statistics of main evaluation criteria in CLERS model (n=2,789)[1].

	Literature				Registrant			
	AFR	CVAFR	RF	CVRF	AFR	CVAFR	RF	CVRF
Mean	4.14	0.30	12.50	0.29	4.28	0.30	7.96	0.27
SD	1.26	0.05	4.92	0.13	1.26	0.05	2.98	0.13

[1] Abbreviation: AFR = the revised attenuation factor, CV = the coefficient of variance, i.e., uncertainty band, RF = the retardation factor, SD = the standard deviation, and n = the number of soil polygons.

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Appendix A. Additional runs of the CLERS model for remaining islands in Hawaii.
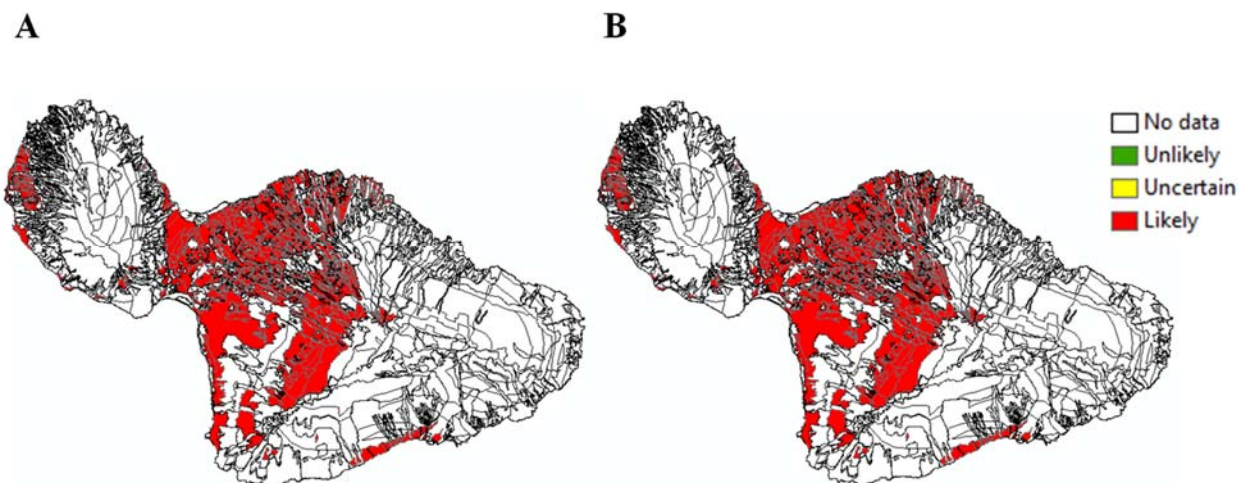
A1. Maui Island, Hawaii

Figure A1. Leaching potential of the parent compound (on Maui Island, Hawaii) using (a) literature and (b) registrant' recommended values in the CLERS model.
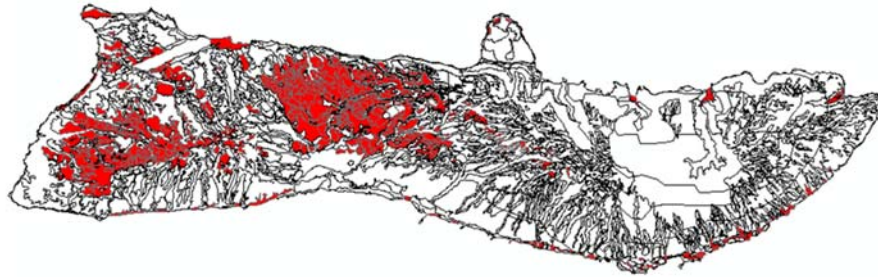
Table A1. Summary statistics of the main evaluation criteria in the CLERS model for Maui Island, Hawaii (*n*=1,095) [1].

	Literature				Registrant			
	AFR	CVAFR	RF	CVRF	AFR	CVAFR	RF	CVRF
Mean	4.24	0.29	16.26	0.25	4.38	0.29	10.23	0.24
SD	0.80	0.03	7.68	0.13	0.80	0.03	4.64	0.12

[1] Abbreviation: AFR = the revised attenuation factor, CV = the coefficient of variance, i.e., uncertainty band, RF = the retardation factor, SD = the standard deviation, and *n* = the number of soil polygons.
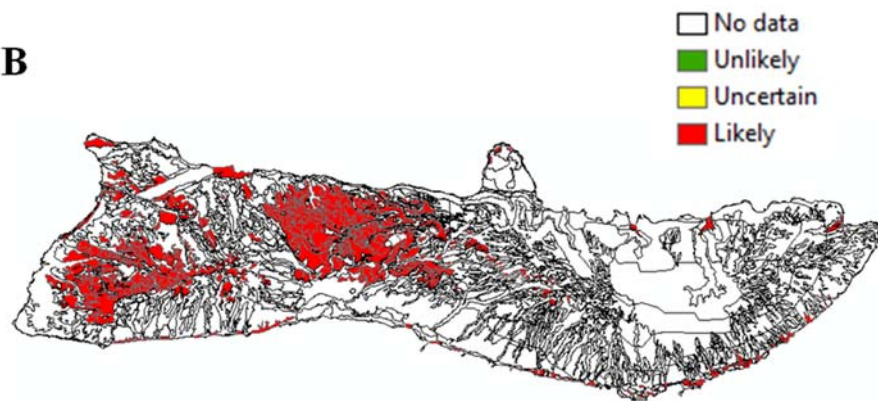
A2. Molokai Island, Hawaii

Figure A2. Leaching potential of the parent compound (on Molokai Island, Hawaii) using (a) literature and (b) registrant' recommended values in the CLERS model.

Table A2. Summary statistics of the main evaluation criteria in the CLERS model for Molokai Island, Hawaii (*n*=515) [1].

	Literature				Registrant			
	AFR	CVAFR	RF	CVRF	AFR	CVAFR	RF	CVRF
Mean	4.47	0.85	12.05	0.27	4.62	0.85	7.68	0.25
SD	0.46	8.15	7.78	0.11	0.46	8.15	4.70	0.10

[1] Abbreviation: AFR = the revised attenuation factor, CV = the coefficient of variance, i.e., uncertainty band, RF = the retardation factor, SD = the standard deviation, and *n* = the number of soil polygons.
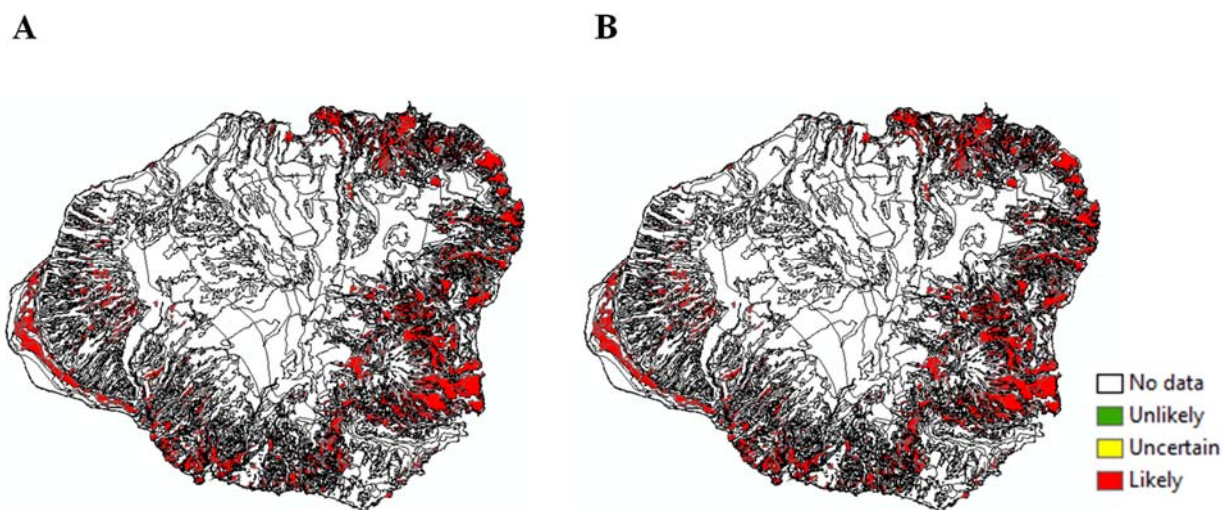
A3. Kauai Island, Hawaii

Figure A3. Leaching potential of the parent compound (on Kauai Island, Hawaii) using (a) literature and (b) registrant' recommended values in the CLERS model.

Table A3. Summary statistics of the main evaluation criteria in the CLERS model for Kauai Island, Hawaii (n=1,236) [1].

	Literature				Registrant			
	AFR	CVAFR	RF	CVRF	AFR	CVAFR	RF	CVRF
Mean	4.86	1.04	16.42	0.22	5.00	1.04	10.33	0.21
SD	0.91	1.70	6.31	0.10	0.90	1.70	3.82	0.10

[1] Abbreviation: AFR = the revised attenuation factor, CV = the coefficient of variance, i.e., uncertainty band, RF = the retardation factor, SD = the standard deviation, and n = the number of soil polygons.
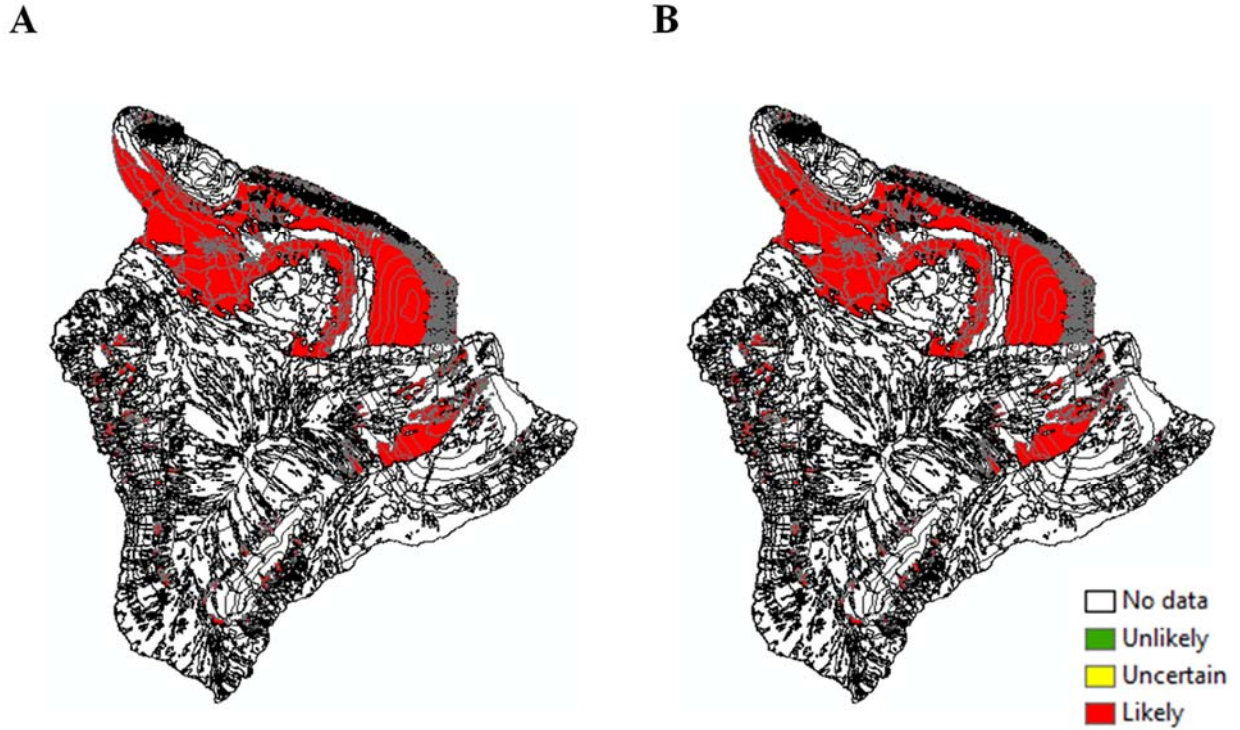
A4. Hawaii Island, Hawaii

Figure A4. Leaching potential of the parent compound (on Hawaii Island, Hawaii) using (a) literature and (b) registrant' recommended values in the CLERS model.

Table A4. Summary statistics of the main evaluation criteria in the CLERS model for Hawaii Island, Hawaii (*n*=2,101)[1].

	Literature				Registrant			
	AFR	CVAFR	RF	CVRF	AFR	CVAFR	RF	CVRF
Mean	3.29	0.07	17.29	0.38	3.42	0.07	10.85	0.37
SD	1.53	0.09	6.56	0.14	1.53	0.09	3.97	0.14

[1] Abbreviation: AFR = the revised attenuation factor, CV = the coefficient of variance, i.e., uncertainty band, RF = the retardation factor, SD = the standard deviation, and *n* = the number of soil polygons.