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OFFICE OF
PREVENTION, PESTICIDES
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MEMORANDUM

SUBJECT: Tier I Drinking Water Assessment for the Section 3 Proposed Registration of Pyrasulfotole on Wheat, Oats, Barley and Triticale

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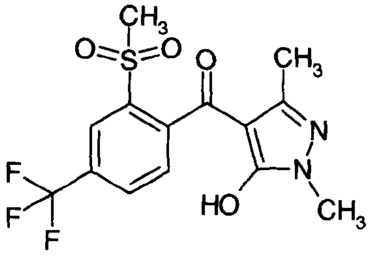
Attached is the drinking water exposure assessment for proposed pyrasulfotole use on wheat, oats, barley and triticale. If additional refinements are necessary, please contact Marietta Echeverria at 703-305-8578 or echeverria.marietta@epa.gov.

Drinking Water Exposure Assessment for the Section 3 Proposed Registration of Pyrasulfotole on Wheat Oats, Barley and Triticale



Pyrasulfotole
(5-hydroxy-1,3-dimethyl-1*H*-pyrazol-4-yl)[2-(methylsulfonyl)-4-(trifluoromethyl)phenyl]methanone
CAS No. 365400-11-9

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1 EXECUTIVE SUMMARY

This document reports the drinking water exposure assessment for pyrasulfotole that has been conducted to support the human health risk assessment for the Section 3 proposed new registration. Pyrasulfotole is a post emergence herbicide for proposed use on wheat, oats, barley and triticale. Foliar spray applications, aerial and ground spray application and sprinkler irrigation, are being proposed. Tier 1 surface water and groundwater modeling was conducted for the labeled cereal grain use with a single annual application at a rate of 0.045 lbs. a.i./A. The recommended estimated drinking water concentrations (EDWCs) for the human health risk assessment are in Table 1. There was one environmental degradate, pyrasulfotole-benzoic acid (AE 197555), identified in the soil metabolism and terrestrial field dissipation studies. Drinking water exposure to the benzoic acid degradate is not considered in this assessment based on discussions with the HED.

Table 1. Tier I EDWCs for pyrasulfotole for aerial spray applications to wheat, barley, oats or triticale

Drinking Water Source	Model	Use rate (lbs ai/A/year)	Acute (ppb)	Chronic (ppb)
Surface water	FIRST	0.045	4.0	2.8
Groundwater	SCI-GROW	0.045	1.4	1.4

2 PROBLEM FORMULATION

This is a Tier I drinking water assessment that uses modeling and available monitoring data to estimate the groundwater and surface water concentrations in drinking water sources (pre-treatment) resulting from pesticide use on sites that are vulnerable. This initial tier screens out chemicals with low potential risk and allows OPP to focus resources on more refined risk assessments for chemicals which potentially present more significant risks. This drinking water assessment reports potential exposure concentrations for the human health dietary risk assessment and provides a description of how those concentrations were determined.

3 ANALYSIS

3.1 Use Characterization

Pyrasufotole is a post emergence herbicide that is applied as a foliar spray (via ground, aerial, or sprinkler irrigation) one time a year at a maximum application rate of 0.045 lb a.i./A. There are two pyrasulfotole end-use products being proposed for registration in the United States for use on wheat, barley, oats, and triticale. The two proposed formulations are AE 0317309 + Bromo Herbicide (an emuslsifiable concentrate containing 3.3% pyrasulfotole) and AE 0317309 SE06 Herbicide (a suspo-emulsion containing 4.4% pyrasulfotole). According to the proposed labels, pyrasulfotole can be applied at a maximum application rate/year of 0.045 lb a.i./acre for ground and aerial applications and 0.037 lb a.i./acre for sprinkler irrigation application (limited to use on wheat and barley) (**Table 2**). Only one application per year is allowed.

Table 2. Proposed maximum use patterns for pyrasulfotole

Product (% a.i.)	Uses	Application methods	Maximum application rate/year	Maximum number of applications/year
AE 0317309 + Bromo Herbicide (3.3%)	Wheat	Ground Aerial Sprinkler Irrigation	0.037 lb a.i./acre[1]	1
	Barley	Ground Aerial Sprinkler Irrigation		
	Oats	Ground Aerial		
	Triticale	Ground Aerial		
AE 0317309 SE06 Herbicide (4.4%)	Wheat	Ground Aerial	0.045 lb a.i./acre[2]	1
	Barley	Ground Aerial		
	Oats	Ground Aerial		
	Triticale	Ground Aerial		

[1] The application rate on the label was converted to lbs a.i./acre based on the following: The formulated product density = 1.1417 g/cc; the formulation is 3.3% pyrasulfotole and a max application rate of 15 oz of formulated product/acre is allowed.

[2] The application rate on the label was converted to lbs a.i./acre based on the following: The formulated product density = 1.1411 g/cc; the formulation is 4.4% pyrasulfotole and a max application rate of 13.7 oz of formulated product/acre is allowed.

3.2 Environmental Fate and Transport Characterization

Pyrasulfotole is expected to be persistent and mobile to moderately mobile (FAO classification) in the environment. Major routes of dissipation include microbial degradation in soils, formation of non-extractable residues in soils and sediments, and dilution.

Under aerobic conditions pyrasulfotole degraded in 3 soils (loamy sand, silt loam, sandy loam) according to an apparent bi-phasic pattern with observed DT_{50}s ranging from 4-65 d and observed DT_{90}s ranging from >120->358 d. A 2-compartment, 4-parameter exponential model, also known as Double First Order Parallel (DFOP), was used to fit the data and resulted in modeled DT_{50}s ranging from 6-63 d and DT_{90}s ranging from 208-1424 d (MRIDs 46801709, 406801710, 46801711). Degradation products included pyrasulfotole-benzoic acid (AE 197555), CO_2 and non-extractable residues. Non-extractable residues were identified at maximums of 35-62% of applied radioactivity in the 3 soils. The non-extractable residues are uncharacterized and it is uncertain whether they consist of degradates of risk concern. Under sterile conditions, however, the formation of non-extractable residues (as well as the formation of CO_2 and the benzoic acid degradate) were negligible. In terrestrial field dissipation studies pyrasulfotole dissipated from the whole soil profile with modeled (DFOP) DT_{90}s ranging 44-531 d and the amount of parent pyrasulfotole carry over to the following growing season ranged from 4.7 to 37% (MRIDs 46801716, 46801717, 46801718, 46801719).

In aquatic systems, pyrasulfotole is stable to hydrolysis and photolysis (MRIDs 46801705, 46801706). In aerobic aquatic metabolism studies, pyrasulfotole partitioned to the sediment and formed non-extractable residues but there was no evidence of degradation. Pyrasulfotole is considered stable to microbial degradation in aquatic systems (MRID 46801713). Under anaerobic conditions pyrasulfotole is also stable (MRIDs 46801712, 4681714, 46801715).

Batch equilibrium studies resulted in organic carbon sorption coefficients (K_{oc}) ranging 20-345 ml/g_{oc} with a median value of 68 ml/g_{oc} (MRID 46801703). In terrestrial field dissipation studies pyrasulfotole showed variable downward migration in the soil profile under bare soil conditions. In some studies pyrasulfotle was confined to 0-15 cm whereas in others it was detected at quantifiable levels as deep as 75-90 cm (MRIDs 46801716, 46801717, 46801718, 46801719). Since pyrasulfotole has a K_d less than 5 in most soils and is persistent (hydrolysis half-life greater than 25 weeks, photolysis half-life greater than 1 week, aerobic soil metabolism half-life greater than 2-3 weeks), not volatile (Henry's Law constant less than 10^{-2} atm*m^{-3}/mol), and shows movement to 45 cm during some field dissipation studies, there is indication for potential groundwater contamination (Cohen 1984). Depending on soil, site and meteorological conditions pyrasulfotole may be transported off-site to drinking water sources via runoff, leaching and spray drift. Table 3 summarizes the registrant-submitted environmental fate and transport properties of pyrasulfotole. Further details on the environmental fate and transport studies are found in Appendix A.

There was one major degradate, pyrasulfotole-benzoic acid (AE 197555) detected in the aerobic soil metabolism and terrestrial field dissipation studies. Based on discussions with HED, drinking water exposure to pyrasulfotole-benzoic acid is not assessed because it is not of risk concern.

Table 3 Summary of environmental chemistry and fate properties of pyrasulfotole

Parameter	**Value**	**Reference/Comments**
Selected Physical/Chemical Parameters		
PC code	000692	
CAS No.	365400-11-9	
Chemical name	(5-hydroxy-1,3-dimethylpyrazol-4-yl)(α,α,α-trifluoro-2-mesyl-*p*-tolyl)methanone	
Chemical formula	$C_5H_{13}Cl_2N$	
Molecular weight	362.3 g/mol	
Water solubility (20 °C) pH 4 pH 7 pH 9	 4.2 g/L 69 g/L 49 g/L	Product chemistry
Vapor pressure	2.7×10^{-7} Pa (20°C) 6.8×10^{-7} Pa (25°C)	Product chemistry
log K_{OW} pH 4 pH 7 pH 9	 0.276 -1.36 -1.58	Product chemistry
Persistence		
Hydrolysis	Stable (pH = 5, 7, 9)	MRID 46801705
Photolysis in water	Stable	MRID 46801706

Table 3 Summary of environmental chemistry and fate properties of pyrasulfotole

Parameter	**Value**				**Reference/Comments**
Photolysis in soil	$t_{1/2}$ = 227 d				MRID 46801707 Environmental phototransformation half-life based on sunlight expected in Pheonix, AZ (33.26° N)
Aerobic soil metabolism	**Soil Type**	**DT_{50} (d)**	**DT_{90} (d)**	**R^2**	MRIDs 46801709, 46801710, 46801711 2 compartment, 4 parameter exponential model (DFOP)
	Loamy sand	5.8	749	0.977	
	Silt loam	63	1424	0.998	
	Sandy loam	23	208	0.990	
Anaerobic soil metabolism	Stable				MRID 46801712
Aerobic aquatic metabolism	Stable				MRID 46801713
Anaerobic aquatic metabolism	Stable				MRIDs 46801714, 46801715
Mobility					
Batch equilibrium	**Soil Type**	**K_f**[1]	**1/N**	**K_{oc}**[2]	MRID 46801703
	Silt loam	0.98	0.93	21	
	Loamy sand	1.2	0.91	100	
	Clay loam	0.34	0.98	20	
	Sandy loam	0.39	0.95	35	
	Silt loam	3.2	0.93	213	
	Sandy loam	16	0.83	345	
Laboratory volatility	NA				Volatility not likely based on low vapor pressure
Field Dissipation					
Terrestrial field dissipation	**Location**	**DT_{50}**	**DT_{90}**	**% carry over**	MRIDs 46801716, 46801717, 46801718, 46801719
	Kansas	8.9 d	45 d	4.7	
	North Dakota	5.7 d	44 d	7.7	
	Washington	5.7 d	213 d	11	
	Saskatchewan	10 d	260 d	37	
	Manitoba	9.2 d	531 d	19	
	Ontario	18 d	178 d	8.9	
Bioaccumulation					
Accumulation in fish, BCF	No data				Bioaccumulation is not expected based on low log K_{ow}

1. Units of $(mg/kg)/(mg/L)^{1/N}$, where 1/N is the Freundlich exponent.
2. Approximation calculated from the Freundlich coefficient, per standard EFED guidance.

3.3 Drinking Water Exposure Modeling

Tier 1 modeling was used to estimate the drinking water exposure for use in the dietary risk assessment of pyrasulfotole. The following is a description of the models used, the selection of the model input parameters, and a characterization of the output from these simulations.

3.3.1 Models

Tier 1 EDWCs for surface water were generated using FIRST, dated August 5, 2001. FIRST is a screening model designed by the Environmental Fate and Effects Division (EFED, 2001a) of the Office of Pesticide Programs to estimate the concentrations found in drinking water from surface water sources for use in human health risk assessment. As such, it provides upper bound values on the concentrations that might be found in drinking water due to the use of a pesticide. FIRST is a single-event model (one runoff event), but can account for spray drift from multiple applications. FIRST is hardwired to represent the Index Reservoir, a standard water body used by the Office of Pesticide Programs to assess drinking water exposure (Office of Pesticide Programs, 2002). It is based on a real reservoir, Shipman City Lake in Illinois, that is known to be vulnerable to pesticide contamination. The single runoff event moves a maximum of 8% of the applied pesticide into the reservoir. This amount can be reduced due to degradation on the field and the effects of binding to soil in the field. FIRST also uses a Percent Cropped Area (PCA) factor to adjust for the area within the watershed that is planted to the modeled crop. The national default PCA of 0.87 was applied in this assessment.

Tier 1 EDWCs for groundwater were generated with SCIGROW 2.3, dated July 29, 2003 (EFED, 2001b). SCIGROW is a regression model used as a screening tool for ground water used as drinking water. SCIGROW was developed by regressing the results of Prospective Ground Water studies against the Relative Index of Leaching Potential (RILP). The RILP is function of aerobic soil metabolism and the soil-water partition coefficient. The output of SCIGROW represents the concentrations that might be expected in shallow unconfined aquifers under sandy soils.

3.3.2 Modeling Approach and Input Parameters

Tables 4 and 5 summarize the model input parameter values used in FIRST and SCIGROW, respectively. These parameters were selected in accordance with EFED's input parameter guidance (Environmental Fate and Effects Division, 2002). To estimate first order half-lives (rate constants) for exposure modeling, the modeled DT_{90} was divided by 3.32 (the expected ratio between DT_{50} and DT_{90} for first order reactions). An aerobic soil metabolism first order half-life of 439 d (the upper 90th percentile confidence bound on the mean) was used for surface water modeling with FIRST and the median value, 226 d, was used for groundwater modeling with SCIGROW. The soil-water partitioning coefficient used in FIRST and SCIGROW was 20 ml/g_{oc}, the lowest non-sand K_{oc}. The lowest K_{oc} value was used in SCIGROW because there was greater than 3-fold variability in the available data.

Table 4. FIRST (v 1.0) input parameter values for pyrasulfotole applied by aerial spray

Parameter	Value	Source	Comments
Application Rate (lb a.i./A)	0.045	AE 0317309 SE06 Herbicide (4.4%)	

Table 4. FIRST (v 1.0) input parameter values for pyrasulfotole applied by aerial spray			
Parameter	**Value**	**Source**	**Comments**
Number of Applications	1	AE 0317309 SE06 Herbicide (4.4%)	
Soil Partitioning Coefficient (K_{oc}; ml/g_{oc})	20	MRID 46801703	lowest non-sand value
Aerobic Soil Metabolism $t_{1/2}$ (d)	439	MRIDs 46801709, 46801710, 46801711	90th percentile upper confidence bound on the mean where $t_{1/2}$ is estimated by DT90/3.32
Wetted in?	No	foliar applied	
Depth of Incorporation (inches)	0	foliar applied	
Method of Application	aerial spray	AE 0317309 SE06 Herbicide (4.4%)	
Percent Cropped Area	0.87	National default	
Solubility in Water (mg/L)	6.9×10^4	Product chemistry data	
Aerobic Aquatic Metabolism $t_{1/2}$ (d)	0	MRID 46801713	Stable to aquatic metabolism
Hydrolysis $t_{1/2}$	0	MRID 46801705	Stable to hydrolysis
Aquatic Photolysis $t_{1/2}$ (d)	0	MRID 46801706	Stable to photolysis

Table 5. SCIGROW 2.3 input parameter values for pyrasulfotole applied by aerial spray.			
Parameter	**Value**	**Source**	**Comments**
Maximum Application Rate (lb a.i./A/application)	0.045	AE 0317309 SE06 Herbicide (4.4%)	
Maximum Number of Applications per Year	1	AE 0317309 SE06 Herbicide (4.4%)	
Aerobic Soil Metabolism Half-life (d)	226	MRIDs 46801709, 46801710, 46801711	median value where $t_{1/2}$ is estimated by DT90/3.32
Organic Carbon Partition Coefficient (K_{oc}, ml/g_{oc})	20	MRID 46801703	Lowest value; > 3x variability in data

3.3.3 Modeling Results

The FIRST and SCI-GROW output files are located in Appendix B. Based on the results of these simulations, EFED recommends an acute surface water EDWC of **4.0 µg/L** and a chronic EDWC of **2.8 µg/L** for use in the human health risk assessment. These recommendations are based on the use of pyrasulfotole on cereal grains (wheat, barley, oats, and triticale) at an annual application rate of 0.045 lb a.i./A/year. The recommended EWDC for groundwater is **1.4 µg/L** and is also based on the use of pyrasulfotole on cereal grains at the previously stated rate.

3.4 Monitoring Data

There were no national-scale monitoring data available for this assessment.

3.5 Drinking Water Treatment

There is no available information on the drinking water treatment effects on pyrasulfotole.

4 CONCLUSIONS

The estimated concentrations provided in this assessment are conservative estimates of pyrasulfotole concentrations in untreated drinking water. A major source of uncertainty is the nature of the non-extractable residues formed during degradation in soils. Non-extractable residues were identified at maximums of 35-62% of applied radioactivity in 3 soils. The non-extractable residues are uncharacterized and it is uncertain whether they consist of degradates of risk concern. Under sterile conditions these non-extractables were not formed suggesting that the formation of them is microbially mediated.

If dietary risks require refinement, higher tiered models and modeling scenarios can be utilized upon request.

References

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Appendix A. Environmental Fate and Transport Study Details

Abiotic Degradation

Hydrolysis

In an **acceptable** study (MRID 46801705), the hydrolysis of pyrasulfotole at 0.14 mg a.i./L, was studied in the dark at 24.9 ± 0.02°C in sterile aqueous buffered pH 5, pH 7, and pH 9 solutions for 30 days. [^{14}C]Pyrasulfotole averaged 98.4-100.4% of the applied in the pH 5 solutions and 98.6-100.3% in the pH 7 solutions throughout the experiment. In the pH 9 solution, [^{14}C]pyrasulfotole averaged 96.6-98.1% of the applied through 22 days posttreatment and 95.7% at 30 days. Half-lives were not calculated because pyrasulfotole was stable to hydrolysis.

Aqueous Photolysis

In an **acceptable** study (MRID 46801706), the aqueous phototransformation of pyrasulfotole at *ca.* 1 mg a.i./L, was studied in sterile pH 7 buffer (0.01M phosphate) at 25 ± 1°C under continuous irradiation using a UV-filtered xenon arc lamp for 212 hours. [^{14}C]Pyrasulfotole (both labels) did not degrade in either the irradiated or dark control solutions. In the irradiated solutions, [^{14}C]pyrasulfotole ranged from an average of 97.7% to 100.7% of the applied with no pattern of decline during the 9-day experiment. In the dark controls, [^{14}C] pyrasulfotole ranged from an average 99.6% to 102.0% of the applied with no pattern of decline. A half-life was not calculated because pyrasulfotole was stable in both the irradiated and dark control solutions.

Soil Photolysis

In an **acceptable** study (MRID 46801707), the phototransformation of pyrasulfotole, at 0.51 mg/kg (equivalent to 75 g a.i./ha), was studied on silt loam soil [pH 7.4, organic matter 7.1%] from North Dakota that was irradiated continuously using a UV-filtered xenon lamp for 9 days at 25 ± 0.1°C. The intensity of the lamp was 680 W/m^2, and 7.0 hours of irradiation with the artificial light was reported to be equivalent to 1 solar day in late June in Phoenix, Arizona. [^{14}C]Pyrasulfotole decreased from an average of 104.2% of the applied at time 0 to 87.2% in the irradiated samples and 89.9% in the dark controls at study termination (9 days posttreatment). Concentrations were variable and were affected by overall recoveries of [^{14}C]residues; [^{14}C]pyrasulfotole comprised 97.9% of the recovered at time 0 and 90.0% and 93.6% in the irradiated and dark controls, respectively, at 9 days posttreatment. No major transformation products were isolated from either the irradiated or dark control soils. No minor transformation products, which averaged ≤1.0% of the applied, were identified in either the irradiated or dark control soils. Based on first order linear regression analysis, pyrasulfotole dissipated with half-lives of 32.5 days in the irradiated samples (continuous irradiation) and 64.2 days in the dark controls. The half-lives are of uncertain value because they are extrapolated well beyond the duration of the study, between replicate variability at some intervals is *ca.* 5% of the applied, and the calculations are based on the assumption that degradation follows a linear pattern. The **phototransformation half-life** for pyrasulfotole, was 66 days based on the continuous irradiation used in the study. The study author stated that 7.0 hours of continuous irradiation with the artificial light was equivalent to 1 day of natural sunlight in Phoenix, Arizona (33.26° N latitude). Therefore, the **environmental phototransformation half-life** is expected to be *ca.* 227 days in Phoenix, AZ.

Metabolism

Aerobic Soil Metabolism

In an **acceptable** aerobic soil metabolism study (MRID 46801709), $[^{14}C]$pyrasulfotole dissipated in a loamy sand soil (pH 5.6-6.2, organic carbon 1.2%) from North Carolina following a biphasic pattern decreasing quickly from 96.4-97.5% of the applied at day 0 posttreatment to 53.8-54.8% at 4 days and was 40.0-40.7% at 7 days, then dissipation significantly slowed with $[^{14}C]$pyrasulfotole comprising 20.2-22.8% at study termination. The reviewer-calculated **log-linear half-life** was 240 days ($r^2 = 0.4428$) and the **nonlinear half-life** was 69 days ($r^2 = 0.441$). Based on a 2-compartment, 4-parameter exponential model (DFOP) the **DT_{50} and DT_{90}** estimates were 5.8 and 749 days, respectively ($r^2 = 0.977$). The **observed DT_{50}** and **DT_{90}** values were 4-7 days and >358 days, respectively.

2-Methylsulfonyl-4-trifluoromethylbenzoic acid (AE B197555) was a major transformation product in phenyl-label treated soil detected at a maximum 12.2% of the applied at 7 days posttreatment and was 4.2% at study termination. No minor transformation products were identified for either label. Non-extractable $[^{14}C]$residues increased from 1.7-1.9% at day 0 to maximums of 49.7-50.1% at 100-120 days and were 43.2-44.8% at 358 days. At study termination, volatilized $^{14}CO_2$ totaled 17.3%-18.6% of the applied.

Under **sterile** (autoclaved soil, both labels) conditions, parent pyrasulfotole comprised 94.8-95.4% of the applied at 120 days (final interval), with AE B197555 in phenyl-label treated soil detected at ≤3.2% at any interval. At study termination, extractable and nonextractable $[^{14}C]$residues were 95.6-99.3% and 2.7-3.5% of the applied, respectively, with volatilized $^{14}CO_2$ and volatile $[^{14}C]$organic compounds ≤0.2%.

In an **acceptable** aerobic soil metabolism study (MRID 46801710), $[^{14}C]$pyrasulfotole dissipated in a silt loam soil (pH 7.0-7.3, organic carbon 4.7%) from North Dakota following a biphasic pattern with a steady decline during the initial 2 months posttreatment, decreasing from 94.3-97.1% of the applied at day 0 to 47.2-50.0% at 65 days, then dissipation slowed with $[^{14}C]$pyrasulfotole comprising 22.0-24.9% at study termination. The reviewer-calculated **log-linear half-life** for both radiolabels was 161 days ($r^2 = 0.8227$) and the **nonlinear half-life** was 95 days ($r^2 = 0.9144$). The reviewer-calculated **DT_{50} and DT_{90}** estimates based on a 2-compartment, 4-paramter exponential model (DFOP) were 63 and 1424 days, respectively ($r^2 = 0.998$). The **Observed DT_{50} and DT_{90}** and values were 50-65 days and >358 days, respectively.

2-Methylsulfonyl-4-trifluoromethylbenzoic acid (AE B197555) was a minor transformation product in phenyl-label treated soil detected at a maximum 3.8% of the applied; no other minor or major products were identified for either label. Nonextractable $[^{14}C]$residues increased from 0.4-1.1% at day 0 to maximums of 31.3-35.2% at 155-190 days and were 30.1-30.7% at 358 days. At study termination, volatilized $^{14}CO_2$ totaled 33.5-40.5% of the applied.

Under **sterile** (autoclaved soil, both labels) conditions, parent pyrasulfotole comprised 93.6-94.2% of the applied at 120 days (final interval), with AE B197555 in phenyl-label treated soil detected at a maximum 3.7% at study termination. At 120 days, extractable and nonextractable [^{14}C]residues were 93.6-97.9% and 3.8-5.2% of the applied, respectively, with volatilized $^{14}CO_2$ and volatile [^{14}C]organic compounds ≤0.4%.

In a **supplemental** aerobic soil metabolism study (MRID 46817011), phenyl-labeled pyrasulfotole dissipated in a sandy loam soil (pH 5.9-6.6, organic carbon 1.4%) from Germany from a mean 100.0% of the applied at day 0 to 48.0% at 29 days and was 19.0% at 120 days. Pyrazole-labeled pyrasulfotole reached the observed DT$_{50}$ somewhat faster decreasing from 98.4% at day 0 to 48.9% at 21 days and was 17.3% at study termination. The reviewer-calculated **log-linear half-life** for both radiolabels was 48 days ($r^2 = 0.9127$) and the **nonlinear half-life** was 32.4 days ($r^2 = 0.9503$). The reviewer-calculated **DT$_{50}$ and DT$_{90}$** estimates based on a 2-compartment, 4-parameter exponential model (DFOP)were 23 and 208 days, respectively ($r^2 = 0.990$). The **observed DT$_{50}$ and DT$_{90}$** values were 14 – 29 and >120 days, respectively.

2-Methylsulfonyl-4-trifluoromethylbenzoic acid (AE B197555) was a minor transformation product in phenyl-label treated soil detected at a maximum 8.9 ± 0.4% of the applied; no other minor or major products were identified for either label. Nonextractable [^{14}C]residues increased from 2.1-2.7% at day 0 to 60.1-62.1% at study termination (120 days). At study termination, volatilized $^{14}CO_2$ comprised total means of 16.3-18.0% of the applied, while volatile [^{14}C]organic compounds were ≤0.1% at all intervals.

Table A1 summarizes the various modeled used to describe the degradation kinetics in the aerobic soil metabolism studies.

Table A1. Summary of models used to fit degradation data in aerobic soil metabolism studies

Model	**Half-life (d)**	**Model equation**	**r^2**	**DT$_{50}$ (d)**	**DT$_{90}$ (d)**
Loamy sand, North Carolina (MRID 46801709)					
Log-linear	240	$y = -0.0029x + 3.7590$	0.443	--	--
Nonlinear	68.6	$y = 58.6*\exp(-0.0101*x)$	0.441	--	--
DFOP	--	$y = 69.0*\exp(-0.24*x) + 33.1*\exp(-0.0016*x)$	0.977	5.8	747
Observed DT$_{50/90}$	--	--	--	4-7	>358
Silt loam, North Dakota (MRID 46801710)					
Log-linear	161	$y = -0.0043x + 4.2958$	0.823	--	--
Nonlinear	95.0	$y= 87.2*\exp(-0.0073*x)$	0.914		
DFOP	--	$y= 66.6*\exp(-0.019*x)+31.2*\exp(-0.0008*x)$	0.998	63	1424
Observed DT$_{50/90}$	--	--	--	50-65	>358
Sandy loam, Germany (MRID 46810711)					
Log-linear	47.6	$y = -0.01456 + 4.3854$	0.913	--	--
Nonlinear	32.4	$y = 91.4*\exp(-0.0214*x)$	0.950	-	-
DFOP	--	$y = 58.5*\exp(-0.0538*x)+37.7*\exp(-0.0064*x)$	0.990	23	208
Observed DT$_{50/90}$	--	--	--	14-29	>120

Anaerobic Soil Metabolism

In an **acceptable** anaerobic soil metabolism study (MRID 46801712), [^{14}C]pyrasulftole-residues partitioned between the soil and water layer with mean (n = 2) distribution ratios (water:soil) of 1:22-28 immediately after flooding (30 days posttreatment), decreasing to 1:5 after 33 days (63 days posttreatment) and were 1:7-11 at study termination (150 days posttreatment). The dissipation rate of [^{14}C]pyrasulfotole significantly slowed with the conversion to anaerobic conditions. [^{14}C]Pyrasulfotole comprised means of 93.5-97.3% of the applied in the soil at day 0 posttreatment, then at day 0 post-flooding (30 days posttreatment) was detected at 66.0-68.4% in the total system and was 62.2-64.1% at 120 days post-flooding (150 days posttreatment). In the water layer, [^{14}C]pyrasulfotole increased from means of 2.4-3.1% at day 0 post-flooding (30 days posttreatment) to 11.7-14.2% at 33 days (63 days posttreatment) and was 7.2-7.7% at study termination. In the soil, [^{14}C]pyrasulfotole decreased from means of 93.5-97.3% at day 0 posttreatment to 62.9-66.0% at day 0 post-flooding (30 days posttreatment) and was 53.3-56.5% at 90-120 days post-flooding (120-150 days posttreatment). In the water layer, [^{14}C]pyrasulfotole dissipated with a combined (both labels) **linear half-life** of 127 days and nonlinear **half-life** of 116 days. **Observed DT50** values for pyrasulfotole in the soil and total system were >120 days and *ca.* ≥120 days in the water layer. Calculated dissipation half-lives for [^{14}C]pyrasulfotole in the soil and total system could not be determined due to insufficient dissipation post-flooding. **Pyrasulfotole is therefore considered to be stable under anaerobic soil conditions.**

2-Methylsulfonyl-4-trifluoromethylbenzoic acid (AE B197555) was the sole transformation product detected at maximum means of 5.1% (15 days post-flooding), 7.7% (day 0 post-flood) and 9.9% (15 and 61 days post-flood) of the applied in the water, soil and total system, respectively, of phenyl-label [^{14}C]pyrasulfotole treated soil and was 4.1%, 5.1% and 9.2%, respectively, at study termination.

Phenyl-label nonextractable [^{14}C]residues increased from 0.8% at day 0 to 22.5% at study termination. Pyrazole-label nonextractable [^{14}C]residues increased from 2.0% at day 0 to 24.9% at study termination. Maximum mean levels of volatilized $^{14}CO_2$ (identity not confirmed) detected were 2.6% and 6.6% of the applied for the phenyl- and pyrazole-label treated soils, respectively, while volatile [^{14}C]organic compounds were ≤0.1% (both labels) at all sampling intervals.

Aerobic Aquatic Metabolism

In an **acceptable** aerobic aquatic metabolism study (MRID 46801713), the biotransformation of pyrasulfotole was studied in a pond water-sandy loam sediment (water pH 4.8, sediment pH 4.5-5.4, organic carbon 4.1%) from North Carolina and a pond water-silty clay sediment (water pH 7.5, sediment pH 6.9-7.5, organic carbon 0.81%) from Kansas for 131-132 days under aerobic conditions.

In sandy loam systems (both labels), following application of [^{14}C]pyrasulfotole to the water layer, [^{14}C]residues partitioned from the water layer to the sediment with average (n = 2) distribution ratios (water:sediment) of *ca.* 100:1 at day 0, 2:1 at 11-55 days, 1:4 at 81 days and were 1:>10 thereafter. [^{14}C]Pyrasulfotole in the total system decreased from a mean 97.6% of the applied at day 0 to 44.5% at 81 days and was 16.3-18.2% thereafter. In the water layer, [^{14}C]pyrasulfotole decreased from a mean 97.6% at day 0 to 61.8-68.3% at 11-55 days, 22.9% at

81 days and was 5.2-5.5% thereafter. In the sediment, [^{14}C]pyrasulfotole increased from a mean 0.9% at day to 25.0% at 26 days, then decreased to 11.1-12.7% at 109-132 days. **Linear half-lives** for pyrasulfotole in the water, sediment and total system were 30, 90 and 48 days, respectively, and **nonlinear half-lives** were 46, 99 and 69 days, respectively. **Observed DT50** values were 55-81 days in the water, 81-≥132 days in the sediment and 55-109 days in the total system. However, these fitted transformation models do not adequately fit the observed dissipation pattern of parent residues. Extractable [^{14}C]residues in the sediment increased from a mean 0.9% of the applied at day 0 to a maximum 25.1% at 26 days, then decreased to 11.1-13.1% at 109-132 days. Nonextractable [^{14}C]residues were detected at means of 8.1-15.0% at 11-55 days, then sharply increased to 50.7% at 81 days and were 72.6% at study termination. **Pyrasulfotole does not appear to be transforming in this sandy loam system, but rather rapidly partitions from the water to an unextractable sediment-bound phase between Days 55 – 81. Pyrasulfotole is therefore considered to be stable under conditions of this aerobic aquatic system.**

In silty clay loam systems (both labels), following application of [^{14}C]pyrasulfotole to the water layer, [^{14}C]residues partitioned from the water layer to the sediment with average (n = 2) distribution ratios (water:sediment) of *ca.* 100:1 at day 0, 3:1 at 21 days and were 2:1 thereafter. [^{14}C]Pyrasulfotole dissipated slowly in the total system decreasing from a mean 101.4% of the applied at day 0 to 82.3-87.8% at 104-131 days. In the water layer, [^{14}C]pyrasulfotole decreased from a mean 100.9% of the applied at day 0 to 63.9% at study termination, while increasing in the sediment from 0.5% to 23.9% at the same respective intervals. **Observed DT50** values were >131 days in the water, sediment and total system. Linear/nonlinear half-lives for pyrasulfotole in the sediment and total system were not determined because levels of parent in the sediment were still increasing at study termination, and there was insufficient dissipation of parent in the total system. **Pyrasulfotole is considered to be stable under conditions of this aerobic aquatic system.** Extractable [^{14}C]residues in the sediment increased from a mean 1.0% of the applied at day 0 to 24.4% at 131 days. Nonextractable [^{14}C]residues increased from a mean 0.5% at day 0 to 13.1% at 104 days and were 10.6% at study termination.

Anaerobic Aquatic Metabolism

In an **acceptable** study (MRID 46801714), the biotransformation of phenyl-U-^{14}C-labeled pyrasulfotole was studied in a pond water-silty clay sediment (water pH 7.5, dissolved organic carbon 11.7 mg/L; sediment pH 6.6-7.0, organic carbon 1.1%) systems from Kansas for 365 days under anaerobic (static, nitrogen atmosphere) conditions in darkness at 20 ± 1°C. Following application of [^{14}C]pyrasulfotole to the water-sediment systems, [^{14}C]residues partitioned from the water layer to the sediment with average (n = 2) distribution ratios (water:sediment) of 100:1 at day 0, 4:1 at 3 days, 2:1 at 10 days and were 1:1 thereafter. [^{14}C]Pyrasulfotole dissipated slowly in the total system decreasing from a mean 99.2% of the applied at day 0 to 65.1% at 31 days and was 60.4%-65.6% thereafter. In the water layer, [^{14}C]pyrasulfotole decreased from a mean 99.2% at day 0 to 49.7% at 31 days and was 38.3-40.0% at 183-365 days. In the sediment, [^{14}C]pyrasulfotole increased to a mean 25.5% at study termination.

Calculated linear and nonlinear first-order half-lives for pyrasulfotole in the water layer and total system are of limited use given the low correlation coefficient values (r^2 = ≤0.51), and the half-lives for pyrasulfotole in the total system were extrapolated significantly beyond the final sampling interval. Levels of [^{14}C]pyrasulfotole in the sediment were still increasing at study termination; consequently, calculated half-lives could not be determined. **Observed DT50** values of pyrasulfotole were 22-31 days in the water layer and >365 days in the sediment and total system. Non-first order DT50 and DT90 estimates for the total system were estimated at 6000 and 46000 days, respectively using a multi-compartment non-linear regression model (r^2 = 0.95). **Pyrasulfotole is considered stable in the whole system under these anaerobic aquatic conditions.**

Extractable and nonextractable sediment [^{14}C]residues increased to maximum means of 25.5% and 33.9% of applied, respectively, at 365 days. The maximum level of volatilized $^{14}CO_2$ detected at any sampling interval was 2.8% of the applied, with volatile [^{14}C]organic compounds <0.1%.

In an **acceptable** study (MRID 46801715), the biotransformation of pyrazole-3-^{14}C-labeled pyrasulfotole was studied in a pond water-silty clay sediment (water pH 7.5, dissolved organic carbon 11.7 mg/L; sediment pH 7.0, organic carbon 1.1%) systems from Kansas for 365 days under anaerobic (static, nitrogen atmosphere) conditions in darkness at 20 ± 1°C. Following application of [^{14}C]pyrasulfotole to the water-sediment systems, [^{14}C]residues partitioned from the water layer to the sediment with average (n = 2) distribution ratios (water:sediment) of 100:1 at day 0, 4:1 at 3 days, 1:1 at 14-184 days and were 1:2 thereafter. [^{14}C]Pyrasulfotole dissipated slowly in the total system decreasing from a mean 100.0% of the applied at day 0 to 54.9% at 275 days and was 59.7% at 365 days. In the water layer, [^{14}C]pyrasulfotole decreased from a mean 100.0% at day 0 to 49.9% at 17 days and was 37.3% at study termination. In the sediment, [^{14}C]pyrasulfotole increased to a mean 22.7% at 63 days and was 19.1-22.9% thereafter.

Calculated linear and nonlinear half-lives for pyrasulfotole in the water layer and total system are of limited use given the low correlation coefficient values (r^2 = <0.45), and the half-lives for pyrasulfotole in the total system were extrapolated significantly beyond the final sampling interval. Since concentrations of [^{14}C]pyrasulfotole in the sediment remained at steady levels from 63 days posttreatment through study termination, calculated half-lives could not be determined. **Observed DT50** values of pyrasulfotole were 14-28 days in the water layer and >365 days in the sediment and total system. Non-first order DT50 and DT90 estimates for the total system were estimated at 722 and 4745 days, respectively using a multi-compartment non-linear regression model (r^2 = 0.95). **Pyrasulfotole is considered stable in the whole system under these anaerobic aquatic conditions.**

Extractable sediment [^{14}C]residues increased to a maximum mean 22.9% of applied at 120 days and were 22.4% at 365 days. Nonextractable sediment [^{14}C]residues increased to a maximum mean 36.4% at study termination. Volatilized $^{14}CO_2$ totaled a mean 1.9% of the applied at study termination, with volatile [^{14}C]organic compounds ≤0.1% at any interval.

Mobility and Persistence

Batch Equilibrium

In an **acceptable** study (MRID 46801703), the adsorption/desorption characteristics of pyrasulfotole were studied in definitive experiments using three US soils: a silt loam [HCB, pH 7.7, organic carbon 4.7%], a loamy sand [Pikeville, pH 6.4, organic carbon 1.2%], and a silt loam [Carlyle, pH 5.2, organic carbon 1.5%]; two German soils: a clay loam [CL6S, pH 7.5, organic carbon 1.7%] and a sandy loam [SL2.3, pH 6.7, organic carbon 1.1%]; and a German sandy loam sediment [Nidda, pH 5.8, organic carbon 4.6%], in a batch equilibrium experiment. After 24 hours of equilibration, 55.7-63.3%, 60.3-71.0%, 26.4-32.3%, 30.1-35.2%, 43.9-52.2%, and 50.4-73.5% of the applied [^{14}C]pyrasulfotole was adsorbed to the HCB silt loam, Pikeville loamy sand, CL6S clay loam, SL2.3 sandy loam, and Carlyle silt loam soils, and the Nidda sandy loam sediment, respectively (reviewer-calculated). Registrant-calculated adsorption K_d values averaged 1.32, 1.77, 0.367, 0.47, 4.25, and 32.9 for the HCB silt loam, Pikeville loamy sand, CL6S clay loam, SL2.3 sandy loam, and Carlyle silt loam soils, and the Nidda sandy loam sediment, respectively; corresponding adsorption K_{oc} values averaged 28.1, 148, 21.6, 42.7, 283, and 715. Registrant-calculated Freundlich adsorption K_F values were 0.980, 1.20, 0.341, 0.386, 3.20, and 15.9 for the HCB silt loam, Pikeville loamy sand, CL6S clay loam, SL2.3 sandy loam, Carlyle silt loam soils, and the Nidda sandy loam sediment, respectively; corresponding Freundlich adsorption K_{Foc} values were 20.8, 100, 20.0, 35.1, 213, and 345. At the end of the desorption phase, 55.0%, 49.7%, 70.4% 69.0% 65.6%, and 61.1% of the applied [^{14}C]pyrasulfotole desorbed from the HCB silt loam, Pikeville loamy sand, CL6S clay loam, SL2.3 sandy loam, and Carlyle silt loam soils, and the Nidda sandy loam sediment, respectively (reviewer-calculated). Registrant-calculated desorption K_d values averaged 2.26, 3.67, 0.923, 1.51, 10.4, and 56.6 for the HCB silt loam, Pikeville loamy sand, CL6S clay loam, SL2.3 sandy loam, and Carlyle silt loam soils, and the Nidda sandy loam sediment, respectively; corresponding adsorption K_{oc} values averaged 48.2, 306, 54.3, 137, 696, and 1230. Registrant-calculated Freundlich desorption K_F values were 1.37, 2.30, 0.678, 1.13, 8.46, and 30.9 for the HCB silt loam, Pikeville loamy sand, CL6S clay loam, SL2.3 sandy loam, and Carlyle silt loam soils, and the Nidda sandy loam sediment, respectively; corresponding Freundlich desorption K_{Foc} values were 29.2, 192, 40, 103, 564, and 672.

Terrestrial Field Dissipation

In an **acceptable** study (MRID 46801716), soil dissipation/accumulation of pyrasulfotole under US field conditions was conducted in three replicate bare plots and three replicate cropped plots (wheat) of loam soil in Kansas. In the bare test plot, the measured zero-time recovery of pyrasulfotole in the 0-15 cm soil layer was 19.80 ppb or 63.9% of the theoretical based on the target application rate (reviewer-calculated based on a theoretical day-0 recovery of 31 µg/kg). Pyrasulfotole decreased to 11.20 ppb by 7 days, 6.54 ppb by 14 days, 1.36 ppb by 58 days, and was last detected above the LOQ at 0.69 ppb at 257 days posttreatment. Pyrasulfotole was detected at levels below the LOQ in the 15-30 cm soil depth, and was not detected below 30 cm. The major transformation product **AE B197555** was detected in the 0-15 cm soil depth at a maximum concentration of 6.15 ppb at 4 days (which is equivalent to 8.31 ppb parent equivalents or 26.8% of the theoretical applied pyrasulfotole based on the target application rate), then decreased to 3.25 ppb by 14 days, was below the LOQ by 58 days, and was not detected by 257 days posttreatment. AE B197555 was not detected below the 0-15 cm soil depth at any sampling intervals.

Under field conditions in the bare test plot, pyrasulfotole had a reviewer-calculated half-life value of 87.7 days in soil ($r^2 = 0.6814$; based on all available replicate data in the top 15 cm soil layer, using linear regression and the equation $t_{½} = ln\ 2 / k$, where k is the rate constant); however, dissipation was bi-phasic with a more rapid decline phase occurring through the 58-day sampling interval. The reviewer-calculated half-life based on 0-58 day data in the top 15 cm soil layer was 14.9 days ($r^2 = 0.9250$). The reviewer-calculated DT_{50} and DT_{90} values for pyrasulfotole in the whole soil column using a double first order regression model were 8.9 and 45 days, respectively ($r^2 = 0.97$). Reviewer calculated DT_{50} and DT_{90} values for the strongly bi-phasic dissipation pattern of AE B197555 residues in the whole soil column were 17 and 45 days following initial application, respectively ($r^2 = 0.87$). In the bare test plot, residue carryover (i.e., percentage of the total amount of parent equivalent material in the whole soil column relative to Day 0 concentrations) was 4.7% at the beginning of the following growing season (i.e., at 257 days post treatment), and 1.2% at the end of the study (i.e., 526 days post treatment).

In an **acceptable** study (MRID 46801717), soil dissipation/accumulation of pyrasulfotole under US field conditions was conducted in three replicate bare plots and three replicate cropped plots (wheat) of clay loam/loam soil in North Dakota. In the bare test plot, the measured zero-time recovery of pyrasulfotole in the 0-15 cm soil layer was 24.4 ppb or 71.8% of the theoretical based on the target application rate (reviewer-calculated based on a theoretical day-0 recovery of 34 µg/kg). Pyrasulfotole decreased to 11.9 ppb by 7 days, 4.0 ppb by 27 days, and was last detected above the LOQ at 0.5 ppb at 377 days posttreatment. Pyrasulfotole was not detected above the LOQ in soil below the 0-15 cm soil depth. The major transformation product **AE B197555** was initially detected in the 0-15 cm soil depth at 1.2 ppb at day 0, increased to a maximum of 13.5 ppb by 7 days (which is equivalent to 18.2 ppb parent equivalents or 53.6% of the theoretical applied pyrasulfotole based on the target application rate), then decreased to 5.7 ppb by 27 days, 1.0 ppb by 317 days, and was below the LOQ by 377 days posttreatment. AE B197555 was not detected below the 0-15 cm soil depth.

Under field conditions in the bare test plot, pyrasulfotole had a reviewer-calculated half-life value of 84.5 days in the top 15 cm soil layer ($r^2 = 0.8107$; based on all available replicate data, using linear regression and the equation $t_{½} = ln\ 2 / k$, where k is the rate constant); however, dissipation was bi-phasic, and the observed half-life was approximately 7 days. The reviewer calculated DT50 and DT90 values for pyrasulfotole in the whole soil column were 6 and 44 days, respectively (two compartment non-linear regression model; $r^2 = 0.96$). The reviewer calculated DT50 and DT90 values for AE B197555 in the whole soil column were 25 and 227 days, respectively (two-compartment, non-linear regression model; $r^2 = 0.81$).Carryover of total residues in the soil column was 7.7 and 1.8% of the applied pyrasulfotole at the beginning of the following growing season (i.e. Day 317) and at the end of the study period (i.e. Day 498), respectively, based on observed Day 0 concentrations.

In an **acceptable** study (MRID 46801718), soil dissipation/accumulation of pyrasulfotole under US field conditions was conducted in three replicate bare plots and three replicate cropped plots (wheat) of sandy loam soil in Washington. In the bare test plot, the measured zero-time recovery of pyrasulfotole in the 0-15 cm soil layer was 27.18 ppb or 109% of the theoretical based on the target application rate (reviewer-calculated based on a theoretical day-0 recovery of 25 µg/kg). Pyrasulfotole decreased to 17.51-18.59 ppb by 1-3 days, 12.35 ppb by 7 days, was last detected above the LOQ at 1.10 ppb at 28 days, and was not detected following 175 days posttreatment. Pyrasulfotole moved into deeper soil layers over time, reaching the 45-60 cm layer at 28 days, the 75-90 cm layer at 58 days, and the 105-120 cm layer by 175 days.

Pyrasulfotole was detected in the 15-30, 30-45, 45-60, 60-75, and 75-90 cm soil layers at maximum concentrations of 3.26 ppb (28 days), 1.84 ppb (28 days), 1.99 ppb (175 days), 1.24 ppb (58 days), and 0.57 ppb (58 days), respectively; residues were detected below the LOQ in the 90-105 and 105-120 cm soil layers. The major transformation product **AE B197555** was detected in the 0-15 cm soil depth at a maximum of 3.86 ppb at 7 days (which is equivalent to 5.21 ppb parent equivalents or 20.8% of the theoretical applied pyrasulfotole based on the target application rate), then decreased to below the LOQ by 28-58 days, and was not detected by 120 days posttreatment. AE B197555 was detected in the 15-30 cm soil depth at a maximum concentration of 0.94 ppb at 14 days, in the 30-45 cm soil depth at a maximum of 1.59 ppb at 28 days, and in the 45-60 cm soil depth at a maximum of 0.57 ppb at 28 days. AE B197555 was not detected above the LOQ in soil below the 45-60 cm depth; however, residues were detected below the LOQ to 120 cm, the maximum depth analyzed.

Under field conditions in the <u>bare test plot</u>, pyrasulfotole had a reviewer-calculated half-life value of 41.5 days in soil ($r^2 = 0.5835$; based on all available replicate data, using linear regression and the equation $t_{½} = \mathit{ln}\ 2 / k$, where k is the rate constant); however, dissipation was bi-phasic, with a more rapid decline phase occurring through the 58-day sampling interval. The reviewer-calculated half-life based on 0-58 day data from the top 15 cm soil layer was 8.2 days ($r^2 = 0.9462$). The reviewer calculated DT50 and DT90 values for pyrasulfotole in the whole soil column were 6 and 213 days, respectively (two compartment non-linear regression model; $r^2 = 0.94$). The reviewer calculated half-life value for AE B197555 residues in the whole soil column was 42.0 days (first order regression; $r^2 = 0.94$), or an estimated DT_{50} of 49 days following initial application. Carryover of total residues in the soil column was 11.1 and 3.3% of the applied pyrasulfotole at the beginning of the following growing season (i.e. Day 269) and at the end of the study period (i.e. Day 526), respectively, based on observed Day 0 concentrations.

In an **acceptable** study (MRID 46801719), soil dissipation/accumulation of pyrasulfotole under Canadian field conditions was conducted in four replicate bare plots in Saskatchewan (Site 1), Manitoba (Site 2), and Ontario (Site 3) on clay loam soils.

At <u>Site 1 (Saskatchewan)</u>, the measured zero-time recovery of pyrasulfotole in the 0-7.5 cm soil layer was 65.5 ppb or 58.0% of the theoretical based on the target application rate (reviewer-calculated based on a theoretical day-0 recovery of 113 µg/kg). Pyrasulfotole decreased to 32.8-37.0 ppb by 7-14 days, 20.2-20.8 ppb by 21-30 days, 6.42 ppb by 120 days, and was 1.52-2.13 ppb from 402 to 449 days posttreatment. Pyrasulfotole was detected at ≤2.83 ppb in the 7.5-15 cm soil depth, ≤1.46 ppb in the 15-30 cm depth, and ≤0.65 ppb in the 30-45 cm depth, and was detected only below the LOQ in the 45-60 cm and 60-75 cm depths. The major transformation product **AE B197555** was detected in the 0-7.5 cm soil depth at a maximum of 36. 9 ppb at 14 days (which is equivalent to 49.8 ppb parent equivalents, or 67.3% of the total parent equivalents in the soil column at Day 0 after application), ranged from 32.1 to 34.9 ppb from 21 to 56 days, then decreased to 8.63 ppb by 120 days, and was 0.90 ppb at 449 days posttreatment. AE B197555 was detected in the 7.5-15 cm soil depth at a maximum of 4.63 ppb at 120 days and in the 15-30 cm depth at a maximum of 2.60 ppb at 343 days. AE B197555 was not detected above the LOQ in soil below the 15-30 cm depth.

At <u>Site 2 (Manitoba)</u>, the measured zero-time recovery of pyrasulfotole in the 0-15 cm soil layer was 112.99 ppb or 90.4% of the theoretical based on the target application rate (reviewer-calculated based on a theoretical day-0 recovery of 125 µg/kg). Pyrasulfotole decreased to 44.8-56.2 ppb from 7 to 61 days, 16.9 ppb by 121 days, 8.34 ppb by 349 days, and was 4.60 ppb at 462 days posttreatment. Pyrasulfotole was detected at ≤7.53 ppb in the 7.5-15 cm soil depth, ≤3.51 ppb in the 15-30 cm depth, and ≤1.14 ppb in the 30-45 cm depth, and was only detected below the LOQ in the 45-60 cm depth. The major transformation product **AE B197555** was detected in the 0-7.5 cm soil depth at a maximum of 26.7 ppb at 29 days (which is equivalent to 36.1 ppb parent equivalents, or 29.0% of the total parent equivalents in the soil column at Day 0 after application), decreased to 16.1 ppb by 61 days, and ranged from 1.17 to 1.80 ppb from 121 to 462 days posttreatment. AE B197555 was detected in the 7.5-15 cm soil depth at a maximum of 3.40 ppb at 7 days and was not detected above the LOQ in soil below the 7.5-15 cm depth, but was detected at levels below the LOQ in all soil depths analyzed (0-75 cm) at 462 days posttreatment.

At Site 3 (Ontario), the measured zero-time recovery of pyrasulfotole in the 0-15 cm soil layer was 58.1 ppb or 63.1% of the theoretical based on the target application rate (reviewer-calculated based on a theoretical day-0 recovery of 92 μg/kg). Pyrasulfotole decreased to 32.4 ppb by 14 days, 20.4 ppb by 30 days, 4.91 ppb by 139 days, and was 0.75 ppb at 458 days posttreatment. Pyrasulfotole was detected at ≤4.10 ppb in the 7.5-15 cm soil depth and was detected below the LOQ in the 15-30, 30-45, 45-60, and 60-75 cm depths. The major transformation product **AE B197555** was detected in the 0-7.5 cm soil depth at a maximum of 27.8 ppb at 14 days (which is equivalent to 37.6 ppb parent equivalents, or 56.7% of the total parent equivalents in the soil column at Day 0 after application), then decreased to 15.7 ppb by 30 days, 5.20 ppb by 56 days, and was last detected above the LOQ at 0.85 ppb at 350 days posttreatment. AE B197555 was detected in the 7.5-15 cm soil depth at a maximum of 2.40 ppb at 7 days and in the 15-30 cm depth at a maximum of 1.01 ppb at 30 days, and was detected at levels below the LOQ in the 30-45, 45-60, and 60-75 cm depths.

Under field conditions at Site 1 (Saskatchewan), pyrasulfotole had a reviewer-calculated half-life value of 106.6 days in soil ($r^2 = 0.8609$; based on all available replicate data, using linear regression and the equation $t_{½} = ln\ 2 / k$, where k is the rate constant); however, dissipation was bi-phasic, with a more rapid decline phase occurring through the 21-day sampling interval. The reviewer-calculated half-life based on 0-21 day data from the top 7.5 cm soil layer was 14.4 days ($r^2 = 0.6241$). The registrant-calculated DT50 and DT90 values were 7 and 313 days, respectively for pyrasulfotole (DFOP model). The reviewer calculated DT50 and DT90 values for whole-soil column pyrasulfotole residues were 10 and 260 days, respectively (2 compartment non-linear model, $r^2 = 0.86$). The reviewer-calculated half-life value for AE B197555 in the top 7.5 cm of the soil column was 82.5 days following the maximum detection at 14 days. The reviewer calculated half-life value for AE B197555 residues in the whole soil column was 121.6 days ($r^2 = 0.86$), or an estimated DT_{50} of 136 days following initial application.

Under field conditions at Site 2 (Manitoba), pyrasulfotole had a reviewer-calculated half-life value of 115.5 days in soil ($r^2 = 0.8344$; based on all available replicate data from the top 7.5 cm soil layer, using linear regression and the equation $t_{½} = ln\ 2 / k$, where k is the rate constant); however, dissipation was bi-phasic, with >50% of the test material dissipating by the second sampling interval at 7 days posttreatment, after which concentrations were level through 2 months posttreatment before decreasing again. The registrant-calculated DT50 and DT90 values were 31 and 568 days, respectively for pyrasulfotole (DFOP model). The reviewer calculated DT50 and DT90 values for whole-soil column pyrasulfotole residues were 9.2 and 531 days, respectively (2 compartment non-linear model, $r^2 = 0.89$). The reviewer-calculated half-life value for AE B197555 in the top 7.5 cm of the soil column was 21.8 days following the maximum detection at 29 days posttreatment. The reviewer calculated half-life value for AE B197555 residues in the whole soil column was 35.0 days ($r^2 = 0.82$), or an estimated DT_{50} of 64 days following initial application.

Under field conditions at Site 3 (Ontario), pyrasulfotole had a reviewer-calculated half-life value of 84.5 days in soil ($r^2 = 0.8946$; based on all available replicate data, using linear regression and the equation $t_{½} = \mathit{ln}\ 2 / k$, where k is the rate constant); however, dissipation was bi-phasic, with a more rapid decline phase occurring through the 56-day sampling interval. The reviewer-calculated half-life based on 0-56 day data from the top 7.5 cm soil layer was 22.7 days ($r^2 = 0.9146$). The registrant-calculated DT50 and DT90 values were 15 and 160 days, respectively for pyrasulfotole (DFOP model). The reviewer calculated DT50 and DT90 values for whole-soil column pyrasulfotole residues were 18 and 178 days, respectively (2 compartment non-linear model, $r^2 = 0.96$). The reviewer-calculated half-life value for AE B197555 in the top 7.5 cm of the soil column was 27.6 days following the maximum detection at 14 days posttreatment. The reviewer calculated half-life value for AE B197555 residues in the whole soil column was 26.8 days ($r^2 = 0.94$), or an estimated DT_{50} of 41 days following initial application.

Carryover of residues at the start of the following growing season (i.e., at 343-350 days post treatment), was 37.2%, 18.9% and 8.9% of the applied pyrasulfotole for sites in Saskatchewan, Manitoba and Ontario respectively (the majority of residues were detected as parent at all sites; total parent-equivalent residues in the soil column were compared to observed levels at Day 0). By the end of the study period (i.e., 449-462 days post treatment), 13.7, 16.2 and 2.0% of the applied pyrasulfotole was present in the Saskatchewan, Manitoba and Ontario sites, respectively.

Appendix B: Input/Output Modeling Files

FIRST File

```
RUN No.   1 FOR pyrasulfotole    ON   wheat         * INPUT VALUES *
   --------------------------------------------------------------------
    RATE (#/AC)    No.APPS &    SOIL  SOLUBIL  APPL TYPE  %CROPPED INCORP
     ONE(MULT)     INTERVAL     Koc   (PPM )   (%DRIFT)     AREA    (IN)
   --------------------------------------------------------------------
   .045(   .045)    1   1       20.0 6900.0    AERIAL(16.0)  87.0     .0


   FIELD AND RESERVOIR HALFLIFE VALUES (DAYS)
   --------------------------------------------------------------------
   METABOLIC  DAYS UNTIL  HYDROLYSIS   PHOTOLYSIS   METABOLIC  COMBINED
    (FIELD)  RAIN/RUNOFF  (RESERVOIR)  (RES.-EFF)   (RESER.)   (RESER.)
   --------------------------------------------------------------------
    439.00        2          N/A        .00-     .00        .00       .00


   UNTREATED WATER CONC (MICROGRAMS/LITER (PPB)) Ver 1.1.0 DEC 12, 2005
   --------------------------------------------------------------------
        PEAK DAY  (ACUTE)       ANNUAL AVERAGE (CHRONIC)
          CONCENTRATION              CONCENTRATION
   --------------------------------------------------------------------
              4.011                         2.791
```

SCIGROW File

```
                   SCIGROW
                  VERSION 2.3
      ENVIRONMENTAL FATE AND EFFECTS DIVISION
         OFFICE OF PESTICIDE PROGRAMS
       U.S. ENVIRONMENTAL PROTECTION AGENCY
                SCREENING MODEL
         FOR AQUATIC PESTICIDE EXPOSURE

SciGrow version 2.3
chemical:pyrasulfotole
time is  1/12/2007  13:55: 0
-------------------------------------------------------------------------
 Application    Number of     Total Use    Koc     Soil Aerobic
 rate (lb/acre) applications  (lb/acre/yr) (ml/g)  metabolism (days)
-------------------------------------------------------------------------
    0.045          1.0          0.045     2.00E+01     226.0
-------------------------------------------------------------------------
groundwater screening conc (ppb) =   1.36E+00
*****************************************************************************
```