UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, D.C. 20460

OFFICE OF
PREVENTION, PESTICIDES, AND
TOXIC SUBSTANCES

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MEMORANDUM   **August 30, 2007**

SUBJECT: **Pyroxsulam (Section 3: Wheat Use)**
Tier II Drinking Water Exposure Assessment for Pyroxsulam on
Spring and Winter Wheat (including Durum).

TO: James Stone/Joanne Miller
Registration Division (7505P)

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FROM: Greg Orrick, Environmental Scientist   *Greg Orrick 9-5-07*
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THROUGH: Elizabeth Behl, Branch Chief   *EBehl 8-5-07*
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EXECUTIVE SUMMARY

This assessment provides estimated drinking water concentrations (EDWC) of
pyroxsulam (XDE-742) in surface water and in ground water in support of human health
risk assessment. Tier II EDWCs (**Table 1**) of pyroxsulam were generated with the
coupled models PRZM and EXAMS for surface water and SCI-GROW for ground water.
Modeled application rates represent the maximum use pattern of two proposed labels for
use on wheat (EPA Reg. No. pending). Remaining model input parameters were chosen
according to current guidance (USEPA, 2002). EDWCs reflect exposure to pyroxsulam
and all potential degradates of concern (USEPA, 2007). If the screening Estimated
Drinking Water Concentrations (EDWC) listed in this memo result in dietary risk
exceedances, contact Greg Orrick (703-305-6140) of Environmental Risk Branch IV
(7507P) to request a refined drinking water exposure assessment.

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Table 1. Tier II Drinking Water Exposure Estimates for Pyroxsulam Use on Wheat.			
Source	1-in-10-year Peak Exposure (µg/L)	1-in-10-year Annual Mean Exposure (µg/L)	30-year Mean Exposure (µg/L)
Surface water	0.320	0.164	0.102
Ground water[1]	0.465	0.465	<0.465

[1] Ground water concentrations calculated by SCI-GROW do not distinguish between peak, annual mean, and 30-year mean concentrations.

Pyroxsulam is a new systemic post-emergence cereals herbicide for selective control of wild oat, winter annual brome species, annual ryegrass, and other annual grass and broadleaf weeds in winter and spring wheat (including durum). The compound has low volatility and is increasingly soluble in water with increasing pH. Pyroxsulam weakly sorbs to soil, is mobile to highly mobile, and may readily move into surface water through runoff and/or present a ground water concern, depending on the permeability of the soil. Low application rates may limit the extent to which the compound runs into surface water or leaches into ground water.

Pyroxsulam may be moderately persistent in the environment. Primary routes of degradation include aqueous photolysis, aerobic soil metabolism, and possibly aerobic aquatic metabolism. Pyroxsulam appears to persist under anaerobic conditions and was stable to the abiotic processes of soil photolysis and hydrolysis.

Major degradates include the demethylated products 5-OH-XDE-742, 7-OH-XDE-742, 6-Cl-7-OH-XDE-742, and 5,7-diOH-XDE-742 and the further degraded products XDE-742 ATSA, XDE-742 sulfinic acid, XDE-742 ADTP, and carbon dioxide. The toxicities of pyroxsulam's degradates are not determined; the Office of Pesticide Programs (OPP) assumes in the circumstances that the organic degradates are of equal or less toxicity than the parent (USEPA, 2007). EDWCs reflect exposure to pyroxsulam and its organic degradates in order to include any potential residues of concern.
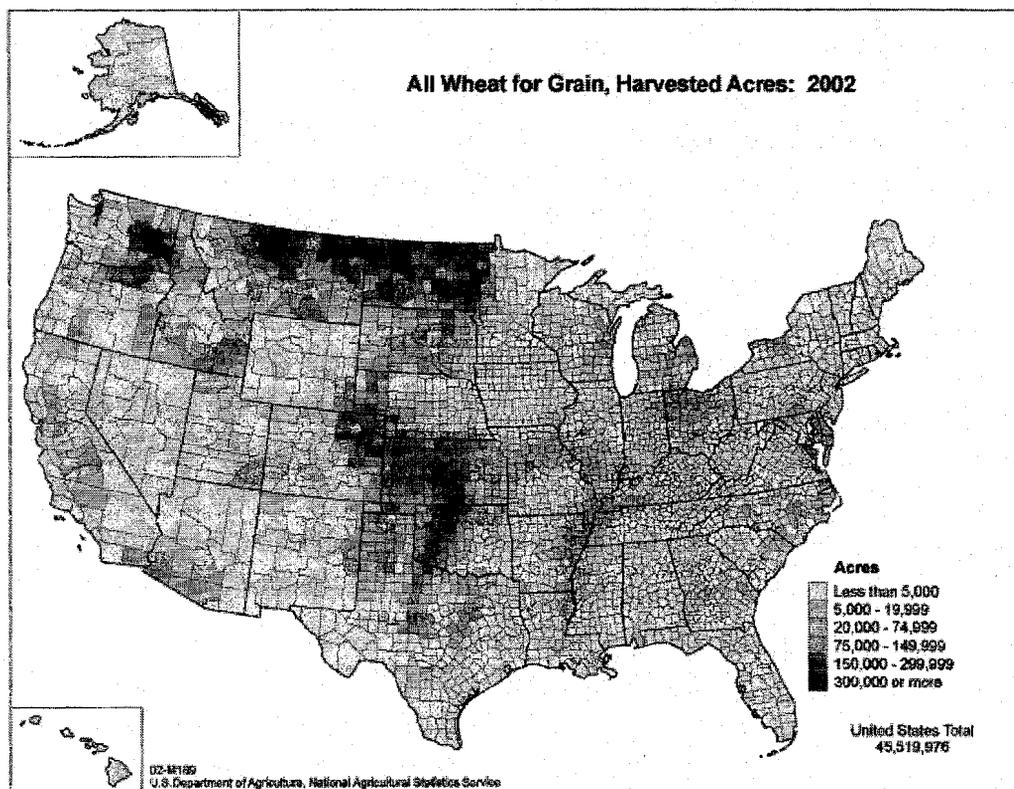

PROBLEM FORMULATION

This drinking water assessment uses environmental modeling to provide estimates of surface water and ground water concentrations in drinking water source water (pre-treatment) resulting from pyroxsulam use on vulnerable sites. Estimates reflect drinking water exposure to residues of concern for pyroxsulam, which include the parent compound and its organic degradates on a per molar basis (USEPA, 2007). Primary routes of transport to source water include runoff, erosion, leaching, and spray drift. Due to their crop-specificity, the coupled models PRZM and EXAMS were used to assess exposure in surface water due to runoff, erosion, and spray drift from the proposed pyroxsulam uses. Exposure in ground water due to leaching was accessed with the screening model SCI-GROW.

ANALYSIS

Use Characterization

Pyroxsulam [N-(5,7-dimethoxy[1,2,4]triazolo[1,5-α]pyrimidin-2-yl)-2-methoxy-4-(trifluoromethyl)-3-pyridinesulfonamide], also known as XDE-742, is a new systemic post-emergence cereals herbicide in the class of compounds known as triazolopyridine sulfonamides. The compound inhibits acetolactate synthesis (ALS) enzyme and is used to achieve selective control of wild oat, winter annual brome species, annual ryegrass, and other annual grass and broadleaf weeds in winter and spring wheat (including durum).

Key winter wheat producing areas in the United States include the High Plains states, extending from South Dakota south to Texas, and the Pacific Northwest states. Winter wheat is also an important rotational crop grown in most Midwestern and Southeastern states. Key spring wheat and durum producing states include Idaho, Minnesota, Montana, North Dakota, South Dakota and Washington. **Figure 1** displays the spatial extent in 2002 of wheat harvested for grain.

All Wheat for Grain, Harvested Acres: 2002

Acres
Less than 5,000
5,000 - 19,999
20,000 - 74,999
75,000 - 149,999
150,000 - 299,999
300,000 or more

United States Total
45,519,976

02-ME189
U.S. Department of Agriculture, National Agricultural Statistics Service

Figure 1. Acres of wheat for grain harvested in 2002 (USDA, 2007).

Two formulations of pyroxsulam are proposed for registration; these include GF-1274 (7.5% a.i.), a water dispersible granule (WDG) formulation for use on winter wheat, and

GF-1674 (2.87% a.i.), an oil dispersion (OD) formulation for use on both spring and winter wheat. Both formulations are to be mixed with water and applied as a post-emergence foliar application with aerial and ground-spray equipment.

The maximum proposed application rates per use and per growing season are the same, limited at 0.0164 lbs a.i./A for GF-1274 and 0.0132 lbs a.i./A, for GF-1674. Therefore, the maximum annual application rate of 0.0164 lbs a.i./A characterizes the maximum use pattern for pyroxsulam on wheat, as only one growing season occurs per year. Because no uses of pyroxsulam have yet been registered, the proposed use on winter wheat is the maximum use pattern from which EDWCs were generated in order to characterize national drinking water exposure from pyroxsulam use.

Fate and Transport Characterization

Our understanding of the environmental fate and transport properties of pyroxsulam is limited by the quality of the available data set. Many environmental fate parameters of pyroxsulam listed in **Table 2** are based on single, supplemental studies. Acceptable anaerobic aquatic metabolism data are not available, as anaerobic conditions were not maintained in the submitted study. The extraction method of the aerobic aquatic metabolism study was inadequate, which increases uncertainty in the reported half-lives. Model parameters listed in **Tables 4 and 5** were generated from the fate and transport properties given below.

Table 2. General chemical properties and environmental fate parameters of pyroxsulam.		
Parameter	Value	Source
Selected Physical/Chemical Parameters		
Molecular mass	434.4	MRID 46908334
Vapor pressure (20°C)	$<10^{-9}$ torr	MRID 46908327
Water solubility (20°C)	16.4 mg/L (pH 4) 3.20×10^3 mg/L (pH 7) 1.37×10^4 mg/L (pH 9)	MRID 46908327
Henry's Law Constant (20°C)	$<1.36 \times 10^{-8}$ Pa m^3/mol	MRID 46908334
pKa at 25°C	4.51	MRID 46908327
Log octanol-to-water partition coefficient (K_{OW})	1.08 (pH 4) -1.01 (pH 7) -1.60 (pH 9)	MRID 46908327
Persistence		
Hydrolysis half life (20°C)	No significant degradation (pH 5, 7, and 9)	MRID 46908326
Aqueous photolysis half life (parent; total residues)	4.5 d; no significant degradation	MRID 46908327
Soil photolysis half-life	No significant degradation	MRID 46908328

Table 2. General chemical properties and environmental fate parameters of pyroxsulam.		
Parameter	**Value**	**Source**
Aerobic soil metabolism half-life range (parent; total residues)	2.64–14.6 d; 59.0–186 d	MRID 47202701
Aerobic aquatic metabolism half-life range (parent; total residues)	14.5–18.8 d; 53.3–128 d	MRID 46908336
Anaerobic aquatic metabolism half-life	No significant degradation	MRID 46908331
Mobility		
Range of Freundlich soil-to-water partition coefficients (K_F) for adsorption	0.18 (1/n=0.93) – 1.60 (1/n=0.96)	MRID 47159601
Range of Freundlich organic carbon normalized partition coefficients (K_{FOC})	7.1–68.0 L/kg_{OC}	MRID 47159601
Field Dissipation		
Terrestrial field dissipation half-life range	4.6–23 d	MRID 46908334

Transport and Mobility

Pyroxsulam will not significantly volatilize due to a low vapor pressure ($<10^{-9}$ torr at 20°C) and solubility in water that increases with increasing pH (16.4 mg/L (pH 4) to 1.37 x 10^4 mg/L (pH 9) at 20°C). Ranges of solubility in water and K_{OW} across pH values indicate that the compound exhibits acid/base behavior, with a pKa of 4.51 at 25°C.

Pyroxsulam weakly sorbs to soil; however, the compound displays affinity to organic matter, as the coefficient of variation (CV) across ten soils for K_{FOC} (69%) is less than that for K_F (87%). Pyroxsulam is mobile to highly mobile (K_{FOC} of 7.1 to 68.0 L/kg_{OC}) and may readily move into surface water through runoff and/or present a ground water concern, depending on the permeability of the soil. Low application rates may limit the extent to which the compound runs into surface water or leaches into ground water.

Degradation

Pyroxsulam may be moderately persistent in the environment. The compound was stable to the abiotic processes of soil photolysis and hydrolysis. Primary routes of degradation include aqueous photolysis ($t_{1/2}$ of 4.5 days) and aerobic soil metabolism ($t_{1/2}$ range of 2.64-14.6 days). Aerobic aquatic metabolism may also be a primary route of degradation ($t_{1/2}$ range of 14.5-18.8 days); however, the submitted data are uncertain and half-life estimates may be overestimated because residues were inadequately extracted.

The total residues of pyroxsulam were stable under aqueous photolysis, as carbon dioxide was not evolved. Total residue half-lives in aerobic soil and aerobic aquatic systems increased to relatively similar ranges of 59.0-186 days and 53.3-128 days, respectively.

Pyroxsulam appears to persist under anaerobic conditions. The submitted anaerobic aquatic metabolism study indicates that pyroxsulam was stable through the first 30 days,

when redox potentials were the lowest (E_h 7 range -10.2 to -143.3 mV). Degradation occurred suddenly after 30 days, coinciding with an increase in aqueous redox potential (range +8.5 to -80.0 mV), suggesting that changes in aerobicity in the test system may have lead to rapid biodegradation.

Field Studies

A terrestrial field dissipation study was conducted for pyroxsulam using four sites in Canada with three bare ground plots each. Two of the sites, SK2 (loam soil) and MB (clay loam soil), were found in Ecoregions relevant to use sites in the U.S. The plots were irrigated to a target of 110% of the 30-year precipitation normal. Soil samples (0-90 cm depth) were collected through 126-359 days post-treatment. Pyroxsulam dissipated in the loam and clay loam soils with half-lives of 4.6 days (0-30 cm depth) and 23 days (0-60 cm depth), respectively.

Test sites were analyzed for 5-OH-XDE-742, 7-OH-XDE-742, and 6-Cl-7-OH-XDE-742. No major degradates were detected. 6-Cl-7-OH-XDE-742 was initially detected in the loam soil at 3% of the applied on day 14, with a 5-day half-life, and was not detected in the clay loam soil. 7-OH-XDE-742 was detected at up to 4% of the applied (day 14) in the loam soil and up to 8% of the applied (day 28) in the clay loam soil; no pattern of decline could be calculated in either soil. 5-OH-XDE-742 was below detection limits in all samples from the loam and clay loam soils.

Degradates

Major identified degradates include 5-OH-XDE-742, 7-OH-XDE-742, 6-Cl-7-OH-XDE-742, 5,7-diOH-XDE-742, XDE-742 ATSA, XDE-742 sulfinic acid, XDE-742 ADTP, and carbon dioxide (IUPAC names in **Table 3**; structures in **Table II.2** of **Appendix II**); the first four listed are most structurally similar to the parent compound. The maximum reported amounts of pyroxsulam degradation products are reported in **Table II.1** of **Appendix II**. XDE-742 sulfinic acid and XDE-742-ADTP were photodegradates identified at up to 79.2% and 39.8% of the applied, respectively. 5-OH-XDE-742, 7-OH-XDE-742, 6-Cl-7-OH-XDE-742, and carbon dioxide were major biodegradates in aerobic soil at up to 24.1%, 13.7%, 26.2%, and 15.6% of the applied, respectively. 7-OH-XDE-742 and XDE-742 ATSA were major biodegradates in aerobic aquatic systems, forming up to 58.4% and 12.9% of the applied, respectively.

Table 3. Chemical Names for the Transformation Products of Pyroxsulam.	
Synonym	**IUPAC Chemical Name**
Major Degradates	
5-OH-XDE-742	N-(5-hydroxy-7-methoxy[1,2,4]triazolo[1,5-α]pyrimidin-2-yl)-2-methoxy-4-(trifluoromethyl)-3-pyridinesulfonamide
7-OH-XDE-742	N-(7-hydroxy-5-methoxy[1,2,4]triazolo[1,5-α]pyrimidin-2-yl)-2-methoxy-4-(trifluoromethyl)-3-pyridinesulfonamide
6-Cl-7-OH-XDE-742	N-(6-chloro-7-hydroxy-5-methoxy[1,2,4]triazolo[1,5-α]pyrimidin-2-yl)-2-methoxy-4-(trifluoromethyl)pyridine-3-sulfonamide

Table 3. Chemical Names for the Transformation Products of Pyroxsulam.	
Synonym	**IUPAC Chemical Name**
5,7-diOH-XDE-742	N-(5,7-dihydroxy[1,2,4]triazolo[1,5-α]pyrimidin-2-yl)-2-methoxy-4-(trifluoromethyl)-3-pyridinesulfonamide
XDE-742 ATSA	N-(5-amino-1H-1,2,4-triazol-3-yl)-2-methoxy-4-(trifluoromethyl)pyridine-3-sulfonamide
XDE-742 sulfinic acid	2-methoxy-4-(trifluoromethyl)pyridine-3-sulfinic acid
XDE-742 ADTP	5,7-dimethoxy[1,2,4]triazolo[1,4-α]pyrimidin-2-amine
Minor Degradates	
XDE-742 CSF	N-cyano-2-methoxy-4-(trifluoromethyl)pyridine-3-sulfonamide
XDE-742 PSA	2-methoxy-4-(trifluoromethyl)pyridine-3-sulfonic acid

Minor biodegradates formed in aerobic soil include XDE-742 CSF and XDE-742 PSA at up 8.1% and 5.9% of the applied, respectively.

The toxicities of the major degradates of pyroxsulam are not determined; however, none are expected to be more toxic than the parent (USEPA, 2007). EDWCs were modeled to reflect exposure to pyroxsulam and all of its organic degradates on a per molar basis so as to include any potential residues of concern.

Drinking Water Exposure Modeling

Models

Pesticide Root Zone Model (PRZM v3.12.2, May 12, 2005) and Exposure Analysis Modeling System (EXAMS v2.98.04.06, Apr. 25, 2005) are simulation models coupled with the input shell PRZM/EXAMS (PE v5.0, Nov. 15, 2006) to generate EDWCs of pyroxsulam residues that may occur in surface water used as drinking water. The PRZM model simulates pesticide movement and transformation from crop application through soil residue processes. The EXAMS model simulates pesticide loading via runoff, erosion, and spray drift assuming a standard watershed of 172.8 ha that drains into an adjacent standard drinking water index reservoir of 5.26 ha, an average depth of 2.74 m. A more detailed description of the index reservoir watershed can be found in Jones *et al.*, 1998. The coupled PRZM/EXAMS model and users manuals may be downloaded from the U.S. Environmental Protection Agency (EPA) Water Models web-page (USEPA, 2007a). EDWCs produced by PRZM/EXAMS must be manually modified by agricultural Percent Cropped Areas (PCA) to account for the maximum area within a watershed that may be planted with the modeled crop.

Screening Concentration in Ground Water (SCI-GROW v2.3, Jul. 29, 2003) is a regression model used as a screening tool to estimate pesticide concentrations found in ground water used as drinking water. SCI-GROW was developed by fitting a linear model to ground water concentrations with the Relative Index of Leaching Potential (RILP) as the independent variable. Ground water concentrations were taken from 90-day average high concentrations from Prospective Ground Water studies. The RILP is a

function of aerobic soil metabolism and the soil-water partition coefficient. The output of SCI-GROW represents the concentrations of pyroxsulam residue that might be expected in shallow unconfined aquifers under sandy soils, which is representative of the ground water most vulnerable to pesticide contamination and likely to serve as a drinking water source. The SCI-GROW model and user's manual may also be downloaded from the EPA Water Models web-page (USEPA, 2007a). Both PRZM/EXAMS and SCI-GROW were run to estimate screening-level exposure of drinking water sources to total residues of concern of pyroxsulam.

Input Parameters

Input parameters for the PRZM/EXAMS models follow in **Table 4**; data source and justification descriptors accompany values for each parameter.

Table 4. PRZM/EXAMS Model Input Parameters for Pyroxsulam Use on Wheat. Source Data are in Table 3.

Input Parameter	Value	Justification	Source
Application Rate in lbs a.i./A (kg a.i./ha)	0.0132 (0.0148)	Label directions	Proposed labels
Applications per Year	1	Label directions	Proposed labels
Date of Application	Apr. 1st	Application occurs in Fall or Spring.	USDA crop profiles (USDA, 2007a), and label directions
Application Method	Aerial	Label directions	Proposed labels
CAM Input	Foliar applied (CAM=2)	Label directions	Proposed labels
IPSCND Input	1	Foliar residue after harvest is applied to the field.	USDA crop profiles (USDA, 2007a)
Spray Drift Fraction	0.16	Default drinking water assessment value for aerial spray	Input parameter guidance (USEPA, 2002) and Spray Drift Task Force studies[1]
Application Efficiency	0.95	Default value for aerial spray	Input parameter guidance (USEPA, 2002)
Molecular Mass (g/mol)	434.4	Product chemistry data	MRID 46908334
Vapor Pressure (torr)	1×10^{-9}	Maximum reported value at 20°C	MRID 46908327
Solubility in Water (mg/L)	32000	Represents 10x the measured water solubility value at pH 7, 20°C.	MRID 46908327
Organic Carbon Partition Coefficient (K_{OC}) (mL/g_{OC})	30.4	Represents the average K_{FOC} from ten soils.	MRID 47159601
Aerobic Soil Metabolism Half-life (days)	167	Represents the high-end confidence bound on the mean total residue half-life.	MRID 47202701
Aerobic Aquatic Metabolism Half-life (days)	206	Represents the high-end confidence bound on the mean total residue half-life.	MRID 46908336

Table 4. PRZM/EXAMS Model Input Parameters for Pyroxsulam Use on Wheat. Source Data are in Table 3.			
Input Parameter	Value	Justification	Source
Anaerobic Aquatic Metabolism Half-life (days)	0	Represents no significant degradation.	MRID 46908331
Hydrolysis Half-lives (days)	0 (pH 5) 0 (pH 7) 0 (pH 9)	Represents stability to hydrolysis.	MRID 46908326
Aqueous Photolysis Half-life (days)	0	Represents no significant degradation of total residues.	MRID 46908327

1. Spray Drift Task Force studies were reviewed by the FIFRA Scientific Advisory Panel (SAP meeting, Dec 10-11, 1997); online at: http://www.epa.gov/scipoly/sap/1997/index.htm.

Scenario Inputs. The currently approved and nationally protective North Dakota wheat scenario was used to model use on winter wheat, as it is the lone scenario available for modeling applications to wheat. The maximum application method and rate were obtained from the proposed labels for pyroxsulam. The application date was selected in the Spring, when weed pressures may increase as temperatures rise.

Environmental Fate. Chemical property input values were chosen in accordance with current input parameter guidance (USEPA, 2002). Based on analysis of total residues of concern, the high-end confidence bound on the mean was selected for the aerobic soil metabolism half-life (167 d) and the aerobic aquatic metabolism half-life (206 d).

Percent Cropped Area. A standard percent cropped area (PCA) of 0.56 was used as an estimate of the extent of watershed on which wheat is grown in North Dakota (Effland *et al.*, 1999). Actual fractions of cropped area are likely to be less in other areas of the country. The PRZM/EXAMS model does not include PCA inputs. Therefore, modeled exposure estimates were manually multiplied by the appropriate PCA to yield reported EDWC values.

Input parameters for the SCI-GROW model appear in **Table 5**. Data source and justification descriptors accompany values for each parameter.

Table 5. SCI-GROW input parameters for pyroxsulam. Source data are in Table 2.			
Input Parameter	Value	Justification	Source
Application Rate (lbs a.i./A)	0.0164	Label directions	Proposed label
Applications per Year	1	Label directions	Proposed label
Organic Carbon Partition Coefficient (K_{OC}) (mL/g_{OC})	7.1	Represents the lowest reported K_{OC}, as values show greater than three-fold variation.	MRID 4715960 1
Aerobic Soil Metabolism Half-life (days)	124	Represents the median total residue half-life in four soils.	MRID 4720270 1

The lowest reported Freundlich organic carbon partition coefficient ($K_{FOC} = 7.1$ mL/g_{OC}) was selected because the range of values from ten soils showed greater than three-fold variation. The median total residue half-life (124 d) from four aerobic soils was selected

to approximate the biodegradation kinetics of the residues of concern in aerobic soil environments.

Modeling Results

Screening estimates generated for drinking water exposure assessment are listed in **Table 6**. The surface water estimates were adjusted by a Percent Cropped Area (PCA) factor of 56%. The proposed use pattern for the GF-1274 formulation for use on winter wheat was the maximum use pattern modeled for surface water and ground water exposure estimates, as described above. Modeled estimates are 1-in-10-year peak, 1-in-10-year annual mean, and 30-year mean exposure values. Model input/output data for these estimates are attached in **Appendix I**.

Table 6. Tier II Drinking Water Exposure Estimates for Pyroxsulam Use on Wheat.			
Source	1-in-10-year Peak Exposure (μg/L)	1-in-10-year Annual Mean Exposure (μg/L)	30-year Mean Exposure (μg/L)
Surface water	0.320	0.164	0.102
Ground water[1]	0.465	0.465	<0.465

[1] Ground water concentrations calculated by SCI-GROW do not distinguish between peak, annual mean, and 30-year mean concentrations.

The biodegradation data for pyroxsulam are uncertain. Acceptable aerobic aquatic metabolism and anaerobic aquatic metabolism data would increase confidence in and refine surface water exposure estimates. Other factors inherent in the modeling that may have affected the accuracy and precision of this analysis include the ability of the models to represent the real world and the use of maximum label practices that can be greater than actual agricultural practices. Screening models are not designed to simulate real events or typical exposure. These models should simply indicate which chemicals surpass high-end levels of concern and warrant refinement of dietary risk.

Drinking Water Treatment

The Office of Pesticide Programs (OPP) does not have direct data on the effects of drinking water treatment on pyroxsulam. Flocculation and sedimentation removal may be effective at reducing pyroxsulam concentrations. Carbon filtering may also reduce pyroxsulam concentrations due to the compound's moderate affinity to organic carbon. Because of the absence of data on pyroxsulam, the effects of drinking water treatment were not considered in this assessment.

CONCLUSIONS

Tier II drinking water exposure estimates for pyroxsulam use on wheat are represented by the maximum use pattern on winter wheat (**Tables 1 and 6**). Select environmental fate data used to generate these estimates are uncertain. Acceptable aerobic aquatic metabolism and anaerobic aquatic metabolism data would increase confidence in and

enable refinement of surface water exposure estimates. The total residues of concern of pyroxsulam include pyroxsulam parent and all organic degradates, which are assumed to have similar toxicity to pyroxsulam parent.

LITERATURE CITATIONS

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Submitted Studies

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Appendix I. SCI-GROW and PRZM/EXAMS Input/Output Data.

SCI-GROW Input/Output File.

SciGrow version 2.3
chemical:Orthosulfamuron
time is 9/21/2006 14:16:23

Application rate (lb/acre)	Number of applications	Total Use (lb/acre/yr)	Koc (ml/g)	Soil Aerobic metabolism (days)
0.069	1.0	0.069	2.21E+02	10000.0

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groundwater screening cond (ppb) = 6.11E-01
****

PRZM/EXAMS Input File.

Output File: XDE_IR
Metfile: w14914.dvf
PRZM scenario: NDwheatSTD.txt
EXAMS environment file: ir298.exv
Chemical Name: Pyroxsulam

Description	Variable Name	Value	Units	Comments
Molecular weight	mwt	434.4	g/mol	
Henry's Law Const.	henry		atm-m^3/mol	
Vapor Pressure	vapr	1e-9	torr	
Solubility	sol	32000	mg/L	
Kd	Kd		mg/L	
Koc	Koc	30.4	mg/L	
Photolysis half-life	kdp	0	days	Half-life
Aerobic Aquatic Metabolism	kbacw	206	days	Halfife
Anaerobic Aquatic Metabolism	kbacs	0	days	Halfife
Aerobic Soil Metabolism	asm	167	days	Halfife
Hydrolysis:	pH 5	0	days	Half-life
Hydrolysis:	pH 7	0	days	Half-life
Hydrolysis:	pH 9	0	days	Half-life
Method:	CAM	2	integer	See PRZM manual
Incorporation Depth:	DEPI	0	cm	
Application Rate:	TAPP	0.0148	kg/ha	
Application Efficiency:	APPEFF	.95	fraction	
Spray Drift	DRFT	.16		fraction of application rate applied to pond
Application Date	Date	01-04		dd/mm or dd/mmm or dd-mm or dd-mmm
Record 17:	FILTRA			
	IPSCND	1		
	UPTKF			
Record 18:	PLVKRT			
	PLDKRT			
	FEXTRC	0.5		
Flag for Index Res. Run	IR	Reservoir		
Flag for runoff calc.	RUNOFF	total		none, monthly or total(average of entire run)

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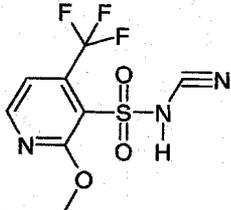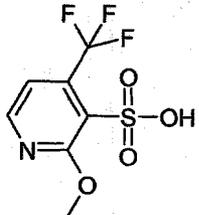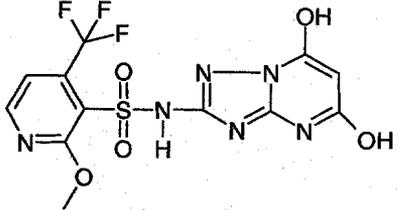## Appendix II. Chemical Names, Structures, and Maximum Reported Amounts of Pyroxsulam and Its Degradates.

Table II.1. Maximum Reported Amounts of Pyroxsulam Degradation Products.			
Degradate	**Maximum % of Applied**	**Study Type**	**MRID**
XDE-742 sulfinic acid	79.2% (3.8 d)	Aqueous photolysis	MRID 46908327
XDE-742-ADTP	39.8% (3.8 d)	Aqueous photolysis	MRID 46908327
5-OH-XDE-742	24.1% (3 d) 2% (7 d)[1]	Aerobic soil metabolism Terrestrial Field dissipation	MRID 46908329 MRID 46908334
7-OH-XDE-742	13.7% (3 d) 76.5% (58 d) 58.4% 17 d) 41% (68 d)[1]	Aerobic soil metabolism Anaerobic aquatic metabolism[2] Aerobic aquatic metabolism Terrestrial Field dissipation	MRID 46908329 MRID 46908331 MRID 46908336 MRID 46908334
6-Cl-7-OH-XDE-742	26.2% (7 d) 5-7% (68-462 d)[1]	Aerobic soil metabolism Terrestrial Field dissipation	MRID 46908329 MRID 46908334
XDE-742 CSF	8.1 (21 d)	Aerobic soil metabolism	MRID 46908329
XDE-742 PSA	5.9% (29 d)	Aerobic soil metabolism	MRID 46908329
5,7-diOH-XDE-742	27.3% (126 d)	Anaerobic aquatic metabolism[2]	MRID 46908331
XDE-742-ATSA	12.9% 54 d)	Aerobic aquatic metabolism	MRID 46908336
CO_2	1.2% (15 d) 15.6% (133 d) 0.1% (14-126 d) 2.3% (75 d)	Aqueous photolysis Aerobic soil metabolism Anaerobic aquatic metabolism[2] Aerobic aquatic metabolism	MRID 46908327 MRID 46908329 MRID 46908331 MRID 46908336
Unidentified/non-extracted residues	69.9% (14.9 d) 31.0% (15 d) 94.1% (29 d) 76.5% (54 d)	Aqueous photolysis Soil photolysis Aerobic soil metabolism Aerobic aquatic metabolism	MRID 46908327 MRID 46908328 MRID 46908329 MRID 46908336

[1] Terrestrial field dissipation values are expressed in percent of initial measured parent concentration.
[2] Anaerobic conditions were not maintained in the anaerobic aquatic metabolism study. The degradates identified were likely the result of aerobic biodegradation.

Table II.2. Chemical Names and Structures of Pyroxsulam and its Degradates.	
Chemical Name	**Structure**
Pyroxsulam, XDE-742 N-(5,7-dimethoxy[1,2,4]triazolo[1,5--α]]pyrimidin-2-yl)-2-methoxy-4-(trifluoromethyl)-3-pyridinesulfonamide	
XDE-742 sulfinic acid 2-methoxy-4-(trifluoromethyl)pyridine-3-sulfinic acid	
XDE-742 ADTP 5,7-dimethoxy[1,2,4]triazolo[1,4-α]pyrimidin-2-amine	
5-OH-XDE-742 N-(5-hydroxy-7-methoxy[1,2,4]triazolo[1,5-α]pyrimidin-2-yl)-2-methoxy-4-(trifluoromethyl)-3-pyridinesulfonamide	
7-OH-XDE-742 N-(7-hydroxy-5-methoxy[1,2,4]triazolo[1,5-α]pyrimidin-2-yl)-2-methoxy-4-(trifluoromethyl)-3-pyridinesulfonamide	
6-Cl-7-OH-XDE-742 N-(6-chloro-7-hydroxy-5-methoxy[1,2,4]triazolo[1,5-α]pyrimidin-2-yl)-2-methoxy-4-(trifluoromethyl)pyridine-3-sulfonamide	

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Table H.2. Chemical Names and Structures of Pyroxsulam and its Degradates.

Chemical Name	Structure
XDE-742 CSF, **XDE-742 cyanosulfonamide** N-cyano-2-methoxy-4-(trifluoromethyl)pyridine-3-sulfonamide	
XDE-742 PSA, **XDE-742 sulfonic acid** 2-methoxy-4-(trifluoromethyl)pyridine-3-sulfonic acid	
5,7-diOH-XDE-742 N-(5,7-dihydroxy[1,2,4]triazolo[1,5-α]pyrimidin-2-yl)-2-methoxy-4-(trifluoromethyl)-3-pyridinesulfonamide	
XDE-742-ATSA N-(5-amino-1H-1,2,4-triazol-3-yl)-2-methoxy-4-(trifluoromethyl)pyridine-3-sulfonamide	

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