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OFFICE OF
PREVENTION, PESTICIDES AND
TOXIC SUBSTANCES

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MEMORANDUM

SUBJECT: Prothioconazole Tier II Estimated Drinking Water Concentrations (EDWCs) for Use in the Human Health Risk Assessment.

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TO: Barry O'Keefe, Biologist
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This memo summarizes the Tier II estimated drinking water concentrations (EDWCs) for prothioconazole (2-[2-(1-Chlorocyclopropyl)-3-(2-chlorophenyl)-2-hydroxypropyl]-1,2-dihydro-3H-1,2,4-triazole-3-thione; CAS Registry Number 178928-70-6) in surface water and in groundwater for use in the human health risk assessment to support a new chemical registration. Prothioconazole has the potential to reach surface water via runoff, erosion, and spray drift, and, as a result of the moderate to slight mobility of prothioconazole's degradates, may reach groundwater because of its aerobic soil persistence. Due to uncertainties in the fate data, this exposure assessment summarizes the upper and lower bounds of Tier II estimated drinking water concentrations (EDWC) for prothioconazole total toxic residues.

The time series for upper and lower bounds on each crop scenario have been provided to HED (**113961 D324659 Prothioconazole DWA time series.xls**). Please contact Roxolana Kashuba (703.308.7772) with questions.

Attachment

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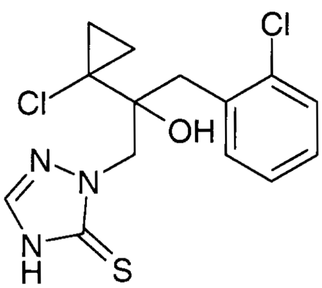
Office of Prevention, Pesticides,
and Toxic Substances

Prothioconazole Tier II Drinking Water Exposure Assessment



Prothioconazole, 2-[2-(1-Chlorocyclopropyl)-3-(2-chlorophenyl)-2-hydroxypropyl]-1,2-dihydro-3H-1,2,4-triazole-3-thione
CAS Registry Number 178928-70-6
PC Code 113961

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EXECUTIVE SUMMARY

This document reports the drinking water exposure assessment for prothioconazole that has been conducted to support the human health risk assessment for the registration of prothioconazole. Prothioconazole is a broad-spectrum, systemic fungicide to be used as ground and aerial foliar spray treatment for fungal disease control in wheat, barley, lentils, canola, oilseed subgroup, chickpeas, dried peas and beans, peanuts and rice. Prothioconazole's mode of action is the inhibition of demethylation of two precursors of sterols in fungi (lanosterol and 24-methylene dihydrolano-sterol). Based on available data, prothioconazole together with its major degradates appear to be persistent (*ie.*, prothioconazole relatively quickly degrades to two major persistent degradates of similar toxicity to parent). Prothioconazole's mobility is unable to be characterized due to quick degradation in mobility studies, but one major degradate formed in large amounts (prothioconazole-desthio) is moderately mobile while the other major degradate formed in smaller amounts (prothioconazole-S-methyl) is slightly mobile.

This exposure assessment summarizes the upper and lower bounds of Tier II estimated drinking water concentrations (EDWC) for prothioconazole total toxic residues in surface water and in groundwater for use in the human health risk assessment. The Screening Concentration in Ground Water (SCIGROW) model is used to estimate ground water concentrations and the Pesticide Root Zone Model (PRZM) and Exposure Analysis Modeling System (EXAMS) models are used to estimate surface water concentrations. Additionally, the Interim Rice Model is used to generate screening level rice paddy water concentrations resulting from pesticide use on rice.

As there were two major degradates (prothioconazole-desthio and prothioconazole-S-methyl) detected in major amounts in almost all fate laboratory studies, it is assumed that these degradates are likely to result in significant environmental concentrations. In addition, prothioconazole-desthio and prothioconazole-S-methyl are likely to exhibit similar toxicity to the parent prothioconazole, based on submitted toxicological studies on these degradates, and HED has concern regarding the hazard associated with these environmental metabolites. Therefore, estimated environmental concentrations are based on total toxic residues, ie., the parent prothioconazole compound plus prothioconazole-desthio and prothioconazole-S-methyl. Two other major degradates were not included in this assessment: prothioconazole-thiazocine (not considered considered a degradate of concern) and 1,2,4-triazole (as it is being assessed separately as a common degradates in the ongoing, conazole aggregate risk assessment).

There are two major uncertainties in drinking water modeling: inclusion versus exclusion of unextracted residues in half-life calculations and use of prothioconazole-desthio versus prothioconazole-S-methyl K_{OC}. Estimated concentrations of prothioconazole in groundwater and surface water that could be used as drinking water as provided for each crop in **Tables 1a and 1b**, respectively. Ranges of upper and lower bound concentration estimates represent differences in input parameter assumptions and differences in PCA, as footnoted. This is explained in greater detail in the body of the document (and estimated concentrations resulting from each individual input parameter combination are reported in **Tables 8a-8i**). For surface water, peak values represent acute concentrations, 1-in-10-year averages represent chronic concentrations, and 30-year average represents lifetime concentrations.

Table 1a. Ranges of Tier I Estimated Drinking Water Concentrations (EDWCs) for groundwater based on aerial application of prothioconazole.

DRINKING WATER SOURCE (MODEL USED)	USE SCENARIO (rate modeled)	ESTIMATED DRINKING WATER CONCENTRATION (EDWC) (ppb)	
Groundwater (SCIGROW)	Wheat and Canola[1]	Acute and Chronic	0.015 - 0.33
	Bean[1]	Acute and Chronic	0.023 - 0.50
	Peanut[1]	Acute and Chronic	0.030 – 0.67

[1]Represents ranges in input parameters (aerobic soil metabolism half-life and K_{OC}).

Table 1b. Ranges of Tier II Estimated Drinking Water Concentrations (EDWCs) for surface water based on aerial application of prothioconazole.

DRINKING WATER SOURCE (MODEL USED)	USE SCENARIO (rate modeled)	ESTIMATED DRINKING WATER CONCENTRATION (EDWC) (ppb)		
		Acute	Chronic	Lifetime
Surface water (PRZM/EXAMS)	NATIONAL PERCENT CROPPED AREA (PCA)			
	Wheat[1]	7.1 - 28	4.4 - 25	3.5 - 20
	Canola[1]	8.6 - 27	4.6 - 23	3.6- 17
	Bean[1]	20- 70	14 - 65	11 - 49
	Peanut[1]	27- 73	15 - 63	12 - 52
	Rice[2]	45 - 115	N/A	N/A
	REGIONAL PERCENT CROPPED AREA (PCA)			
	Canola[1]	8.2 - 26	4.4 - 22	3.4 - 16
	Bean[3]	14 - 67	10 - 62	8.0 - 47
	Peanut[3]	12 - 56	6.4 - 49	5.1 - 40
	Rice[4]	21 - 112	N/A	N/A

[1]Represents ranges in input parameters (aerobic soil, aerobic aquatic, and anaerobic aquatic metabolism half-lives and K_{OC}).
[2]Represents range in K_d input parameter.
[3]Represents ranges in input parameters (aerobic soil, aerobic aquatic, and anaerobic aquatic metabolism half-lives and K_{OC}) as well as ranges in regional PCAs.
[4]Represents range in K_d input parameter as well as ranges in regional PCAs.

Prothioconazole has the potential to reach surface water via runoff, erosion, and spray drift. Prothioconazole's degradates are moderately to slightly mobile and may reach groundwater because of their aerobic soil persistence.

PROBLEM FORMULATION

For most crops, this is a Tier II drinking water assessment that uses modeling to estimate the ground water and surface water concentrations of prothioconazole total toxic residues in drinking water source water (pre-treatment) resulting from pesticide use on sites that are highly vulnerable. A total toxic residues approach was used because prothioconazole degrades quickly to two major degradates which are both of toxicological concern. Aerial application is allowed for all crops, in addition to ground application, and was modeled in this assessment. Because prothioconazole is a new chemical, monitoring data are not available. Concentrations from use on rice were estimated using the Interim Rice screening model, which generates an acute point estimate instead of a distribution and does not take degradation into account.

There are two major uncertainties in drinking water modeling. First, some prothioconazole residue remained in the bound phase in studies used to characterize persistence. To address this uncertainty, modeling was bound based on inclusion and exclusion of unextracted residues in half-life calculations. Second, the two major degradates of prothioconazole formed rapidly after application have different mobility. To address this uncertainty, modeling was conducted using K_{OC}s for prothioconazole-desthio and prothioconazole-S-methyl.

To further refine EDWCs for canola, beans, peanuts, and rice, regional default Percent Cropped Area factors (PCA) have been applied to estimated concentrations. Because wheat is grown across the country, and a crop-specific national PCA is available, wheat EDWCs are not further refined with regional PCAs. Canola is grown within a single regional basin and, therefore, only one default regional PCA was used in canola refinement. Alternately, most beans and peanuts are grown in two regional basins each and, therefore, two default regional PCAs were used in bean and peanut refinement. Similarly, EDWCs for rice are reported with two (lower and higher end) regional PCAs.

ANALYSIS

Use Characterization

Prothioconazole is proposed for use as a pre- or post-infection fungicide on barley, canola, chickpea, dried shell peas and beans, lentils, oilseed crop, peanut, rice and numerous varieties of wheat. It is formulated as flowable formulation and applied via ground spray or aerially. Based on current proposed labels, the maximum proposed single application rates among all uses range from 0.134 to 0.178 lbs. a.i./A. Maximum seasonal applications vary predominantly based on the number of applications allowed. For example, the total yearly maximum proposed rate is 0.712 lbs a.i./A for use on peanuts and would result from 4 applications of 0.178 lbs a.i./A. Complete use rates and management practices by crop based on proposed labels are presented in **Table 2** are based on the Petition for Tolerances submitted by Bayer Crop Science (March 31, 2004). The maximum proposed use is highlighted.

Table 2. Summary use information for prothioconazole, based on PROLINE® 480SC Fungicide label.

USE	SINGLE APP. RATE (lbs. a.i./A)	NUMBER OF APPS.	MAX SEASONAL APP. RATE (lbs. a.i./A)	INTERVAL BETWEEN APPS. (days)	APPLICATION METHOD	INCORP. DEPTH (inches)
Peanut	0.156-0.178	4	0.712	14	Aerial and Ground spray	0

USE	SINGLE APP. RATE (lbs. a.i./A)	NUMBER OF APPS.	MAX SEASONAL APP. RATE (lbs. a.i./A)	INTERVAL BETWEEN APPS. (days)	APPLICATION METHOD	INCORP. DEPTH (inches)
Chickpea	0.134-0.178	3	0.534	10 to 14	Aerial and Ground spray	0
Dried shell pea & bean	0.134-0.178	3	0.534	5 to 14	Aerial and Ground spray	0
Lentil	0.134-0.178	3	0.534	10 to 14	Aerial and Ground spray	0
Barley	0.088-0.178	2	0.293	7 to 14	Aerial and Ground spray	0
Canola	0.134-0.178	2	0.356	5 to 7	Aerial and Ground spray	0
Oilseed crop subgroup	0.134-0.178	2	0.356	5 to 7	Aerial and Ground spray	0
Wheat	0.134-0.178	2	0.293	7 to 14	Aerial and Ground spray	0
Rice	0.143	2	0.285	Not specified	Aerial and Ground spray	0

Fate and Transport Characterization

Prothioconazole appears to degrade relatively quickly in the environment, however its degradates, primarily prothioconazole-desthio, are persistent and have been included in drinking water exposure estimates due to their toxicity. This quick degradation in concert with poor extraction methods in soil and sediment metabolism studies leads to great uncertainty in composition and bioavailability of large amounts of unextracted material. It cannot be determined which portions of the unextracted material are composed of potentially bioavailable parent, which are composed of potentially bioavailable prothioconazole-desthio or other degradates, and which are composed of legitimately unextractable, non-bioavailable material. Due to this uncertainty, biotic degradation rates are unable to be calculated for prothioconazole alone. Therefore, a total toxic residues method, including unextracted material, is utilized for higher bound environmental exposure estimate modeling. For lower bound estimate modeling, it is assumed that unextracted material is non-bioavailable and non-toxic. There is evidence that the prothioconzazole-desthio degradate is moderately mobile (K_ds of 4.13 to 13.38 mL/g in four soils, stability to hydrolysis, long half-lives to other environmental degradation processes and multiple detections at 15-30 cm and one detection at 30-45 cm in terrestrial field dissipation studies). **Table 3** provides a detailed summary table of physical/chemical and environmental fate/transport properties of prothioconazole combined residues of concern. **Tables 4a and 4b** summarize the major and minor degradation products, respectively, formed by each degradation process in the studies reviewed.

Table 3. Summary of physical/chemical and environmental fate and transport properties of prothioconazole combined residues of concern.

PARAMETER	VALUE(S) (units)	SOURCE MRID	COMMENT
Chemical Name	Prothioconazole: 2-[2-(1-Chlorocyclopropyl)-3-(2-chlorophenyl)-2-hydroxypropyl]-1,2-dihydro-3H-1,2,4-triazole-3-thione;	46246003 46477401	Prothioconazole-desthio: 2-[2-(1-Chlorocyclopropyl)-3-(2-chlorophenyl)-2-hydroxy-propyl]-1,2-dihydro-3H-1,2,4-triazole Prothioconazole-S-methyl: alpha-1(1-chlorocyclopropyl)-alpha-[(2-chlorophenyl)methyl]-3-(methylthio)-1H-1,2,4-triazole-1-ethanol
Molecular Weight	Prothioconazole: 344.264	46246003 46477401	Prothioconazole-desthio: 312.2 Prothioconazole-S-methyl: 358.3
Solubility (pH 4 (20 °C)) (pH 8 (20 °C)) (pH 9 (20 °C))	Prothioconazole: 5 mg/L or ppm 300 mg/L or ppm 2000 mg/L or ppm	46246003	Moderately solubility at acidic pH, highly soluble at alkaline pHs.
Vapor Pressure (20 °C and 25 °C)	Prothioconazole: <<4 x 10^{-7} Pa	46246003	Relatively non-volatile under field conditions.
Henry's Law constant (20 °C)	Prothioconazole: <2.96 x 10^{-10} atm-m^3/mol	46246003	Estimated from vapor pressure and water solubility.
pKa (20 °C)	Prothioconazole: 6.9	46246003	Weak acid, anion at neutral and alkaline pHs.
Octanol-Water Partition Coefficient (log K_{OW}, at 20 °C) Unbuffered pH 4 pH7 pH9	Prothioconazole: 4.05 4.16 3.82 2.00	46246003	Potential for bioaccumulation at neutral and acidic pH.
Hydrolysis Half-life (pH 4, 7, 9; (25 °C))	Prothioconazole and Prothiconazole-desthio: stable (Prothioconazole-S-methyl is not formed from prothioconaozle hydrolysis.)	46246505 46246506	Study (46246505) conducted on prothioconazole at 50 °C; results extrapolated to 25 °C. Phenyl label only. Stable at all three pHs. Study (46246506) conducted on prothioconazole-desthio as "parent" at 25 °C. Degradation slopes not significantly different from zero; phenyl label only.
Aqueous Photolysis Half-life (pH 7, at 25 °C)	Prothioconazole: $t_{1/2}$ = 9.7 days Prothioconazole-desthio: Increasing at study termination Prothioconazole and Prothiconazole-desthio: $t_{1/2}$ = 101.9 days (Prothioconazole-S-methyl is not formed from prothioconaozle aqueous photolysis.)	46246507	Value corrected to represent natural sunlight at 40°N latitude; uncorrected laboratory half-life of 19.9 days for both phenyl and triazole labels (continuous irradiation; xenon lamp). Concentration of prothioconazole-desthio was still increasing at prothioconazole aqueous photolysis study termination.

<table>
<tr><th>PARAMETER</th><th colspan="5">VALUE(S) (units)</th><th>SOURCE MRID</th><th>COMMENT</th></tr>
<tr><td>Soil Photolysis Half-life</td><td colspan="5">Prothioconazole and Prothiconazole-desthio:

stable

(Prothioconazole-S-methyl is not formed from prothioconaozle soil photolysis.)</td><td>46246510</td><td>Half-life could not be calculated as parent degraded faster in dark samples than in irradiated samples. Phenyl label only. Concentration of prothioconazole-desthio was still increasing at study termination.</td></tr>
<tr><td>Aerobic Soil Metabolism Half-life</td><td colspan="5">Prothioconazole combined residues of concern:
$t_{1/2}$ = 533.2 days (silt; phenyl),
866.4 days (silt; triazole).
990.2 days (loamy sand; phenyl),
1386.3 days (loamy sand; triazole),
866.4 days (sandy loam; phenyl) ,
462.1 days (silty clay loam; phenyl).</td><td>46246511
46246512</td><td>Half-lives are calculated via linear regression on log-transformed data, combining amounts of prothioconazole, prothioconazole-desthio, and prothioconazole-S-methyl per sampling interval. Phenyl and triazole labels treated separately, labeled accordingly. Non-extractable residues included.</td></tr>
<tr><td>Anaerobic Aquatic Metabolism Half-life</td><td colspan="5">Prothioconazole combined residues of concern:
$t_{1/2}$ = stable (total system);
56.8 days (water layer).</td><td>46246516</td><td>Fuquay, GA pond sediment/water system. Sandy clay loam/water, phenyl label only. Half-lives are calculated via linear regression on log-transformed data, combining amounts of of prothioconazole, prothioconazole-desthio, and prothioconazole-S-methyl per sampling interval. Non-extractable residues included.</td></tr>
<tr><td>Aerobic Aquatic Metabolism Half-life</td><td colspan="5">Prothioconazole combined residues of concern:
$t_{1/2}$ = 433.2 days (H, total system, p),
346.6 days (H, total system, t),
106.6 days (A, total system, p),
67.3 days (A, total system, t).
$t_{1/2}$ = 17.2 days (H, water layer, p),
16.2 days (H, water layer, t),
23.3 days (A, water layer, p),
21.7 days (A, water layer, t).</td><td>46246515</td><td>Two systems tested: (H) Honniger Weiher pond (loam/water) and (A) Anglerweiher lake (loamy sand/water). Both phenyl (p) and triazole (t) labels in each system. Half-lives are calculated via linear regression on log-transformed data, combining amounts of prothioconazole, prothioconazole-desthio, and prothioconazole-S-methyl per sampling interval. Non-extractable residues included.</td></tr>
<tr><td rowspan="4">Organic Carbon Partition Coefficient (K_{OC})</td><td>(mL/g_{OC})</td><td>LS</td><td>SCL</td><td>SL</td><td>S</td><td></td><td></td></tr>
<tr><td>Prothioconzole</td><td>--</td><td>--</td><td>--</td><td>--</td><td>46246539
46246504</td><td>Parent mobility cannot be determined due to instability and low column resolution; very high sorption estimated, lower mobility than transformation products</td></tr>
<tr><td>Prothioconzole -desthio</td><td>523</td><td>536</td><td>617</td><td>625</td><td>46246450</td><td>Conducted on prothioconazole-desthio as "parent." Used four soils: loamy sand (LS) at 0.79%OC, silty clay loam (SCL) at 1.66%OC, sandy loam (SL) at 2.02%OC, silt (S) at 2.14%OC.</td></tr>
<tr><td>Prothioconzole -S-methyl</td><td>1973</td><td>2484</td><td>2772</td><td>2995</td><td>46246501</td><td>Conducted on prothioconazole-S-methyl as "parent." Used same soils as MRID: 46246450.</td></tr>
</table>

PARAMETER	VALUE(S) (units)					SOURCE MRID	COMMENT
Soil Partition Coefficient (K_d)	(mL/g)	LS	SCL	SL	S		
	Prothioconzole	--	--	--	--	46246539 46246504	Same as for K_{OC}.
	Prothioconzole -desthio	4.13	8.90	12.46	13.38	46246450	Same as for K_{OC}.
	Prothioconzole -S-methyl	15.6	41.2	56.0	64.1	46246501	Same as for K_{OC}.
Terrestrial Field Dissipation Half-life[1]	**California (sandy loam/loam):** Prothioconazole: $t_{1/2}$ (in surface soil)= 2.2 days; Not detected above LOD below a depth of 15 cm nor after 7DAT. Prothioconazole-desthio: $t_{1/2}$ (in surface soil)= 84.5 days; Detected above LOD to a depth of 45 cm and through 307DAT. **Georgia (sand/sandy loam):** Prothioconazole: $t_{1/2}$ (in surface soil)= 4.7 days; Not detected above LOD below a depth of 15 cm nor after 14DAT. Prothioconazole-desthio: $t_{1/2}$ (in surface soil)= 96.3 days; Detected above LOD to a depth of 30 cm through 7DAT. **New York (loamy sand):** Prothioconazole: $t_{1/2}$ (in surface soil)= 96.3 days; Not detected above LOD below a depth of 15 cm nor after 211DAT. Prothioconazole-desthio: $t_{1/2}$ (in surface soil)= 315.1 days; Not detected above LOD below a depth of 15 cm (except for one sampling interval (211DAT) where detected above LOD to 30 cm); detected above LOD through study completion (567DAT).					46246517 46246518 46246519	Studies conducted on prothioconazole as parent. For half-lives calculated for degradates from parent dissipation studies, day of max concentration of degradate is used as day zero in regression.
Aquatic Field Dissipation Half-life[1]	**California (clay):** Prothioconazole: $t_{1/2}$ (in sediment)= 203.9 days; $t_{1/2}$ (in paddy water)= 1.7 days. Prothioconazole-desthio: $t_{1/2}$ (in sediment)= 122 days. **Arkansas (loam):** Prothioconazole: $t_{1/2}$ (in sediment)= too few detections; $t_{1/2}$ (in paddy water)= 0.9 days. Prothioconazole-desthio: $t_{1/2}$ (in sediment)= 121.6 days. **Arkansas-cropped (loam):** Prothioconazole: $t_{1/2}$ (in sediment)= too few detections; $t_{1/2}$ (in paddy water)= 0.6 days. Prothioconazole-desthio: $t_{1/2}$ (in sediment)= 90.0 days.					46246522 46246523 46246524	Studies conducted on prothioconazole as parent. For half-lives calculated for degradates from parent dissipation studies, day of max concentration of degradate is used as day zero in regression.
Bioconcentration Factor (BCF)	Prothioconazole and prothioconazole-desthio do not appear to bioaccumulate.					46246034 46246035	BCF cannot be calculated due to lack of a clear accumulation plateau.

[1]DAT= days after treatment.

Table 4a. Summary of major degradate formation from degradation of prothioconazole.

STUDY TYPE	MAJOR DEGRADATE and MAXIMUM CONCENTRATION				SOURCE
	Prothioconazole-desthio (SXX0665) (% applied)	Prothioconazole-S-methyl (WAK7861) (% applied)	Prothioconazole-thiazocine (% applied)	1,2,4-triazole (% applied)	
Hydrolysis	5.7% at 168 days	–	–	Not able to be detected.	MRID: 46246505.
Aqueous Photolysis	55.7% at 11 days (triazole label)	–	14.1% at 5 days (phenyl label)	11.9% at 18 days (triazole label)	MRID: 46246507.
Soil Photolysis	39.0 % at 15 days (29.4% max at 15 days in dark control)	–	–	Not able to be detected.	MRID: 46246510.
Aerobic Soil Metabolism	49.4% at 7 days (triazole label)	14.6% at 7 days (triazole label)	–	<2.0% at 120, 272, & 365 days (triazole label)	MRID: 46246511, 46246512.
Aerobic Aquatic Metabolism	26.9% at 14 days in sediment (both labels) 32.3% at 7 days in water (phenyl label) 54.6% at 7 days in total system (phenyl label)	9.6% at 7 days in sediment (triazole label) 3.1% at 7 days in water (triazole label) 12.7 % at 7 days in total system (triazole label)	–	6.1% at 121 days in sediment (triazole label) 37.2% at 121 days in water (triazole label) 41.8 % at 121 days in total system (triazole label)	MRID: 46246515.
Anaerobic Aquatic Metabolism	Not determined; -desthio formation determined to be artifact of storage and, therefore, added to parent (parent+desthio at 95.2% in total system at 0 days)	78.2% at 240 days in sediment 9.9% at 30 days in water 78.2% at 240 days in total system	–	Not able to be detected.	MRID: 46246516.
Terrestrial Field Dissipation	223.9 ug/kg soil at 3 days, 0-15 cm soil depth (CA) 84.9 ug/kg soil at 3 days, 0-15 cm soil depth (GA) 273.0 ug/kg soil at 28 days, 0-15 cm soil depth (NY)	15.9 ug/kg soil at 3 days, 0-15cm soil depth (CA) 12.3 ug/kg soil at 7 days, 0-15 cm soil depth (GA) 58.9 ug/kg soil at 28 days, 0-15 cm soil depth (NY)	–	7.3 ug/kg soil at 29 days, 0-15cm soil depth (CA) 5.3 ug/kg soil at 120 days, 0-15cm soil depth (GA) 3.5 ug/kg soil at 422 days, 0-15 cm soil depth (NY)	MRID: 46246517, 46246518, 46246519.
Aquatic Field Dissipation	32.7 ug/kg sediment at 14 days, 0-3 in.; 50.3 ug/L paddy water at 3 days (CA)	10.2 ug/kg sediment at 122 days, 0-3 in.; 1.04 ug/L paddy water at 3 days (CA)	–	3.3 ug/kg sediment at 364 days, 0-3 in.; 0.13 ug/L paddy water at 7 days (CA)	MRID: 46246522, 46246523, 46246524.

Data are reported in single replicates.
Studies conducted with both phenyl and triazole radiolabels include: aerobic soil metabolism (MRID: 46246511 only), aerobic aquatic metabolism, and aqueous photolysis. All other studies are conducted with phenyl radiolabel only (ie., hydrolysis, soil photolysis, other aerobic soil metabolism (MRID: 46246512 only), anaerobic aquatic metabolism). The 1,2,4-triazole degradate is not able to be detected in studies using the phenyl radiolabel. (The 1,2,4-triazole degradate column for studies which did not use the triazole label are designated "Not able to be detected.")
Field studies not radiolabelled. The only degradates tracked in field studies are: prothioconazole-desthio, prothioconazole-S-methyl, prothioconazole-thiazocine, and 1,2,4-triazole. Maximum concentrations in the field studies are determined after the 6^{th} (CA, NY) or 2^{nd} (GA) application. (DAT= days after 6^{th} or 2^{nd} treatment); 800 ug/kg, 400 ug/kg, and 1000 ug/kg total prothioconazole applied in CA, GA, and NY, respectively. Blank boxes represent degradates which are not detected above MDL.

Table 4b. Summary of minor degradate formation from degradation of prothioconazole.

STUDY TYPE	MINOR DEGRADATE and MAXIMUM CONCENTRATION					SOURCE
	Prothioconazole-sulfonic acid (JAU6726) **(% applied)**	**Prothioconazole-triazolinone (WAK7860** **(% applied)**	**Prothioconazole-3, 4, 5, and 6-hydroxy-desthio (3, 4, 5, and 6-HO-SXX0665** **(% applied)**	**2-chlorobenzoic acid** **(% applied)**	**JAU6476-triazolylketone (WAK4995)** **(% applied)**	
Hydrolysis	–	–	–	–	–	MRID: 46246505.
Aqueous Photolysis	–	–	–	–	–	MRID: 46246507.
Soil Photolysis	3.6 % at 15 days (<1.0% max at all days in dark control)	2.7 % at 7 days (3.2% max at 15 days in dark control)	–	–	–	MRID: 46246510.
Aerobic Soil Metabolism	8.3% at 181 days (triazole label)	3.1% at 63 days (phenyl label)	2.1% at 14 days (triazole label) for 3-OH; <3.3% in mixture at 63 days (triazole label) for both 4 and 5-OH; 4.6% at 120 days (triazole label) for 6-OH	2.2% at 272 days (triazole label)	–	MRID: 46246511, 46246512.
Aerobic Aquatic Metabolism	–	6.1% at 59 days in sediment (triazole label) 2.2% at 59 days in water (triazole label) 6.7% at 59 days in total system (triazole label)	–	–	5.8% at 121 days in sediment (triazole label) 8.0% at 59 days in water (triazole label) 9.1% at 59 days in total system (triazole label)	MRID: 46246515.
Anaerobic Aquatic Metabolism	–	78.2% at 240 days in sediment 9.9% at 30 days in water 78.2% at 240 days in total system	–	–	–	MRID: 46246516.

Data are reported in single replicates.
Studies conducted with both phenyl and triazole radiolabels include: aerobic soil metabolism (MRID: 46246511 only), aerobic aquatic metabolism, and aqueous photolysis. All other studies are conducted with phenyl radiolabel only (ie., hydrolysis, soil photolysis, other aerobic soil metabolism (MRID: 46246512 only), anaerobic aquatic metabolism). The 1,2,4-triazole degradate is not able to be detected in studies using the phenyl radiolabel. (The 1,2,4-triazole degradate column for studies which did not use the triazole label are designated "Not able to be detected.")
Minor degradates were not tracked in field dissipation studies.

Drinking Water Exposure Modeling

This section describes the models used, the selection of model input parameter values, and the model output.

Models

SCIGROW (Screening Concentration in Ground Water, v2.3) is a regression model used as a screening tool to estimate pesticide concentrations found in ground water used as drinking water. SCIGROW was developed by fitting a linear model to groundwater concentrations with the Relative Index of Leaching Potential (RILP) as the independent variable. Groundwater 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 SCIGROW represents the concentrations that might be expected in shallow unconfined aquifers under sandy soils, which is representative of the ground water most vulnerable to pesticide contamination likely to serve as a drinking water source. **(Ref. 2)**

PRZM-EXAMS (Pesticide Root Zone Model (PRZM, v3.12 beta) and Exposure Analysis Modeling System (EXAMS, v2.98.04)) is used as a Tier II screening tool to estimate pesticide concentrations found in surface water used as drinking water. PRZM simulates pesticide application to an agricultural field and its transport to an adjacent reservoir by storm events with runoff and eroded sediment. EXAMS estimates the concentration over time in the index reservoir per crop scenario during 30 years of simulated weather. The Index Reservoir is 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 (albeit not currently in active use as a drinking water supply), Shipman City Lake in Illinois, that is known to be vulnerable to pesticide contamination. Additionally, PRZM-EXAMS can account for spray drift and adjusts for the area within a watershed that is planted with the modeled crop (Percent Cropped Area). Spray drift (modeled as direct deposition of the pesticide into the reservoir) is assumed to be 16% of the applied active ingredient for aerial application and 6.4% for other ground spray application.

Pesticide concentrations in water from application to rice paddies are estimated by applying the total annual application to the paddy and partitioning the pesticide between the water and the paddy sediment according to a linear or K_d partitioning model (Interim Rice Model; 10/29/2002). The EDWC ($\mu g. L^{-1}$) represents the dissolved concentration occurring in the water column and the concentration in water released from the paddy. Movement of pesticide on suspended sediment is not considered. This is intended to be an interim measure until a more complete rice modeling method becomes available.

Scenario Selection

Four crop scenarios were used to assess impacts of new uses of prothioconazole listed in **Table 2**. Each scenario represents the most vulnerable of areas used to grow the respective crops. Application dates were chosen based on label information compared to scenario crop emergence, maturation, and harvest dates, as follows:

WHEAT (North Dakota):

Crop emergence date—	May 15
Crop maturation date—	July 25
Crop harvest date—	August 5

From label: For fusarium head blight, apply from at least 75% of the wheat heads on the main stem are fully emerged to when 50% of the heads on the mainstem are in flower (ie., between about May 20 to July 1). Do not apply within 30 days of harvest (ie., before July 5).
Therefore, June 18 was chosen as the wheat scenario application date.
This scenario represents application to wheat (**Figure 1**) at a site that is vulnerable to runoff. The same scenario is used to represent barley (**Figure 2**). While a reasonable surrogate for small

grains, barley growing areas are more spatially concentrated than wheat. Another minor difference is that the minimum application interval allowed for wheat is 5 days while that allowed for barley is 10 days.

CANOLA (North Dakota):

Crop emergence date— May 15
Crop maturation date— August 15
Crop harvest date— August 25

From label: Apply when canola crop is in 20-50% bloom stage, which is 4-8 days after the canola crop begins to flower. Best protection will be achieved if prothioconazole is applied prior to petals beginning to fall (ie., about June 15 through August 1).

Therefore, June 17 was chosen as the canola scenario application date.

This scenario represents application to canola (**Figure 3**) at a site that is vulnerable to runoff. The same scenario is used to represent oilseed subgroup composed of rapeseed, Indian rapeseed, Indian mustard, field mustard, black mustard, crambe and borage.

BEAN (Michigan):

Crop emergence date— June 5
Crop maturation date— July 27
Crop harvest date— September 4

From label: Apply at first sign of disease (ie., post emergence, post June 5). Do not apply within 7 days of harvest (ie., before August 28).

Therefore, June 29 was chosen as the bean scenario application date.

This scenario represents application to dried shelled peas (**Figure 4**) and beans (**Figure 5**) subgroup (except soybeans) at a site that is vulnerable to runoff. The same scenario is used to represent chickpeas and lentils. A minor difference is that the minimum application interval allowed for dried shelled peas and beans subgroup (except soybeans) is 5 days while that allowed for chickpeas and lentils is 10 days.

PEANUT (North Carolina):

Crop emergence date— May 10
Crop maturation date— October 1
Crop harvest date— October 10

From label: Preventative spray schedule—prothioconazole for sprays 3, 4, 5, and 6 of 7 spray application program, starting 30-40 days after planting (ie., Spray 1= June 11, Spray 2= June 25, Spray 3= July 9). When using Leaf Sport Advisory Program, spray prothioconazole in the first advisory spray in July and continue at 14 day intervals.

Therefore, July 9 was chosen as the peanut scenario application date.

This scenario represents application to peanuts (**Figure 6**) at a site that is vulnerable to runoff.

Figure 1. Wheat grown in United States.

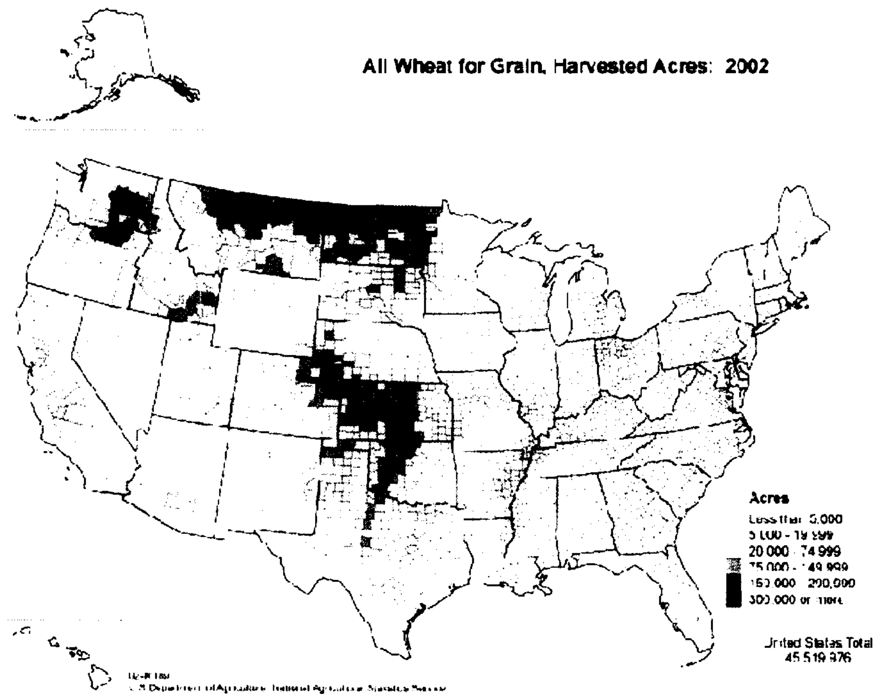


Figure 2. Barley grown in United States.

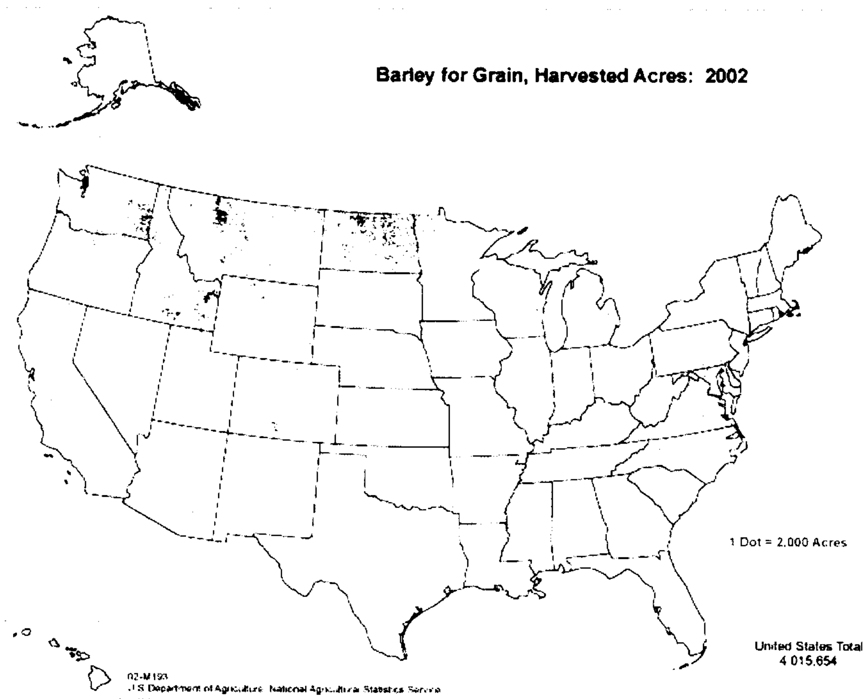


Figure 3. Canola grown in United States.

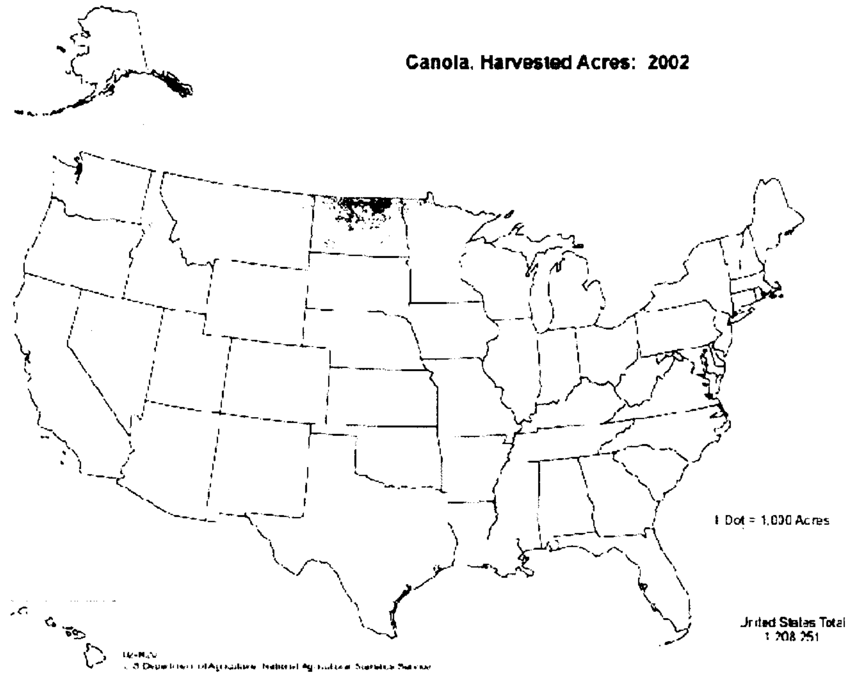


Figure 4. Dry edible peas grown in United States.

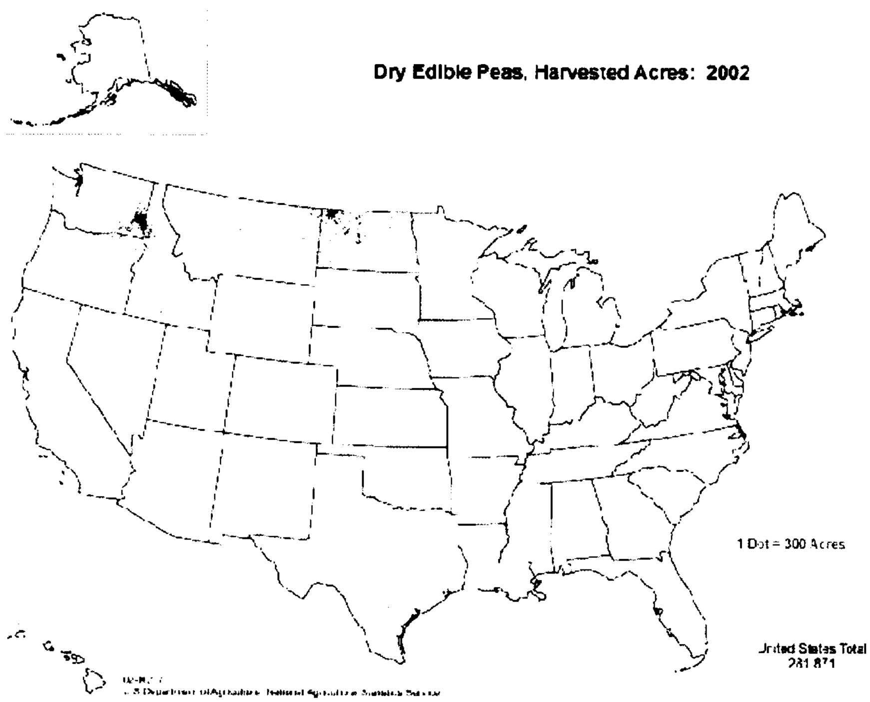


Figure 5. Dry edible beans grown in United States.

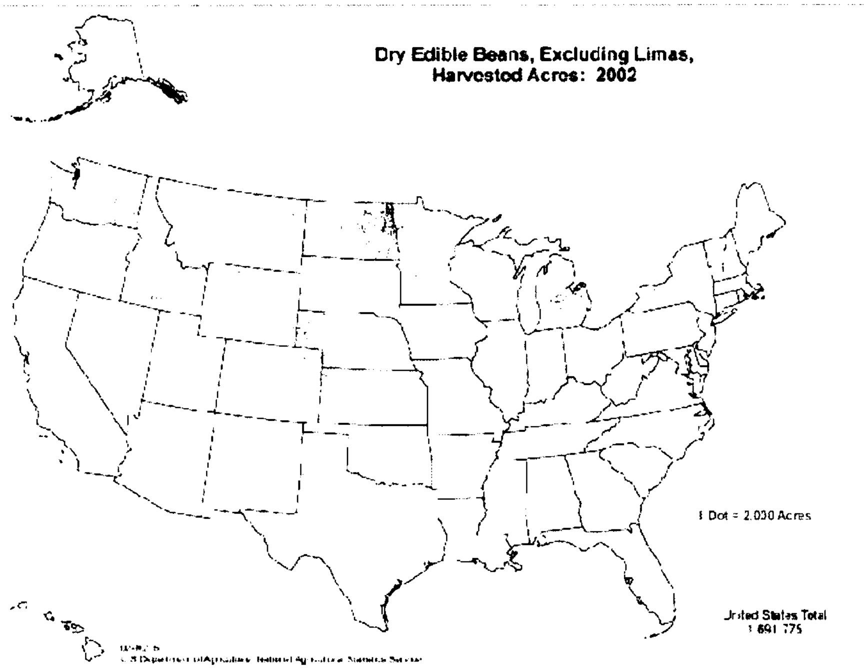
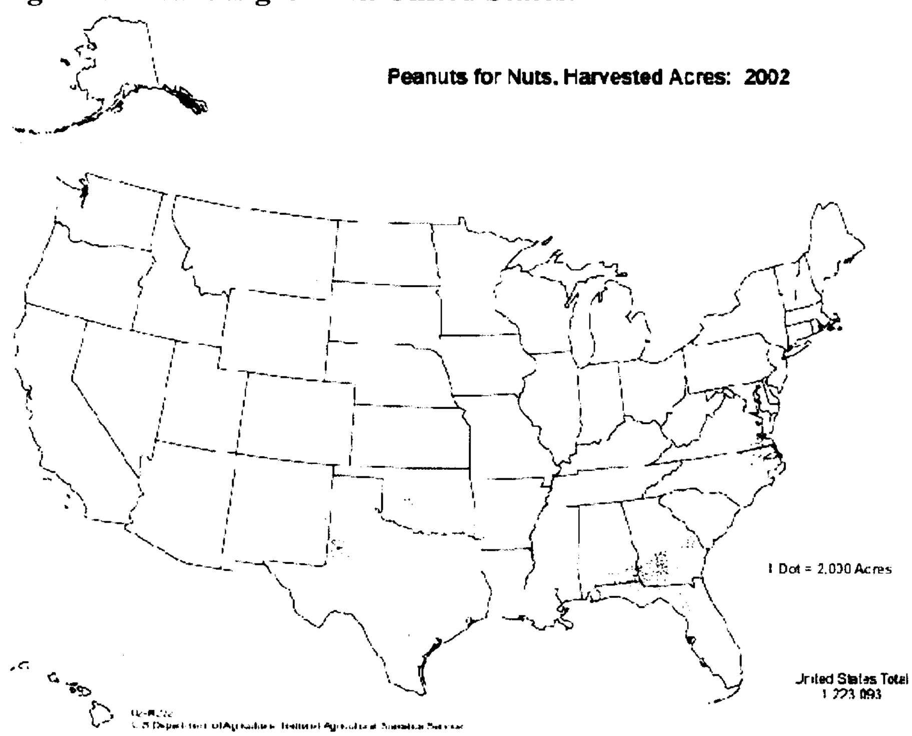


Figure 6. Peanuts grown in United States.



For regional PCA refinement, wheat (**Figure 1**) is grown nationally and, therefore, does not warrant regional refinement (national PCA: 56%). Barley (**Figure 2**) is grown in the northwest of the United States but is modeled together with wheat and, therefore, a barley-specific regional PCA is not applied. Canola (**Figure 3**) is grown in the north half of North Dakota, a portion of the Souris-Red-Rainy section of the Mississippi river basin (basin 9, regional PCA: 83%). Dry edible peas and beans (**Figures 4 and 5**) are also grown in the north half of North Dakota, a portion of the Souris-Red-Rainy section of the Mississippi river basin (basin 9, regional PCA: 83%) and Pacific Northwest basin West of the Western Divide (basin 17, regional PCA: 63%). Peanuts (**Figure 6**) are grown in the Texas Gulf section of the Mississippi river basin (basin 12, regional PCA: 67%) and in the south of Virginia/north of North Carolina and southern Georgia and Alabama sections of the South Atlantic Gulf basin East of the Eastern Divide (basin 3, regional PCA: 38%). Rice is grown in Southwest Louisiana, Texas, and California (lower estimate regional PCA: 41%) and in the lower Mississippi river encompassing Arkansas and parts of Louisiana and Mississippi (higher estimate regional PCA: 85%).

Modeling Approach and Input Parameters

Tables 5 and 6 list modeling parameter input values for SCIGROW and PRZM-EXAMS, respectively. Input parameters were selected in accordance with EFED's "Guidance for Selecting Input Parameters in Modeling the Environmental Fate and Transport of Pesticides," Version II (2-28-02).

Modelling was conducted using total toxic residues, including parent **prothioconazole** and degradates **prothioconazole-desthio** and **prothioconazole-S-methyl**. These contaminants of concern, which are formed quickly and at greater than 10% of applied through all routes of degradation of prothioconazole (except aqueous and soil photolysis for prothioconazole-S-methyl), were identified in coordination with the Health Effects Division as being of toxicological concern based on toxicity studies conducted on these degradates indicating that they exhibit similar levels of toxicity to that of parent. Major degradate **prothioconazole-thiazocine**, is not considered in the drinking water assessment, as recommended by HED, because it is not considered a degradate of concern in any human health effects metabolism studies. Major degradate **1,2,4-triazole** is formed at maximums of 41.8%, 11.9% and <2.0% of applied via aerobic aquatic metabolism, aqueous photolysis, and aerobic soil metabolism, respectively, and is not radiolabelled (and, therefore, not reported) in the remainder of the environmental fate studies. However, it is not considered in the prothioconazole drinking water exposure assessment because its predicted environmental concentrations and toxicity are taken into account in the ongoing, current conazole aggregate risk assessment. Additional minor identified degradates (**Table 4b**) are not considered in the drinking water exposure assessment due to their apparently low levels expected in drinking water.

For PRZM-EXAMS surface water modeling inputs, the organic carbon partition coefficient (K_{OC}) was used instead of the soil partition coefficient (K_d) because K_d was related to organic carbon for the four soils tested. Therefore, the partition coefficient corrected for organic carbon (K_{OC}), was assumed to better represent partitioning in soil. Given the total toxic residue modeling approach, because it is not possible, given data constraints, to calculate one overall adsorption coefficient, the K_{OC} of prothioconazole-desthio was chosen for use in modeling because it is the most conservative, most mobile parameter of prothioconazole, prothioconazole-desthio, and prothioconazole-S-methyl. However, in reality, each of the compounds represented in the total toxic residues approach has a different mobility in the soil and there is thus some uncertainty in the exposure estimates as a single K_{oc} must be used to represent the suite. In order to gauge the effect this uncertainty in mobility has on the drinking water concentration estimates, modeling was also conducted using the K_{OC} of prothioconazole-S-methyl in order to test the effect of this higher estimated soil binding on concentrations.

Degradation half-lives were adjusted for use in the PRZM-EXAMS model according to the input-parameter guidelines. The aerobic soil metabolism half-lives and aerobic aquatic metabolism half-lives were calculated by linear regression on log-transformed data (prothioconazole total toxic residues plus unextracted residues), and then the 90th percentile confidence bound on the mean of those six and four values, respectively, was used in modeling. The anaerobic aquatic metabolism half-life value, calculated by linear regression on log-transformed data (prothioconazole total toxic residues plus unextracted residues) was not significantly different than zero and was assumed to be stable for the purposes of modeling. Again, in order to bound drinking water concentration estimates, modeling was also conducted using half-lives excluding unextracted residues. This would reflect the EDWCs that would occur if all the unextracted material in these studies was in fact unavailable and/or non-toxic degradates.

While the proposed label allows for both ground and aerial application, aerial spray was modeled as the method of application in order to be protective of all application scenarios. When all other parameters remain the same, as tested on all four scenarios including unextracted and using low K_{OC}, PRZM-EXAMS calculated 6-16% higher acute surface water concentrations for aerial spray than for ground spray due to default drift assumptions (see **113961 D324659 Prothioconazole DWA.zip** for output).

Table 5. SCI-GROW (v2.3) input parameter values for prothioconazole use on wheat, canola, beans, and peanuts (total toxic residues)[1].

PARAMETER (units)	VALUE(S)	SOURCE	COMMENT
Maximum Application Rate (lb a.i./A)	0.178	Proposed label.	Represents the maximum possible single application rate per crop season (year).
Number of Applications per Year	4, 3, 2	Proposed label.	Represents the maximum possible applications per crop season (year) for peanuts, beans, and wheat and canola, respectively.
Organic Carbon Partition Coefficient (K_{oc}; mL/g)	576.6 2628	MRID: 46246450. MRID: 46246501.	Represents the median of four values ranging from 523.0 to 625.3 mL/g for prothioconazole-desthio. Represents the median of four values ranging from 1973 to 2995 mL/g for prothioconazole-S-methyl.
Aerobic Soil Metabolism Half-life (days)	866.4 (include unextracted) 288.8 (not include unextracted)	MRID: 46246511, 46246512.	Represents the median of six values (range: 462.1-1386.3) for the aerobic soil metabolism of prothioconazole total toxic residues, except 1,2,4-triazole degradate. Non-extractable residues are included and not included as parent as noted.

[1] Parameters are selected as per Guidance for Selecting Input Parameters in Modeling the Environmental Fate and Transport of Pesticides; Version I, February 28, 2002.

Table 6. PRZM (v3.12 beta) and EXAMS (2.98.04) input parameter values for prothioconazole use on wheat, canola, beans, and peanuts (total toxic residues)[1].

PARAMETER (units)	VALUE(S)	SOURCE	COMMENT
Application Rate (kg a.i./ha)	0.2	Proposed label.	Represents the maximum possible single application rate per crop season (year) for all uses. Equivalent to 0.178 lb a.i./A.
Number of Applications	Wheat: 2 Canola: 2 Beans: 3 Peanuts: 4	Proposed label.	Represents the maximum possible applications per crop season (year) for each use.
Interval between Applications (days)	Wheat: 7 Canola: 5 Beans: 5 Peanuts: 14	Proposed label.	Represents the minimum possible interval between applications per crop season (year) for each use.
Molecular weight (g/mol)	344.264	MRID: 46246003, 46477401.	For parent prothioconazole only.
Henry's Law Constant (atm-m^3/mol)	2.96×10^{-10}	MRID: 46246003.	For parent prothioconazole only.
Vapor Pressure (torr)	3×10^{-9}	MRID: 46246003.	For parent prothioconazole only.
Solubility in Water @ 20 °C, pH 8 (mg/L or ppm)	300	MRID: 46246003.	–
Soil Partition Coefficient (K_{OC} (mL/g_{OC}))	523 1973	MRID: 46246450. MRID: 46246501.	Represents the lowest non-sand K_{OC} value among four values ranging from 523.0 to 625.3 mL/ g_{OC} for prothioconazole-desthio. Represents the lowest non-sand K_{OC} value among four values ranging from 1973 to 2995 mL/ g_{OC} for prothioconazole-S-methyl.
CAM (Chemical Application Method)	2	Proposed label.	Linear foliar based on crop canopy: proposed label allows aerial spray and ground spray.
Depth of Incorporation (inches)	0	Proposed label.	–
Application efficiency (decimal)	Ground spray: 0.99 Aerial spray: 0.95	Input Guidance.	Modeled one test case ground application for each scenario and only aerial application for assessment.
Spray drift fraction (decimal)	Ground spray: 0.064 Aerial spray: 0.16	Input Guidance.	Modeled one test case ground application for each scenario and only aerial application for assessment.
Percent Cropped Area (decimal)	National: Wheat: 0.56 Canola: 0.87 Beans: 0.87 Peanuts: 0.87 Regional: Canola: 0.83 Beans: 0.63 and 0.83 Peanuts: 0.38 and 0.67	Proposed label.	National-scale wheat and national and regional-scale default values.
Application date (day/month)	Wheat: 18/June Canola: 17/June Beans: 29/June Peanuts: 9/July	Proposed label and PRZM scenarios.	–

PARAMETER (units)	VALUE(S)	SOURCE	COMMENT
Hydrolysis Half-life @ pH 4, 7, 9 (days)	0	MRIDs: 46246505, 46246506.	Two studies show that both prothioconazole and prothioconazole-desthio are stable to hydrolysis.
Aqueous Photolysis Half-life @ pH 7 (days)	101.9	MRID: 46246507.	Maximum, dark-controlled, value for prothioconazole total toxic residues, corrected to represent natural sunlight at 40°N latitude.
Water Half-Life, ie., Aerobic Aquatic Metabolism Half-life (days)	385.2 (with unextracted) 78.0 (no unextracted)	MRID: 46246515.	Represents the 90th percentile confidence bound on the mean of four total system half-life values (238.4, range: 67.3-346.6 with unextracted; 61.5, range: 42.5-83.5 no unextracted) calculated using prothioconazole total toxic residues, except 1,2,4-triazole degradate.
Benthic Half-life, ie., Anaerobic Aquatic Metabolism Half-life (days)	0 (with unextracted) 4158 (no unextracted)	MRID: 46246516.	Represents one total system half-life value (stable with unextracted) or three times one total system half-life value (1386.3 no unextracted) calculated using prothioconazole total toxic residues, except 1,2,4-triazole degradate
Soil Half-life, ie., Aerobic Soil Metabolism Half-life (days)	1052.2 (with unextracted) 360.3 (no unextracted)	MRIDs: 46246511, 46246512.	Represents the 90th percentile confidence bound on the mean of six values (850.8, range: 462.1-1386.3 with unextracted; 281.0, range: 123.8-462.1) for the aerobic soil metabolism of prothioconazole total toxic residues, except 1,2,4-triazole degradate.

[1] Most parameters are selected as per Guidance for Selecting Input Parameters in Modeling the Environmental Fate and Transport of Pesticides; Version I, February 28, 2002.

Inputs into the rice model included 0.320 kg a.i./ha total mass applied (equivalent to 0.286 (0.143 x 2) lbs. a.i./A), 1.067 x10^6 L ha^{-1} volume of water in a paddy 4 inches deep (including the pore space in a 1 cm sediment interaction zone), 130,000 kg ha^{-1} mass of sediment in the top 1 cm interaction zone (when the sediment bulk density was assumed to be 1.3 kg L^{-1}), and K_d values of 10.46 and 39.46 (from prothioconazole-desthio K_{OC} of 523 and prothioconazole-S-methyl K_{OC} of 1973, respectively, assuming 2.0% organic carbon content). An organic carbon content of 2% represents a typical value for a high clay soil that might be used to grow rice in the US. (*Policy for Estimating Aqueous Concentrations from Pesticides Labeled for Use on Rice (10/29/2002)*). Rice application was modeled at 0% crop coverage, given label directions on the timing of prothioconazole application. Rice application was initially modeled at 87% national default PCA, and was refined to represent regional PCAs in rice-growing areas.

Modeling Results

Prothioconazole has the potential to reach surface water via runoff, erosion, and spray drift, and, as a result of the moderate to slight mobility of prothioconazole's degradates, may reach groundwater because of its aerobic soil persistence. The concentrations provided in this assessment (**Tables 7a-7c**) represent upper and lower bounds on estimates in drinking water for aerial applications of prothioconazole. The full distributions of these estimates (30 years of daily values) have been provided to HED. The highest surface water concentrations estimated using the tier II model were for crops with higher number of applications per season (beans, three applications; peanuts, four applications). Overall, the highest surface water exposure was estimated for use on rice (two applications) using a screening model, which has a higher degree of uncertainty than estimates for other crops.

SCIGROW concentration (ppb) represents the groundwater concentration that might be expected in shallow unconfined aquifers under sandy soils. Output is used for both acute and chronic endpoints.

PRZM-EXAMS concentrations (ppb) represent untreated surface water concentrations, which have been adjusted for percent crop treated. The one-in-10-year peak day concentration is used for acute endpoints, the one-in-10-year annual average concentration is used for chronic endpoints, and the 30-year annual average is used for lifetime (cancer) endpoints.

Table 7a. Upper-bound Tier II Estimated Drinking Water Concentrations for prothioconazole (including unextracted residues and using lower K_{OC}).

DRINKING WATER SOURCE (MODEL USED)	USE SCENARIO (rate modeled)	National PCA (Regional PCA range)	ESTIMATED DRINKING WATER CONCENTRATION (EDWC) (ppb)		
Groundwater (SCIGROW)	Wheat and Canola (0.178 lb a.i./A x 2)	N/A	Acute and Chronic	0.33	
	Bean (0.178 lb a.i./A x 3)	N/A	Acute and Chronic	0.50	
	Peanut (0.178 lb a.i./A x 4)	N/A	Acute and Chronic	0.67	
Surface water (PRZM/EXAMS)	ND Wheat (0.178 lb a.i./A x 2)	56%		National PCA	Regional PCA
			Acute (1-in-10-year)	28	N/A
			Chronic (1-in-10-year)	25	N/A
			30-year Daily Average	20	N/A
	ND Canola (0.178 lb a.i./A x 2)	87% (83%)	Acute (1-in-10-year)	27	26
			Chronic (1-in-10-year)	23	22
			30-year Daily Average	17	16
	MI Beans (0.178 lb a.i./A x 3)	87% (63% - 83%)	Acute (1-in-10-year)	70	51 - 67
			Chronic(1-in-10-year)	65	47 – 61
			30-year Daily Average	49	35 - 47
	NC Peanut (0.178 lb a.i./A x 4)	87% (38% - 67%)	Acute (1-in-10-year)	73	32 - 56
			Chronic (1-in-10-year)	62	27 - 48
			30-year Daily Average	52	23 - 40

Table 7b. Lower-bound Tier II Estimated Drinking Water Concentrations for prothioconazole (not including unextracted residues and using higher K_{OC}).

DRINKING WATER SOURCE (MODEL USED)	USE SCENARIO (rate modeled)	National PCA (Regional PCA range)	ESTIMATED DRINKING WATER CONCENTRATION (EDWC) (ppb)		
Groundwater (SCIGROW)	Wheat and Canola (0.178 lb a.i./A x 2)	N/A	Acute and Chronic	0.015	
	Beans (0.178 lb a.i./A x 3)	N/A	Acute and Chronic	0.023	
	Peanut (0.178 lb a.i./A x 4)	N/A	Acute and Chronic	0.030	
Surface water (PRZM/EXAMS)	ND Wheat (0.178 lb a.i./A x 2)	56%		National PCA	Regional PCA
			Acute (1-in-10-year)	7.1	N/A
			Chronic (1-in-10-year)	4.4	N/A
			30-year Daily Average	3.5	N/A
	ND Canola (0.178 lb a.i./A x 2)	87% (83%)	Acute (1-in-10-year)	8.6	8.2
			Chronic (1-in-10-year)	4.6	4.4
			30-year Daily Average	3.6	3.4
	MI Beans (0.178 lb a.i./A x 3)	87% (63% - 83%)	Acute (1-in-10-year)	20	14 - 19
			Chronic(1-in-10-year)	14	10 – 13
			30-year Daily Average	11	8.0 - 11
	NC Peanut (0.178 lb a.i./A x 4)	87% (38% - 67%)	Acute (1-in-10-year)	27	12 - 21
			Chronic (1-in-10-year)	16	6.8 - 12
			30-year Daily Average	12	5.3 – 9.3

Table 7c. Estimated Drinking Water Concentrations for prothioconazole on rice.

DRINKING WATER SOURCE (MODEL USED)	USE SCENARIO (rate modeled)	PCA	EDWC (ppb)		
			Acute	Chronic	Lifetime
Rice paddy surface water (Interim Rice Model)	Rice[1] (0.134 lb a.i./A x 2)	National (87%)	45 - 115	N/A	N/A
	Rice[2] (0.134 lb a.i./A x 2)	Regional (41%-85%)	21 - 112	N/A	N/A

[1]Represents range in K_d input parameter.

[2]Represents range in K_d input parameter as well as ranges in regional PCAs.

APPENDIX B reports individual EDWCs for 8 different permutations of model runs using different combinations of environmental fate parameters and adjusting by national and regional PCAs.

Monitoring Data

Because prothioconazole is a new chemical, monitoring data were not available.

Characterization

Because of the uncertainties with unextracted residues and K_{OC}, EFED has provided HED with upper and lower bound Tier II estimated drinking water concentrations in order to characterize how this uncertainty affects the EDWCs. Generally, upper and lower EDWCs differed by a factor of 3 to 6 as a result of these bounding assumptions. Inclusion or exclusion of unextracted residues made a much larger difference in concentrations than use of a high or low K_{OC}.

The treatment of unextracted residues as parent is warranted due to insufficient extraction methods. The registrant used 80:20 acetonitrile:water for a neutral organic; extraction with something more neutral and organic, like hexane, would have been more effective. Given the poor acetonitrile:water extraction, there is not enough evidence to allow exceedance of the standard 20% bound material criterion. Unextracted residues may be toxic and bioavailable and, therefore, should not be considered dissipated, and therefore there is low confidence without this assumption that estimated drinking water exposure would be adequately conservative EDWCs calculated including unextracted residues and EDWCs calculated not including unextracted residues differ by a factor of 2 to 3.

The second major uncertainty in this assessment is due to differences in partitioning for different degradates, and inability to calculate parent partitioning. Because a total toxic residues method was used for this assessment, a single K_{OC} has to be selected to represent the suite of compounds considered as part of the 'total toxic residues', as there is only one input parameter available to describe the suite. In most cases, the parent partition coefficient is selected, but as noted above, it could not be estimated for prothioconazole. Since the desmethyl degradate is the primary degradate, and also has the lowest K_{OC} of the major degradates, it was chosen to represent the suite. To identify the limits on the uncertainty due this selection, additional EDWC's were calculated using the K_{OC} for the S-methyl degradate. EFED found there to be a 1-28% difference between predicted concentrations when using a high (prothioconazole-S-methyl) instead of a low (prothioconazole-desthio) K_{OC}.

EDWCs refined using regional PCAs were not substantially lower for canola and beans grown in the Souris-Red-Rainy portion (north part of North Dakota) of the Mississippi River Basin (decrease of only 4% in concentrations). However, EDWCs for beans grown in the Pacific Northwest basin (southeast Washington and northern Idaho) decreased by 24%, EDWCs for peanuts grown in the Texas Gulf basin (north Texas and southwest Oklahoma) decreased by 20%, and EDWCs for peanuts grown in the South Atlantic Gulf basin (southern Virginia, northern North Carolina, southern Georgia and southern Alabama) decreased by 49%.

APPENDIX A: Molecular structure of prothioconazole's major degradates.

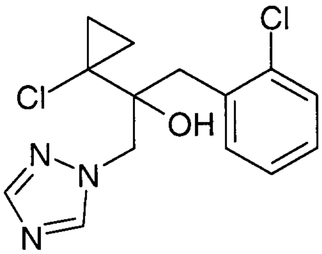


Figure 6. Prothioconazole-desthio

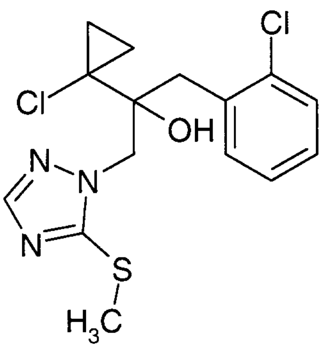


Figure 7. Prothioconazole-S-methyl

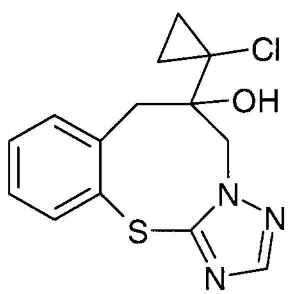


Figure 8. Prothioconazole-thiazocine

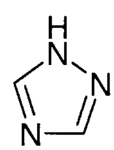


Figure 9. 1,2,4-triazole

APPENDIX B: Modeling results from individual fate parameter combinations.

Estimated drinking water concentrations (EDWCs) are estimated for all four permutations of the two major uncertainties (unextracted residue inclusion and K_{OC}), adjusted for national Percent Cropped Areas (PCAs), and are reported in **Tables 8a-8d**. Upper and lower bound concentrations are noted in red and blue, respectively. EDWCs for canola, beans, and peanuts are further refined by applying regional Percent Cropped Areas (PCAs) and are reported in **Tables 8e-8h**. Wheat is grown nationally and is, therefore, not refined by region in a national assessment. Again, upper and lower bound concentrations are noted in red and blue, respectively. Estimated EDWCs for rice with national PCA and lower and higher end regional PCAs are reported in **Table 8i**.

Table 8a. Tier II Estimated Drinking Water Concentrations (EDWCs) for drinking water assessment based on aerial application of prothioconazole: not including unextracted residues and using lower K_{OC}.

DRINKING WATER SOURCE (MODEL USED)	USE SCENARIO (rate modeled)	NATIONAL PERCENT CROPPED AREA (PCA)	ESTIMATED DRINKING WATER CONCENTRATION (EDWC) (ppb)		
Groundwater (SCIGROW)	Wheat and Canola (0.178 lb a.i./A x 2)	N/A	Acute and Chronic		0.14
	Bean (0.178 lb a.i./A x 3)	N/A	Acute and Chronic		0.22
	Peanut (0.178 lb a.i./A x 4)	N/A	Acute and Chronic		0.29
DRINKING WATER SOURCE (MODEL USED)	**USE SCENARIO (rate modeled)**	**NATIONAL PERCENT CROPPED AREA (PCA)**	**ESTIMATED DRINKING WATER CONCENTRATION (EDWC) (ppb)**		
			Acute	Chronic	Lifetime
Surface water (PRZM/EXAMS)	ND Wheat (0.178 lb a.i./A x 2)	56%	9.9	5.4	4.3
	ND Canola (0.178 lb a.i./A x 2)	87%	10.	5.6	3.9
	MI Bean (0.178 lb a.i./A x 3)	87%	24	15	11
	NC Peanut (0.178 lb a.i./A x 4)	87%	31	**15**	**12**

Table 8b. Tier II Estimated Drinking Water Concentrations (EDWCs) for drinking water assessment based on aerial application of prothioconazole: including unextracted residues and using lower K_{OC}.

DRINKING WATER SOURCE (MODEL USED)	USE SCENARIO (rate modeled)	NATIONAL PERCENT CROPPED AREA (PCA)	ESTIMATED DRINKING WATER CONCENTRATION (EDWC) (ppb)		
Groundwater (SCIGROW)	Wheat and Canola (0.178 1b a.i./A x 2)	N/A	Acute and Chronic [redacted]		
	Bean (0.178 1b a.i./A x 3)	N/A	Acute and Chronic [redacted]		
	Peanut (0.178 1b a.i./A x 4)	N/A	Acute and Chronic [redacted]		
DRINKING WATER SOURCE (MODEL USED)	**USE SCENARIO (rate modeled)**	**NATIONAL PERCENT CROPPED AREA (PCA)**	**ESTIMATED DRINKING WATER CONCENTRATION (EDWC) (ppb)**		
			Acute	Chronic	Lifetime
Surface water (PRZM/EXAMS)	ND Wheat (0.178 1b a.i./A x 2)	56%	[redacted]	[redacted]	[redacted]
	ND Canola (0.178 1b a.i./A x 2)	87%	[redacted]	[redacted]	[redacted]
	MI Bean (0.178 1b a.i./A x 3)	87%	[redacted]	64	[redacted]
	NC Peanut (0.178 1b a.i./A x 4)	87%	[redacted]	62	[redacted]

Table 8c. Tier II Estimated Drinking Water Concentrations (EDWCs) for drinking water assessment based on aerial application of prothioconazole: not including unextracted residues and using higher K_{OC}.

DRINKING WATER SOURCE (MODEL USED)	**USE SCENARIO** **(rate modeled)**	**NATIONAL PERCENT CROPPED AREA (PCA)**	**ESTIMATED DRINKING WATER CONCENTRATION (EDWC) (ppb)**	
Groundwater (SCIGROW)	Wheat and Canola (0.178 lb a.i./A x 2)	N/A	Acute and Chronic	0.015
	Bean (0.178 lb a.i./A x 3)	N/A	Acute and Chronic	0.023
	Peanut (0.178 lb a.i./A x 4)	N/A	Acute and Chronic	0.030

DRINKING WATER SOURCE (MODEL USED)	**USE SCENARIO** **(rate modeled)**	**NATIONAL PERCENT CROPPED AREA (PCA)**	**ESTIMATED DRINKING WATER CONCENTRATION (EDWC) (ppb)**		
			Acute	Chronic	Lifetime
Surface water (PRZM/EXAMS)	ND Wheat (0.178 lb a.i./A x 2)	56%	7.1	4.4	3.5
	ND Canola (0.178 lb a.i./A x 2)	87%	8.6	4.6	3.6
	MI Bean (0.178 lb a.i./A x 3)	87%	20.	14	11
	NC Peanut (0.178 lb a.i./A x 4)	87%	27	16	12

Table 8d. Tier II Estimated Drinking Water Concentrations (EDWCs) for drinking water assessment based on aerial application of prothioconazole: including unextracted residues and using higher K_{OC}.

DRINKING WATER SOURCE (MODEL USED)	**USE SCENARIO (rate modeled)**	**NATIONAL PERCENT CROPPED AREA (PCA)**	**ESTIMATED DRINKING WATER CONCENTRATION (EDWC) (ppb)**		
Groundwater (SCIGROW)	Wheat and Canola (0.178 lb a.i./A x 2)	N/A	Acute and Chronic	0.022	
	Bean (0.178 lb a.i./A x 3)	N/A	Acute and Chronic	0.034	
	Peanut (0.178 lb a.i./A x 4)	N/A	Acute and Chronic	0.045	
DRINKING WATER SOURCE (MODEL USED)	**USE SCENARIO (rate modeled)**	**NATIONAL PERCENT CROPPED AREA (PCA)**	**ESTIMATED DRINKING WATER CONCENTRATION (EDWC) (ppb)**		
			Acute	Chronic	Lifetime
Surface water (PRZM/EXAMS)	ND Wheat (0.178 lb a.i./A x 2)	56%	24	21	15
	ND Canola (0.178 lb a.i./A x 2)	87%	23	21	14
	MI Bean (0.178 lb a.i./A x 3)	87%	69	[redacted]	45
	NC Peanut (0.178 lb a.i./A x 4)	87%	72	[redacted]	51

Table 8e. Tier II Estimated Drinking Water Concentrations (EDWCs) with Regional PCAs applied for drinking water assessment based on aerial application of prothioconazole: not including unextracted residues and using lower K_{OC}.

DRINKING WATER SOURCE (MODEL USED)	USE SCENARIO (rate modeled)	REGIONAL PERCENT CROPPED AREA (PCA)	ESTIMATED DRINKING WATER CONCENTRATION (EDWC) (ppb)		
			Acute	Chronic	Lifetime
Surface water (PRZM/EXAMS)	ND Canola (0.178 lb a.i./A x 2)	83% (basin 9)	9.9	5.3	3.8
	MI Bean (0.178 lb a.i./A x 3)	83% (basin 9)	23	14	11
		63% (basin 17)	17	11	8.2
	NC Peanut (0.178 lb a.i./A x 4)	67% (basin 12)	24	11	9.1
		38% (basin 3)	14	6.4	5.1

Table 8f. Tier II Estimated Drinking Water Concentrations (EDWCs) with Regional PCAs applied for drinking water assessment based on aerial application of prothioconazole: including unextracted residues and using lower K_{OC}.

DRINKING WATER SOURCE (MODEL USED)	USE SCENARIO (rate modeled)	REGIONAL PERCENT CROPPED AREA (PCA)	ESTIMATED DRINKING WATER CONCENTRATION (EDWC) (ppb)		
			Acute	Chronic	Lifetime
Surface water (PRZM/EXAMS)	ND Canola (0.178 lb a.i./A x 2)	83% (basin 9)	[redacted]	[redacted]	[redacted]
	MI Bean (0.178 lb a.i./A x 3)	83% (basin 9)	[redacted]	61	[redacted]
		63% (basin 17)	51	47	35
	NC Peanut (0.178 lb a.i./A x 4)	67% (basin 12)	[redacted]	48	[redacted]
		38% (basin 3)	32	27	23

Table 8g. Tier II Estimated Drinking Water Concentrations (EDWCs) with Regional PCAs applied for drinking water assessment based on aerial application of prothioconazole: not including unextracted residues and using higher K_{OC}.

DRINKING WATER SOURCE (MODEL USED)	USE SCENARIO (rate modeled)	REGIONAL PERCENT CROPPED AREA (PCA)	ESTIMATED DRINKING WATER CONCENTRATION (EDWC) (ppb)		
			Acute	Chronic	Lifetime
Surface water (PRZM/EXAMS)	ND Canola (0.178 lb a.i./A x 2)	83% (basin 9)	8.2	4.4	3.4
	MI Bean (0.178 lb a.i./A x 3)	83% (basin 9)	19	13	11
		63% (basin 17)	14	10	8.0
	NC Peanut (0.178 lb a.i./A x 4)	67% (basin 12)	21	12	9.3
		38% (basin 3)	12	6.8	5.3

Table 8h. Tier II Estimated Drinking Water Concentrations (EDWCs) with Regional PCAs applied for drinking water assessment based on aerial application of prothioconazole: including unextracted residues and using higher K_{OC}.

DRINKING WATER SOURCE (MODEL USED)	USE SCENARIO (rate modeled)	REGIONAL PERCENT CROPPED AREA (PCA)	ESTIMATED DRINKING WATER CONCENTRATION (EDWC) (ppb)		
			Acute	Chronic	Lifetime
Surface water (PRZM/EXAMS)	ND Canola (0.178 lb a.i./A x 2)	83% (basin 9)	22	20	14
	MI Bean (0.178 lb a.i./A x 3)	83% (basin 9)	66	[redacted]	43
		63% (basin 17)	50	47	32
	NC Peanut (0.178 lb a.i./A x 4)	67% (basin 12)	56	[redacted]	39
		38% (basin 3)	32	28	22

Table 8i. Tier II Estimated Drinking Water Concentrations (EDWCs) with National and Regional PCAs applied for drinking water assessment based on aerial application of prothioconazole to rice.

APPLICATION RATE (lbs. a.i./A)	Kd (mL/g)	ESTIMATED DRINKING WATER CONCENTRATION (EDWC) (ppb)		
		National PCA (0.87)	Higher Regional PCA (0.85)	Lower Regional PCA (0.41)
0.286 (0.143 x 2)	10.46 (from K_{OC} of 523)	45	44	21
	39.46 (from K_{OC} of 1973)	115	112	54

Higher estimate PCA associated mostly with lower Mississippi river encompassing Arkansas and parts of Louisiana and Mississippi.
Lower estimate PCA associated with rice grown in Southwest Louisiana, Texas, and California.

APPENDIX C: PRZM-EXAMS input filenames.

WDwA.pzr (ND Wheat, aerial application, including unextracted, low K_{OC})
WDwG.pzr (ND Wheat, ground application, including unextracted, low K_{OC})
WDwAnNR.pzr (ND Wheat, aerial application, not including unextracted, low K_{OC})
WDwAhK.pzr (ND Wheat, aerial application, including unextracted, high K_{OC})
WDwAnNRk.pzr (ND Wheat, aerial application, not including unextracted, high K_{OC})

CDwA.pzr (ND Canola, aerial application, including unextracted, low K_{OC})
CDwG.pzr (ND Canola, ground application, including unextracted, low K_{OC})
CDwAnNR.pzr (ND Canola, aerial application, not including unextracted, low K_{OC})
CDwAhK.pzr (ND Canola, aerial application, including unextracted, high K_{OC})
CDwAnNRk.pzr (ND Canola, aerial application, not including unextracted, high K_{OC})

BDwA.pzr (MI Bean, aerial application, including unextracted, low K_{OC})
BDwG.pzr (MI Bean, ground application, including unextracted, low K_{OC})
BDwAnNR.pzr (MI Bean, aerial application, not including unextracted, low K_{OC})
BDwAhK.pzr (MI Bean, aerial application, including unextracted, high K_{OC})
BDwAnNRk.pzr (MI Bean, aerial application, not including unextracted, high K_{OC})

PDwA.pzr (NC Peanut, aerial application, including unextracted, low K_{OC})
PDwG.pzr (NC Peanut, ground application, including unextracted, low K_{OC})
PDwAnNR.pzr (NC Peanut, aerial application, not including unextracted, low K_{OC})
PDwAhK.pzr (NC Peanut, aerial application, including unextracted, high K_{OC})
PDwAnNRk.pzr (NC Peanut, aerial application, not including unextracted, high K_{OC})

See file 113961 D324659 Prothioconazole DWA.zip for input files and output summary.

APPENDIX D: SCIGROW model output files.

```
                         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:Prothioconazole(**wheat/canola**, not including unextracted, low K_{OC})
time is 2/13/2006 12:23:15

Application rate (lb/acre)	Number of applications	Total Use (lb/acre/yr)	Koc (ml/g)	Soil Aerobic metabolism (days)
0.178	2.0	0.356	5.77E+02	288.8

groundwater screening cond (ppb) = **1.44E-01**
****

SciGrow version 2.3
chemical:Prothioconazole(**bean**, not including unextracted, low K_{OC})
time is 2/13/2006 12:23:42

Application rate (lb/acre)	Number of applications	Total Use (lb/acre/yr)	Koc (ml/g)	Soil Aerobic metabolism (days)
0.178	3.0	0.534	5.77E+02	288.8

groundwater screening cond (ppb) = **2.16E-01**
****

SciGrow version 2.3
chemical:Prothioconazole(**peanut**, not including unextracted, low K_{OC})
time is 2/13/2006 12:24:05

Application rate (lb/acre)	Number of applications	Total Use (lb/acre/yr)	Koc (ml/g)	Soil Aerobic metabolism (days)
0.178	4.0	0.712	5.77E+02	288.8

groundwater screening cond (ppb) = **2.89E-01**
****

SciGrow version 2.3
chemical:Prothioconazole(**wheat/canola**, including unextracted, low K_{OC})
time is 2/13/2006 12:32:02

Application rate (lb/acre)	Number of applications	Total Use (lb/acre/yr)	Koc (ml/g)	Soil Aerobic metabolism (days)
0.178	2.0	0.356	5.77E+02	866.4

groundwater screening cond (ppb) = **3.33E-01**
****

SciGrow version 2.3
chemical:Prothioconazole(**bean**, including unextracted, low K_{OC})
time is 2/13/2006 12:32:32

Application rate (lb/acre)	Number of applications	Total Use (lb/acre/yr)	Koc (ml/g)	Soil Aerobic metabolism (days)
0.178	3.0	0.534	5.77E+02	866.4

groundwater screening cond (ppb) = **5.00E-01**

****

SciGrow version 2.3
chemical:Prothioconazole(**peanut**, including unextracted, low K_{OC})
time is 2/13/2006 12:32:57

Application rate (lb/acre)	Number of applications	Total Use (lb/acre/yr)	Koc (ml/g)	Soil Aerobic metabolism (days)
0.178	4.0	0.712	5.77E+02	866.4

groundwater screening cond (ppb) = **6.66E-01**

****

SciGrow version 2.3
chemical:Prothioconazole(**wheat/canola**, not including unextracted, high K_{OC})
time is 4/13/2006 11:31:57

Application rate (lb/acre)	Number of applications	Total Use (lb/acre/yr)	Koc (ml/g)	Soil Aerobic metabolism (days)
0.178	2.0	0.356	2.63E+03	288.8

groundwater screening cond (ppb) = **1.51E-02**

****

SciGrow version 2.3
chemical:Prothioconazole(**bean**, not including unextracted, high K_{OC})
time is 4/13/2006 11:31:45

Application rate (lb/acre)	Number of applications	Total Use (lb/acre/yr)	Koc (ml/g)	Soil Aerobic metabolism (days)
0.178	3.0	0.534	2.63E+03	288.8

groundwater screening cond (ppb) = **2.26E-02**

****

SciGrow version 2.3
chemical:Prothioconazole(**peanut**, *not including unextracted, high* K_{OC})
time is 4/13/2006 11:31:20

Application rate (lb/acre)	Number of applications	Total Use (lb/acre/yr)	Koc (ml/g)	Soil Aerobic metabolism (days)
0.178	4.0	0.712	2.63E+03	288.8

groundwater screening cond (ppb) = **3.01E-02**

****

SciGrow version 2.3
chemical:Prothioconazole(**wheat/canola**, including unextracted, high K_{OC})
time is 4/13/2006 11: 0:58

Application rate (lb/acre)	Number of applications	Total Use (lb/acre/yr)	Koc (ml/g)	Soil Aerobic metabolism (days)
0.178	2.0	0.356	2.63E+03	866.4

groundwater screening cond (ppb) = **2.23E-02**

****

SciGrow version 2.3
chemical:Prothioconazole(**bean**, including unextracted, high K_{OC})
time is 4/13/2006 11: 0:45

Application rate (lb/acre)	Number of applications	Total Use (lb/acre/yr)	Koc (ml/g)	Soil Aerobic metabolism (days)
0.178	3.0	0.534	2.63E+03	866.4

groundwater screening cond (ppb) = **3.35E-02**

****

SciGrow version 2.3
chemical:Prothioconazole(**peanut**, including unextracted, high K_{OC})
time is 4/13/2006 11: 0:13

Application rate (lb/acre)	Number of applications	Total Use (lb/acre/yr)	Koc (ml/g)	Soil Aerobic metabolism (days)
0.178	4.0	0.712	2.63E+03	866.4

groundwater screening cond (ppb) = **4.46E-02**

****