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OFFICE OF
PREVENTION, PESTICIDES AND
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MEMORANDUM

SUBJECT: Drinking Water Assessment for the Section 3 New Use Petitions for the Use of Prothioconazole on Soybeans and Sugar Beets

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1. EXECUTIVE SUMMARY

The Environmental Fate and Effects Division (EFED) has completed a drinking water assessment for the Section 3 new use petitions for the use of prothioconazole on soybeans and sugar beets. Prothioconazole is used as a pre- or post-infection fungicide on barley, canola, chickpeas, dried shell peas and beans, lentils, oilseed crop, peanut, and numerous varieties of wheat. The previously completed drinking water assessment (DWA) for these registered uses can be found in the June 21, 2006 memo, "Prothioconazole Tier II Estimated Drinking Water

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Concentrations (EDWCs) for Use in the Human Health Risk Assessment. [Second revision]" (DP Barcode D330265).

This memo provides estimated drinking water concentrations (EDWCs) for the Health Effects Division to use in their dietary risk assessment for the use of prothioconazole on soybeans and sugar beets. In HED's previous Dietary Risk Assessment, surface water EDWCs for beans were used for both the acute and chronic risk analyses. However, the ranges of regional PCAs applied in previous drinking water assessment have been re-evaluated based on the most current Agricultural Census which provides national-scale information on where crops are grown. The ranges have been revised and consequently the highest acute exposure results from modeled application to peanuts and the highest chronic and cancer exposure results from modeled applications to sugar beets. These values are recommended for use in HED's risk assessment and are listed in **Table 1**. The full distributions of these estimates (30 years of daily values) were previously provided to HED (June 21, 2006). More complete information on the determination of the previous EDWCs can be found in the June 21, 2006 memo (DP Barcode D324659).

Table 1. Upper-bound estimated drinking water concentrations for prothioconazole (including unextracted residues and using lower K_{oc}). Values in bold are recommended for HED's risk assessment.

DRINKING WATER SOURCE (MODEL USED)	USE SCENARIO (rate modeled)	Regional PCA range	ESTIMATED DRINKING WATER CONCENTRATION (EDWC) (ppb)	
Groundwater (SCIGROW)	Peanut (0.178 lb a.i./A x 4)	N/A	Acute and Chronic	**0.67**
Surface water (PRZM/EXAMS)	NC Peanut (0.178 lb a.i./A x 4)	38% - 87%	Acute (1-in-10-year)	13 - **29**
			Chronic(1-in-10-year)	4.4 - 10
			30-year Daily Average	3.6 – 8.3
	MN Sugar beets (0.178 lb a.i./A x 3)	56-87%	Acute (1-in-10-year)	13 - 20
			Chronic(1-in-10-year)	8.4 - **13**
			30-year Daily Average	6.4 - **10**

2. USE CHARACTERIZATION

Prothioconazole is used as a pre- or post-infection fungicide on barley, canola, chickpea, dried shell peas and beans, lentils, oilseed crop, peanut, and numerous varieties of wheat. Application rates for the proposed new uses are presented below in **Table 2,** and application rates for the previously registered uses assessed in the June 2006 DWA are presented in **Table 3**.

Table 2. Summary use information for the proposed new uses of prothioconazole.

Crop Type	Maximum Rate per Application (lbs a.i./A) and Max. Number of Applications	Maximum Seasonal Application Rate (lbs a.i./A/season)	Application Interval (days)	Pre-Harvest Interval (days)
Soybeans	0.09375 (3)	0.2813	10-21	21
Sugar beets	0.1781 (3)	0.5343	14-30	7

Table 3. Summary use information for previously assessed prothioconazole uses, based on PROLINE® 480SC Fungicide label.

Crop Type	Max. Application Rate (lbs. a.i./A)	Max. No. of Applic.	Max. Seasonal Applic. Rate (lbs. a.i./A)	Applic. Interval (days)	Application Method(s)
Peanut	0.1781	4	0.7124	14	Aerial and ground spray
Chickpea	0.1781	3	0.5343	10 to 14	Aerial and ground spray
Dried shell pea & bean	0.1781	3	0.5343	5 to 14	Aerial and ground spray
Lentil	0.1781	3	0.5343	10 to 14	Aerial and ground spray
Barley	0.1781	2	0.2928	7 to 14	Aerial and ground spray
Canola	0.1781	2	0.3563	5 to 7	Aerial and ground spray
Oilseed crop subgroup	0.1781	2	0.3563	5 to 7	Aerial and ground spray
Wheat	0.1781	2	0.2928	7 to 14	Aerial and ground spray

3. ENVIRONMENTAL FATE AND TRANSPORT CHARACTERIZATION

Prothioconazole is stable to hydrolysis and degrades by aqueous photolysis ($t_{1/2}$ = 9 d) to prothioconazole-desthio which appears to resist further photolytic degradation (combined $t_{1/2}$ = 101 d). Prothioconazole and its degradates are not expected to volatilize (vapor pressure < 4 x10^{-7} Pa). Based on available data, prothioconazole together with its major degradates appear to be persistent to microbial degradation in soil ($t_{1/2}$ = 462 – 1386 d) and water ($t_{1/2}$ = 67 – 433 d). Prothioconazole degrades relatively quickly to two major persistent degradates which are of similar toxicity to that of the parent, prothioconazole-desthio and prothioconazole-S-methyl. 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 (K_{oc} = 523 – 625 ml/g_{oc}). The other major degradate formed in smaller amounts (prothioconazole-S-methyl) is slightly mobile (K_{oc} = 1973 – 2993 ml/g_{oc}). Because these two

major degradates are considered to be of similar toxicity to the parent, they are included in the drinking water exposure estimates. Also, ineffective extraction methods in soil and aquatic metabolism studies resulted in large amounts of unextracted material, leading to uncertainties in the composition and bioavailability of such and precluding accurate determinations of the biotic degradation rate for parent prothioconazole. Therefore, a total toxic residues method, including unextracted material, was utilized for environmental exposure modeling. This adds considerable uncertainty to the assessment regarding the bioavailability and the biotic degradation rates for prothioconazole residues. If additional data regarding the persistence of the degradates and the nature of the unextracted residues become available, the exposure estimates may be refined. Additional details regarding the environmental fate and transport of prothioconazole and its degradates can be found in the June 21, 2006 Drinking Water Assessment (DP 324659). **Table 4** provides a detailed summary table of physical/chemical and environmental fate/transport properties of prothioconazole combined residues of concern. **Tables 5** summarize the major degradation products formed by each degradation process in the studies reviewed.

Table 4. 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	
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.

PARAMETER	VALUE(S) (units)	SOURCE MRID	COMMENT
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	
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;
Soil Photolysis Half-life	Prothioconazole and Prothiconazole-desthio: stable (Prothioconazole-S-methyl is not formed from prothioconaozle soil photolysis.)	46246510	Half-life could not be calculated as parent degraded faster in dark samples than in irradiated samples.
Aerobic Soil Metabolism Half-life	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).	46246511 46246512	Half-lives are calculated combining amounts of prothioconazole, prothioconazole-desthio, and prothioconazole-S-methyl per sampling interval. Non-extractable residues included.
Anaerobic Aquatic Metabolism Half-life	Prothioconazole combined residues of concern: $t_{1/2}$ = stable (total system); 56.8 days (water layer).	46246516	Half-lives are combining amounts of prothioconazole, prothioconazole-desthio, and prothioconazole-S-methyl per sampling interval. Non-extractable residues included.
Aerobic Aquatic Metabolism Half-life	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).	46246515	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 combining amounts of prothioconazole, prothioconazole-desthio, and prothioconazole-S-methyl per sampling interval. Non-extractable residues included.

Organic Carbon Partition Coefficient (K_{OC})	(mL/g_{OC})	LS	SCL	SL	S		
	Prothioconzole	--	--	--	--	46246539 46246504	Parent mobility cannot be determined due to instability

PARAMETER	VALUE(S) (units)					SOURCE MRID	COMMENT
	Prothioconzole -desthio	523	536	617	625	46246450	Conducted on prothioconazole-desthio 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.
	Prothioconzole -S-methyl	1973	2484	2772	2995	46246501	Conducted on prothioconazole-S-methyl Used same soils as MRID: 46246450.
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.

PARAMETER	VALUE(S) (units)	SOURCE MRID	COMMENT
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 5. 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 6th (CA, NY) or 2nd (GA) application. (DAT= days after 6th or 2nd 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.

4. DRINKING WATER MODELING

The original estimated drinking water concentrations (EDWC) for prothioconazole in surface water and groundwater were calculated using the Tier II model PRZM-EXAMS (Pesticide Root Zone Model (PRZM, v3.12 beta dated May 24, 2001) and Exposure Analysis Modeling System (EXAMS, v2.98.04 dated July 18, 2002) and the regression model SCI-GROW (Screening Concentration in Ground Water, v.2.3; dated 7/29/2003), respectively. The surface water modeling for the proposed new uses was conducted with updated versions of PRZM (3.12.2 dated May 12, 2005) and EXAMS (2.98.04.06 dated April 25, 2005). The upper and lower bound acute and chronic groundwater and surface water EDWCs determined for the previously registered uses are presented in **Tables 6a** and **6b** and the upper bound (only) EDWCs for the proposed new uses are in **Table 6c**. The model inputs are presented in **Tables 7** and **8**.

The concentrations provided in this assessment (**Tables 6a-6c**) represent upper and lower bounds on estimates in drinking water for aerial applications of prothioconazole based on uncertainties in the metabolism degradation and binding coefficients. The full distributions of these estimates (30 years of daily values) were previously provided to HED (June 21, 2006). 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 beans (acute) and sugar beets (chronic and cancer).

Because of the uncertainties associated with high levels of unextracted residues, modeling was conducted using bounding assumptions based on inclusion and exclusion of unextracted residues in half-life calculations. Also, because the two major degradates of prothioconazole that are formed rapidly after application have different mobilities, modeling was conducted using K_{oc}s for prothioconazole-desthio and prothioconazole-S-methyl. Generally, upper and lower EDWCs differed by a factor of 1.3-2.6x as a result of these bounding assumptions. Inclusion or exclusion of unextracted residues made a larger difference in concentrations than use of a high or low K_{oc}.

To further refine EDWCs for canola, beans, peanuts, and sugar beets a range of regional default Percentage Cropped Area (PCA) factors have been applied to estimated concentrations. Note that the ranges of regional PCAs have been reassessed since the previous drinking water assessment and the numbers are therefore slightly different than what was previously reported (DP 324659). Because wheat and soybeans have crop-specific PCAs, the EDWCs for these uses are not further refined.

Table 6a. 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)	11	N/A
			Chronic (1-in-10-year)	6.0	N/A
			30-year Daily Average	4.8	N/A
	ND Canola (0.178 lb a.i./A x 2)	87% (13% - 87%)	Acute (1-in-10-year)	14	2.1 – 14
			Chronic (1-in-10-year)	9.1	1.4 – 9.1
			30-year Daily Average	6.7	1.0 – 6.7
	MI Beans (0.178 lb a.i./A x 3)	87% (13% - 87%)	Acute (1-in-10-year)	23	3.4 - 23
			Chronic(1-in-10-year)	12	1.8 - 12
			30-year Daily Average	9.5	1.4 – 9.5
	NC Peanut (0.178 lb a.i./A x 4)	87% (38% - 87%)	Acute (1-in-10-year)	29	13 - 29
			Chronic (1-in-10-year)	10	4.4 - 10
			30-year Daily Average	8.3	3.6 – 8.3

Table 6b. 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)	5.4	N/A
			Chronic (1-in-10-year)	2.6	N/A
			30-year Daily Average	2.0	N/A
	ND Canola (0.178 lb a.i./A x 2)	87% (13% - 87%)	Acute (1-in-10-year)	7.5	1.1 – 7.5
			Chronic (1-in-10-year)	3.5	0.5 – 3.5
			30-year Daily Average	2.6	0.4 – 2.6
	MI Beans (0.178 lb a.i./A x 3)	87% (13% - 87%)	Acute (1-in-10-year)	14	2.1 – 14
			Chronic(1-in-10-year)	6.7	1.0 – 6.7
			30-year Daily Average	5.2	0.8 – 5.2
	NC Peanut (0.178 lb a.i./A x 4)	87% (38% - 87%)	Acute (1-in-10-year)	21	9.2 – 21
			Chronic (1-in-10-year)	6.2	2.7 – 6.2
			30-year Daily Average	4.8	2.1- 4.8

Table 6c. Upper-bound Tier II Estimated Drinking Water Concentrations for prothioconazole (including unextracted residues and using lower K_{oc}) proposed new uses.

DRINKING WATER SOURCE (MODEL USED)	USE SCENARIO (rate modeled)	National PCA (Regional PCA range)	ESTIMATED DRINKING WATER CONCENTRATION (EDWC) (ppb)		
Groundwater (SCIGROW)	Sugar beets (0.178 1b a.i./A x 3)	N/A	Acute and Chronic	0.50	
	Soybeans (0.09375 1b a.i./A x 3)	N/A	Acute and Chronic	0.26	
Surface water (PRZM/EXAMS)	MN Sugar beets (0.178 1b a.i./A x 3)	87% (56-87%)		National PCA	Regional PCA
			Acute (1-in-10-year)	20	13 - 20
			Chronic (1-in-10-year)	13	8.4 - 13
			30-year Daily Average	10	6.4 - 10
	MS Soybeans (0.09375 1b a.i./A x 3)	56% (soybean-wheat specific PCA)	Acute (1-in-10-year)	5.7	NA
			Chronic (1-in-10-year)	1.4	NA
			30-year Daily Average	0.89	NA

Table 7. Input values used for prothioconazole Tier I groundwater modeling with SCI-GROW2.

Model Input Parameter	Input Value and Unit	Source	Comments
Aerobic Soil Metabolism Half-life	866.4 (including unextracted) 288.8 (not including unextracted)	MRIDs 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.
Organic - Carbon Normalized Partition Coefficient K_{oc}	576.6 mL/g 2628 mL/g	MRID 46246450 MRID 46246451	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 523.0 to 625.3 mL/g for prothioconazole-S-methyl.
Application Rate	0.1781 lb a.i./A/application 0.09375 lb a.i./A/application	Label	Represents the maximum possible single application rate per crop season (year).
Maximum No. of Applic./Year	4, 3, 2	Label	Represents the maximum possible applications per crop season (year) for peanuts, beans, and wheat and canola, respectively.

Table 8. Input values used for prothioconazole Tier II surface water modeling with PRZM/EXAMS.

Parameter (units)	Value (s)	Source	Comments
Application Rate (kg a.i./ha)	0.2 0.105 (soybeans)	Proposed label.	Represents the maximum possible single application rate per crop season (year) for all uses.
Number of Applications	Wheat: 2 Canola: 2 Beans: 3 Peanuts: 4 Sugar beets: 3 Soybeans: 3	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 Sugar beets: 14 Soybeans: 10	Proposed label.	Represents the minimum possible interval between applications per crop season (year) for each use.
Molecular weight (g/mol)	344.3	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 ^{o}C, pH 8 (mg/L or ppm)	300	MRID: 46246003.	–
Soil Partition Coefficient (K_{OC} (mL/g_{OC}))	523.0 1973.0	MRID: 46246450. MRID: 46246451.	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 523.0 to 625.3 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)	Aerial spray: 0.95	Input Guidance.	–
Spray drift fraction (decimal)	Aerial spray: 0.16	Input Guidance.	–

Parameter (units)	Value (s)	Source	Comments
Percent Cropped Area (decimal)	Wheat: 0.56 Canola: 0.87 Beans: 0.87 Peanuts: 0.87 Sugar beets: 0.87 Soybeans: 0.56	Proposed label.	National-scale wheat and default values.
Application date (day/month)	Wheat: 18/June Canola:17/June Beans: 29/June Peanuts: 9/July Sugar beets: 24/August Soybeans: 15/May	Proposed label and PRZM scenarios.	–
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.
Aerobic Aquatic Metabolism Half-life (days)	385.2 (include unextracted) 78.0 (not include 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) calculated using prothioconazole total toxic residues.
Anaerobic Aquatic Metabolism Half-life (days)	0 (include unextracted) 4158 (not include unextracted)	MRID: 46246516.	Represents one total system half-life value (stable) or three times one total system half-life value (1386.3) calculated using prothioconazole total toxic residues.
Aerobic Soil Metabolism Half-life (days)	1052.2 (including unextracted) 360.3 (not including unextracted)	MRIDs: 46246511, 46246512.	Represents the 90th percentile confidence bound on the mean of six values for the aerobic soil metabolism of prothioconazole total toxic residues.

Appendix A. Modeling Input and Output

stored as MNsugarbeets.out
Chemical: prothioconazole
PRZM environment: MNsugarbeetSTD.txt modified Tueday, 29 May 2007 at 12:57:22
EXAMS environment: ir298.exv modified Thuday, 29 August 2002 at 16:34:12
Metfile: w14914.dvf modified Wedday, 3 July 2002 at 10:05:52
Water segment concentrations (ppb)

Year	Peak	96 hr	21 Day	60 Day	90 Day	Yearly
1961	5.178	5.1	4.825	4.535	4.31	1.345
1962	7.911	7.831	7.538	7.127	6.852	4.969
1963	9.076	8.989	8.649	8.215	7.952	6.405
1964	12.14	12.06	11.67	11.25	10.98	8.941
1965	16.91	16.74	16.06	15.04	14.36	11.97
1966	12.37	12.32	12.08	11.74	11.47	10.83
1967	12.18	12.09	11.8	11.25	10.82	9.754
1968	11.98	11.88	11.63	11.09	10.7	9.709
1969	15.54	15.43	14.85	13.78	13.62	11.87
1970	21.45	21.22	20.37	18.9	18.03	13.44
1971	20.95	20.76	20.31	19.55	18.74	14.47
1972	17.11	17.02	16.64	15.88	15.66	14.06
1973	19.44	19.23	18.61	17.44	16.61	11.98
1974	18.08	17.94	17.45	16.43	15.78	13.96
1975	16.03	15.94	15.4	15.08	14.9	14
1976	13.16	13.11	12.88	12.48	12.44	10.66
1977	22.64	22.36	21.31	20.87	20.49	16.24
1978	19.07	18.98	18.58	17.77	17.3	15.84
1979	20.6	20.43	19.79	18.59	17.36	15.38
1980	17.88	17.72	17.26	16.59	16	14.29
1981	13.57	13.51	13.27	12.77	12.42	11.76
1982	25.07	24.78	23.64	21.64	20.19	12.48
1983	17.7	17.59	17.16	16.31	15.99	13.82
1984	22.51	22.26	21.37	19.8	18.21	12.59
1985	16.7	16.6	16.2	15.43	15.04	13.96
1986	15.99	15.87	15.49	14.84	14.52	13.08
1987	12.23	12.18	11.97	11.53	11.25	10.19
1988	13.48	13.34	12.81	11.93	11.37	8.941
1989	14.71	14.58	14.1	13.61	13.12	10.79
1990	11.3	11.21	10.86	10.7	10.48	9.765

Sorted results

Prob.	Peak	96 hr	21 Day	60 Day	90 Day	Yearly		
0.032258064516129			25.07	24.78	23.64	21.64	20.49	16.24
0.0645161290322581			22.64	22.36	21.37	20.87	20.19	15.84
0.0967741935483871			22.51	22.26	21.31	19.8	18.74	15.38
0.129032258064516			21.45	21.22	20.37	19.55	18.21	14.47
0.161290322580645			20.95	20.76	20.31	18.9	18.03	14.29
0.193548387096774			20.6	20.43	19.79	18.59	17.36	14.06
0.225806451612903			19.44	19.23	18.61	17.77	17.3	14
0.258064516129032			19.07	18.98	18.58	17.44	16.61	13.96
0.290322580645161			18.08	17.94	17.45	16.59	16	13.96
0.32258064516129		17.88	17.72	17.26	16.43	15.99	13.82	
0.354838709677419			17.7	17.59	17.16	16.31	15.78	13.44
0.387096774193548			17.11	17.02	16.64	15.88	15.66	13.08
0.419354838709677			16.91	16.74	16.2	15.43	15.04	12.59
0.451612903225806			16.7	16.6	16.06	15.08	14.9	12.48
0.483870967741936			16.03	15.94	15.49	15.04	14.52	11.98
0.516129032258065			15.99	15.87	15.4	14.84	14.36	11.97
0.548387096774194			15.54	15.43	14.85	13.78	13.62	11.87
0.580645161290323			14.71	14.58	14.1	13.61	13.12	11.76

0.612903225806452		13.57	13.51	13.27	12.77	12.44	10.83
0.645161290322581		13.48	13.34	12.88	12.48	12.42	10.79
0.67741935483871	13.16	13.11	12.81	11.93	11.47	10.66	
0.709677419354839		12.37	12.32	12.08	11.74	11.37	10.19
0.741935483870968		12.23	12.18	11.97	11.53	11.25	9.765
0.774193548387097		12.18	12.09	11.8	11.25	10.98	9.754
0.806451612903226		12.14	12.06	11.67	11.25	10.82	9.709
0.838709677419355		11.98	11.88	11.63	11.09	10.7	8.941
0.870967741935484		11.3	11.21	10.86	10.7	10.48	8.941
0.903225806451613		9.076	8.989	8.649	8.215	7.952	6.405
0.935483870967742		7.911	7.831	7.538	7.127	6.852	4.969
0.967741935483871		5.178	5.1	4.825	4.535	4.31	1.345

0.1	22.404	22.156	21.216	19.775	18.687	15.289

Average of yearly averages: 11.5829666666667

Inputs generated by pe5.pl - Novemeber 2006

Data used for this run:
Output File: MNsugarbeets
Metfile: w14914.dvf
PRZM scenario: MNsugarbeetSTD.txt
EXAMS environment file: ir298.exv
Chemical Name: prothioconazole

Description	Variable Name	Value	Units	Comments
Molecular weight	mwt	344.3	g/mol	
Henry's Law Const.	henry	2.96e-10	atm-m^3/mol	
Vapor Pressure	vapr	3e-9	torr	
Solubility	sol	300	mg/L	
Kd	Kd		mg/L	
Koc	Koc	523	mg/L	
Photolysis half-life	kdp	101.9	days	Half-life
Aerobic Aquatic Metabolism	kbacw	385.2	days	Halfife
Anaerobic Aquatic Metabolism	kbacs	0	days	Halfife
Aerobic Soil Metabolism	asm	1052.2	days	Halfife
Hydrolysis:	pH 7	0	days	Half-life
Method: CAM	2	integer	See PRZM manual	
Incorporation Depth:		DEPI	cm	
Application Rate:	TAPP	0.2	kg/ha	
Application Efficiency:		APPEFF	0.95	fraction
Spray Drift	DRFT	0.16	fraction of application rate applied to pond	
Application Date	Date	24/8	dd/mm or dd/mmm or dd-mm or dd-mmm	
Interval 1 interval	14	days	Set to 0 or delete line for single app.	
app. rate 1	apprate		kg/ha	
Interval 2 interval	14	days	Set to 0 or delete line for single app.	
app. rate 2	apprate		kg/ha	
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)

stored as MSSoybeans.out
Chemical: prothioconazole
PRZM environment: MSsoybeanSTD.txt modified Tueday, 29 May 2007 at 12:58:06
EXAMS environment: ir298.exv modified Thuday, 29 August 2002 at 16:34:12
Metfile: w03940.dvf modified Wedday, 3 July 2002 at 10:05:46
Water segment concentrations (ppb)

Year	Peak	96 hr	21 Day	60 Day	90 Day	Yearly
1961	5.565	5.362	4.644	3.87	3.267	1.205
1962	2	1.932	1.747	1.433	1.385	0.8182
1963	8.812	8.492	7.321	5.461	4.712	1.922
1964	3.15	3.065	2.745	2.416	2.305	1.283
1965	3.011	2.909	2.538	1.963	1.662	0.9639
1966	5.199	5.02	4.712	3.848	3.531	1.765
1967	5.071	4.902	4.586	4.249	3.875	1.791
1968	3.779	3.65	3.418	2.699	2.349	1.21
1969	2.552	2.468	2.157	1.81	1.694	0.9859
1970	2.241	2.164	1.889	1.517	1.397	0.9188
1971	2.69	2.601	2.365	2.016	1.988	1.001
1972	1.943	1.877	1.677	1.435	1.372	0.7693
1973	2.111	2.037	1.78	1.464	1.26	0.7102
1974	7.133	6.876	5.935	4.429	3.823	1.618
1975	4.891	4.765	4.223	3.761	3.473	1.616
1976	5.919	5.719	5.095	4.73	4.325	1.895
1977	3.94	3.81	3.396	3.052	2.96	1.507
1978	3.307	3.195	2.874	2.477	2.357	1.294
1979	12.55	12.16	10.79	9.062	8.42	3.384
1980	4.119	3.988	3.795	3.539	3.234	1.758
1981	10.19	9.957	8.642	6.514	5.899	2.585
1982	10.64	10.26	8.927	7.647	6.59	2.729
1983	6.127	5.923	5.611	4.573	3.99	1.968
1984	3.334	3.26	2.867	2.717	2.534	1.341
1985	3.512	3.394	2.963	2.4	2.254	1.202
1986	9.087	8.762	7.923	6.409	5.545	2.205
1987	9.974	9.615	8.543	6.504	5.496	2.266
1988	2.916	2.829	2.531	2.262	2.187	1.417
1989	10	9.648	8.766	6.941	5.955	2.511
1990	3.154	3.048	2.719	2.309	1.995	1.169

Sorted results

Prob.	Peak	96 hr	21 Day	60 Day	90 Day	Yearly	
0.032258064516129		12.55	12.16	10.79	9.062	8.42	3.384
0.0645161290322581		10.64	10.26	8.927	7.647	6.59	2.729
0.0967741935483871		10.19	9.957	8.766	6.941	5.955	2.585
0.129032258064516		10	9.648	8.642	6.514	5.899	2.511
0.161290322580645		9.974	9.615	8.543	6.504	5.545	2.266
0.193548387096774		9.087	8.762	7.923	6.409	5.496	2.205
0.225806451612903		8.812	8.492	7.321	5.461	4.712	1.968
0.258064516129032		7.133	6.876	5.935	4.73	4.325	1.922
0.290322580645161		6.127	5.923	5.611	4.573	3.99	1.895
0.32258064516129	5.919	5.719	5.095	4.429	3.875	1.791	
0.354838709677419		5.565	5.362	4.712	4.249	3.823	1.765
0.387096774193548		5.199	5.02	4.644	3.87	3.531	1.758
0.419354838709677		5.071	4.902	4.586	3.848	3.473	1.618
0.451612903225806		4.891	4.765	4.223	3.761	3.267	1.616
0.483870967741936		4.119	3.988	3.795	3.539	3.234	1.507
0.516129032258065		3.94	3.81	3.418	3.052	2.96	1.417
0.548387096774194		3.779	3.65	3.396	2.717	2.534	1.341
0.580645161290323		3.512	3.394	2.963	2.699	2.357	1.294
0.612903225806452		3.334	3.26	2.874	2.477	2.349	1.283
0.645161290322581		3.307	3.195	2.867	2.416	2.305	1.21
0.67741935483871	3.154	3.065	2.745	2.4	2.254	1.205	

0.709677419354839		3.15	3.048	2.719	2.309	2.187	1.202
0.741935483870968		3.011	2.909	2.538	2.262	1.995	1.169
0.774193548387097		2.916	2.829	2.531	2.016	1.988	1.001
0.806451612903226		2.69	2.601	2.365	1.963	1.694	0.9859
0.838709677419355		2.552	2.468	2.157	1.81	1.662	0.9639
0.870967741935484		2.241	2.164	1.889	1.517	1.397	0.9188
0.903225806451613		2.111	2.037	1.78	1.464	1.385	0.8182
0.935483870967742		2	1.932	1.747	1.435	1.372	0.7693
0.967741935483871		1.943	1.877	1.677	1.433	1.26	0.7102

0.1	10.171	9.9261	8.7536	6.8983	5.9494	2.5776

Average of yearly averages: 1.59361

Inputs generated by pe5.pl - Novemeber 2006

Data used for this run:
Output File: MSSoybeans
Metfile: w03940.dvf
PRZM scenario: MSsoybeanSTD.txt
EXAMS environment file: ir298.exv
Chemical Name: prothioconazole

Description	Variable Name	Value	Units	Comments
Molecular weight	mwt	344.3	g/mol	
Henry's Law Const.	henry	2.96e-10	atm-m^3/mol	
Vapor Pressure	vapr	3e-9	torr	
Solubility	sol	300	mg/L	
Kd	Kd		mg/L	
Koc	Koc	523	mg/L	
Photolysis half-life	kdp	101.9	days	Half-life
Aerobic Aquatic Metabolism	kbacw	385.2	days	Halfife
Anaerobic Aquatic Metabolism	kbacs	0	days	Halfife
Aerobic Soil Metabolism	asm	1052.2	days	Halfife
Hydrolysis:	pH 7	0	days	Half-life
Method: CAM	2	integer	See PRZM manual	
Incorporation Depth:		DEPI	cm	
Application Rate:	TAPP	0.105	kg/ha	
Application Efficiency:		APPEFF	0.95	fraction
Spray Drift	DRFT	0.16	fraction of application rate applied to pond	
Application Date	Date	15-5	dd/mm or dd/mmm or dd-mm or dd-mmm	
Interval 1 interval	10	days	Set to 0 or delete line for single app.	
app. rate 1	apprate		kg/ha	
Interval 2 interval	10	days	Set to 0 or delete line for single app.	
app. rate 2	apprate		kg/ha	
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)