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

OFFICE OF CHEMICAL SAFETY
AND POLLUTION PREVENTION

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MEMORANDUM

SUBJECT: **Propoxycarbazone-sodium:** Drinking Water Exposure Assessment for Registration Review

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ERB2/EFED (7507P)

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This assessment provides estimated drinking water concentrations (EDWC) of propoxycarbazone in surface water and in ground water in support of human health risk assessment for registration review. Screening EDWCs (**Table 1**) of propoxycarbazone were generated with the Surface Water Concentration Calculator (SWCC) and with the Pesticide Root Zone Model for Ground Water (PRZM-GW). Modeled application rates represent the maximum use patterns of proposed end-use labels and current registered labels. Remaining model input parameters were chosen according to current guidance (USEPA, 2009)[1]. EDWCs reflect exposure to propoxycarbazone residues of concern in drinking water, which include the parent compound and propoxycarbazone-carboxylic acid. If the screening EDWCs listed in this memo result in dietary risk exceedances, contact James Lin (703-308-9591) of Environmental Risk Branch II (7507P) to request a refined drinking water exposure assessment.

[1] USEPA. 2009. Guidance for Selecting Input Parameters in Modeling the Environmental Fate and Transport of Pesticides. Version 2.1. U.S. Environmental Protection Agency, Office of Pesticide Programs, Environmental Fate and Effects Division, Oct. 22, 2009. http://www.epa.gov/oppefed1/models/water/input_parameter_guidance.htm

Table 1. Maximum Screening Drinking Water Exposure Estimates for Propoxycarbazone Residues of Concern*

Source (Model)	Use (Maximum Rate)	Peak Exposure (µg/L)	Annual Mean Exposure (µg/L)
Surface water (SWCC)	2 @ 0.02625 lb a.i./acre	**4.16**	1.07
Ground water (PRZM-GW)	1 @ 0.0525 lb a.i./acre	3.47	**2.8**

*Maximum values in bold.

The Environmental Fate and Effects Division (EFED) has produced two drinking water assessments for propoxycarbazone:

1. DP 284671 – Tier 1 Drinking Water Assessment for Propoxycarbazone-sodium (Olympus™) (November 2003)

2. DP 348511 - Drinking Water Assessment and Ecological Risk Summary for Tier 1 Drinking Water Assessment for Propoxycarbazone-sodium (Olympus™) use on Rangeland (August 2008)

Due to recent updated modeling approaches, EFED is required to use new tools: the Surface Water Concentration Calculator (SWCC)[2] for surface water and the Pesticide Root Zone Model for Ground Water (PRZM-GW)[3] for ground water.

USE INFORMATION

Propoxycarbazone-sodium (which dissociates in the presence of moisture to form propoxycarbazone) is a sulfonyl-amino-carbonyl-triazolinone herbicide (a type of ALS inhibitor similar to the sulfonylureas) used for the selective post-emergence control of grasses and broad-leaved plants in wheat, triticale, rangeland, pastures, and agricultural fallow/conservation reserve. The only commercial available formulation is water dispersible granules (dry flowable). It can be applied by either aerial or ground spray equipment. **Table 2** lists the maximum use patterns for the labeled use sites. The table is a summary of the "EFED Table 1 Report", which is a part of the Biological and Economic Analysis Division's (BEAD) Label Use Report Package for registration review (August 2014).

[2] USEPA, 2014. Implementation of the Surface Water Concentration Calculator for use in the Environmental Fate and Effects Division (EFED)

[3] USEPA. 2012. Guidance for Using PRZM-GW in Drinking Water Exposure Assessments. U.S. Environmental Protection Agency, Office of Pesticide Programs, Environmental Fate and Effects Division, Oct. 15, 2012.

Table 2. Maximum Use Patterns for Current Registered Use Sites of Propoxycarbazone-sodium (PC 122019)

Use Site	Single Max. Rate (lbs/Acre)	Max. Rate per Crop Cycle	Max. Rate per Year (lbs/Acre)	Application Methods
Agricultural Fallow / Conservation Reserve	0.0525	NS	0.0525	Broadcast - Aerial Broadcast – Ground Spot Treatment - Ground
Pastures	0.0525	NS	0.0525	Broadcast - Aerial Broadcast – Ground Spot Treatment - Ground
Rangeland	0.0525	NS	0.0525	Broadcast - Aerial Broadcast – Ground Spot Treatment - Ground
Triticale	0.0148	0.0148	0.0395	Broadcast - Aerial Broadcast – Ground
	0.0395	NS		
Wheat	0.0263	0.0525	0.0525	Broadcast - Aerial Broadcast – Ground
	0.0394	0.0525		
	0.0175	0.0175		Spray - Aerial Spray – Ground

FATE AND TRANSPORT CHARACTERIZATION

Transport and Mobility

Propoxycarbazone has a high water solubility (42,000 mg/L in pH 7 water) and a low vapor pressure (7.1×10^{-11} torr at 20ºC). The calculated Henry's Law Constant of 9.35×10^{-16} atm-m^3/mol) indicates that propoxycarbazone is not expected to be volatile under field conditions and from water. The high water solubility and low soil partitioning coefficients (K_d = 0.22 to 1.07) indicate that it is very mobile in soil. Due to its low K_{OW} value of 0.028, bioaccumulation is not likely to occur.

Degradation

Propoxycarbazone degradation in the environment appears to be variable. The compound hydrolyzes at relatively slow rates, the half-lives at pH 7 are 495 and 433 days, with an average of 464 days. In pH 7 buffered water, the photolysis half-lives of propoxycarbazone are 93.5 and 37 days, with an average of 65 days. For photodegradation on soil, the half-lives are 70 and 38 days, with an average of 54 days. Several aerobic soil metabolism studies show a range of half-life values: 8.7, 16, 21, 47, 77, 83, 103, and 224 days. Aerobic aquatic metabolism study half-lives are 107, 110, 193, and 210 days. The anaerobic aquatic metabolism study has the longest half-life of 1155 days.

Table 3 summaries the product chemistry and environmental fate properties of propoxycarbazone.

Table 3. Product Chemistry and Environmental Fate Properties of Propoxycarbazone

Parameter	Value	Source
Selected Physical/Chemical Parameters		
Molecular mass (molecular formula)	420 g/mol ($C_{15}H_{17}N_4O_7SNa$)	(Calculated)
Vapor pressure (20 °C)	7.1x 10^{-7} torr	Product Chemistry
Aqueous solubility (20°C, pH 7)	42000 mg/L	
Henry's Law Constant (20°C)	9.35x10^{-16} atm-m^3/mol	(Calculated)
Log octanol-to-water partition coefficient (log K_{OW}) (20°C, pH 7)	-1.55	Product Chemistry
Dissociation constant (pKa)	2.1	
Persistence in Water		
Hydrolysis half-life (20°C)	pH 4: 110 day, pH 7: 495 day, pH 9: 408 day	MRID 45012733 MRID 45012740
	pH 4: 154 day, pH 7: 433 day, pH 9: 385 day	MRID 45012724 MRID 45012725
Aqueous photolysis half-life (20°C) (pH 7)	93.5 day 37 day	MRID 45012703 MRID 45012702
Persistence in Soil		
Photodegradation half-life on soil	70 day 38 day	MRID 45012729 MRID 45012728
Aerobic soil metabolism half-life (20°C)	77 day	MRID 45012720 MRID 45012736
	103 day	MRID 45012723
	21day, 16 day, 83 day	MRID 45012721 MRID 45012735
	8.7 day, 46.5 day, 223.6 day	MRID 45012722 MRID 45012736
Aerobic aquatic metabolism half-life (20 °C)	110 day, 107 day, 193 day, 210 day	MRID 4512704
Anaerobic aquatic metabolism half-life (20 °C)	1155 days	MRID 45012708 MRID 45012707
Mobility		
Freundlich Adsorption coefficient (K_d) (Koc) (20 °C)	0.2504, 0.4968, 0.2239, 0.2134, 1.0747 L/kg 10.1, 18.7, 26, 57.7, 66.7	MRID 45012634
Terrestrial Field Dissipation		
Field Dissipation half-life	22.4 day 16.8 day 44.4 day	MRID 45012716 MRID 45012719 MRID 45012715

Parameter	Value	Source
Fish Bioconcentration		
Not required - Kow (0.028) is less than 1,000		

Environmental Degradates

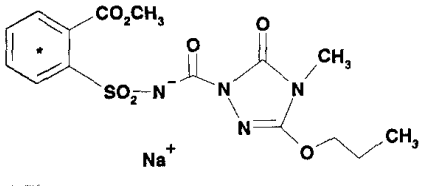
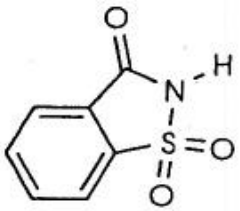
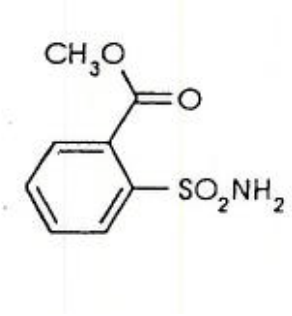
The most prominent degradate of propoxycarbazone is propoxycarbazone-carboxylic acid (MKH 7018 or MKH 8394), which results from the loss of a methyl ester group, but has the intact sulfonylurea bridge. This degradate was quite stable in aerobic and anaerobic aqueous metabolism studies, forming 50% or more of the applied test compound at the end of 100-day or 365-day experiments. However, this was a minor degradate in soil. This degradate may persist and accumulate in ponds, lakes, and reservoirs.

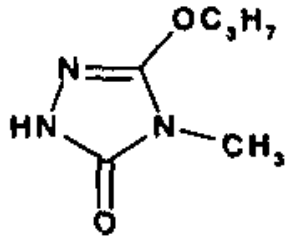
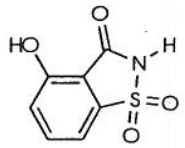
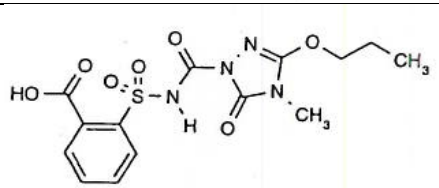
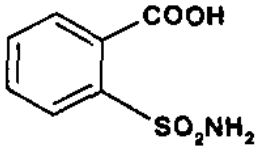
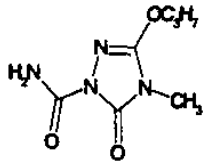
There are two sets of degradates that result from the cleaving of the sulfonylurea bridge. These include the triazolinones, and the sulfonamide/saccharins. The former set includes N-methylpropoxytriazolinone amide and N-methylpropoxytriazolinone (MKH 7017), which was a major degradate in all soil metabolism studies. The latter set includes propoxycarbazone-sulfonamide methyl ester (STJ 4934), sulfonamide acid (MKH 7283), saccharin (MKH 7284) and 4-hydroxysaccharin. All of these were major metabolites in soil or aquatic metabolism experiments. With the exception of 4-hydroxysaccharin, all are of equal or greater mobility than the parent compound. The available chemical names and structures are listed in **Table 4**.

Residues of Concern

The modeled residues of concern include the parent compound plus propoxycarbazone-carboxylic acid (MKH 8394), which has the intact sulfonylurea bridge (Report of the Metabolism Assessment Review Committee – MARC, DP 299170, April 2004). The other degradates are assumed less toxic than the parent compound and are not of concern because the sulfonylurea bridge is cleaved.

Table 4. Propoxycarbazone-sodium and Its Environmental Transformation Products

Code Name/ Synonym	Chemical Name	Chemical Structure	Study Type	MRID	Maximum %AR (day)	Final %AR (study length)
PARENT						
Propoxycarbazone **MKH 6561**	Methyl 2-(4,5-dihydro-4-methyl-5-oxo-3-propoxy-1H-1,2,4-triazol-1-yl) carboxamidosulfonylbenzoate, sodium salt CAS Reg. No. 181274-15-7 (sodium salt); 145026-81-9 (acid) **Formula: $C_{15}H_{18}N_4O_7S$ Na** **MW: 420 g/mol (sodium salt)** **398 g/mol (acid, MKH 5554)**					
TRANSFORMATION PRODUCTS						
Saccharin **MKH 7284**	1,2-Benzisothiazol-3(2H)-one,1,1-dioxide **Formula: $C_7H_5NO_3S$** **MW: 183 g/mol**		Hydrolysis	45012733 45012740	1.19% (30 d) @ pH 4 3.26% (30 d) @ pH 7 3.78% (30d) @ pH 9	1.19% (30 d) @ pH 4 3.26% (30 d) @ pH 7 3.78% (30d) @ pH 9
			Soil photolysis	45012729	4.7% (18 d)	4.7% (18 d)
			Aqueous photolysis	45012702	**22.26%** (19 d)	22.265 (19 d)
			Aerobic soil	45012720 45012736	1.4% (88 d)	1.4% (361 d)
				45012722 45012736	**26.6%** (14 d)	15.65 (180 d)
MKH 6561 sulfonamide methyl ester **STJ 4934**	2-carbomethoxybenzene-sulfonamide **Formula: $C_8H_9NO_4S$** **MW: 215 g/mol**		Hydrolysis	45012733 45012740	**16.61%** (30 d)	16.61% (30 d)
			Aqueous photolysis	45012702	5.8% (7 d)	4.165 (19 d)
			Soil photolysis	45012729	9.7% (11 d)	8.7% (18 d)
			Aerobic soil	45012720 45012736	4.1% (13 d)	< 0.5% (163 d)
				45012722 45012736	**20.9%** (6 d)	4.6% (180 d)
			Aerobic Aquatic	45012704	**11.3%** (100 d)	11.3% (100 d)

N-methyl propoxy triazolinone **MKH 7017**	3H-1,2,4-Triazol-3-one, 2,4-dihydro-4-methyl-5-propoxy **Formula: $C_6H_{11}N_3O_2$** **MW: 157 g/mol**		Hydrolysis	45012724 45012725	**13.92%** (33 d) @ pH 4 4.15% (33 d) @ pH 7 4.72% (33 d) @ pH 9	13.92% (33 d) @ pH 4 4.15% (33 d) @ pH 7 4.72% (33 d) @ pH 9
			Aqueous photolysis	45012703	**13.6%** (19 d)	13.6 % (19 d)
			Soil photolysis	45012728	8.57% (18 d)	8.57% (18 d)
			Aerobic soil	45012723	**28.7%** (365 d)	28.7% (365 d)
				45012721 45012735	**32%** (28 d) **43.9%** (29 d) **55.2%** (182 d)	14% (182 d) 19.9% (182 d) 55.2% (182 d)
			Anaerobic Aquatic	45012708	**20.5%** (196 d)	15.1% (365 d)
			Aerobic Aquatic	45012704	**34.4%** (100 d)	34.4% (100 d)
4-Hydroxy Saccharin	1,2-Benzisothiazol-3(2H)-one,4-hydroxy-,1,1-dioxide **Formula: $C_7H_5NO_4S$** **MW: 199 g/mol**		Aerobic soil	45012720 45012736	**13.8%** (361 d)	13.8% (161 d)
				45012722 45012736	**21.9%** (180 d)	21.9% (180 d)
MKH 6151 Carboxylic Acid **MKH 8394**	Benzoic acid, 2-(((4,5-dihydro-4-methyl-5-oxo-3-propoxy-1H-1,2,4-triazol-1-yl) carbonyl)amino)sulfonyl **Formula: $C_{14}H_{16}N_4O_7S$** **MW: 384 g/mol**		Aerobic soil	45012720 45012736	1.2% (88 d)	0.5% (361 d)
				45012722 45012736	3.7% (180 d)	3.7% (180 d)
			Anaerobic Aquatic	45012708	**87.8%** (90 d)	76.1% (365 d)
				45012707	**84.9%** (120 d)	68.8% (365 d)
			Aerobic Aquatic	45012704	**71.6%** (62 d)	48.3% (100 d)
MKH 6151 Sulfonamide Acid **MKH 7283**	Benzoic acid, 2-(aminosulfonyl) **Formula: $C_7H_7NO_4S$** **MW: 201 g/mol**		Aerobic soil	45012722 45012736	5.0% (14 d)	ND (180 d)
			Anaerobic Aquatic	45012707	**24.6%** (365 d)	24.6% (365 d)
			Aerobic Aquatic	45012704	**19.4%** (100 d)	19.4% (100 d)
N-Methyl propoxy triazolinones amide	3H-1,2,4-Triazol-3-one-2-carboxamide-2,4-dihydro-4-methyl-5-propoxy **Formula: $C_7H_{12}N_4O_3$** **MW: 200 g/mol**		Aerobic soil	45012723	**16.1%** (313 d)	16% (365 d)
				45012721 45012735	8% (93 d)	7.1% (182 d)

Drinking Water Exposure Assessment

Drinking water exposure to the residues of concern is estimated using available chemical properties and environmental fate data.

Drinking Water from Surface Water Sources

The Surface Water Concentration Calculator (SWCC v1.106) was used to calculate EDWCs from surface water sources. Based on the use site table, the modeling effort is focusing on two maximum annual rate scenarios: (1) a single application rate of 0.0525 lb ai/ac for agricultural fallow/conservation reserve, pastures, and rangeland, and (2) a fall application of 0.02625 lb ai/ac, followed by a spring application of 0.02625 lb ai/ac for wheat.

There are two rangeland modeling scenarios in the SWCC database. They are for California rangeland hay and Texas Barton Springs range. For the wheat use site, two applicable scenarios are for North Dakota and Texas. **Table 5** presents some background information of these modeling scenarios. **Table 6** lists the chemical modeling input parameters. **Table 7** lists the application related information and assumptions. Since propoxycarbazone is used to control post-emergence grass weeds, the application dates were assumed during the heavy weed growing time.

Table 5. Modeling Scenarios Used for Surface Water Concentration Calculator

Modeling Scenario	Met. File (.dvf)	Emergency Date	Maturation Date	Harvest Date
California Rangeland Hay	23232	Nov. 1	April 1	May 1
Texas Barron Spring Range	13958	March 1	June 15	Nov. 15
North Dakota Wheat	14914	Oct. 16	April 30	June 17
Texas Wheat	13958	May 16	July 25	August 5

Table 6. Chemical Model Inputs for Propoxycarbazone Residues of Concern

Parameter	**Value**	**Source**
Molecular Weight (g/mol)	420	$C_{15}H_{17}N_4O_7SNa$
Water Solubility (mg/L)	42000	Product Chemistry
Vapor Pressure (torr)	7.1×10^{-7}	
Hydrolysis half-life (day) @pH 7	495, 433 (use the higher value: 495)	MRID 45012733, 45012740 MRID 45012724, 45012725
Aqueous photolysis half-life (day)	37 and 93.5 (use the higher value 93.5)	MRID 45012703 MRID 45012702
Aerobic soil metabolism half-life (day)	107 (upper 90th percentile on eight values of 77, 103, 21, 16, 83, 8.7, 46.5, and 224)	MRID 45012720, 45012736 MRID 45012723, 45012721 MRID 45012735, 45012722 MRID 45012736
Aerobic aquatic metabolism half-life (day)	199 (upper 90th percentile on four values of 110, 107, 193, and 210)	MRID 4512704

Parameter	Value	Source
Anaerobic aquatic metabolism half-life (day)	1155 (the single available value was not multiplied by 3 because it is large)	MRID 45012708 MRID 45012707
Adsorption coefficients (K_d)	0.4518 (Mean of five values:0.2504, 0.4968, 0.2239, 0.2134 and 1.0747)	MRID 45012634

Table 7. Application Information Related to Propoxycarbazone Use on Modeling Scenarios

Model Input Variable	Input Value	Comments
Application Date(s)	December 1 for California Rangeland Hay April 1 for Texas Barron Spring Range April 1 and November 16 for North Dakota Wheat June 16 and October 1 for Texas Wheat	Post-emergence (after emergence date)
Maximum Application Rate (maximum) and Number of Application	1 @ 0.0525 lb a.i./acre	Range land use
	2 @ 0.02625 lb a.i./acre	Wheat use
Application method, App. Efficiency / Spray Drift	Ground, 0.99 / 0.066	USEPA, 2013 [4]
	Aerial, 0.95/0.135	

Standard percent cropped areas (PCA) are used as conservative default estimates of the extent of watershed on which agricultural crops of unknown specific PCA are grown.[5] Considering the many use sites of propoxycarbazone, the PCA value of 1 was used to represent the national default PCA for all agricultural land. The SWCC results are tabulated in **Table 8**.

[3] USEPA. 2013. Guidance on Modeling Offsite Deposition of Pesticides via Spray Drift for Ecological and Drinking Water Assessments. U.S. Environmental Protection Agency, Office of Pesticide Programs, Environmental Fate and Effects Division. Internal memorandum. Dec. 20, 2013.

[5] USEPA. 2014. Development of Community Water System Drinking Water Intake. Percent Cropped Area Adjustment Factor for use in Drinking Water Exposure Assessments: 2014 Update

Table 8. Propoxycarbazone Total Residue of Concern EDWCs from Surface Water Sources

PRZM Scenario	Type of Application	1-in-10-year Peak Exposure (µg/L)	1-in-10-year Annual Mean Exposure (µg/L)	30-year Mean Exposure (µg/L)
CA Rangeland Hay	Aerial	1.19	0.410	0.280
	Ground	1.07	0.353	0.218
TX Barron Spring Range	Aerial	1.57	0.424	0.210
	Ground	1.46	0.390	0.175
ND Wheat	Aerial	0.942	0.420	0.272
	Ground	0.843	0.362	0.208
TX Wheat	Aerial	4.07	1.06	**0.491**
	Ground	**4.16**	**1.07**	0.480

The modeling results of the Texas Wheat scenario with ground applications provided the higher EDWCs of 4.16 µg/L and 1.07 µg/L to represent the 1-in-10-year peak and mean exposure values, respectively.

Drinking Water from Ground Water Sources

PRZM-GW (v1.07) is used to calculate EDWCs from ground water sources. The chemical specific input parameters including hydrolysis half-life, aerobic soil metabolism half-life, and adsorption coefficient (K_d) are taken from **Table 6** and application related inputs are taken from **Table 7**. Only the inputs used for the Texas Barton Springs Range surface water scenario with ground applications were modeled, since they provided more conservative surface water results. All six available ground water scenarios were modeled as surrogates for range land scenarios, with the Florida citrus scenario producing the highest EDWCs as shown in **Table 9**. The EDWCs of 3.47 µg/L and 2.8 µg/L represent the acute and chronic exposure values, respectively.

Table 9. PRZM-GW Output of EDWCs for Propoxycarbazone Total Residue of Concerns

Modeled Scenario	Max. Daily Conc. (µg/L)	Mean Breakthrough Time (years)	Post-breakthrough Mean (µg/L)
DMV corn	2.18	12.706	1.93
FL citrus	**3.47**	7.254	**2.8**
FL potato	1.8	6.020	1.31
GA peanut	0.591	11.059	0.517
NC cotton	0.631	19.258	0.538
WI corn	1.67	26.872	1.48

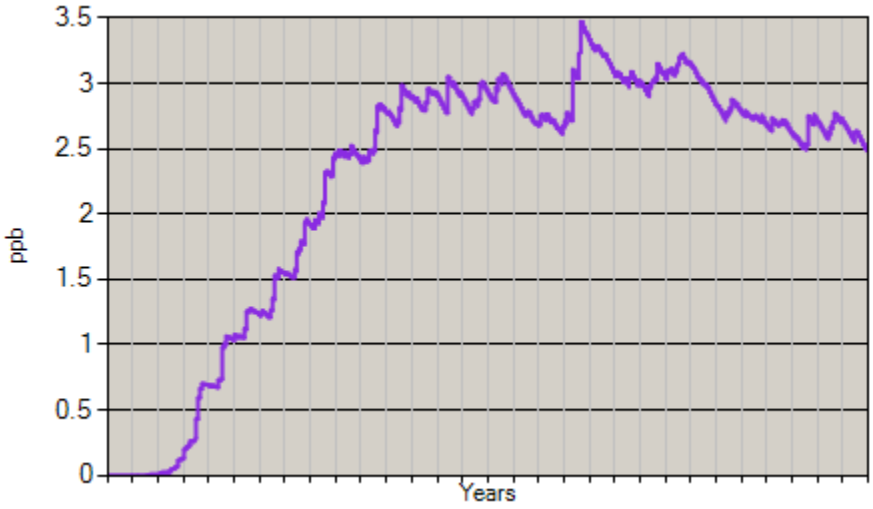


Figure 1. PRZM-GW EDWCs over 30 years for the Florida citrus scenario

Monitoring Data

Propoxycarbazone is not an analyte in the following water monitoring programs: the California Department of Pesticide Regulation (CDPR) surface water database (http://www.cdpr.ca.gov/docs/emon/surfwtr/surfcont.htm, the USGS NAWQA surface and ground water database (http://cida.usgs.gov/nawqa_queries_public/), the USEPA STORET Data Warehouse (http://www.epa.gov/storet/), and the USDA Pesticide Data Program drinking water monitoring analyses (http://www.ams.usda.gov/AMSv1.0/ams.fetchTemplateData.do?template=TemplateG&navID=&rightNav1=&topNav=&leftNav=ScienceandLaboratories&page=PDPDownloadData/Reports&resultType=&acct=pestcddataprg).

Conclusion

The overall estimated drinking water concentrations from surface water sources and ground water sources are summarized in **Table 1**. The surface water concentrations are on the same order of magnitude as the ground water concentrations. For acute exposure, the surface water concentration (**4.16 µg/L**) is higher than that for ground water, whereas for chronic exposure, the ground water value (**2.8 µg/L**) is higher. These results are similar to previous drinking water assessment results, with an increase in ground water estimates relative to previous estimates (DP 348511): surface water acute, 4.59 µg/L; surface water chronic, 1.79 µg/L; ground water acute and chronic, 0.36 µg/L.