UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
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MEMORANDUM

SUBJECT: Tier I Estimated Surface Drinking Water Concentrations and Estimated Ground Water Concentrations (EDWCs) for Picoxystrobin Use on Sweet Corn for Use in Human Health Risk Assessment (PP# 0F7722).

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12/1/2011

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This memo presents the Tier I Estimated Surface Drinking Water Concentrations and Estimated Ground Water Concentrations (EDWCs) for picoxystrobin calculated using the Tier I aquatic models FIRST and SCI-GROW, respectively, for use in the human health dietary risk assessment. Although there are other uses, sweet corn application rates were the maximum and EECs generated from such use should cover all of the other uses registered. A PCA of 0.87 was used since there are other uses than corn. The Tier I modeling is not use site-specific but models application rate generically so that as long as the highest rate is modeled it will yield the highest EDWC. For any refinements needed, HED should consult with EFED.

For the proposed action (D377700) and based on the Picoxystrobin; Report of the Residues of Concern Knowledgebase Subcommittee (ROCKS) memo dated (Aug 22, 2011), this assessment uses a total toxic residue (TTR) approach to include parent and the following major environmental degradates: Compound 2, Compound 3, Compound 7, and Compound 8 (see Appendix A).

Table 1 provides a summary of the Tier I modeled drinking water concentrations. Should there be a need for additional refinements; the EFED can perform a Tier II aquatic assessment, for surface waters and groundwater.

Table 1. Tier I modeled surface and groundwater concentrations.

Drinking water (model used)	**Use rate modeled (lb a.i./Acre)**	**Maximum estimated Drinking water Concentration (ppb)**	
Groundwater (SCI-GROW; Version dated)	Sweet corn (0.195 ; 4 applications)	Acute and chronic	0.052
Surface water (FIRST; Version dated)	Sweet corn (0.195 ; 4 applications)	Acute	29.0
	Sweet corn (0.195 ; 4 applications)	Chronic	7.42

Picoxystrobin is a new chemical fungicide (DuPont Aproach fungicide; Methyl (2*E*)-3-methoxy-2-{2-[6-(trifluoromethyl)-2-pyridyloxymethyl]phenyl}acrylate; CAS#: 117428-22-5; PC code: 129200). Picoxystrobin is a broad spectrum cereal fungicide from the strobilurin group. It has systemic, translaminar and preventative properties. Picoxystrobin and other strobilurin analogues inhibit fungal respiration. The picoxystrobin molecule contains a ß-methoxyacrylate moiety, which is common to the naturally occurring strobilurins and is responsible for the binding of picoxystrobin to the bc1 segment of the electron transport chain. This binding causes interference with electron flow at the cytochrome bc1 complex.

This is a Tier I screening drinking water assessment using Tier I aquatic models SCI-GROW and FIRST, and maximum application rates for picoxystrobin and its major degradates, with the minimum interval between applications. It was found that the worst case scenario for picoxystrobin was sweet corn, which had the highest seasonal application rate and the highest PCA.

Fate and Transport Characterization

Table 2 provides a detailed summary of physical/chemical and environmental fate/transport properties of picoxystrobin, including measured parameters, values, data sources, and comments.

Table 2, Summary of physical/chemical and environmental fdte and transport properties of picoxystrobin.

OPPTS Guideline	Data Requirement	Data Summary	Source
835.2120	Hydrolysis $t_{1/2}$ at 50°C	Stable	MRID# 48073834
835.2240	Aqueous photolysis $t_{1/2}$ at 25°C	28.9 days	MRID# 48073835
835.2410	Soil photolysis $t_{1/2}$ at 20°C	11.6 days	MRID# 48073836
835.4100	Aerobic soil metabolism $t_{1/2}$ at 20°C (combined radio-label half-life)	73.7 days (sandy loam) 29.4 days (clay loam) 38.3 days (sand) 34.7 days (sandy loam)	MRID 48073837
835.4200	Anaerobic Soil Metabolism $t_{1/2}$ at 20°C	Waived	MRID 48073838
835.4300	Aerobic aquatic metabolism $t_{1/2}$ at 20°C (sandy clay loam sediment system and sand system, 2 radio-labels)	39.2 days 47.5 days	MRID 48073839
835.4400	Anaerobic aquatic metabolism $t_{1/2}$ at 20°C (,sandy loam soil system combined labels)	83.5 days	MRID 48073840
835.1230	Organic carbon partitioning coefficient (K_{oc}, mL/g oc)	837 (sandy loam) 1089 (silty clay loam) 741 (sandy loam) 933 (sandy loam) 1067 (sand) 878 (Sandy clay loam)	MRID 48073838
	Freundlich adsorption value, K_f,	4.9 (sandy loam)	MRID 48073838

OPPTS Guideline	Data Requirement	Data Summary	Source
	mL/g oc (1/n)	22.4 (silty clay loam) 22.4 (sandy loam) 15.7 (sandy loam) 3.5 (sand) 14 (Sandy clay loam)	
835.6100	Terrestrial field dissipation DT_{50} US soils	41.3 days (Porterville, California/Sandy loam) 34.7 days (Arkansaw, Wisconsin/Sandy loam-loamy)	MRID 48073842 MRID 48073843
	Terrestrial field dissipation DT_{50} Foreign soils	151 days (Manitoba, Canada/Clay loam-loam) 39.4 days (Prince Edward Island, Canada/Sandy loam) 62 days (Grissoles, France/Silty clay loam) 108 days (Maidenhead, UK/Sandy clay loam) 94 days (Saxe-Anhalt, Germany/Sandy clay loam) 80 days (Cessac, France/Clay loam) 53 days (Schleswig-Holstein, Germany/Sandy loam) 80 days (Bracknell, Berkshire, UK/Sandy clay loam)	MRID 48073841 MRID 48073844 MRID 48073846 MRID 48073847 MRID 48073848 MRID 48073849 MRID 48073850 MRID 48073851
850.1730	Fish bioconcentration (BCF) (steady state BCF)	1400 in viscera, 110 in flesh and 170 in the carcass. 290 in whole fish BCF	MRID 48073776

Picoxystrobin is moderately persistent in aerobic and anaerobic conditions, and is moderately mobile based on the FAO Soil mobility classifications (mean Koc = 924; MRID 48073832) (USEPA, 2006). Picoxystrobin is moderately persistent in soil with half-lives ranging from 29 to 73 days in aerobic soil from three studies conducted in four soils (MRID 48073837). There is no evidence of degradation via hydrolysis which was studied across environmental pHs (pH 5, pH 7, and pH 9 @ 25° C; MRID 48073834). Picoxystrobin degraded under the conditions of aerobic aquatic metabolism with half-lives ranging from 39 to 41 days (MRID 48073839); and under anaerobic aquatic systems with a half-life of 83 days (MRID 48073840). The primary route of degradation may include aqueous photolysis (half-life of 16 days; MRID 48073835); however photolysis only plays a significant role in shallow clear waters. Under other conditions, aerobic biometabolism is expected to be the primary route of degradation.

Major degradates Compound 2 (IN-QDY62 R403092), Compound 3 (IN-QDK50 R403814), Compound 4, Compound 7 (IN-QFA35), Compound 12, Compound 8 (IN-QDY63), and CO_2 were identified in the environmental fate studies at concentrations >10% of the applied radioactivity. In all four soils and under aerobic soil conditions, Compounds 2 and 3 were reported at decreasing concentrations at the study termination (119 and 365 days).

Drinking Water Exposure Modeling

Models

SCI-GROW (Screening Concentration in Ground Water) is a regression model used as a screening tool for ground water used as drinking water. SCIGROW was developed by regressing the results of Prospective Ground Water studies against the Relative Index of Leaching Potential (RILP). The RILP is a function of aerobic soil metabolism and the soil-water partition coefficient. The output of SCI-GROW 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.

FIRST (FQPA Index Reservoir Screening Tool) is a screening model designed by the Environmental Fate and Effects Division of the Office of Pesticide Programs to estimate the concentrations found in drinking water from surface water sources for use in human health risk assessment. It provides upper bound values on the concentrations that might be found in drinking water due to the use of a pesticide. FIRST is a single event model, but can account for spray drift from multiple applications. Spray drift (resulting in direct deposition of the pesticide into the reservoir) is assumed to be 16% of the applied active ingredient for aerial application, 6.3% for orchard air blast application, and 6.4% for other ground spray application. FIRST is hardwired to represent the Index Reservoir, a stand rd 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 uses as a drinking water supply), Shipman City Lake in Illinois, that is known to be vulnerable to pesticide contamination. The single runoff event moves a maximum of 8% of the applied pesticide into the reservoir. This amount can be reduced due to

degradation on the field and the effects of binding to soil in the field. FIRST also uses a Percent Cropped Area (PCA) factor to adjust for the area within the watershed that is planted to the modeled crop. The default agricultural PCA is 0.87.

Modeling Approach and Input Parameters

Table 3 provides the input parameter values used for modeling of picoxystrobin using SCIGROW. Model output is shown in Appendix B.

Table 3. SCI-GROW (v2.3) input parameter values for picoxystrobin.

Parameter (units)	Value(s)	Source
Max. application rate (lb a.i./Acre)	0.195	EPA Reg. No. 352-IUN
Number of applications per year	4	EPA Reg. No. 352-IUN
Organic carbon partition coefficient (K_{oc}; mg/L)	799 (mean)	MRID# 408073832; values used: 83.7, 1089, 741, 933, 1067, 878); Model input guidance (2009). K_{oc} model applied.
Aerobic soil metabolism half-life (days)	47.8 (median)	Half-lives are re-calculated as per half-life guidance for a new set of data that combine all components of the stressor (TTR) so that calculated half-lives represent the decline of all of the species of the TTR. MRID# 408073837; half-lives values used: 84.0, 33.8, 45.1, and 50.6 days; Model input guidance (2009)

Table 4 provides the input parameter values used for modeling of picoxystrobin and its major degradates using FIRST. Due to the lack of fate data on degradates; the Total Residue (TR) model was used to calculate half-lives as model inputs. This modeling strategy requires an assumption that all residues of concern have similar physical, chemical, and partitioning characteristics. Application rates for the parent pesticide are used to represent the total mass loading of pesticide and its transformation product.

The sweet corn scenario was used as a conservative approach because it has highest rate. Tier I does not make geographic distinctions like Tier II will, and needed refinements would use more use site specific scenarios.

The Percent Cropped Area (PCA) used in this drinking water assessment was 0.87 since corn was not the only use. It is the default value for "other crops" for which there is no PCA. It is also the maximum PCA available.

Table 4. FIRST (Version 1.1.1, March 26, 2008) input parameter values for picoxystrobin and its four major degradates (Compound 2, Compound 3, Compound 7, and Compound 8) when used on sweet corn.

PARAMETER (units)	VALUE (S)	SOURCE	COMMENT
Application Rate (lb a. i . /A)	0.195	Proposed label. EPA Reg No. 352-IUN	Maximum value proposed for the use on sweet corn.
Number of Applications	4	Proposed label. EPA Reg No. 352-IUN	Maximum value proposed for the use on sweet corn.
Interval between Applications (days)	7	Proposed label. EPA Reg No. 352-IUNNo. 352-IUN	Lowest value; Input parameter guidance V. 2.1.(2009).
Percent Cropped Area (decimal)	0.87	Development and Use of Percent Cropped Area Adjustment Factors in Drinking Water Exposure Assessments (2010).	All Agricultural Land (default national because there are multiple uses)
Soil Partition Coefficient K_{OC}, (mL/g)	799	MRID# 48073838	Mean of six Koc values: 83.7, 1089, 741, 933, 1067, and 878; Input

			parameter guidance V. 2.1.(2009).
Aerobic Soil Metabolism Half-life (days)	65.2	MRID# 48073837	Half-lives are re-calculated as per half-life guidance for a new set of data that combine all components of the stressor (TTR) so that calculated half-lives represent the decline of all of the species of the TTR. Represents the 90th percentile of the upper confidence bound on the mean of 4 half-life values: 84.0, 33.8, 45.1, and 50.6 days; mean 53.4 days, std. dev, 21.6
Wetted in?	No		Input parameter guidance V. 2.1.(2009).
Depth of Incorporation (inches)	0		
Method of Application	Aerial	Proposed label. EPA Reg No. 352-IUN	
Solubility in Water @ 20 ^{o}C (mg/L)	3	MRID# 48073834	
Aerobic Aquatic Metabolism Half-life (days)	2079	MRID# 48073839	Half-lives are re-calculated as per half-life guidance for a new set of data that combine all components of the stressor (TR) so that calculated half-lives represent the decline of all of the species of the TR. Single value of 693.1 days multiplied by 3;

			Input parameter guidance V. 2.1.(2009).
Hydrolysis Half-life @ pH 7 (days)	stable	MRID# 48073834	Stable. Input parameter guidance V. 2.1.(2009).
Aquatic Photolysis Half-life @ pH 7 (days)	28.9	MRID# 48073835	Input parameter guidance V. 2.1.(2009).

SCI-GROW 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.

FIRST concentrations (ppb) represent untreated surface water concentrations. The peak day concentration (over 30 years) is used for acute endpoints and the annual average concentration (over 30 years) is used for chronic endpoints. The estimated concentrations provided in this assessment are conservative estimates of concentrations in drinking water. If dietary risks require refinement, higher tiered crop specific and location-specific models and modeling scenarios can be utilized.

Monitoring Data

Monitoring data usually provide different kinds of information than modeling (e.g., monitoring reflects current use pattern, underestimates frequency of occurrence, often misses peaks, inputs cannot be adjusted as modeled ones can, usually done for purposes other than character zing exposure from a particular pesticide), and, consequently, tend to complement the modeling rather than refine it. In general, a useful interpretation of monitoring values requires in-depth assessment of the data, which is beyond the scope of a Tier I assessment.

For the new chemical (picoxystrobin) no monitoring data is available.

Drinking Water Treatment

There are no data available on the effects of water treatment on the possible increasing dissipation and or the transformation into products that may be less or more toxic than the parent.

CONCLUSIONS

In this assessment it has been assumed that the reported value is the total of picoxystrobin and its major degradates (Compound 2, Compound 3, Compound 7, and Compound 8) in drinking water. The results yielded an acute estimated surface water concentration of 29.0

ppb and a cancer/chronic drinking water concentration of 7.42 ppb. The groundwater EDWC suitable for acute and chronic exposure is 0.055 ppb.

References

1. Policy Establishing Current Versions of Exposure Models and Responsibility for Model Maintenance (11/06/2002)

2. SCIGROW: Users Manual (1 1/01/2001, revised 08/23/2002)

3. FIRST Users Manual (08/01/2001)

4. FIRST: A Screening Model to Estimate Pesticide Concentrations in Drinking Water (05/01/2001)

5. Guidance for Selecting Input Parameters in Modeling the Environmental Fate an Transport of Pesticides (2009) .

6 The Incorporation of Water Treatment Effects on Pesticide Removal and Transformations in Food Quality Protection Act (FQPA) Drinking Water Assessments (10/25/01)

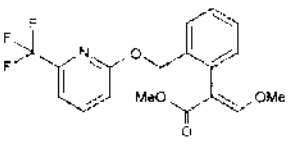
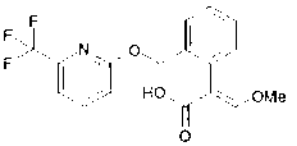
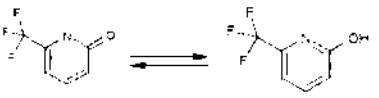
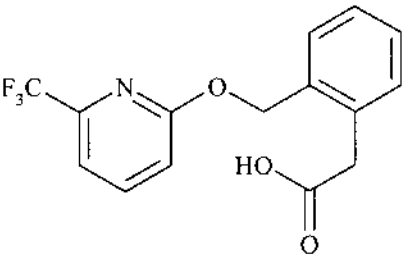
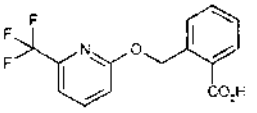
7. Tomlin, CDS (ed.) The Pesticide Manual-World Compendium, 11th edition, British Crop Protection Council, Surrey, England 1997, p. 416.

8. Food and Agriculture Organization of the United Nations. FA0 PESTICIDE DISPOSAL Parameters of pesticides that influence processes in the soil. Editorial Group, FA0 Information Division: Rome, 2000. http://www.fao.orgJDOCREP/003/X2570E00.

9. Development and Use of Percent Cropped Area Adjustment Factors in Drinking Water Exposure Assessments. 2010. R. David Jones, Kevin Costello, Jim Hetrick, Jim Lin, Ron Parker, Nelson Thurman, Chuck Peck, Greg Orrick@ http://www.epa.gov/oppefed1/models/water/pca_adjustment_dwa.html#literature.

APPENDIX A

Structures of Picoxystrobin Major Metabolites and Degradates

Code Name	Chemical Abstracts Name (IUPAC Name)	Structure
Picoxystrobin	methyl *(E)*-2-{2-[6-(trifluoromethyl)pyridin-2-yloxymethyl]phenyl}-3-methoxyacrylate	
Compound 2 IN-QDY62 (R403092)	4-(cyclopropylhydroxymethylene)-3,5-dioxocyclohexanecarboxylic acid	
Compound 3 IN-QDK50 (R403814)	6-(trifluoromethyl)pyridin-1H-2-one (6-(trifluoromethyl) pyrindin-2-ol (preferred name))	
Compound 7 (R408631)	2-[2-[6-trifluoromethyl) pyridin-2-yloxymethyl] phenyl] acetic acid	
Compound 8 IN-QDY63 (R408509)	2-[6-(trifluoromethyl)pyridin-2-yloxymethyl]phenyl]benzoic acid	

Appendix B

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:picoxystrobin

time is 11/30/2011 15:36: 8

Application rate (lb/acre)	Number of applications	Total Use (lb/acre/yr)	Koc (ml/g)	Soil Aerobic metabolism (days)
0.195	4.0	0.780	7.99E+02	47.8

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groundwater screening cond (ppb) = 5.50E-02

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FIRST Output File

RUN No. 1 FOR picoxystrobin ON corn * INPUT VALUES *

RATE (#/AC) ONE(MULT)	No.APPS & INTERVAL	SOIL Koc	SOLUBIL (PPM)	APPL TYPE (%DRIFT)	%CROPPED AREA	INCORP (IN)
0.195(0.700)	4 7	799.0	3.0	AERIAL(16.0)	87.0	0.0

FIELD AND RESERVOIR HALFLIFE VALUES (DAYS)

METABOLIC (FIELD)	DAYS UNTIL RAIN/RUNOFF	HYDROLYSIS (RESERVOIR)	PHOTOLYSIS (RES.-EFF)	METABOLIC (RESER.)	COMBINED (RESER.)
65.20	2	0.00	28.90- 3583.60	******	1315.70

UNTREATED WATER CONC (MICROGRAMS/LITER (PPB)) Ver 1.1.1 MAR 26, 2008

PEAK DAY (ACUTE) CONCENTRATION	ANNUAL AVERAGE (CHRONIC) CONCENTRATION
29.023	7.417