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OFFICE OF
CHEMICAL SAFETY AND
POLLUTION PREVENTION

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MEMORANDUM

SUBJECT: Boscalid Drinking Water Assessment in Support of Registration Review

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1 Executive Summary

This assessment provides Estimated Drinking Water Concentrations (EDWCs) for the use of the fungicide boscalid (2-chloro-N-(4'-chloro[1,1'-biphenyl]-2-yl)- 3-pyridinecarboxamide, CAS Registry Number 188425-85-6, PC Code 128008) in support of the human health dietary risk assessment for Registration Review. Boscalid is in the anilide, carboxamide, and pyridine and chemical classes and is registered for use on several agricultural crops and residential use patterns.

Boscalid is non-volatile, moderately mobile in soil (FAO, 2000), and not likely to bioconcentrate (log octanol-water partition coefficient, K_{OW} = 2.96). Aerobic soil metabolism time to 50% degradation (DT50) range from 390 to 680 days and boscalid is classified as persistent using the Goring persistence scale[1]. Anaerobic aquatic metabolism DT50 range from 284 to 320-days and aerobic aquatic metabolism DT50 range from 545-days to essentially stable. Boscalid is stable to abiotic degradation. Terrestrial field dissipation studies have been conducted at a total of fourteen different sites. Dissipation half-lives ranged from 1.0 to greater than 360 days with residue carryover being observed at all sites. Boscalid may be transported to surface water and groundwater via runoff, leaching, or spray drift.

New fate data available for this assessment includes aerobic soil and anaerobic aquatic metabolism studies. These studies reduced uncertainty in the unextracted residues, and the fate analysis was updated based on these newly available data. Additionally, degradation kinetic calculations were updated using the North American Free Trade Agreement (NAFTA) procedure (USEPA, 2015a). See fate discussion for additional details.

In this drinking water assessment boscalid is the only residue of concern. Previous Estimated Drinking Water Concentrations (EDWCs) reflected residues of parent plus unextracted residues.

The Pesticide in Water Calculator (PWC version 1.52) was used to obtain EDWCs in surface water and groundwater. The PWC was not available when the previous drinking water assessment was completed in 2013 (USEPA, 2013, DP Barcode 409880); however, the PWC relies on the same base models (*e.g.*, the Pesticide Root Zone Model [PRZM]) as previous drinking water assessments. A new policy finalized in 2017 also recommended using 24-hour mean concentrations as acute concentrations for drinking water (USEPA, 2017); whereas, instantaneous (initial) concentrations had been used previously. Use patterns summarized in the Pesticide Label Use Summary (PLUS) report (USEPA, 2018) developed to support the Registration Review Process were considered in this drinking water assessment. The use patterns with the highest application rates (ornamentals) and that resulted in the highest EDWCs previously (turf) were simulated in modeling.

The EDWCs for both surface and groundwater recommended for use in Health Effects Division (HED) human health dietary risk assessment is summarized in **Table 1-1.** The highest EDWCs were obtained for groundwater and therefore, EFED recommends use of the highest daily value of 470 µg/L for the acute assessment and the post-breakthrough average value of 436 µg/L for

[1] Goring et al. (1975) provides the following persistence scale for aerobic soil metabolism half-lives:

- Non-persistent less than 15 days
- Slightly persistent for 15-45 days
- Moderately persistent for 45-180 days, and
- Persistent for greater than 180 days.

the chronic and cancer assessment. These EDWCs are based on the proposed maximum annual application rate of 2.10 lb pounds active ingredient per acre per year (lbs a.i./A/yr) reflecting use on ornamentals. These EDWCs are lower than the EDWCs for surface and groundwater in the previous drinking water assessments for boscalid because unextracted residues are no longer considered an uncertainty in the fate data.

Table 1-1: Highest Estimated Drinking Water Concentrations (EDWCs) for Boscalid Across Registered Uses

Use, Scenario, Source	Application Rate lbs a.i./A, # of Apps, RTI	EDWCs[1,2,3] in µg/L		
		Acute	Chronic	Cancer
Ornamentals, FLnurserySTD/ CAnurserySTD Surface Water	0.70 lbs. a.i./A, 3x, 7-day	**88.7**	**56.8**	**35.7**
Ornamentals, Wisconsin Sand, Groundwater		**470**	**436**	**436**

RTI=retreatment interval

[1] Previously estimated acute and annual average surface water concentrations for turf were 97.3 and 26.4 µg/L, respectively. Previously estimated groundwater concentrations were 773 and 697 µg/L (USEPA, 2013, DP Barcode 409880; USEPA, 2014b).

[2]For surface water modeling, the acute concentration is the 1-in-10 year 24-hour mean, the chronic concentration is the 1-in-10-year annual average, and the cancer chronic number is the 30-year average concentration. For groundwater simulations, the acute number is the highest daily value and the chronic and cancer EDWCs is the post breakthrough average concentration.

[3] For surface water modeling FLnurseySTD scenario EDWCs were the highest for acute assessment while the CAnurserySTD scenario EDWCs were highest for chronic and cancer assessments.

The Water Quality Portal (http://www.waterqualitydata.us/portal.jsp) was searched for monitoring information for boscalid in June 2019. There were 737 reported detections found in surface water samples and 23 detections reported for groundwater. The maximum detected concentration in surface water was 36 µg/L and the maximum detected concentration in groundwater was 2.12 µg/L. The sampling frequency of the monitoring indicates that these measured concentrations are not likely to capture the full range of concentrations (e.g., the peak concentration) that may occur at the sites.

Two open literature studies are available in which boscalid was monitored. Reilly *et al*. (2012) analyzed for boscalid in first-order streams, ponds, and shallow groundwater (< 10 m from the surface) draining agricultural areas of the United States with intense fungicide use. Sites were chosen based on fungicide use on potatoes. Boscalid was detected in 72% of surface water samples, with a maximum detected concentration of 110 ng/L. Boscalid was detected in 62% of groundwater samples with a maximum detected concentration of 2120 ng/L. Smalling and Orlando (2011) collected water and sediment (both bed and suspended) from January 2008 through October 2009 from 12 locations within three of the largest watersheds along California's Central Coast (Pajaro, Salinas, and Santa Maria Rivers) and analyzed for a suite of pesticides including boscalid. Boscalid was detected in 85% of samples, at a maximum concentration of 36 µg/L.

2 Use Characterization

Boscalid is a carboxamide fungicide registered for use on several row and orchard crops and as a seed treatment. Boscalid may be used on ornamentals (outdoor residential, greenhouse, and terrestrial non-food uses) and on greenhouse tomato. There are no registered indoor (other than greenhouse and on endive) or aquatic uses for boscalid. Boscalid may be formulated as a single active ingredient pesticide or co-formulated with the fungicides pyraclostrobin and chlorothalonil and with the insecticide lambda-cyhalothrin. Based on the labels boscalid will be applied as a ground spray, airblast spray, aerial spray, chemigation, handheld, or seed treatment equipment. Formulations include water soluble packets (WSG), aerosol, or flowable concentration (FC). Boscalid use patterns were evaluated based on the March 2018 Pesticide Label Use Summary (PLUS) report and considering use patterns with the highest max single rate (lb a.i./A/application) and the max annual rate (lbs a.i./A/year). Simulations were selected based on use patterns that previously resulted in the highest EDWCs for turf and the current highest max single rate for ornamentals. The maximum labeled use pattern for turf is 0.35 lbs a.i./A applied three times with a 14-day minimum retreatment interval (**Table 2-1**). The maximum labeled use pattern allowed for ornamentals is 0.70 lbs a.i./A applied up to three times with a 7-day minimum retreatment interval.

Table 2-1: Summary of the Selected Maximum Labeled Use Patterns for Boscalid

Use Site/ Location	Form	App Target	App Type	App Equip	App Time	Max Single Rate lbs ai/A	Max # App/yr*	Max Annual Rate lbs ai/A/yr	MRI (d)	PHI (d)	Comments	Drift Restrictions
Turf[1]/ Golf Course Turf Only	DF	Foliar	Broad	G	All	0.35	NS (6)*	2.1	14	NS	Not for use on residential turfgrass, turfgrass	None outside of standard restrictions.
Ornamentals, Trees[2]/ Ag and Residential	DF	Foliar/ plant, soil, containerized plant	Banded, Broad	G, BP, HS, A, C	All	0.70	NS (3)*	2.1	7	NS	National label not allowed in CA.	None outside of standard restrictions.

App=application; equip=equipment; Broad=broadcast; NS=not specified; DF=dry flowable; MRI = Minimum retreatment interval; PHI=preharvest interval; A=aerial; C=chemigation; G=ground; ai=active ingredient; d=day; BP= backpack; HS= hand sprayer; All=indicates that the product may be applied during any crop status. Typically, this occurs when the product is applied based on disease pressure. NS=not specified

*Turf and ornamental labels did not specify a maximum number of apps per year and these were calculated by dividing the maximum annual rate by the max single rate to obtain the maximum number of apps per year.

[1]Previously resulted in the highest number for EECs.

[2]Ornamentals includes uses on coniferous/evergreen and softwood trees, deciduous/broadleaf hardwood trees, and various other ornamentals.

3 Environmental Fate and Transport Characterization

Table 3-1 summarizes the physical, chemical, and bioconcentration properties of boscalid. Boscalid has a water solubility of 4.64 mg/L at 20°C and is classified as moderately mobile in soil based the Food and Agriculture Organization of the United Nations (FAO) soil mobility classification (FAO, 2000). Boscalid may be transported to surface water and groundwater via runoff, leaching, and spray drift. While boscalid is classified as non-volatile based on the classification scheme in the terrestrial field dissipation guideline (USEPA, 2008) and its vapor pressure and air-water partition coefficient; it has been measured in air monitoring studies both in the vapor phase and associated with particles at low concentrations (Schumer *et al.*, 2010). Boscalid has a log K_{ow} of 2.96 at 20°C and does not dissociate. Organic-carbon normalized Freundlich distribution coefficients (K_{FOC}) range from 507 to 1110 (mg/L) $(mg/kg)^{-1/n}$ measured in six soils (MRID 45405216). Boscalid is unlikely to bioconcentrate in terrestrial or aquatic organisms.

Table 3-1: Summary of Physical-Chemical and Mobility of Boscalid

<table>
<tr><th>Parameter</th><th colspan="3">Value[1]</th><th>Source/
Study Classification/
Comment</th></tr>
<tr><td>Molecular Weight (g/mol)</td><td colspan="3">343.21</td><td>--</td></tr>
<tr><td>Water Solubility at 20°C mg/L</td><td colspan="3">4.64 ± 0.06</td><td>(Mathur, 2002, DP Barcode 285692)</td></tr>
<tr><td>Vapor Pressure
25°C</td><td colspan="3">2×10^{-6} Pa
2×10^{-8} Torr</td><td>(Mathur, 2002, DP Barcode 285692)
Non-volatile under field conditions</td></tr>
<tr><td>Henry's Law constant at 20°C (atm-m^3/mole)</td><td colspan="3">1×10^{-9}, estimated</td><td>Estimated from vapor pressure at 25°C and water solubility at 20°C</td></tr>
<tr><td>Log Dissociation Constant (pKa)</td><td colspan="3">No dissociation at environmental relevant pH 4 to 9</td><td>(Mathur, 2002, DP Barcode 285692)</td></tr>
<tr><td>Octanol-water partition coefficient (K_{ow}) at 20°C (unitless)</td><td colspan="3">912 (log K_{OW} 2.96)</td><td>(Mathur, 2002, DP Barcode 285692)
Not likely to bioconcentrate</td></tr>
<tr><td>Air-water partition coefficient (K_{AW}) (unitless)</td><td colspan="3">7.96×10^{-8} (log K_{AW} = -7), estimated</td><td>(Mathur, 2002, DP Barcode 285692)
Estimated from vapor pressure at 25°C and water solubility at 20°C.
Non-volatile from surface water.</td></tr>
<tr><td rowspan="6">Organic-carbon normalized Freundlich Solid-Water Distribution Coefficient (K_{FOC}) in $(mg/L)(mg/kg)^{-1/n}$</td><td>Soil/Sediment</td><td>K_F</td><td>K_{FOC}</td><td rowspan="6">MRID 45405216.Supplemental. Kd and K_{OC} were not previously calculated. The Freundlich exponent ranged from 0.71 to 0.89 and the equilibrium concentration could have an impact on the resulting sorption</td></tr>
<tr><td>Sand/loamy sand</td><td>28</td><td>1110</td></tr>
<tr><td>Sandy loam</td><td>7.6</td><td>507</td></tr>
<tr><td>Loamy sand</td><td>6.5</td><td>594</td></tr>
<tr><td>Loamy sand</td><td>3.9</td><td>987</td></tr>
<tr><td>Loam</td><td>3.3</td><td>655</td></tr>
</table>

Parameter	Value[1]			Source/ Study Classification/ Comment
Freundlich solid-water distribution coefficients (K_F) in (mg/L)(mg/kg)$^{-1/n}$ Freundlich Exponent (1/n)	Sandy clay loam	26	776	coefficient. The coefficient of variation for K_{FOC} and K_F were 90% and 30%, respectively.
	Mean	13	772	
	CV	90	30	
Steady State Bioconcentration Factor (BCF) L/kg-wet weight fish	**Species**	**BCF**	**Depuration Half-Life**	MRID 45405007. Acceptable. Based on total radioactivity. Value reflects total radioactivity. Rapid depuration with half-life of 1 day.
	Rainbow Trout (*Oncorhynchus mykiss*)	70	1.0-day half-life	

CV=Coefficient of Variation

[1] All estimated values were calculated according to "*Guidance for Reporting on the Environmental Fate and Transport of the Stressors of Concern in Problem Formulations for Registration Review, Registration Review Risk Assessments, Listed Species Litigation Assessments, New Chemical Risk Assessments, and Other Relevant Risk Assessments*" (USEPA, 2010).

Table 3-2 summarizes representative degradation half-life data and time to 50% and 90% loss (DT_{50} and DT_{90}) for boscalid that were determined to be appropriate for the current analysis. In laboratory studies, the primary routes of degradation are anaerobic aquatic metabolism (DT_{50} 284-320 d), and aerobic soil metabolism (aerobic DT_{50} 390-680 d). Some studies previously used in the fate analysis were reclassified to be supplemental and still had uncertainties in the unextracted residues and thus, were not included in the fate summary (additional details will be discussed below). The rate of degradation from aerobic soils for boscalid is classified persistent using the Goring persistence scale (Goring *et al.*, 1975). Based on previously submitted studies boscalid is stable to hydrolysis, aqueous photolysis, and soil photolysis (1 soil). In aerobic aquatic metabolism (2 pond systems) studies, DT50 values ranged from 545-days to essentially stable and anaerobic aquatic metabolism DT50 values range from 284 to 320 days.

Current recommended NAFTA degradation kinetics calculations were not available in previous studies and degradation kinetics for previously completed studies were updated to using current recommended procedures. Previously EDWCs were calculated with and without unextracted residues. Unextracted residues were considered because a range of polar and nonpolar solvents used for extracting residues were not explored to determine if the amount of unextracted residues could potentially be available for exposure.

The unextracted residue guidance recommends the use of three solvents in the extraction procedures of laboratory studies: one polar solvent with dielectic constants between 18 to 80, one polar solvent with a lower dielectic constant between 6.0 to 9.1; and one nonpolar solvent with dielectic constants between 1.9 to 4.8 (USEPA, 2014c). A new aerobic soil (MRID 50564601) and anaerobic aquatic (MRID 50564602) study were received since the last drinking water assessment was completed. These new studies utilized a range of polar and nonpolar solvents and collectively a weight of evidence exists to determine that unextracted residues are not available for exposure for these new studies.

The summary of solvents used in laboratory studies is available in **Appendix B**. While the unextracted residues in the new studies are not an uncertainty, there is still some uncertainty associated with the previously submitted aerobic soil and anaerobic aquatic metabolism studies. The extraction solvents used in previous studies (MRID 45643802, MRID 45405208, & MRID 45405213) included methanol and methanol: water 1:1 only. Newly submitted studies included six extraction steps for time points where unextracted residues began to increase. An additional 10 to 15% applied radioactivity (AR) (~1/5 to ½ of the max unextracted residues observed in the study were removed in the later extraction steps, which included ethyl acetate and hexane).

The newly submitted aerobic soil metabolism study (MRID 50564901) had a maximum amount of 27% unextracted residues and a DT_{50} of 680-days. The previously completed aerobic soil metabolism studies, using mainly methanol and water as extraction solvents, had maximum unextracted residues ranging from 24 to 45% applied radioactivity with DT_{50} values ranging from 90 to 562-days. There is uncertainty in whether some of the unextracted residues of the previously completed studies as a range of solvents were not used in those studies; however, if we only rely on data from the new study, modeling may be overly conservative as a threefold uncertainty factor would be applied. Therefore, it was decided to consider the aerobic soil metabolism study results with the unextracted residues in the same range as those observed in the newly submitted study for use in modeling. These studies had DT_{50} values of 390 and 562-days and have similar results to the result observed in the new study. Previously submitted aerobic soil metabolism studies with greater than 30% unextracted residues were considered to be uncertain.

The newly submitted anaerobic aquatic metabolism study had a maximum of 51% unextracted residues and a DT_{50} of 284-days. While the previously submitted anaerobic aquatic metabolism, study did not use a range of solvents, the maximum unextracted residues of 55% were similar to the newly submitted study and the DT_{50} is 320-day, longer than the newly submitted study. While there is uncertainty in the unextracted residues in this study, this study was still included in the fate analysis.

Acetonitrile and acetonitrile: water 1:1 were the extraction solvents utilized in the previously submitted aerobic aquatic metabolism study (MRID 45405214) and unextracted residues were below 13.5% applied radioactivity. The DT_{50} values ranged from 545-days to essentially stable Therefore, unextracted residues were not a major uncertainty in the aerobic aquatic metabolism study.

Table 3-2: Summary of Environmental Degradation Data for Boscalid

Study	System Name/ Characteristics	Kinetics Model Fitted Value		Representative Half-life --Used to Derive Model Input (days)[2]	Source/ Study Classification/ Comment
		DT50 (days)	DT90 (days)		
Abiotic Hydrolysis	pH 4, 7, 9 (25°C)	Stable			MRID 45405205. Acceptable. Does not hydrolyze.
Atmospheric Degradation	Hydroxyl Radical	1 day			Estimated Using EPIWeb Version 4.1. Appendix A
Aqueous Photolysis	pH 5, 22°C, 40°N sunlight	Stable			MRID 45405206. Acceptable. Adjusted for sunlight intensity at 40°N latitude.
Soil Photolysis	pH 7.3, 22°C, 40°N sunlight	Stable			MRID 45405207. Acceptable. Adjusted for sunlight intensity at 40°N latitude.
Aerobic Soil Metabolism	ID Clay loam, (27°C pH 6.8)	562	2137	678 DFOP	MRID 45643802, Acceptable. Replicate data were not available for all time points. While there is some uncertainty in the unextracted residues for the ID clay loam and IL silt loam, unextracted residues reached a maximum of 26%, and the results are similar to MRID 50564901, without uncertainties in the unextracted residues.[3]
	IL Silt loam, (27°C pH 6.5)	390	1297	390 SFO	
	ND Sandy clay loam, (20°C, pH 8.1)	680	2257	680 SFO	50564901[N], Supplemental; maximum amount of 27% unextracted residues
Aerobic Aquatic Metabolism	German Loamy sand pond, (20°C, water pH 8.5, sediment pH 6.8)	545	1810	545 SFO	45405214, Supplemental; System was flooded prior to addition of the parent compound. However, boscalid was essentially stable in the test system.
	German Loam pond-like, (20°C, water pH 8.1, sediment pH 7.5)	Essentially Stable		1.38×10^{33} SFO	
Anaerobic Aquatic Metabolism	Pond water: sediment (20°C, water pH 8.4, sediment pH 7.3)	320	2774	1060 DFOP	45405213, Acceptable; Half-life reflects formation of unextracted residues. See text above table for additional information.
	Golden lake water: loamy, ND	284	1562	470 IORE	50564902[N], Supplemental

Study	System Name/ Characteristics	Kinetics Model Fitted Value		Representative Half-life --Used to Derive Model Input (days)[2]	Source/ Study Classification/ Comment
		DT50 (days)	DT90 (days)		
	(20°C, water pH 7.9, sediment pH 8.3)				

SFO=single first order; DFOP=double first order in parallel; IORE=indeterminate order (IORE); SFO DT_{50}=single first order half-life; T_{IORE}=the half-life of an SFO model that passes through a hypothetical DT_{90} of the IORE fit; DFOP slow DT_{50}=slow rate half-life of the DFOP fit.
Studies designated with an N value were submitted after the problem formulation was complete.
[1] The value used to estimate a model input value is the calculated SFO DT_{50}, T_{IORE}, or the DFOP slow DT_{50} from the DFOP equation. The model chosen is consistent with that recommended using the, *Guidance for Evaluating and Calculating Degradation Kinetics in Environmental Media* (NAFTA, 2012; USEPA, 2015a).
[2] Study was determined to be supplemental mainly due to the presence of unextracted residues and the individual study did not use the range of recommended solvents; however, based on the weight of evidence across studies, it was determined that the unextracted residues may be assumed to be unavailable for exposure.
[3] For MRID 45643802, the CA Clay loam and ND loam soils had unextracted residues greater than 30% and are likely overestimate degradate rates. Results for MRID 45405208 are not used quantitatively due to uncertainty in the unextracted residues and only one replicate was utilized in the study.

Transformation products resulting from the environmental degradation of boscalid are listed below.

- **M510F47:** 2-chloronicotinic acid
- **M510F49:** (2-hydroxy-N-(4’-chlorobiphenyl-2-yl)-nicotonamide)
- **M510F50:** Unknown 2
- **M510F01:** 2-Chloro-N-(4'-chloro-5-hydroxy-[1,1'-biphenyl]-2-yl)nicotinamide
- **M510F62:** 4'-Chloro-[1,1'-biphenyl]-2-amine

In previous studies there was one major degradate M510F49 (2-hydroxy-N-(4’-chlorobiphenyl-2-yl)nicotinamide))[2] and one minor degradate M510F47 (2-chloronicotinic acid)[3] were observed in aerobic soil metabolism studies. M510F47 is similar to a degradate (6-chloronicotinic acid) that occurs with the neonicotinoid insecticides (acetamiprid and imidacloprid) and a butenolide insecticide (flupyradifurone). The degradate M510F49 was classified as a major degradate in one soil sample (MRID45643802) with a maximum amount of applied radioactivity associated with it being 14.4%; its aerobic soil metabolism half-life was estimated as 1.7 days. The two degradates observed in the aerobic soil metabolism studies were also found in most terrestrial field dissipation studies. All other boscalid degradates were classified as minor degradates. Known degradates were not included in the exposure calculations in previous risk assessments because they occurred in small amounts and were not expected to significantly alter EECs.

Additional information on the degradates are in the discussion of the residues of concern section and in **Appendix C**.

[2] Observed in all five soils.
[3] Observed in four of five soils.

Table 3-3 summarizes data from the terrestrial field dissipation studies. Terrestrial field dissipation studies have been conducted on several U.S. sites on various cropped (peach/almond) and bare ground plots, and on bare ground plots in Canada. Dissipation half-lives ranged from 1.0 to greater than 360 days, and carryover of residues was observed at all 14 sites from one application to the next, and from year to year. Most boscalid was observed in the top soil layer, however boscalid was also detected at the deepest depth sampled (45 cm) at 2 of 14 sites. The two degradates observed in the aerobic soil metabolism studies (2-chloronicotinic acid and 2-hydroxy-N-(4'-chlorobiphenyl-2-yl) nicotinamide) were also found in most terrestrial field dissipation studies.

Table 3-3: Summary of Terrestrial Field Dissipation Data for Boscalid

Site	System Name/ Characteristics	Half-life		Kinetic Equation	Deepest Core Boscalid Found (cm)	Reference or (MRID #), Study classifications and comment
		DT50 (days)	DT90 (days)			
Georgia, Sandy Loam	Bare plot	264	877	SFO	15-30	45405218. Supplemental. Applications were made direction to the bare soil between orchard/vineyard rows at all three test sites (bare ground plots) and to the orchard canopy at the Georgia and California test sites.
	Cropped (peach) plot	282	937	SFO	7.5-15	
New York, Loamy sand	Bare plot	356	1183	SFO	7.5-15	
California, Sandy loam	Bare plot	150	498	SFO	30-45	
	Cropped (almond) plot	>360	NA	SFO	15-30	
New Jersey, Loam soil	Bare plot	108	359	SFO	30-45	45405219. Acceptable.
	Turf plot	44	146	SFO	0-15	
Illinois, Silt loam	Bare plot	244	811	SFO	7.5-15	
	Turf plot	155	515	SFO	15-30	
Texas, Sandy loam	Bare plot	143	475	SFO	7.5-15	
	Turf plot	108	359	SFO	0-15	
California, Sandy loam	Bare plot	77	256	SFO	7.5-15	45405220. Acceptable.
Idaho, Loam soil	Bare plot	333	1106	SFO	7.5-15	
Florida, Fine sand	Bare plot	27	90	SFO	30-45	
North Dakota, Silt clay	Bare plot	1	3.32	SFO	0-7.5	45405221. Acceptable. High variability in measured concentrations.
Colorado, Loam soil	Bare plot	119	395	SFO	7.5-15	
Ontario, Brant soil series	Bare plot	30	100	SFO	7.5-15	45405222. Supplemental. High variability in measured concentrations.
Manitoba, Clay loam	Bare plot	316	1050	SFO	7.5-15	
Alberta, PGL soil association	Bare plot	372	1236	SFO	0-7.5	

PGL=Peoria-Gage-Landry

4 Residues of concern

The Metabolism Assessment Review Committee (MARC) reported that the residue of concern for boscalid in drinking water is the parent compound only (Nelson *et al.*, 2003). The 2010 "*Tier I Drinking Water Assessment for Boscalid used as seed treatment on Rapeseed (cultivars, varieties, and/or hybrids, including canola and crambe)*" was conducted for boscalid and unextracted residues (Lieu, 2010, D380018). The previous assessment considers boscalid plus unextracted residues, and parent boscalid only, in order to bracket the uncertainty caused by the presence of high amounts of unextracted residues in fate studies. The current assessment considers parent boscalid only because the uncertainty in the potential exposure to unextracted residues was resolved with the newly submitted fate data. See fate and transport characterization discussion for additional details. New degradates that were not previously identified were observed in new fate studies; however, they are all present at less than 2% applied radioactivity and are also not likely to substantially change the EDWCs.

5 Drinking Water Exposure Modeling

5.1 Models

EDWCs in surface water were determined using the Pesticides in Water Calculator (PWC v1.52), comprised of a user interface, a field model (Pesticide Root Zone Model; PRZM v.5.02), and a water body model (Variable Volume Water Model; VVWM v.1.02). The models generate multi-decadal daily concentration time series and corresponding 1-in-10-year daily average, 1-in-10-year annual average, and 30-year average EDWCs of boscalid in surface water bodies adjacent to application sites receiving runoff and spray drift. The index reservoir conceptual model for surface water assumes a standard 172.8 ha watershed that drains into an adjacent drinking water "index" reservoir of 5.26 ha surface area, and a mean depth of 2.74 m. A more detailed description of the index reservoir and its watershed can be found in Jones *et al*. (USEPA, 1998).

The latest version of PWC also utilizes PRZM to estimate potential concentrations of boscalid in groundwater sources of drinking water. Groundwater modeling simulates leaching through the soil profile to generate a groundwater concentration daily time series file, with maximum and post-breakthrough average concentrations being the main output products. Pesticide soil sorption and degradation during vertical transport are simulated. The aerobic soil biotic degradation rate is assumed to decline linearly with distance from the surface, to a value of zero at soil depth of one meter. Hydrolysis by contrast is assumed to proceed at a depth-invariant rate throughout the soil profile. Model output concentrations represent a vertical average of depth-variable concentrations in the simulated aquifer, from the water table to the bottom of the well screen. Currently, six scenarios of vulnerable soil are used for groundwater modeling.

Descriptions, documentation, and links for running EFED's exposure models can be found at: https://www.epa.gov/pesticide-science-and-assessing-pesticide-risks/about-water-exposure-models-used-pesticide.

5.2 Input Parameters

Model input parameters were developed in accordance with the EFED *Guidance for Selecting Input Parameters in Modeling the Environmental Fate and Transport of Pesticides*, Version 2.1, NAFTA degradation kinetics guidelines, and PRZM-GW input parameter guidance (USEPA, 2009; USEPA, 2014a; USEPA, 2015b; USEPA and Health Canada, 2012). Physical/chemical properties and environmental fate source data from submitted studies were presented previously in **Table 3-1**. New fate data (aerobic soil and anaerobic aquatic metabolism studies) were submitted for this assessment. Some studies previously used in the fate analysis were reclassified to be supplemental and still had uncertainties in the unextracted residues and were not included in the fate summary. Therefore, data was used form selected results to develop the model inputs. See Section 3 for a description on why selected soil systems were assumed to be useful in modeling. The updated model input values calculated for the chemical tab are shown in **Table 5-1.**

Table 5-1: PWC Input Parameters for Boscalid Modeling

Parameter (units)	Value (s)	Source	Comments
K_{OC} (mL/g)	772	MRID 45405216, 45405217	Average of 6 values for parent. The K_{FOC} was utilized because K_d and K_{oc} were not previously calculated. Coefficient of variation is 30% for the K_{FOC} versus 90% for K_F. The Freundlich exponent ranged from 0.71 to 0.89 and the equilibrium concentration could influence the sorption coefficient.
Water Column Metabolism Half-life (days) at 20°C	0	MRID 45405214	Boscalid was essentially stable in both systems.
Benthic Metabolism Half-life (days) at 20°C	1673	MRID	Represents the 90 percent upper confidence bound on the mean of 2 representative half-life values from anaerobic aquatic metabolism studies.
Aqueous Photolysis Half-life (days)@ pH 5 (stable)	0	--	Boscalid was essentially stable to photolysis.
Hydrolysis Half-life (days)	0	MRID 45405205	Boscalid was essentially stable to hydrolysis.
Soil Half-life (days) at 27°C	668	MRID 45643802 50564901	Represents the 90 percent upper confidence bound on the mean of 3 representative half-life values from aerobic soil metabolism studies. The temperature of one value was converted from 20°C to 27°C.
Foliar Half-life	0	--	No Data
Molecular Weight (g/mol)	343.21	--	--

Parameter (units)	Value (s)	Source	Comments
Vapor Pressure (Torr) at 25ºC	2×10^{-8}	(Mathur, 2002, DP Barcode 285692)	Vapor pressure for parent
Solubility in Water (mg/L)	4.64	(Mathur, 2002, DP Barcode 285692)	20ºC and measured value for parent

Standard PWC surface water and groundwater scenarios were used in modeling. Maximum application rates were simulated as recommended on the labels. Application dates were chosen to occur in the wettest month within the recommended application window for each scenario when the crop was on the field. Use pattern and application timing assumptions are shown in **Table 5.2**. Standard assumptions were made for the application efficiency (0.99 for ground applications and 0.95 for aerial applications) and spray drift (0.066 for ground applications and 0.135 for aerial applications) based on the most recent EPA guidance (USEPA, 2013). Applications were assumed to occur "above the crop".

5.3 Modeling Results

Modeling results are presented in **section 5.3** with maximum EDWCs given in bold. Output files for both surface water and groundwater are provided in **Appendix D**. The default percent cropped area (PCA) of 1.0 was used according to the guidance titled "*Development and Use of Community Water System Drinking Water Intake Percent Cropped Area Adjustment Factors for use in Drinking Water Exposure Assessments: 2014 Update* (USEPA, 2014a) because boscalid has use patterns across agricultural, residential, and commercial use sites. PCAs are applied to concentrations generated for surface water only.

5.3.1 Surface Water Exposure

The highest EDWCs were calculated for simulations of applications to ornamentals (0.70 lbs a.i./A applied 3x for a total of 2.10 lb a.i./A/year). The scenarios that provided the highest 1-in-10-year daily average, 1-in-10-year annual average, and 30-year simulation average are highlighted in bold in **Table 5-2**.

Table 5-2: Summary of Estimated Drinking Water Concentrations of Surface Water for Boscalid

Use	PWC Scenario	Application Type	Application Dates	Use Rate, Applications, Retreatment Interval	Concentrations (μg/L)[1]		
					1-Day mean (Acute)	Annual Mean (Chronic)	Overall Mean (Cancer)
Ornamentals	**CAnurserySTD**	Aerial	**3/1, 3/8, 3/15**	0.70 lbs. a.i./A (0.78 kg/ha) 3x, 7 days, Foliar	66.7	**56.8**	**35.7**
	FLnurserySTD		**6/1, 6/8, 6/15**		**88.7**	24.7	14.4
	MInurserySTD		9/1, 9/8, 9/15		48.9	25.5	19.4
	NJnurserySTD		3/15, 3/22, 3/29		60.3	23.2	16
	ORnurserySTD		12/1, 12/8, 12/15		61.3	33.8	24
	TNnurserySTD		3/16, 3/23, 3/30		63.1	21.1	12.5
	ORchristmas trees		12/1, 12/8, 12/15		61.9	44.5	36
Turf	FLturf	Ground	9/1, 9/15, 9/29, 10/12, 10/26, 11/9	0.35 lbs. a.i./A (0.39 kg/ha)6x,14 days, Ground	36.2	26.4	19.2
	PAturf		**5/1, 5/15, 5/29, 6/12, 6/26, 7/9**		**63.1**	**51.6**	**28.7**

Bold values indicate maximum concentrations for each use pattern. All values represent residues of parent alone.

5.3.2 Groundwater Exposure

Groundwater EDWCs were calculated for the six standard PWC groundwater scenarios. Ground water modeling results for boscalid are provided in **Table 5-3.** The range of highest daily and post-breakthrough average concentrations range from 18.1 to 470 μg/L and 16.6 to 436 μg/L, respectively and resulted from simulations for ornamentals. Three scenarios had to be simulated for 100 years to get throughputs[4] greater than 1.0.

[4] When estimating concentrations in groundwater, the simulation is initially run for 30-years. When throughputs are less than one, the simulation is extended to 100-years. Once throughputs are greater than one, the concentrations in groundwater will remain relatively constant. When throughputs are less than one, concentrations will continue to increase over time. A "throughput" is the number of void volumes in the vadose zone that must be flushed through to get the main pulse of contaminant into the saturated zone. For a simulation with one application, this is the time right before the first peak of the concentration occurs. This does not indicate that it takes 100-years for the chemical to move into groundwater.

Table 5-3: Estimated Groundwater Concentrations of Boscalid

Use Pattern, App Rate, # of Apps, RTI	Scenario	Break-through Time (years)	Concentrations in µg/L		
			Highest Daily	Post Breakthrough Average	Simulation Average
Ornamentals 0.70 lbs. a.i./A (0.78 kg/ha), 3x, 7-day	Florida Central Ridge	23	263	261	125
	Florida, Jacksonville[3]	40	18.1	16.7	12.3
	Georgia[3]	36	106	99.2	67.1
	North Carolina Coastal Plain	24	276	271	95.3
	Delmarva	28	170	158	36.5
	Wisconsin, Central sand region[3]	34	**470**	**436**	**301**

[1]Bold values indicate maximum concentrations and are recommended for use in the human health risk assessment· All values represent residues of parent alone.

[2] These scenarios are regional vulnerable sites for groundwater evaluation.

[3] Simulation extended to 100-years.

6 Water Monitoring

The Water Quality Portal ((http://www.waterqualitydata.us/portal.jsp)) was searched for monitoring information for boscalid in June 2019. Results from monitoring are summarized in **Table 6-1**.

In the Water Quality Portal, there were 737 reported detections (13%) of boscalid out of 6,592 surface water samples collected between 2002 and 2018 with the maximum detection of 36 µg/L. There were 4,152 groundwater samples collected between 2000 and 2018 and analyzed for boscalid with a maximum detected concentration of 2.12 µg/L. There were 23 (0.5%) detections reported. The limit of detection ranged from 0.020 to 0.05 µg/L. It is unknown whether samples were collected in areas where boscalid is used and this monitoring is unlikely to reflect the potential range of exposure concentrations in surface water and groundwater.

Boscalid has also been detected in soil at concentrations ranging from 6.66 to 274 µg/kg-soil and 0.3 to 45 µg/kg-sediment. The minimum reporting limit for soil and sediment ranged from 1.2 to 1.7 ug/kg.

Two studies were found in the open literature, in which boscalid was monitored in surface and groundwater. Reilly *et al*. (2012) analyzed for boscalid in first-order streams, ponds, and shallow groundwater (< 10 m from the surface) draining agricultural areas of the United States with intense fungicide use. Sites were chosen based on fungicide use on potatoes. Twelve surface water and 12 groundwater sites were sampled in Maine, Idaho, and Wisconsin for several fungicides and other current use pesticides every three weeks from three weeks after the first application to after harvest (7 sampling events per site). All samples were grab samples collected from the center of flow, or vertically integrated from a point within four feet of the water's edge in the case of a pond sample. Shallow groundwater wells were located in the field with samples taken near the water table. Sampled surface water watershed areas ranged from 7 to 20,589 hectares. Samples were filtered (0.7 µm glass fiber filter) prior to extraction. Boscalid was detected in 72% of surface water samples, with a maximum detected concentration of 0.11 µg/L. Boscalid was detected in 62% of groundwater samples with a maximum detected concentration of 2.120 µg/L. The maximum groundwater concentration was 19-fold greater (2120/110) than the maximum boscalid concentration detected in surface water.

Smalling and Orlando (2011) collected water and sediment (both bed and suspended) from January 2008 through October 2009 from 12 locations within three of the largest watersheds along California's Central Coast (Pajaro, Salinas, and Santa Maria Rivers) and analyzed for a suite of pesticides including boscalid. Water samples were collected from estuaries and major tributaries during four storm events and 11 dry season sampling events between 2008 to 2009. The sites included the following station names: Monterrey drainage ditch, Watsonville Slough, Pajara River below Thurwatcher, Pajaro River estuary upper, Pajaro river estuary lower, Blanco drain, Salinas River at Davis Road, Salinas River estuary upper, Salinas river estuary lower, lower Orcutt Creek, Santa Maria River estuary upper, and Santa Maria River estuary lower. Water samples were filtered prior to extraction (0.7 µm glass fiber filter). Boscalid concentrations were generally higher in samples taken during winter storm events than those taken during the dry summer season. Boscalid was detected in 85% of samples, at a maximum concentration of 36 µg/L.

Predicted boscalid surface water EDWCs using EFED modeling ranged from 14 to 89 µg/L. Maximum modeling and monitoring results are within a similar range. Monitored concentrations are unlikely to represent peak concentrations. Additionally, the use and site parameters modeled are different than what occurred at sites where samples were collected for monitoring.

Predicted boscalid concentrations in groundwater ranged from 18 to 470 µg/L, while the maximum detected concentration in groundwater was 2.12 µg/L (Reilly *et al.*, 2012). Groundwater monitoring occurred after just two applications, whereas the boscalid modeling results reflect 30-100 years of repeated application. Boscalid was detected in the samples in the same year in which it was applied to the field. Therefore, the sampled concentrations may not reflect maximum groundwater concentrations that may occur if boscalid was used for multiple years. While monitored groundwater concentrations were generally lower than monitored surface water concentrations, in the study wherein both surface water and groundwater sampling occurred, detected groundwater concentrations exceeded surface water concentrations. This result is consistent with what was predicted using tier I modeling. Additionally, surface water modeling for boscalid is available for more sites than groundwater monitoring. Finally, the use and site parameters modeled are different than what occurred at sites where samples were collected for monitoring and the monitoring results and modeling results are not expected to be similar.

Table 6-1: Surface Water Monitoring Results for Boscalid

Sites (Dataset Source)	Year	Study Type	Maximum Conc. (µg/L)	Detection frequency (Detects/samples)	Limit of Detection µg/L	Source
Surface Water						
ID, ME, and WI streams and pond (potato)	2009-2012	Targeted to fungicide use areas	0.11	72%	0.009 – 0.012	(Reilly *et al.*, 2012)
California Streams and Estuaries	2008-2009	Non-targeted	36 (wet) 0.64 (dry)	85%	0.005	(Smalling and Orlando, 2011)
Water Quality Portal	2002-2018	Non-targeted	36	75% (724/5724)	0.020 – 0.05	Water Quality Portal
Groundwater						
ID, ME, and WI (potato)	2009-2012	Targeted to fungicide use areas	2.12	62%	0.009 – 0.012	(Reilly *et al.*, 2012)
Water Quality Portal	2002-2018	Non-targeted	2.12	13% (23/4151)	0.3 – 0.05	Water Quality Portal

Det.=detection or reporting limit; Conc=concentration

Atmospheric samples were collected in an intensive farming area (Strasbourg, France) in April and May in 2007 and analyzed for 71 current use pesticides (Schumer *et al.*, 2009). Boscalid was detected in 10 of 10 samples at concentrations ranging from 0.35 to 0.81 ng/m^3. The average concentration was 0.53 ng/m^3. Boscalid residues were associated with both atmospheric particles and the gas phase. These results are summarized in **Table 6-2**.

Table 6-2: Summary of Air Monitoring Studies for Boscalid (10 samples)

Location	Average Concentration (ng/m^3)	Maximum Concentration (ng/m^3)	Frequency of Detections	Limit of Det. (pg/m^3)	Date	Source
Strasbourg, France	0.53	0.81	100%	27.3	2007	(Schumer *et al.*, 2009)

Det.=detection or reporting limit

7 Drinking Water Treatment Effects

The EDWCs in this assessment are representative of concentrations in drinking water source water (pre-treatment). For surface water, the conceptual model assumes that a pesticide reaches surface water via spray drift and/or surface runoff and then is completely mixed throughout the water column. Since boscalid is stable to hydrolysis, the compound is not expected to degrade abiotically during the time that elapses between intake and distribution to the consumer's tap. Data also shows that boscalid is stable to aqueous photolysis; therefore, if ultraviolet light were used as a means of disinfection, degradation of boscalid would not be expected to occur.

The most successful drinking water treatment process for removal of pesticides from drinking water is thought to be treatment with granular activated carbon (GAC), which is mainly used in larger drinking water treatment facilities (USEPA, 2011). Data on the sorption of boscalid to GAC are not available; however, some loss of boscalid due to sorption is expected if GAC is used in drinking water treatment.

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Appendix A. AOPwin output

SMILES: c1ccc(c(c1)c2ccc(cc2)CL)NC(=O)c3c(nccc3)CL
CHEM :
MOL FOR: C18 H12 CL2 N2 O1
MOL WT : 343.21
------------------- SUMMARY (AOP v1.92): HYDROXYL RADICALS (25 deg C) --------
Hydrogen Abstraction = 0.0000 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
**Addition to Aromatic Rings = 9.1458 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 9.1458 E-12 cm3/molecule-sec
HALF-LIFE = 1.169 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 14.034 Hrs
.... ** Designates Estimation(s) Using ASSUMED Value(s)
------------------- SUMMARY (AOP v1.91): OZONE REACTION (25 deg C) -----------

****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database: NO Structure Matches

Appendix B. Methiozolin Solvent Solubility and Solvents Utilized in Laboratory Studies

Table B- 1. Summary of Solvents Used in Laboratory Studies

Study	Reference or (MRID #), Study Classification and Comments	Solvents	Max Unextracted
Soil Photolysis	45405206[1], Acceptable	Samples were analyzed directly. No extraction or clean up concentration methods were used.	--
Aerobic Soil Metabolism	45643802, Acceptable	2-3x methanol 1-3x methanol: water 1:1	23.8% 25.7%
	45405208, Supplemental	3x methanol 3x methanol: water 1:1	32.7%
	50564901, Supplemental	2x Methanol 1x 0.1M Formic acid in methanol. 1x Methanol: water 1:1 1x 0.1M Na_2CO_3 in methanol 1:1 1x Ethyl acetate 1x Hexane - Removed 3% in the ethyl acetate and hexane extractions combined and ~13% in extract 4 -8.	27%
Anaerobic soil Metabolism	45405213, Acceptable;	1-3x methanol: water 1:1 2-3x methanol	55.1%
Aerobic Aquatic	45405214, Supplemental	3x acetonitrile:water 1:1 3x acetonitrile -Removed <0.7%AR total	Loamy Sand 13.4% Loamy pond-like 10.5%
Anaerobic Aquatic	45405213, Acceptable	1-3x methanol:water 1:1 2-3x methanol	50.7%
	50564902, Supplemental	Extract 1= Methanol. Extract 2 = Methanol. Extract 3 = 0.1M Formic acid in methanol. Extract 4 = Methanol:water (1:1, v:v). Extract 5 = 0.1M Na_2CO_3 in methanol (1:1, v:v). Extract 6 = Ethyl acetate. Extract 7 = Hexane. Removed ~10-15%% more with extract 5 - 7	

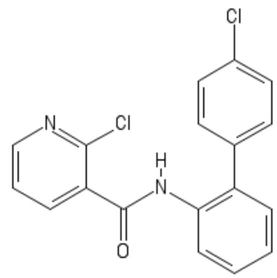
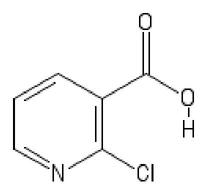
[1]Samples were analyzed directly; no extraction/cleanup/concentration methods were used.

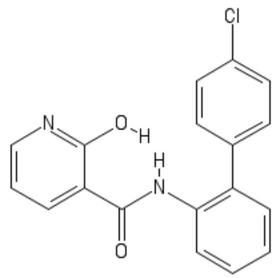
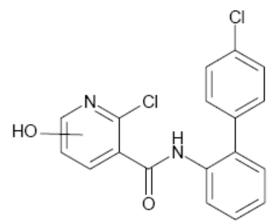
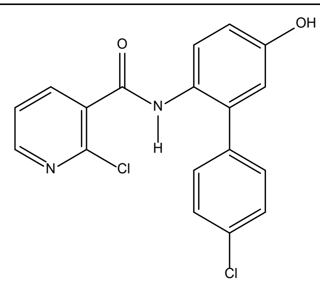
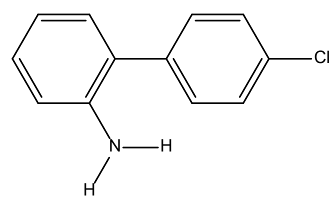
A summary of the solubility of boscalid in different solvents is provided in **Table B- 2**.

Table B- 2. Summary of Solubility Boscalid in Different Solvents

Solvent	Solubility (g/L)
acetone	16.0-20.0
acetonitrile	4.0 - 5.0
dichloromethane	20.2-25.0
N,N-dimethylformamide	> 25.0
ethylacetate	6.7 - 8.0
n-heptane	<1.0
methanol	
1-octanol	<1.0
olive oil	<1.0
2-propanol	<1.0
toluene	2.0 - 2.5

Appendix C. Boscalid and Its Environmental Transformation Products.[A]

Code Name/ Synonym	Chemical Structure	Study Type	MRID	Maximum %AR (day)		Final %AR (study length)
PARENT						
Boscalid, Nicobifen, BAS 510 F **IUPAC:** 2-chloro-N-(4'-chlorobiphenyl-2-yl)-nicotinamide **CAS Number:** 188425-85-6 **SMILES:** C1=CC=CC(=C1C2=CC=C(Cl)C=C2)NC(=O)C3=CC=CN=C3Cl **MW:** 343.21 g/mol		Parent				
TRANSFORMATION PRODUCTS						
M510F47 **IUPAC:** 2-chloronicotinic acid **CAS Number:** 2942-59-8 **Formula:** $C_6H_4ClNO_2$ **MW:** 157.55 g/mol **Smile string:** N1=CC=CC(=C1Cl)C(=O)O		Aerobic Soil	45643802	CL, CL, SCL, L	3.1 (371 d)	3.1 (371 d)
			50564901	SCL	NA	NA
		Anaerobic Aquatic	50564902	Lake	NA	NA
		Terrestrial Field	45405218	SL, SL, SL, SL, LS	<0.01	<0.01 mg/kg (360 d)
		Terrestrial Field	45405219	L, L, SiL, SiL, SL, SL	<0.01	<0.01 mg/kg (359 d)
		Terrestrial Field	45405220	FSL, L FS, LS	0.04 mg/kg (21 d)	<0.01 mg/kg (345 d)
		Terrestrial Field	45405221	SiL, L	0.022 mg/kg (1 d)	<0.01 mg/kg (429 d)
		Terrestrial Field	45405222	L, SiL, L	0.019 mg/kg (1 d)	<0.01 mg/kg (358 d)
M510F49 **IUPAC:** (2-hydroxy-N-(4'-chlorobiphenyl-2-yl)-nicotonamide); **Formula:** $C_{18}H_{13}ClN_2O_2$ **MW:** 324.77 g/mol **SMILES:** C1=CC=CC(=C1C2=CC=C(Cl)C=C2)NC(=O)C3=CC=CN=C3O		Aerobic Soil	45405208	SL	0.2 (364 d)	0.2 (364 d)
			45643802		14.4 (371 d)	14.4 (371 d)
			50564901	SCL	1.8% (0 d)	1.5% (350 d)
		Aerobic Aquatic	45405214	Loamy sand pond, Loamy pond-like	0	0

Code Name/ Synonym	Chemical Structure	Study Type	MRID	Maximum %AR (day)		Final %AR (study length)
		Anaerobic Aquatic	45405213	Pond Water	0	0
			50564902	Lake	1.8% (0 d)	1.4% (308 d)
		Terrestrial Field	45405218	SL, SL, SL, SL, LS	<0.01	<0.01 mg/kg (360 d)
		Terrestrial Field	45405219	L, L, SiL, SiL, SL, SL	<0.01	<0.01 mg/kg (359 d)
		Terrestrial Field	45405220	FSL, L FS, LS	0.04 mg/kg (21 d)	<0.01 mg/kg (345 d)
		Terrestrial Field	45405221	SiL, L	0.022 mg/kg (1 d)	<0.01 mg/kg (429 d)
		Terrestrial Field	45405222	L, SiL, L	0.019 mg/kg (1 d)	<0.01 mg/kg (358 d)
M510F50 Unknown 2		Aerobic Soil	45405208	SCL	0.2 (364 d)	0.2 (364 d)
		Anaerobic Aquatic	45405213	Lake	0	0
M510F01 **IUPAC:** 2-Chloro-N-(4'-chloro-5-hydroxy-[1,1'-biphenyl]-2-yl)nicotinamide **Formula:** $C_{18}H_{12}Cl_2N_2O_2$ **MW:** 359.21 g/mol **SMILES:** ClC1=C(C(N([H])C2=CC=C(O)C=C2C3=CC=C(Cl)C=C3)=O)C=CC=N1		Aerobic Soil	50564901	SCL	NA	NA
		Anaerobic Aquatic	50564902	Lake	1.1% (259 d)	ND (308 d)
M510F62 **IUPAC:** 4'-Chloro-[1,1'-biphenyl]-2-amine **Formula:** C12H10ClN **MW:** 203.67 g/mol **SMILES:** ClC(C=C1)=CC=C1C2=C(N([H])[H])C=CC=C2		Anaerobic Aquatic	50564902	Lake	1.5% (308 d)	1.5% (308 d)

Code Name/ Synonym	Chemical Structure	Study Type	MRID	Maximum %AR (day)		Final %AR (study length)
Unextracted Residues	Not Applicable	Aerobic Soil	45405208	SL	62.7 (266 d)	60.0 (364 d)
		Aerobic Soil	45643802	CL, CL, SCL, L	44.8 (371 d)	44.8 (371 d)
		Aerobic Aquatic	45405214	Loamy sand pond, Loamy pond-like	13.4 (100 d)	13.4 (100 d)
		Anaerobic Aquatic	45405213	Lake	55.1 (361 d)	55.1 (361 d)

[A] ND means “non-detected”, either below limit of detection. NR means “not reported”. AR means “applied radioactivity”. MW means “molecular weight”. Bolded values are laboratory study values >10%AR.

Appendix D. Representative Modeling Output for Surface Water and Groundwater

Summary of Water Modeling of Boscalid and the USEPA Standard Reservoir
Estimated Environmental Concentrations for Boscalid are presented in Table 1 for the USEPA standard reservoir with the FLnurserySTD_V2 field scenario. A graphical presentation of the year-to-year peaks is presented in Figure 1. These values were generated with the Pesticide Water Calculator (PWC), Version 1.52. Critical input values for the model are summarized in Tables 2 and 3. This model estimates that about 2.7% of Boscalid applied to the field eventually reaches the water body. The main mechanism of transport from the field to the water body is by runoff (82.7% of the total transport), followed by spray drift (15.3%) and erosion (1.98%). In the water body, pesticide dissipates with an effective water column half-life of 50.6 days. (This value does not include dissipation by transport to the benthic region; it includes only processes that result in removal of pesticide from the complete system.) The main source of dissipation in the water column is washout (effective average half-life = 50.6 days).
In the benthic region, pesticide dissipation is negligible (1218.1 days). The main source of dissipation in the benthic region is metabolism (effective average half-life = 1218.1 days). The vast majority of the pesticide in the benthic region (98.81%) is sorbed to sediment rather than in the pore water.

Table 1. Estimated Environmental Concentrations (ppb) for Boscalid.

Peak (1-in-10 yr)	89.7
4-day Avg (1-in-10 yr)	87.1
21-day Avg (1-in-10 yr)	81.1
60-day Avg (1-in-10 yr)	66.3
365-day Avg (1-in-10 yr)	24.7
Entire Simulation Mean	14.4

Table 2. Summary of Model Inputs for Boscalid.

Scenario	FLnurserySTD_V2
Cropped Area Fraction	1.0
Koc (ml/g)	772
Water Half-Life (days) @ 20 °C	0
Benthic Half-Life (days) @ 20 °C	1673
Photolysis Half-Life (days) @ 40 °Lat	0
Hydrolysis Half-Life (days)	0
Soil Half-Life (days) @ 27 °C	668
Foliar Half-Life (days)	0
Molecular Weight	343.21
Vapor Pressure (torr)	2.00E-08
Solubility (mg/l)	4.64
Henry's Constant	0.0

Table 3. Application Schedule for Boscalid.

Date (Mon/Day)	Type	Amount (kg/ha)	Eff.	Drift
6/1	Above Crop (Foliar)	0.78	0.95	0.135
6/8	Above Crop (Foliar)	0.78	0.95	0.135
6/15	Above Crop (Foliar)	0.78	0.95	0.135

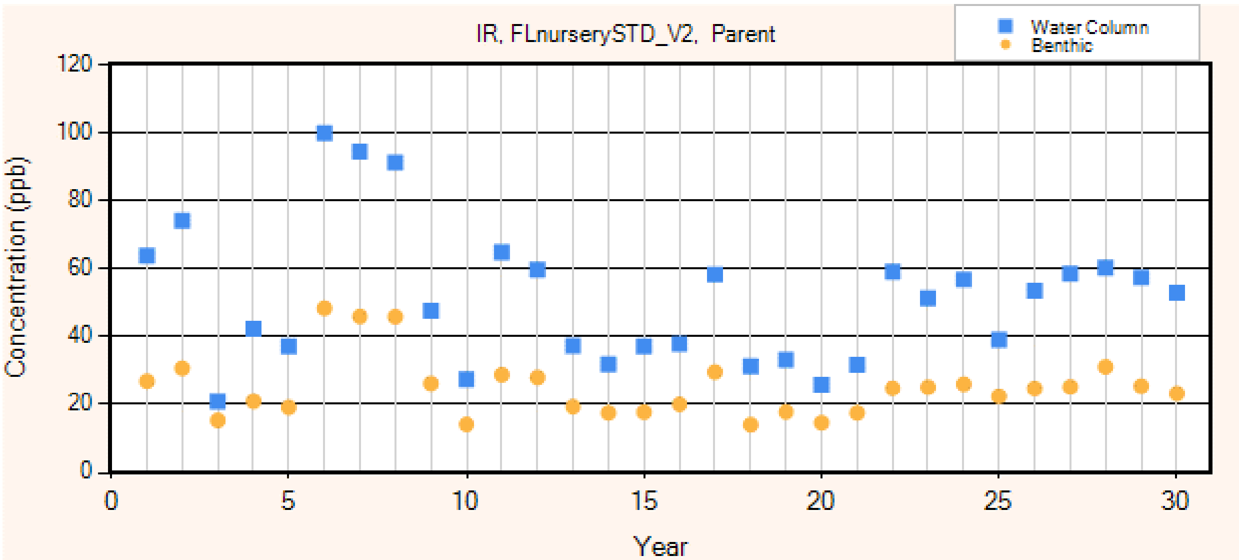


Figure 1. Yearly Peak Concentrations

Table D5. Summary of Groundwater Batch Output for 30-year Simulations

Groundwater Run ID	Peak	Breakthru	Thruput	PostBT Avg	Sim Ave
Delmarva	170.41	10130.6	1.081575	158.2044	36.46441
FL Potato	11.241	**-999999**	0.7506111	-999999	3.127061
FL Citrus	263.16	8460.455	1.295084	261.0685	125.8269
Peanuts	25.255	**-999999**	0.8407854	-999999	3.953142
NC Cotton	276.34	9101.501	1.203867	271.1015	95.34974
WI Sand	162.08	**-999999**	0.8868259	-999999	27.28253

Table D4. Summary of Groundwater Batch Output for 100-year Simulations

Groundwater Run ID	Peak	Breakthru	Thruput	PostBT Avg	Sim Ave
Delmarva	297.32	10339.92	3.49703	274.2648	204.2431
FL Potato	18.065	14553.97	2.484476	16.7565	12.26418
FL Citrus	297.24	8457.49	4.275382	275.4512	231.1686
Peanuts	106.38	12985.1	2.784653	99.25935	67.06194
NC Cotton	309.9	9245.676	3.910909	282.6658	226.4681
WI Sand	470.05	12351.68	2.927456	436.1772	301.6752