UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
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OFFICE OF CHEMICAL SAFETY
AND POLLUTION PREVENTION

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March 16, 2020

MEMORANDUM

SUBJECT: **Pethoxamid:** Drinking Water Exposure Assessment (DWA) for New Herbicide

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1. EXECUTIVE SUMMARY

The Environmental Fate and Effects Division (EFED) has completed the environmental fate and ecological risk assessment in support of the Section 3 New Chemical Registration of the herbicide pethoxamid (2-chloro-N-(2-ethoxyethyl)-N-(2-methyl-1-phenyl-1-propen-1-yl)acetamide; CAS Registry Number: 106700-29-2; PC Code: 090208).

Pethoxamid is an herbicide (pre-emergence and early post-emergence) proposed for control of most annual grasses and certain broad weeds in corn (field, sweet, and popcorn), soybean, cotton, turf (including sod farms), field-grown ornamentals, container-grown ornamentals, and non-crop areas including rights-of-ways, fence rows, production facilities, storage areas, parking areas, and airports (others are listed on the label). This compound is also proposed as a coating on dry granular fertilizer.

Pethoxamid is systemic uptake *via* roots and young shoots. The mode of action of the compound is the inhibition of very long chain fatty acids synthesis (VLCFA, cell division). It is formulated as an emulsifiable concentrate (EC) and two labels are currently proposed for this new chemical: F4044-2 and F4044-2 T&O. The proposed application methods include high and low volume ground and aerial spray. Both the maximum proposed annual and single application rates are 1.5 lbs a.i./A for all the proposed uses. The label specifies a maximum of two applications per year for spring weed control of corn (field, sweet, and popcorn), soybean, and cotton. For ornamentals, multiple applications are proposed if needed, with a proposed annual application rate of 1.5 lbs a.i./A.

Based on the decision of the residues of concern knowledge (ROCKs) committee (DP 442522), the parent molecule (pethoxamid) is the residue of concern (ROC). Therefore, in this assessment the analysis and EDWCs represent the potential exposure to only the parent. More details are provided in the following sections.

Table 1 shows the highest Estimated Drinking Water Concentrations (EDWCs) for pethoxamid across the proposed use patterns. The highest EDWCs were obtained by the MS corn scenario for surface water and therefore, are recommended for used by the Health Effects Division (HED). For surface water sources of drinking water, the acute 1-in-10-year daily average and chronic 1-in-10 year annual average EDWCs are 121 µg/L and 7.45 µg/L, respectively. The cancer 30-year average EDWCs is 2.71 µg/L. A percent crop area (PCA) of 100% was used because current labels include non-agricultural uses (*i.e.* ornamentals).

Table 1. Highest Estimated Drinking Water Concentrations (EDWCs) for Pethoxamid Across Proposed Uses

Use, Scenario	Application Rate lbs a.i./A (kg/ha)	EDWCs[1,2] in µg/L		
		Acute	Chronic	Cancer
All use patterns, MS corn STD Surface Water	One application: 1.5 lbs a.i./A (1.68kg/ha)	**121**	**7.45**	**2.71**
All use patterns, GW Del Marva Ground Water		0.188	0.129	0.129

[1]Bolded values are the recommended EDWCs for use in the Human Health and Effects (HED) drinking water assessment.

[2] For surface water modeling, the acute concentration is provided as 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.

2. USE CHARACTERIZATION

Based on the proposed labels, pethoxamid is formulated as an emulsifiable concentrate (EC) for application via ground or aerial equipment. It is not co-formulated with other pesticides. The end use products are proposed for use on corn (field, sweet, and popcorn), soybean, cotton, turf (including sod farms, residential, commercial, and institutional lawns and landscapes, golf courses, sod farms), field-grown ornamentals, container-grown ornamentals, and non-crop areas including rights-of-ways, fence rows, production facilities, storage areas, parking areas, airports, and others as listed on the proposed label. Pethoxamid is also proposed for use as a coating on dry granular fertilizer granules with restrictions for use on ammonium nitrate, potassium nitrate, sodium nitrate or powdered limestone. Proposed use patterns for pethoxamid products are summarized in **Table 2**. The maximum single and annual application rate for all the uses is 1.5 lb a.i./A. Proposed labels for pethoxamid have spray drift management language, including use of low drift nozzles, application height restrictions, wind speed restrictions, and application buffers in order to reduce the potential of spray drift to non-target areas from aerial applications. The information presented in Table 2 was provided in support of registration of Pethoxamid (PC code 090208) from the Registrant (FMC Corporation) to Registration Division (RD).

The labels do not specify minimum re-treatment interval (MRI) and/or the maximum single application rate for soybeans, corn or cotton when two applications are desired.

Table 2. Summary of the Proposed Labeled Use Patterns for Pethoxamid

Use site	Appl timing	Appl method	Appl rate (lbs a.i./A)	Max single app rate (lbs a.i./A)	Max # of Apps/Year	MRI	Label No.
Corn (field, sweet and pop)	Pre- and post-emerg	A and G	0.5-1.5	1.5	2	NS	F4044-2
Cotton	Pre- and post-emerg	A and G	0.5-1.5	1.5	2	NS	F4044-2
Soybean	Pre- and post-emerg	A and G	0.5-1.5	1.5	2	NS	F4044-2
Turf, sod, etc.	Pre- and post-emerg	A and G	1.0-1.5	1.5	NS	NS	F4044-2 T&O
Ornamentals container and field grown	Pre- and post-emerg	A and G	0.5-1.5	1.5	NS	NS	F4044-2 T&O
Non-crop land	Pre- and post-emerg	A and G	1.0-1.5	1.5	NS	NS	F4044-2 T&O
Dry-fertilizer coating	Pre- and post-emerg	A and G	NS	NS	NS	NS	F4044-2 & F4044-2 T&O

Symbols:
NS: Not Specified
Abbreviations
A=Aerial; App.=application; Broad=broadcast; Emerg=emergence; Equip.=equipment; G=ground boom; L=liquid; MRI=Minimum retreatment interval; PHI=preharvest interval; A=aerial; G=ground; AI=active ingredient; d=day.

3. ENVIRONMENTAL FATE

Table 3 below summarizes the physical chemical properties of pethoxamid. Pethoxamid has high water solubility (400mg/L) and based on its vapor pressure pethoxamid should exist in both vapor and particulate phases in the atmosphere (OPPTS Guideline 835.6100 classification system) and may volatilize from moist soil and water surfaces. Additionally, pethoxamid has a low octanol-water partition coefficient (log K_{ow}= 2.96) and bioconcentration factors (BCF) ranging between 28 – 32 L/kg with depuration rates of greater than 82% of the residues in fish after 56 days, therefore, the compound is not expected to bioaccumulate in aquatic food chains.

Pethoxamid's main route of degradation is aerobic soil metabolism, as it is relatively non-persistent (Goring *et al*., 1975 classification scheme) in the soils tested (half-lives ranged from 5 to 8 days). Also, the compound degrades through both aerobic and anaerobic aquatic metabolism with half-lives ranging from 7 to 13 days. Degradation studies indicated a significant amount of unextracted residues (25-76% of the applied radioactivity) that were further characterized in subsequent extractions. Solvents with different dielectric constants were used and even when harsh polar extractions were performed only 0.5-1.0% of the applied radioactivity was recovered. Uncertainties exist on whether the bound residues are parent or degradates. The degradation studies showed that while pethoxamid degrades, bound residues increased and degradates formed at low percentages of the applied which could indicate that the bound residues consist of parent. However, in later sampling intervals there are multiple degradates forming at low percent of the applied radioactivity (<%10) which can also indicate that the bound residues are a mix of parent and degradates.

Pethoxamid undergoes aqueous photolysis with an environmental half-life of 13.9 days and soil photolysis with a half-life of 79.6 days. This compound is stable in hydrolysis for all the pH values tested (*i.e*., pH 5, 7 and 9 at 50˚C). Pethoxamid is classified as moderately mobile, with an average organic carbon partition coefficient (K_{oc}) of 196 L/Kg (FAO scale). **Table 4** shows the environmental fate values and derived inputs for modeling.

Table 3. Summary of Physical-Chemical, Sorption, and Bioconcentration Properties of Pethoxamid

Parameter	Value[1]	Source/ Study Classification/ Comment
Molecular Weight (g/mole)	295.8	MRID 49813402. Acceptable.
Water Solubility at 20°C mg/L	400	MRID 49813402. Acceptable.
Vapor Pressure (torr)	2.8 x 10^{-3}Pa at 25˚C=2.1x10^{-5} torr	MRID 49813402. Should exist in both vapor and particulate phases in the atmosphere. Acceptable.
Henry's Law constant at 20°C (atm-m^3/mole)	8.35x10^{-7}	Estimated[1] from vapor pressure and water solubility at 20°C. Acceptable.

<table>
<tr><th>Parameter</th><th colspan="3">Value[1]</th><th>Source/
Study Classification/
Comment</th></tr>
<tr><td>Octanol-water partition coefficient (K_{ow}) at 25°C (unitless)</td><td colspan="3">2.96</td><td>MRID 49813402 Supplemental.
Not likely to bioconcentrate.</td></tr>
<tr><td>Air-water partition coefficient (K_{AW}) (unitless)</td><td colspan="3">3.3×10^{-11} (log K_{AW} = -11)</td><td>Estimated[1] from vapor pressure and water solubility at 20°C and pH 7.
Nonvolatile from water.</td></tr>
<tr><td rowspan="5">Soil-Water Distribution Coefficients (K_d in L/kg-soil or sediment)

Organic carbon normalized distribution coefficients (K_{oc} in L/kg-organic carbon)</td><td>Soil/Sediment</td><td>K_d</td><td>K_{OC}</td><td rowspan="5">MRID 49813406.
Acceptable.
Moderately mobile
(FAO classification system).</td></tr>
<tr><td>North Dakota Loam (3.8 % OC, pH 7.5)</td><td>8.66</td><td>228</td></tr>
<tr><td>California loam (0.9 % OC, pH 7.4)</td><td>1.75</td><td>195</td></tr>
<tr><td>Illinois Silt Loam (0.6 % OC, pH 5.8)</td><td>1.03</td><td>171</td></tr>
<tr><td>North Dakota Sandy Clay Loam (2.6 % OC, pH 6.8)</td><td>4.94</td><td>190</td></tr>
<tr><td rowspan="2">Steady State Bioconcentration Factor (BCF) L/kg-wet weight fish</td><td>Species</td><td>BCF</td><td>Depuration</td><td rowspan="2">MRID 49813442. Acceptable.
Identified degradates: MET-30, MET-42, and MET-47.</td></tr>
<tr><td>Rainbow trout</td><td>28 and 32 L/kg in whole fish</td><td>82.1% to 91.8 days depurated by 56 days</td></tr>
</table>

Table 4. Summary of Environmental Fate Properties and Values Used to Derive Model Input Values for Use in Exposure Assessments

Study	System Name/ Characteristics	Kinetics Model Fitted[1] Value		Representative Half-life --Used to Derive Model Input (days)[2]	Reference (MRID), Study Classification and Comments
		DT50 (days)	DT90 (days)		
Abiotic Hydrolysis	pH 5, 50˚C	Stable		Not applicable	49813413, Acceptable
	pH 7, 50˚C	Stable		Not applicable	
	pH 9, 50˚C	Stable		Not applicable	
Direct Aqueous Photolysis	pH 7, 25˚C	13.9	Not Calculated	SFO	49813414, Acceptable; Value is dark control corrected and corrected for 40°N latitude, 12 hours light and dark.
Soil Photolysis	Sandy loam, pH 6.9-7.1, 20 ˚C	79.6	Not Calculated	SFO	49813415, Acceptable; Value is dark control corrected and corrected for 40°N latitude, 12 hours light and dark.
Aerobic Soil Metabolism	loam (UK PT 102) (20°C, pH 6.8)	5.82	19.3	SFO	49811316, Supplemental; it was not determined whether soils were representative of a U.S. use site. Up to 37.6 % of unextracted residues (in PT 103) were not characterized.
	sandy loam (UK PT 103) (20°C, pH 4.6)	6.11	20.3	SFO	

Study	System Name/ Characteristics	Kinetics Model Fitted[1] Value		Representative Half-life --Used to Derive Model Input (days)[2]	Reference (MRID), Study Classification and Comments
		DT50 (days)	DT90 (days)		
	silt loam (UK PT 070) (20°C, pH 5.9)	8.02	26.6	SFO	Met-42 was the major degradate (~10% of the applied).
	clay loam (UK SK 961089) (20°C, pH 7.2)	5.63	18.7	SFO	
Anaerobic soil	NA	NA	NA	NA	49813421, Invalid, No aerobic conditions before anaerobic conditions and flooding
Aerobic Aquatic	ND, USA; Golden Lake water:sand sediment (20°C, water pH 8.7, sediment pH 8.2)	6.96	23.1	SFO	49813422 49813423, Supplemental, Major degradates: Met-06: 12% and 10.3% of the applied)
	ND USA, Goose River water:clay loam sediment (20°C, water pH 8.1, sediment pH 7.8)	13.0	43.1	SFO	
Anaerobic Aquatic	ND, USA Golden Lake water:loamy sand sediment (20°C, water pH 8.6, sediment pH 8.0)	7.85	26.1	SFO	49813424, 49813425, Supplemental
	ND USA Goose River water:clay loam sediment (20°C, water pH 8.4, sediment pH 7.4)	12.1	40.1	SFO	

[1] DT50 and DT90 values were calculated using nonlinear regression and single first-order (SFO), double first-order in parallel (DFOP), or indeterminate-order equation (IORE). For DFOP, the overall DT50 and DT90 values are reported when available. Otherwise, a first and second DT50 are reported. The equations can be found in the document, *Standard Operating Procedure for Using the NAFTA Guidance to Calculate Representative Half-life Values and Characterize Pesticide Degradation,* U.S. Environmental Protection Agency 2012.

[2] The value used to estimate a model input value is the calculated SFO DT_{50}, T_{IORE}, or the 2nd 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*, Health Canada, U.S. Environmental Protection Agency, December 21, 2012. The same model used to estimate the value for deriving a model input is used to describe the DT50 and DT90 results.

The terrestrial field dissipation (TFD) studies showed pethoxamid dissipating relatively fast (within a matter of days to weeks). Refer to **Table 5**. Residues of pethoxamid were detected mostly in the top soil layers (0-5 cm) in all the studies; however, in a few samples pethoxamid was detected at 15 cm layer (deepest layer found). Dissipation half-lives in the TFD studies ranged from 4 to 13 days in soils from Texas, Iowa, California and New York. MET-42 (one of the degradates) was detected in all depths at the sites. Therefore, it has more potential for leaching than parent. Although pethoxamid is moderately mobile, with an average organic-carbon normalized soil-water distribution coefficient (K_{oc}) of 196 L/Kg organic carbon, the degradates MET-42, MET-22, MET-100 and MET-46 are more mobile than the parent and are also more persistent in some soils, with the exception of MET-46.

Table 5. Summary of Field Dissipation Data for Pethoxamid

System Details	Half-life, DT50 (days)	Max Leaching Depth (cm)	Source/ Classification/ Comment
IA, silty clay loam, bareground	12.2 (tR IORE)	5-15 (mainly 0-5)	MRID 49813426 Supplemental Bareground
NY, loamy sand, bareground	6.43 (tR IORE)	5-15 (mainly 0-5)	
TX, sandy clay loam, bareground	13.2 (SFO)	5-15 (mainly 0-5)	
CA, sandy loam, bareground	8.01 (tR IORE)	5-15 (mainly 0-5)	

Degradates of Pethoxamid and Identification of Residues of Concern

Major degradates ($\geq$10% of the applied parent) include MET-6, MET-42 and MET-102 in some of the laboratory and terrestrial field study (see **Appendix A**). The degradate MET-6 is a major degradate in aerobic (maximum formation of 10.3% of the applied) and anaerobic (maximum of 15.2% of the applied) aquatic metabolism studies. MET-42 reached a maximum of 11.5% the applied in the aerobic soil metabolism study. MET-102 was detected at a maximum of 21.5% of the applied in the aqueous photolysis study. Although the applied radioactivity of these degradates were found higher than 10% in the environmental fate studies, the toxicity of MET-42, MET-102 and MET-6 is expected to be lower than parent; therefore, the Residues of concern Knowledgebase Subcommittee (ROCKS) decided that parent alone was the ROC.

Two aerobic soil studies were submitted (MRIDs 50761213 and 50761214) conducted with MET-22 and MER-100 as the test compound, respectively. In the studies, degradation of the compounds was observed however, the mass balances were not determined, extractable and non-extractable radioactivity were not measured as well as the formation/decline of degradates. The study determined half-lives for MET-22 (17.1, 15.2 and 130 days) and MET-100 (16.5, 13.8 and 146 days). These studies are supplemental information only and does not change the parent as the ROC.

Appendix D presents mobility and aerobic soil metabolism data on degradates.

4. DRINKING WATER EXPOSURE MODELING

Modeling Approach and Inputs

Estimation of drinking water concentrations of pethoxamid in surface and ground water were calculated using the Pesticides in Water Calculator (PWC, version 1.52, February 2, 2016), consisting of a graphical user interface shell integrating the Pesticide Root Zone Model (v.5.02) and the Varying Volume Water Model (VVWM, v.1.02.3). The EDWCs were generated using EFED's standard suite of scenarios for all the proposed use patterns as presented in **Table 7**. Chemical input parameters used in modeling are presented in **Table 6** and were calculated for parent alone**.** Input parameters were selected in accordance with EFED's guidance documents (USEPA, 2009; USEPA, 2010; USEPA, 2012; USEPA, 2013a; USEPA, 2013b; USEPA, 2014a; USEPA, 2014b; USEPA and Health Canada, 2013).

The proposed uses on agricultural crops allow for, aerial, and ground broadcast applications of a flowable material. For the proposed agricultural crop uses, EDWCs for broadcast aerial, and ground spray applications were generated using a batch processing input file. The application method resulting in the highest EDWCs for each use scenario is summarized in **Appendix B**. Refer to **Appendix C** to see the output model run for ground water using WI corn.

Simulations for applications as a coated fertilizer were conducted as broadcast applications and assuming spray drift was zero.

Table 6. Aquatic Modeling Input Parameters for Pethoxamid in PWC v1.52

Parameter (units)	Value (s)	Source	Comments
K_{OC} (mL/g)	196	MRID 49813406	Average of 4 values for parent. The coefficient of variation was higher for K_{OC} than for K_d. Therefore, K_{OC} values were used.
Water Column Metabolism Half-life (days) at 20°C	19.3	MRID 49813422 and -23	Represents the 90th percentile upper confidence bound on the mean of 2 representative half-life values from aerobic aquatic metabolism studies.
Benthic Metabolism Half-life (days) at 20°C	16.5	MRID 49813424 and -25	Represents the 90th percentile upper confidence bound on the mean of 2 representative half-life values from anaerobic aquatic metabolism studies.
Aqueous Photolysis Half-life (days)@ pH 7	13.9 at 40°N	MRID 49813414	One measured value for parent.
Hydrolysis Half-life (days)	0	MRID 49813413	No significant degradation observed at 50°C.
Soil Half-life (days) at 20°C	7.3	MRID 49811316	Represents the 90th percentile upper confidence bound on the mean of 4 representative half-life values from aerobic soil metabolism studies.
Foliar Half-life	--	--	No Data
Molecular Weight (g/mol)	295.8	MRID 49813402	--
Vapor Pressure (Torr) at 25°C	2.1×10^{-5} torr	Product Chemistry	--

Parameter (units)	Value (s)	Source	Comments
Solubility in Water (mg/L)	400	Product Chemistry	20°C
Henry's Law Constant	8.35×10^{-7}	--	Estimated from vapor pressure and water solubility at 20°C.
PCA	1.0	PCA guidance, 2014	A PCA of 100% was used because current labels include non-agricultural uses (*i.e.* ornamentals).

[1] Other input parameters for the applications tab are shown in **Table 6.**

Pesticide in Water Calculator (PWC) Scenarios are used to specify soil, climatic, and agronomic inputs in the Pesticide Root Zone Model (PRZM), and are intended to result in high-end water concentrations associated with a particular crop and pesticide within a geographic region. Each PWC scenario is specific to a vulnerable area where the crop is commonly grown. Soil and agronomic data specific to the location are built into the scenario, and a specific climatic weather station providing 30 years of daily weather values is associated with the location. **Table 5** identifies the use sites associated with each surface water PWC scenario. All the scenarios available for each use pattern were modeled. The standard six scenarios for groundwater were also simulated for the use pattern with the highest application rate. Consistent with the pre-emergent early post-emergent application timing recommended on the label, the application time one-day after emergence was chosen for all modeling simulations. A day after the emergence day was selected for all the scenarios as well as one single application of 1.50 lbs a.i./A per year (1.68 kg/ha). The application method selected was above crop with the exception of the dry fertilizer used for which a broadcast application was modeled. The application efficiency and spray drift for most of the crops was 0.95 (for aerial) and 0.135, respectively. However, for dry fertilizer the application efficiency was 0.99 for broadcast with the assumption of no spray drift.

Table 7. Pesticide in Water Calculator (PWC) Input Parameters Specific to Use Patterns for Pethoxamid (Applications Tab and Crop/land Tab)

Use Site	PWC Scenario	App. Rate in lbs a.i./A (kg a.i./ha)	# App. per Year	App. Interval (days)	App Method	Application Efficiency/ Spray Drift
Corn	ILCornSTD	1.50 (1.68)	1	N/A	Above crop	Aerial 0.95/0.135
	INCornSTD					
	IACornSTD					
	KSCornSTD					
	MNCornSTD					
	MSCornSTD					
	NCcornESTD					
	OHCornSTD					
	PACornSTD					
	NECornStd					
Cotton	CAcotton_wirrigSTD	1.50 (1.68)	1	N/A	Above crop	Aerial 0.95/0.135
	MScottonSTD					
	NCcottonSTD					
Turf	PAturfSTD	1.50	1	N/A	Above crop	Aerial

Use Site	PWC Scenario	App. Rate in lbs a.i./A (kg a.i./ha)	# App. per Year	App. Interval (days)	App Method	Application Efficiency/ Spray Drift
	FLturfSTD	(1.68)				0.95/0.135
Ornamentals	CAnurserySTD_V2	1.50 (1.68)	1	N/A	Above crop	Aerial 0.95/0.135
	FLnurserySTD_V2					
	MInurserySTD_V2					
	ORnurserySTD_V2					
	ORXmasTreeSTD					
	TNnurserySTD_V2					
Soybean	MSsoybeanSTD	1.50 (1.68)	1	N/A	Above crop	Aerial 0.95/0.135
Railroad Rights-of-Way	RightOfWayBSS	1.50 (1.68)	1	N/A	Above crop	Aerial 0.95/0.135
	CArightofwayRLF_V2					
Coated Fertilizer	MSsoybeanSTD	1.50 (1.68)	1	N/A	Below Crop	Aerial 1/0

Surface and Ground Water Modeling Output Characterization

The highest EDWCs of pethoxamid across use patterns are summarized in **Table 8**. The highest EDWCs resulted from surface water and not ground water.

Table 8. Highest Estimated Drinking Water Concentrations (EDWCs) for Pethoxamid Across Proposed Uses

Use, Scenario	Application Rate lbs a.i./A (kg/ha)	EDWCs[1],[2] in µg/L		
		Acute	Chronic	Cancer
All use patterns, MS corn STD Surface Water	One application: 1.5 lbs a.i./A (1.68kg/ha)	**121**	**7.45**	**2.71**
All use patterns, GW Del Marva Ground Water		0.188	0.129	0.129

[1]Bolded values are the recommended EDWCs for use in the Human Health and Effects (HED) drinking water assessment.
[2] For surface water modeling, the acute concentration is provided as 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.

For surface water sources of drinking water, the acute 1-in-10-year daily average and chronic 1-in-10 year annual average EDWCs are 121 µg/L and 7.45 µg/L, respectively. The cancer 30-year average EDWCs is 2.71 µg/L.
These groundwater EDWCs are for vulnerable groundwater supplies such as a rural drinking water wells that exist below or are directly influenced by an agricultural field treated yearly at the maximum labeled rates for 30 years.

5. MONITORING DATA

Monitoring data are useful in that they provide some information on the occurrence of pesticides in the environment under existing usage conditions. However, pethoxamid is a new active ingredient; therefore, monitoring data is not yet available.

6. UNCERTAINTIES

The EDWCs in this assessment are representative of concentrations in drinking water source water (pre-treatment). There is no information available examining drinking water treatment impacts on pethoxamid. For surface water, the conceptual model assumes that a pesticide reaches surface water via spray drift and/or surface runoff and it is completely mixed in the water body. Pethoxamid is stable to hydrolysis; therefore, it will not degrade by hydrolysis during the time that elapses from drinking water intake through distribution to the first tap. Photolysis is a relatively unimportant degradation pathway. Therefore, if ultraviolet light were used as a means of disinfection, degradation of pethoxamid would not be expected to be significant. Pethoxamid does degrade via aerobic soil and aquatic metabolism (5.6 to 13 days) and it may degradate during the time in the treatment plant. 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 only used in larger drinking water treatment facilities (USEPA, 2011). The ability of GAC to remove pesticides will vary with the properties of the chemical and whether the sorption sites on GAC have reached capacity (Badriyha *et al.*, 2003; Zhao *et al.*, 1999).

7. Literature Cited

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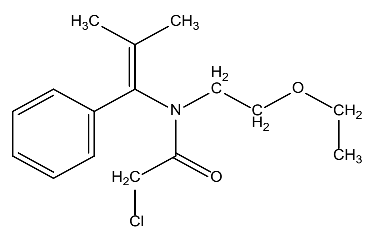
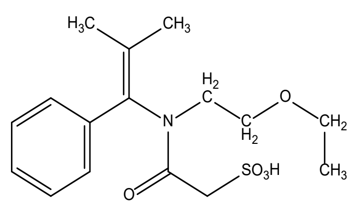
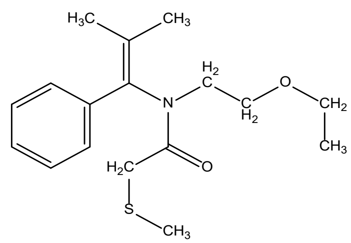
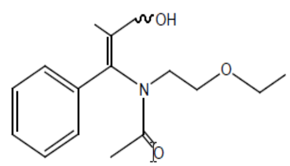
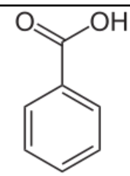
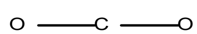
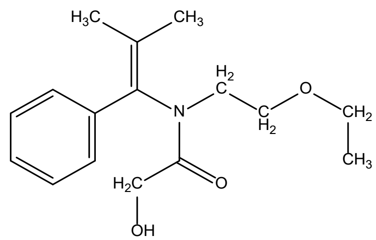
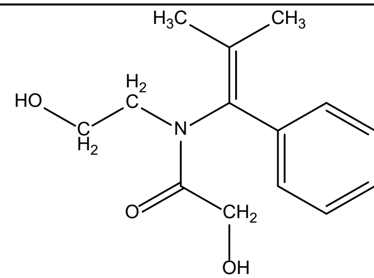
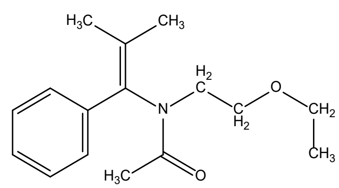
Appendix A. Identified Degradates of Pethoxamid

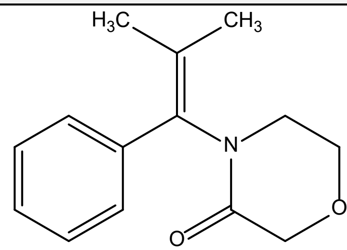
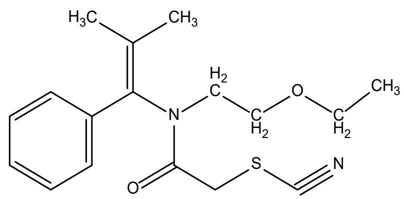
Table A1. Chemical Names and Structures of Pethoxamid and its Transformation Products

Code Name/ Synonym Chemical Name	Chemical Structure	Study Type	MRID	Maximum %AR (day)		Final %AR (Study length)
PARENT						
Pethoxamid (TKC-94) **IUPAC:** 2-Chloro-N-(2-ethoxyethyl)-N-(2-methyl-1-phenylprop-1-enyl)acetamide **CAS:** 2-Chloro-N-(2-ethoxyethyl)-N-(2-methyl-1-phenyl-1-propen-1-yl)acetamide **Cas No.:** 106700-29-2 **Formula:** $C_{16}H_{22}ClNO_2$ **MW:** 295.8 g/mol **SMILES:** C/C(C)=C(N(CCOCC)C(CCl)=O)\C1=CC=CC=C1		Aerobic soil	49813416 49813417 49813418 49813419	Parent		
		Anaerobic soil	49813421			
		Aerobic aquatic	49813422 49813423			
		Anaerobic aquatic	49813424 49813425			
		Hydrolysis	49813413			
		Photolysis in water	49813414			
		Photolysis in soil	49813415			
MAJOR (>10%) TRANSFORMATION PRODUCTS						
MET-42 (TKC-94 sulphonic acid) **IUPAC:** 2-((2-Ethoxyethyl)(2-methyl-1-phenylprop-1-en-1-yl)amino)-2-oxoethane-1-sulfonic acid **Formula:** $C_{16}H_{23}NO_5S$ **MW:** 341.42 g/mol		Aerobic soil	49813416	ssl	**10.38%** (10 d)	4.95% (120 d)
				sl	4.82% (30 d)	2.05% (120 d)
				ssl	5.57% (59 d)	2.91% (120 d)
				cl	7.39% (10 d)	1.71% (120 d)
				ssl	**11.53%** (90 d)	8.41% (120 d)
		Aerobic aquatic	49813422 49813423	Lake	2.6% (102 d)	2.6% (102 d)
				River	2.2% (31, 102 d)	2.2% (102 d)

Code Name/ Synonym Chemical Name	Chemical Structure	Study Type	MRID	Maximum %AR (day)	Final %AR (Study length)	
SMILES: C/C(C)=C(N(CCOCC)C(CS(=O)(O)=O)=O)\C1=CC=CC=C1		Anaerobic aquatic	49813424 49813425	Lake	2.3% (61 d)	1.1% (101 d)
				River	2.9% (101 d)	2.9% (101 d)
		Terrestrial field dissipation study	49813426	IA	68.3 g peq/ha	12.3 g peq/ha
				NY	73 g peq/ha	8 g peq/ha
				CA	161 g peq/ha	22 g peq/ha
				TX	157 g peq/ha	24 g peq/ha
MET-6 **IUPAC:** N-(2-ethoxyethyl)-N-(2-methyl-1-phenylprop-1-en-1-yl)-2-(methylthio)acetamide **Formula:** $C_{17}H_{25}NO_2S$ **MW:** 307.45 g/mol **SMILES:** C/C(C)=C(N(CCOCC)C(CSC)=O)\C1=CC=CC=C1		Aerobic aquatic	49813422 49813423	Lake	**12.0%** (14 d)	5.2% (102 d)
				River	**10.3%** (31 d)	4.5% (102 d)
		Anaerobic aquatic	49813424 49813425	Lake	**9.6%** (61, 101 d)	**9.6%** (101 d)
				River	**15.2%** (101 d)	**15.2%** (101 d)
Met-102 **Formula:** $C_{16}H_{23}NO_3$ **MW:** 277.17 g/mol **SMILES:** C1=CC=CC=C1\C(=C(/C)CO[H])N(CCOCC)C(C)=O		Photolysis in water	49813414	Buffer	**21.5 % (6 d)**	**15.9 % (16 d)**
Benzoic acid **Smiles code:** C1(=CC=CC=C1)C(=O)O **Formula:** C7H6O2 **MW:** 122.12 g/mol		835.2240 Photolysis in water	49813414	Buffer	**31.6 % (16 d)**	**31.6 % (16 d)**
Carbon dioxide **IUPAC:** Carbon dioxide		Aerobic soil	49813416	ssl	**37.60%** (120 d)	**37.60%** (120 d)
				sl	**39.32%** (120 d)	**39.32%** (120 d)

Code Name/ Synonym Chemical Name	Chemical Structure	Study Type	MRID	Maximum %AR (day)	Final %AR (Study length)	
Formula: CO_2 **MW:** 44 g/mol **SMILES:** C(=O)=O				ssl	**38.14%** (120 d)	**38.14%** (120 d)
				cl	**47.84%** (120 d)	**47.84%** (120 d)
				ssl	**25.73%** (120 d)	**25.73%** (120 d)
		Aerobic aquatic	49813422 49813423	Lake	**16.6%** (102 d)	**16.6%** (102 d)
				River	**13.7%** (102 d)	**13.7%** (102 d)
		Anaerobic aquatic	49813424 49813425	Lake	**10.5%** (61 d)	8.4% (101 d)
				River	7.8% (101 d)	7.8% (101 d)
		Photolysis in water	49813414	Buffer	**2.1 % (16 d)**	**2.1 % (16 d)**
Unextracted residues (identified as bound parent compounds in subsequent extractions)	NA	Aerobic soil	49813416	ssl	**36.40%** (120 d)	**36.40%** (120 d)
				sl	**29.37%** (30 d)	**25.06%** (120 d)
				ssl	**33.49%** (30 d)	**31.68%** (120 d)
				cl	**36.34%** (59 d)	**33.66%** (120 d)
				ssl	**32.08%** (120 d)	**32.08%** (120 d)
		Aerobic aquatic	49813422 49813423	Lake	**67.1%** (31 d)	**59.2%** (102 d)
				River	**70.7%** (102 d)	**70.7%** (102 d)
		Anaerobic aquatic	49813424 49813425	Lake	**74.3%** (26 d)	**69.3%** (101 d)
				River	**75.8%** (61 d)	**66.9%** (101 d)
MINOR (<10%) TRANSFORMATION PRODUCTS						
MET-2 **IUPAC:** N-(2-Ethoxyethyl)-2-hydroxy-N-(2-methyl-1-phenylprop-1-en-1-yl)acetamide		Aerobic soil	49813416	ssl	2.28% (30 d)	1.53% (120 d)
				sl	2.47% (6 d)	1.94% (120 d)
				ssl	2.63% (59 d)	1.61% (120 d)
				cl	3.41% (59 d)	2.08% (120 d)

Code Name/ Synonym Chemical Name	Chemical Structure	Study Type	MRID	Maxim um %AR (day)	Final %AR (Study length)	
Formula: $C_{16}H_{23}NO_3$ **MW:** 277.36 g/mol **SMILES:** C/C(C)=C(N(CCOCC)C(CO)=O)\C1=CC=CC=C1				ssl	2.15% (59 d)	2.02% (120 d)
		Aerobic aquatic	49813422 49813423	Lake	3.4% (60 d)	1.9% (102 d)
				River	4.6% (31 d)	1.3% (102 d)
		Anaerobic aquatic	49813424 49813425	Lake	3.5% (26 d)	2.0% (101 d)
				River	7.4% (26 d)	1.3% (101 d)
		Photolysis in water	49813414	buffer	3.3% (16 d)	3.3% (16 d)
MET-3 **IUPAC:** 2-Hydroxy-N-(2-hydroxyethyl)-N-(2-methyl-1-phenylprop-1-en-1-yl)acetamide **Formula:** $C_{14}H_{19}NO_3$ **MW:** 249.31 g/mol **SMILES:** C/C(C)=C(N(CCO)C(CO)=O)\C1=CC=CC=C1		Aerobic soil	49813416	sl	1.27% (30 d)	0.73% (120 d)
		Aerobic aquatic	49813422 49813423	Lake	0.7% (60 d)	0.4% (102 d)
				River	1.1% (102 d)	1.1% (102 d)
		Anaerobic aquatic	49813424 49813425	Lake	1.2% (61 d)	0.1% (101 d)
				River	1.7% (61 d)	0.3% (101 d)
MET-22 (DesCl-PXA) **IUPAC:** N-(2-ethoxyethyl)-N-(2-methyl-1-phenyl-1-propenyl)acetamide **Formula:** $C_{16}H_{23}NO_2$ **MW:** 261.37 g/mol **SMILES:** C/C(C)=C(N(CCOCC)C(C)=O)\C1=CC=CC=C1		Aerobic aquatic	49813422 49813423	Lake	3.0% (102 d)	3.0% (102 d)
				River	3.3% (60 d)	2.5% (102 d)
		Anaerobic aquatic	49813424 49813425	Lake	2.9% (61 d)	2.8% (101 d)
				River	4.7% (101 d)	4.7% (101 d)
MET-27 **IUPAC:** 4-(2-Methyl-1-phenylprop-1-en-1-yl)morpholin-3-one		Aerobic soil	49813416	ssl	1.32% (120 d)	1.32% (120 d)
				sl	1.88% (59 d)	ND (120 d)
				ssl	1.62% (2 d)	ND (120 d)
				cl	0.94% (2 d)	ND (120 d)

Code Name/ Synonym Chemical Name	Chemical Structure	Study Type	MRID	Maximum %AR (day)	Final %AR (Study length)	
Formula: $C_{14}H_{17}NO_2$ **MW:** 231.30 g/mol **SMILES:** C/C(C)=C(N(CCOC1)C1=O)\C2=CC=CC=C2	 			ssl	1.45% (30 d)	ND (120 d)
MET-104 **IUPAC:** N-(2-ethoxyethyl)-N-(2-methyl-1-phenylprop-1-en-1-yl)-2-thiocyanatoacetamide **Formula:** $C_{17}H_{22}N_2O_2S$ **MW:** 318.4 g/mol **SMILES:** C/C(C)=C(N(CCOCC)C(CSC#N)=O)\C1=CC=CC=C1	 	Aerobic aquatic	49813422	Lake	9.3% (31 d)	1.0% (102 d)
			49813423	River	4.6% (14 d)	0.7% (102 d)

Ssl=sandy silt loam; cl=clay loam; sl=sandy loam

[A] AR means "applied radioactivity". MW means "molecular weight". ND means "not detected". NA means "not applicable".

Appendix B. Summary of Surface Water Modeling of Pethoxamid and the USEPA Standard Reservoir

Line Batch Run ID	Peak	1-day	Yr	overall	4-day	21-day	60-day	90-day
1 corn_2_ILCornSTD	21.7	21.4	2.02	1.14	20.5	17.6	11.3	8.06
2 corn_2_INCornStd	26.7	26.2	2.08	0.921	25	21.1	12	8.33
3 corn_2_IAcornstd	21.8	21.4	1.58	0.779	20.4	15.1	8.9	6.31
4 corn_2_KSCornStd	32	31.4	2.18	1.21	29.7	22	12.6	8.76
5 Corn_2_MNCornStd	13.7	13.5	1.3	0.893	13	10.5	7.01	5.11
6 Corn_2_MScornSTD	**123**	**121**	**7.45**	**2.71**	**114**	**82.5**	**43.4**	**30**
7 Corn_2_NCcornESTD	23.4	22.9	1.89	0.911	21.7	16.7	10.4	7.52
8 Corn_2_OHCornSTD	29	28.5	2.37	1.2	27.3	21.1	13.2	9.44
9 Corn_2_PAcornSTD	12.1	12	1.2	0.865	11.5	9.83	6.4	4.74
10 Corn_2_NECornStd	64.6	63	3.98	1.49	58.7	43.7	23.1	16
11 Cotton_2_CAcotton_WirrigSTD	8.28	8.15	0.611	0.559	7.78	6.04	3.45	2.43
12 cotton_2_MScottonSTD	62.7	61.2	3.51	1.51	56.9	40.7	20.7	14.2
13 cotton_2_NCcottonSTD	30.8	30.1	1.76	0.895	28.9	20.1	10.3	7.09
14 turf_2_PAturfSTD	9.31	9.22	1.08	1.01	8.95	7.81	5.48	4.19
15 turf_2_FLturfSTD	10.3	10.2	1.01	0.801	9.78	8.02	5.21	3.89
16 ornamentals_2_CAnurserySTD_V2	18.8	18.5	1.65	1.05	17.7	13.6	8.63	6.4
17 ornamentals_2_FLnurserySTD_V2	32.9	32	2.03	0.836	29.7	20.7	11.9	8.41
18 ornamentals_2_MInurserySTD_V2	12	11.9	2.21	1.83	11.6	10.3	8.23	7.07
19 ornamentals_2_ORnurserySTD_V2	24.9	24.6	4.24	2.27	24.1	21.9	17.1	14.2
20 ornamentals_2_ORXmasTreeSTD	16.1	15.9	2.73	1.97	15.5	13.5	10.5	9.26
21 ornamentals_2_TNnurserySTD_V2	24.5	24.2	2.33	1.46	23.3	19.3	12.8	9.24
22 soybean_2_MSsoybeanSTD	40.7	39.9	2.48	1.27	37.5	27.8	14.6	10
23 ROW_2_RightOfWayBSS	32.4	31.8	2.43	1.24	30.2	23	13.6	9.71
24 ROW_2_CArightofwayRLF_V2	8.27	8.13	0.78	0.706	7.73	5.9	3.78	2.89

Bolded values are the highest and recommended values for HED.

Summary of Water Modeling of Pethoxamid and the USEPA Standard Reservoir

Estimated Environmental Concentrations for Pethoxamid are presented in Table 1 for the USEPA standard reservoir with the MScornSTD 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 2.5% of Pethoxamid applied to the field eventually reaches the water body. The main mechanism of transport from the field to the water body is by runoff (77.8% of the total transport), followed by spray drift (16.3%) and erosion (5.97%).

In the water body, pesticide dissipates with an effective water column half-life of 13.6 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 metabolism (effective average half-life = 20.1 days) followed by washout (43.2 days), photolysis (1724.1 days), and volatilization (17842.3 days).

In the benthic region, pesticide dissipates (17.2 days). The main source of dissipation in the benthic region is metabolism (effective average half-life = 17.2 days). The vast majority of the pesticide in the benthic region (95.49%) is sorbed to sediment rather than in the pore water.

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

Peak (1-in-10 yr)	123.
4-day Avg (1-in-10 yr)	114.
21-day Avg (1-in-10 yr)	82.5
60-day Avg (1-in-10 yr)	43.4
365-day Avg (1-in-10 yr)	7.44
Entire Simulation Mean	2.71

Table 2. Summary of Model Inputs for Pethoxamid.

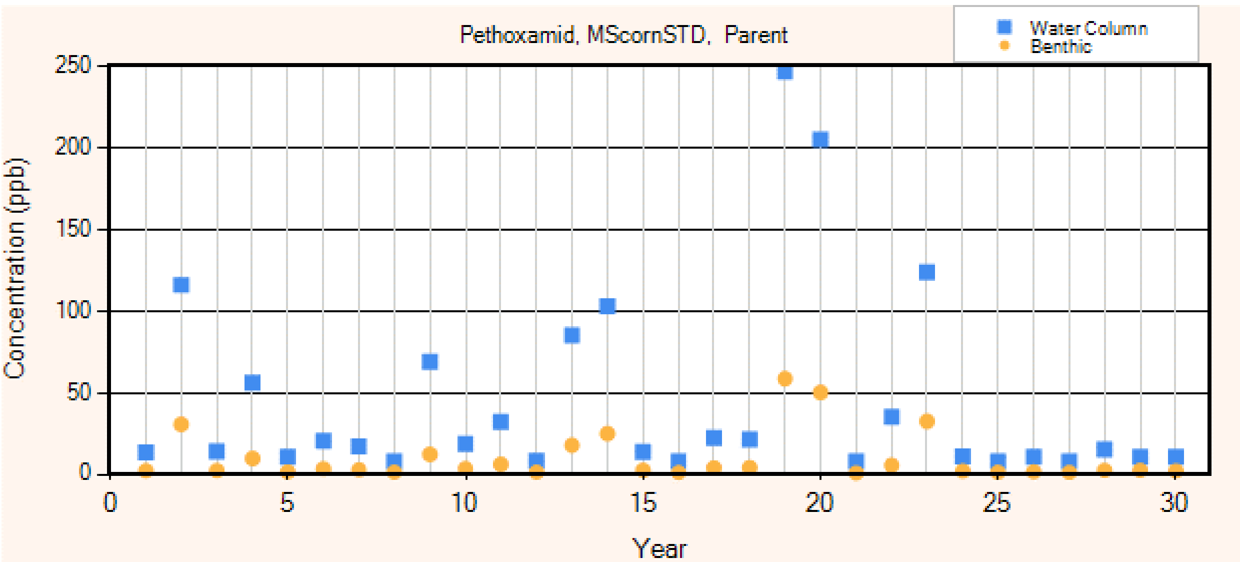
Scenario	MScornSTD
Cropped Area Fraction	1.0
Koc (ml/g)	196
Water Half-Life (days) @ 20 °C	19.3
Benthic Half-Life (days) @ 20 °C	16.5

Photolysis Half-Life (days) @ 40 °Lat	13.9
Hydrolysis Half-Life (days)	0
Soil Half-Life (days) @ 20 °C	7.3
Foliar Half-Life (days)	
Molecular Weight	295.8
Vapor Pressure (torr)	2.1e-5
Solubility (mg/l)	400
Henry's Constant	8.35E-07

Table 3. Application Schedule for Pethoxamid.

Date (Days Since Emergence)	Type	Amount (kg/ha)	Eff.	Drift
1	Above Crop (Foliar)	1.68	0.95	0.135

Figure 1. Yearly Peak Concentrations



Appendix C- Ground water output using all the available scenarios

**** Parent **

GW Run ID	Peak	Breakthru	Thruput	PostBT Avg	Sim Avg
GW_Delmarva_PWC_+0	0.055615	3372.262	3.249155	0.04006551	0.02704413
GW_FL potato_PWC_+0	0.00020413	4040.357	2.711889	5.738877E-05	3.744932E-05
GW_FLCitrus_PWC_+0	0.17471	2680.119	4.088252	0.1126946	0.1033807
GW_GA peanuts_PWC_+0	0.016041	4150.03	2.640222	0.006061846	0.00376555
GW_NCCotton_PWC_+0	0.006724	3768.412	2.90759	0.002925798	0.001891152
GW_WI_corn_PWC_+0	0.18769	4856.824	2.256001	0.1292493	0.07634349

Appendix D. Data on Degradates of Pethoxamid

Transformation Products

Pethoxamid degrades in soil to form MET-42 which is a major degradate in the study; however, this degradate formed as a minor degradate in other studies such as aerobic and anaerobic aquatic studies. In the aerobic and anaerobic aquatic studies, the major degradate was MET-6 (not detected in other studies). MET-102 was a major degradate in aqueous photolysis, but was not observed in any other studies. MET-2 and MET-3 were minor degradates in aerobic soil, aerobic aquatic, and anaerobic aquatic studies, while only MET-2 was observed in the photolysis in water study. MET-27 and MET-22 were minor degradates observed in the aerobic soil studies.

Table D1 presents the mobilities of pethoxamid and its degradates based on submitted batch equilibrium study data and **Table D2** the aerobic soil data of the degradates.

Table D1. Pethoxamid Degradates Mobilities.

Test compound	Koc (L/Kg oc)	FAO Classification	MRID and Classification
Pethoxamid*	227.8, 194.5, 171.3, 190	Moderately mobile	49813406 Acceptable
MET-42[1]	5.26, 10.2, 8.86, 36.0, 9.65, 17.3	Highly mobile to mobile	49813407 Supplemental
MET-22[1]	88.1, 77.4; 128.7, 119.2, 100.4, 92.5	Mobile to moderately mobile	49813408 Supplemental
MET-100[1]	3.67, 13.8, 3.19, 13.8, 1.33, 1.77	Highly mobile to mobile	49813409 Supplemental
MET-46[1]	96,370	Hardly mobile	49813410 Supplemental

*American soil
[1] All soils studied are from Germany.

Table D2. Aerobic Soil Metabolism of Pethoxamid Degradates.[1,2]

Test Compound	Study System	DT_{50} (days)	DT90 (days)	Representative Half-life -- Used to Derive Model Input(days)	Reference or (MRID #), Study Classification and Comments
Aerobic Soil Metabolism **Met-22**	Speyer, Germany LUFA 2.2 loamy sand (20°C, pH 5.5)	93.5	468	Slow $t_{1/2}$ = 162 DFOP	49811317, Supplemental. Samples were analyzed only for the pethoxamid degradate **MET-22**. Volatiles were not trapped, and total extractable and unextracted residues
	Speyer, Germany LUFA 2.3 sandy loam[3] (20°C, pH 6.8)	17.2	85.4	$t_{R\ IORE}$ = 25.7 IORE	

	Speyer, Germany LUFA 2.4 loam[3] (20°C, pH 7.2)	19.2	63.9	SFO	were not measured. Mass balances could not be calculated. Only foreign soils were used.
Aerobic Soil Metabolism **MET-100**	Speyer, Germany LUFA 2.2 loamy sand[3] (20°C, pH 5.5)	85.5	284	SFO	49811318, Supplemental. Volatiles were not trapped, and total extractable and unextracted residues were not measured. Transformation products were not addressed. Mass balances could not be calculated. Only foreign soils were used.
	Speyer, Germany LUFA 2.3 sandy loam (20°C, pH 6.8)	9.06	30.1	SFO	
	Speyer, Germany LUFA 2.4 loam (20°C, pH 7.2)	9.21	30.6	SFO	
Aerobic Soil Metabolism **MET-46**	Speyer, Germany LUFA 2.2 loamy sand[3] (20°C, pH 5.5)	5.45	18.1	SFO	49811319, Supplemental. Volatiles were not trapped, and total extractable and unextracted residues were not measured. Transformation products were not addressed. Mass balances could not be calculated. Only foreign soils were used.
	Speyer, Germany LUFA 2.3 sandy loam (20°C, pH 6.0)	4.34	14.4	SFO	
	Speyer, Germany LUFA 2.4 loam (20°C, pH 7.2)	9.2	30.6	SFO	

1 Calculated half-lives and model parameters in accordance with NAFTA kinetics guidance; Double First Order in Parallel (DFOP), Indeterminate Order Rate Equation (IORE), and Single First Order (SFO)

2 Soil Classification based on USDA system