

Appendix D. Aquatic exposure modeling for vinclozolin and 3,5-DCA

In order to explore uncertainties associated with the total residue approach and relative concentrations of vinclozolin and 3,5-DCA, separate aquatic exposure modeling was conducted for vinclozolin and for 3,5-DCA. These efforts and results are described below.

D.1. Vinclozolin Model Inputs

The appropriate chemical-specific PRZM input parameters are selected from reviewed physical, chemical and environmental fate data submitted by the registrant (Error! Reference source not found. and Error! Reference source not found.) and in accordance with EFED water model input parameter selection guidance (U.S. EPA 2002). The input parameters for relevant to the fate of vinclozolin used in PRZM and EXAMS are in **Table D.1**. Application methods, maximum rates per application and maximum number of applications per year are based on current label directions for use of vinclozolin on turf grass (Table D.2). The application date is not explicitly stated on the label. In order to account for differences in EECs that can be attributed to application timing, applications were simulated on the second day of each month of the year. The selection of the second day of the year was arbitrary.

Table D.1. PRZM/EXAMS input parameters relevant to the fate of vinclozolin.

Input Parameter	Value	Comments
Molecular Wt. (g/mol)	286.11	See Error! Reference source not found.
Henry's Law Constant (atm-m ³ /mol)	3.8×10^{-7}	See Error! Reference source not found.
Vapor pressure (torr)	2.6×10^{-6}	See Error! Reference source not found.
Solubility in water (mg/L @ pH 7, 20°C)	2.6	See Error! Reference source not found.
Hydrolysis half-life (days)	1.3	Based on value for neutral water (pH 7) (See Error! Reference source not found.)
Aqueous photolysis (days)	27.2	See Error! Reference source not found.
Aerobic Soil Metabolism Half-life (days)	201*	Upper confidence bound of mean of available aerobic soil-metabolism half-lives (Error! Reference source not found.).
Aerobic Aquatic Metabolism Half-life (days)	stable	In the case that no aerobic metabolism data are available and the chemical is susceptible to hydrolysis, it is assumed that the chemical is stable to aerobic aquatic metabolism.
Anaerobic Aquatic Metabolism Half-life (days)	402	3 x the available half-life (134 d; See Error! Reference source not found.)
K _{oc} (L/kg _{OC})	582	Mean of non-sand K _{oc} values (Error! Reference source not found.).

Input Parameter	Value	Comments
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* Calculated using the following equation: $t_{input} = (mean\ t_{1/2}) + \frac{t_{90,n-1} * stdev}{\sqrt{n}}$ (USEPA 2002)

Where: $t_{90,n-1}$ = 1.533
Mean $t_{1/2}$ = 107
Stdev = 137
n = 5

Table D.2. PRZM/EXAMS input parameters relevant to the use of vinclozolin.

Input Parameter	Value	Comments
# applications/year	3	Based on label
Maximum rate/application (kg a.i./ha)	1.51	Equivalent to 1.35 lbs a.i./A
CAM	2	For foliar application
IPSCND	1	In cases where CAM 2 is modeled, it is necessary to identify an IPSCND value, which represents the deposition of vinclozolin in the post-season. An IPSCND value of 1 represents conversion of vinclozolin remaining on foliage to surface application to the top soil layer.
Application date	2 nd of each month	This is not explicitly stated on the label. In order to account for differences in EECs that can be attributed to application time, applications were simulated on the second day of each month of the year. The selection of the second day of the year was arbitrary.
Application interval (days)	10	Shortest interval indicated on label.
Spray drift fraction	0.01	Assumption relevant to ground application
Application efficiency	0.99	

D.2. 3,5-DCA Model Inputs

The input parameters relevant to the fate of 3,5-DCA used in PRZM and EXAMS are in

Table D.3. Use specific parameters include application methods and rates (Error! Reference source not found.). Application methods, maximum rates per application and maximum number of applications per year are based on current label directions for use of vinclozolin on turf grass. The application rate is converted to a 3,5-DCA equivalent using the molecular weight of 3,5-DCA. In this approach, available laboratory fate studies indicate that 3,5-DCA is the terminal degradate and that this degradate is stable; as such, it is assumed that 100% of vinclozolin is converted to 3,5-DCA at the time of application. The application date modeled for 3,5-DCA was October 2, which was based on the date where the highest peak EEC was determined from the vinclozolin modeling (Error! Reference source not found. **D.5**).

Table D.3. PRZM/EXAMS input parameters relevant to the fate of 3,5-DCA.

Input Parameter	Value	Comments
Molecular Wt. (g/mol)	162.02	See Table 3
Henry's Law Constant (atm-m ³ /mol)	5.8 x 10 ⁻⁶	See Table 3
Vapor pressure (torr)	2.12 x 10 ⁻²	See Table 3
Solubility in water (mg/L @ pH 7, 20°C)	784	See Table 3
Hydrolysis half-life (days)	stable	Assume stable
Aqueous photolysis (days)	stable	Assume stable
Aerobic Soil Metabolism Half-life (days)	stable	Assume stable
Aerobic Aquatic Metabolism Half-life (days)	stable	Assume stable
Anaerobic Aquatic Metabolism Half-life (days)	stable	Assume stable
Koc (L/kg _{OC})	557	Mean of non-sand Koc values (Table 5).

Table D.4. PRZM/EXAMS input parameters relevant to 3,5-DCA.

Input Parameter	Value	Comments
# applications/year	3	Based on label for vinclozolin
Maximum rate/application (kg a.i./ha)	0.855	On a molar basis, 1.51 kg vinclozolin/ha is equivalent to 5.28 mol/ha. Since it is assumed that 1 mole of vinclozolin results in 1 mole of 3,5-DCA, the molecular weight of 3,5-DCA (162.02 g/mol) is used to determine the maximum application rate of 3,5-DCA that can result from a vinclozolin application (this is assuming that 100% of vinclozolin* is degraded to 3,5-DCA at the time of application).
CAM	2	For foliar application
IPSCND	1	In cases where CAM 2 is modeled, it is necessary to identify an IPSCND value, which represents the deposition of vinclozolin in the post-season. An IPSCND value of 1 represents conversion of vinclozolin remaining on foliage to surface application to the top soil layer.
Application date	October 2	Based on application date resulting in highest peak EEC observed for vinclozolin modeling.
Application interval (days)	10	Shortest interval indicated on label.
Spray drift fraction	0.01	Assumption relevant to ground application
Application efficiency	0.99	

*assumption based on stability of 3,5-DCA as a terminal degradate in laboratory fate studies.

D.3. Results

Peak one-in-ten year aquatic EECs for vinclozolin range 2.61-9.75 µg/L, depending upon the application date. Of the application dates modeled, the highest peak EEC occurred on October 2. One-in-ten year 21-d and 60-d EECs range from 0.296-1.30 µg/L and 0.124-0.491 µg/L, respectively (**Table D.5**). For 3,5-DCA, the peak EEC was 13.2 µg/L and the 21-d and 60-d EECs were 9.83 and 6.98 µg/L, respectively (**Table D.6**).

Table D.5. Vinclozolin EECs (µg/L) predicted using PRZM/EXAMS.

Application date	Peak EEC	21-d EEC	60-d EEC
Jan 2	8.86	1.12	0.491
Feb 2	4.19	0.642	0.317
March 2	2.79	0.480	0.217
April 2	2.61	0.296	0.124
May 2	3.26	0.69	0.140
June 2	4.21	0.497	0.182
July 2	5.55	0.657	0.240
Aug 2	7.16	0.849	0.311
Sept 2	9.14	1.08	0.400
October 2	9.75	1.30	0.482
November 2	6.92	0.779	0.411
December 2	7.65	0.899	0.448

Table D.6. EECs (µg/L) for vinclozolin and 3,5-DCA predicted using PRZM/EXAMS. EECs based on October 2 application date.

Chemical	Peak EEC	21-d EEC	60-d EEC
Vinclozolin	9.75	1.30	0.482
3,5-DCA	13.2	9.83	6.98

D.4. Input/Output files

Vinclozolin

stored as vinclozolin_turf.out

Chemical: vinclozolin

PRZM environment: CATurfRLF.txt modified Tuesday, 20 February 2007 at 12:03:48

EXAMS environment: pond298.exv modified Tuesday, 26 August 2008 at 06:14:08

Metfile: w23234.dvf modified Tuesday, 26 August 2008 at 06:15:38

Water segment concentrations (ppb)

Year	Peak	96 hr	21 Day	60 Day	90 Day	Yearly	
1961	2.161	1.198	0.3493	0.1705	0.13	0.03207	
1962	10.16	5.111	1.365	0.4986	0.3828	0.1283	
1963	4.731	2.378	0.5843	0.2555	0.1777	0.06134	
1964	5.477	2.336	0.5056	0.1782	0.1193	0.0569	
1965	3.577	1.493	0.4629	0.2184	0.1889	0.05644	
1966	1.533	0.7661	0.3909	0.2004	0.1506	0.04761	
1967	11.91	5.192	1.415	0.5059	0.3635	0.1135	
1968	2.359	1.265	0.2908	0.1418	0.1116	0.0552	
1969	2.798	1.334	0.4162	0.222	0.1506	0.06861	
1970	4.281	2.069	0.5235	0.2334	0.185	0.07512	
1971	0.9061	0.3782	0.1636	0.07232	0.05566	0.01996	
1972	2.842	1.518	0.49	0.3265	0.2214	0.05533	
1973	5.052	2.109	0.5388	0.3335	0.2728	0.1101	
1974	1.188	0.4975	0.1641	0.07163	0.06902	0.03081	
1975	2.265	0.9481	0.217	0.1391	0.09541	0.03738	
1976	5.333	1.67	0.3184	0.1291	0.1269	0.04174	
1977	4.092	1.843	0.4239	0.1996	0.1499	0.06661	
1978	1.852	1.06	0.4665	0.2282	0.1876	0.06086	
1979	4.642	2.125	0.5776	0.3117	0.2176	0.1079	
1980	1.849	1.006	0.2634	0.1872	0.1278	0.04859	
1981	6.092	2.544	0.6968	0.3352	0.2977	0.1027	
1982	15.86	6.62	1.486	0.5905	0.4132	0.1891	
1983	3.449	1.531	0.4072	0.2275	0.1983	0.08194	
1984	3.848	1.607	0.5027	0.2915	0.1979	0.05008	
1985	2.512	1.049	0.2378	0.1533	0.1056	0.03836	
1986	2.562	1.452	0.4441	0.233	0.172	0.05461	
1987	1.728	0.9545	0.2114	0.1209	0.08921	0.04258	
1988	1.221	0.6567	0.1978	0.08514	0.1029	0.03433	
1989	1.662	0.7347	0.2356	0.1571	0.1073	0.02923	
1990	0.8815	0.368	0.1637	0.07199	0.0578	0.02339	

Sorted results

Prob.	Peak	96 hr	21 Day	60 Day	90 Day	Yearly	
0.032258064516129	15.86	6.62	1.486	0.5905	0.4132	0.1891	
0.0645161290322581	11.91	5.192	1.415	0.5059	0.3828	0.1283	
0.0967741935483871	10.16	5.111	1.365	0.4986	0.3635	0.1135	
0.129032258064516	6.092	2.544	0.6968	0.3352	0.2977	0.1101	
0.161290322580645	5.477	2.378	0.5843	0.3335	0.2728	0.1079	
0.193548387096774	5.333	2.336	0.5776	0.3265	0.2214	0.1027	
0.225806451612903	5.052	2.125	0.5388	0.3117	0.2176	0.08194	
0.258064516129032	4.731	2.109	0.5235	0.2915	0.1983	0.07512	
0.290322580645161	4.642	2.069	0.5056	0.2555	0.1979	0.06861	

0.32258064516129	4.281	1.843	0.5027	0.2334	0.1889	0.06661
0.354838709677419	4.092	1.67	0.49	0.233	0.1876	0.06134
0.387096774193548	3.848	1.607	0.4665	0.2282	0.185	0.06086
0.419354838709677	3.577	1.531	0.4629	0.2275	0.1777	0.0569
0.451612903225806	3.449	1.518	0.4441	0.222	0.172	0.05644
0.483870967741936	2.842	1.493	0.4239	0.2184	0.1506	0.05533
0.516129032258065	2.798	1.452	0.4162	0.2004	0.1506	0.0552
0.548387096774194	2.562	1.334	0.4072	0.1996	0.1499	0.05461
0.580645161290323	2.512	1.265	0.3909	0.1872	0.13	0.05008
0.612903225806452	2.359	1.198	0.3493	0.1782	0.1278	0.04859
0.645161290322581	2.265	1.06	0.3184	0.1705	0.1269	0.04761
0.67741935483871	2.161	1.049	0.2908	0.1571	0.1193	0.04258
0.709677419354839	1.852	1.006	0.2634	0.1533	0.1116	0.04174
0.741935483870968	1.849	0.9545	0.2378	0.1418	0.1073	
0.03836						
0.774193548387097	1.728	0.9481	0.2356	0.1391	0.1056	
0.03738						
0.806451612903226	1.662	0.7661	0.217	0.1291	0.1029	0.03433
0.838709677419355	1.533	0.7347	0.2114	0.1209	0.09541	
0.03207						
0.870967741935484	1.221	0.6567	0.1978	0.08514	0.08921	
0.03081						
0.903225806451613	1.188	0.4975	0.1641	0.07232	0.06902	
0.02923						
0.935483870967742	0.9061	0.3782	0.1637	0.07199	0.0578	
0.02339						
0.967741935483871	0.8815	0.368	0.1636	0.07163	0.05566	
0.01996						
0.1	9.7532	4.8543	1.29818	0.48226	0.35692	0.11316
Average of yearly averages:						0.064023

Inputs generated by pe5.pl - Novemeber 2006

Data used for this run:

Output File: vinclozolin_turf

Metfile: w23234.dvf

PRZM scenario: CATurfRLF.txt

EXAMS environment file: pond298.exv

Chemical Name: vinclozolin

Description	Variable Name	Value	Units	Comments
Molecular weight	mwt	286.11	g/mol	
Henry's Law Const.	henry	3.8e-7		atm-m ³ /mol
Vapor Pressure	vapr	2.6e-6	torr	
Solubility	sol	2.6	mg/L	
Kd	Kd		mg/L	
Koc	Koc	582	mg/L	
Photolysis half-life	kdp	27.2	days	Half-life
Aerobic Aquatic Metabolism	kbacw	0	days	Halfife
Anaerobic Aquatic Metabolism	kbacs	402	days	Halfife
Aerobic Soil Metabolism	asm	201	days	Halfife
Hydrolysis: pH 7	1.3	days		Half-life
Method:	CAM	2	integer	See PRZM manual
Incorporation Depth:	DEPI	0	cm	
Application Rate:	TAPP	1.51	kg/ha	
Application Efficiency:	APPEFF	0.99	fraction	
Spray Drift	DRFT	0.01	fraction of application rate applied to pond	

Application Date Date 02-10 dd/mm or dd/mm or dd-mm or dd-mm
 Interval 1 interval 10 days Set to 0 or delete line for single app.
 app. rate 1 apprate 1.51 kg/ha
 Interval 2 interval 10 days Set to 0 or delete line for single app.
 app. rate 2 apprate 1.51 kg/ha
 Record 17: FILTRA
 IPSCND 1
 UPTKF
 Record 18: PLVKRT
 PLDKRT
 FEXTRC 0.5
 Flag for Index Res. Run IR EPA Pond
 Flag for runoff calc. RUNOFF none none, monthly or total(average of
 entire run)

3,5-DCA

stored as 3,5-DCA_turf.out
 Chemical: 3,5-DCA
 PRZM environment: CATurfRLF.txt modified Tuesday, 20 February 2007 at
 12:03:48
 EXAMS environment: pond298.exv modified Tuesday, 26 August 2008 at
 06:14:08
 Metfile: w23234.dvf modified Tuesday, 26 August 2008 at 06:15:38
 Water segment concentrations (ppb)

Year	Peak	96 hr	21 Day	60 Day	90 Day	Yearly
1961	4.145	4.016	3.413	2.127	1.714	0.4237
1962	13.4	12.5	9.921	6.658	5.637	2.67
1963	10.72	10.19	8.66	6.37	5.479	2.465
1964	8.246	7.931	6.398	4.207	3.254	1.424
1965	7.256	7.046	3.326	2.336	1.913	1.08
1966	6.784	6.564	5.693	4.835	4.041	1.956
1967	18.89	18.27	16.61	11.61	9.354	3.453
1968	6.101	5.813	4.912	3.768	3.294	1.501
1969	6.155	5.884	5.376	4.596	3.819	1.672
1970	6.528	6.206	5.35	3.86	3.164	1.637
1971	3.436	3.297	2.836	2.088	1.94	0.9588
1972	6.721	6.451	5.506	4.36	3.746	1.091
1973	9.065	8.619	7.259	6.181	5.25	2.727
1974	6.992	6.669	5.693	4.162	3.577	1.563
1975	4.023	3.8	3.052	2.485	2.302	1.13
1976	7.923	4.289	2.018	1.351	1.232	0.6807
1977	11.29	10.78	9.002	6.421	5.309	2.283
1978	7.771	7.435	6.366	5.708	5.288	2.157
1979	7.991	7.641	6.146	5.56	4.764	2.231
1980	8.654	8.272	7.075	6.142	5.644	2.246
1981	9.145	8.647	6.963	5.179	3.931	2.076
1982	26.8	25.37	20.52	14.76	12.22	5.425
1983	9.714	9.318	8.306	7.013	6.362	2.817
1984	6.528	6.14	5.091	3.718	2.957	1.517
1985	3.85	3.664	3.03	2.319	2.164	1.236
1986	8	7.456	5.889	4.894	3.979	1.71
1987	4.228	4.003	3.285	2.238	2.065	1.056
1988	3.176	3.014	1.832	1.511	1.257	0.8144

1989	3.171	3.029	2.584	2.128	1.807	0.9238
1990	2.428	2.31	1.907	1.683	1.551	0.8244

Sorted results

Prob.	Peak	96 hr	21 Day	60 Day	90 Day	Yearly
0.032258064516129	26.8	25.37	20.52	14.76	12.22	5.425
0.0645161290322581		18.89	18.27	16.61	11.61	9.354
0.0967741935483871		13.4	12.5	9.921	7.013	6.362
0.129032258064516	11.29	10.78	9.002	6.658	5.644	2.727
0.161290322580645	10.72	10.19	8.66	6.421	5.637	2.67
0.193548387096774	9.714	9.318	8.306	6.37	5.479	2.465
0.225806451612903	9.145	8.647	7.259	6.181	5.309	2.283
0.258064516129032	9.065	8.619	7.075	6.142	5.288	2.246
0.290322580645161	8.654	8.272	6.963	5.708	5.25	2.231
0.32258064516129	8.246	7.931	6.398	5.56	4.764	2.157
0.354838709677419	8	7.641	6.366	5.179	4.041	2.076
0.387096774193548	7.991	7.456	6.146	4.894	3.979	1.956
0.419354838709677	7.923	7.435	5.889	4.835	3.931	1.71
0.451612903225806	7.771	7.046	5.693	4.596	3.819	1.672
0.483870967741936	7.256	6.669	5.693	4.36	3.746	1.637
0.516129032258065	6.992	6.564	5.506	4.207	3.577	1.563
0.548387096774194	6.784	6.451	5.376	4.162	3.294	1.517
0.580645161290323	6.721	6.206	5.35	3.86	3.254	1.501
0.612903225806452	6.528	6.14	5.091	3.768	3.164	1.424
0.645161290322581	6.528	5.884	4.912	3.718	2.957	1.236
0.67741935483871	6.155	5.813	3.413	2.485	2.302	1.13
0.709677419354839	6.101	4.289	3.326	2.336	2.164	1.091
0.741935483870968	4.228	4.016	3.285	2.319	2.065	1.08
0.774193548387097	4.145	4.003	3.052	2.238	1.94	1.056
0.806451612903226	4.023	3.8	3.03	2.128	1.913	0.9588
0.838709677419355	3.85	3.664	2.836	2.127	1.807	0.9238
0.870967741935484	3.436	3.297	2.584	2.088	1.714	0.8244
0.903225806451613	3.176	3.029	2.018	1.683	1.551	0.8144
0.935483870967742	3.171	3.014	1.907	1.511	1.257	0.6807
0.967741935483871	2.428	2.31	1.832	1.351	1.232	0.4237

0.1	13.189	12.328	9.8291	6.9775	6.2902	2.808
Average of yearly averages:						1.79162666666667

Inputs generated by pe5.pl - Novemeber 2006

Data used for this run:

Output File: 3,5-DCA_turf

Metfile: w23234.dvf

PRZM scenario: CATurfRLF.txt

EXAMS environment file: pond298.exv

Chemical Name: 3,5-DCA

Description	Variable	Name	Value	Units	Comments
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Molecular weight	mwt	162.02	g/mol		
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Henry's Law Const.	henry	5.8e-6	atm-m^3/mol		
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Vapor Pressure	vapr	2.12e-2	torr		
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Solubility	sol	784	mg/L		
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Kd	Kd	mg/L			
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Koc	Koc	557	mg/L		
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Photolysis half-life	kdp	0	days	Half-life	
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Aerobic Aquatic Metabolism	kbacw	0	days	Halfife	
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Anaerobic Aquatic Metabolism	kbacs	0	days	Halfife	
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Aerobic Soil Metabolism asm 0 days Halfife
 Hydrolysis: pH 7 0 days Half-life
 Method: CAM 2 integer See PRZM manual
 Incorporation Depth: DEPI 0 cm
 Application Rate: TAPP 0.855 kg/ha
 Application Efficiency: APPEFF 0.99 fraction
 Spray Drift DRFT 0.01 fraction of application rate applied to pond
 Application Date Date 02-10 dd/mm or dd/mm or dd-mm or dd-mm
 Interval 1 interval 10 days Set to 0 or delete line for single app.
 app. rate 1 apprate 1.51 kg/ha
 Interval 2 interval 10 days Set to 0 or delete line for single app.
 app. rate 2 apprate 1.51 kg/ha
 Record 17: FILTRA
 IPSCND 1
 UPTKF
 Record 18: PLVKRT
 PLDKRT
 FEXTRC 0.5
 Flag for Index Res. Run IR EPA Pond
 Flag for runoff calc. RUNOFF none none, monthly or total(average of
 entire run)