

APPENDIX D. Example output from PRZM/EXAMS, ECOSAR

PE5 example output:

Avocado:

stored as avocado.out

Chemical: Methomyl

PRZM environment: CAAvocadoRLF_V2.txt modified Wedday, 26 March 2008 at 10:28:12

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

Metfile: w23188.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	2.575	2.26	1.52	0.7114	0.4743	0.1169
1962	2.575	2.269	1.428	0.6443	0.4295	0.1211
1963	2.575	2.253	1.386	0.6165	0.411	0.1153
1964	2.575	2.279	1.453	0.668	0.4453	0.1295
1965	10.89	9.569	5.988	2.748	1.832	0.4684
1966	2.575	2.241	1.427	0.6543	0.4362	0.1679
1967	9.741	8.559	5.129	2.3	1.534	0.3906
1968	2.575	2.248	1.387	0.6274	0.4182	0.1421
1969	2.575	2.218	1.306	0.5689	0.3793	0.1127
1970	2.575	2.249	1.49	0.6818	0.4545	0.1202
1971	2.575	2.271	1.51	0.7103	0.4735	0.1309
1972	2.575	2.267	1.78	0.903	0.602	0.1644
1973	2.575	2.261	1.395	0.6179	0.4119	0.1232
1974	3.668	3.277	2.164	1.217	0.8112	0.2112
1975	2.575	2.26	1.406	0.6316	0.421	0.1409
1976	2.575	2.186	1.238	0.5323	0.3549	0.09747
1977	2.575	2.211	1.271	0.5356	0.3571	0.09767
1978	2.604	2.281	1.419	0.6735	0.449	0.1159
1979	2.575	2.239	1.342	0.5822	0.3881	0.1113
1980	2.575	2.233	1.331	0.5777	0.3851	0.1169
1981	3.5	3.028	2.158	1.008	0.6719	0.1726
1982	2.575	2.236	1.35	0.5973	0.3982	0.116
1983	2.575	2.241	1.342	0.5773	0.3849	0.1032
1984	2.575	2.36	1.494	0.6677	0.4451	0.1158
1985	5.792	5.093	3.31	1.557	1.038	0.267
1986	2.575	2.233	1.384	0.6311	0.4207	0.1308
1987	2.575	2.244	1.592	0.8492	0.5661	0.1531
1988	3.26	2.869	2.06	0.9641	0.6427	0.1837
1989	2.575	2.23	1.333	0.6315	0.421	0.1247
1990	2.575	2.234	1.355	0.6088	0.4058	0.1386

Sorted results

Prob.	Peak	96 hr	21 Day	60 Day	90 Day	Yearly
0.032258064516129	10.89	9.569	5.988	2.748	1.832	0.4684
0.0645161290322581	9.741	8.559	5.129	2.3	1.534	0.3906
0.0967741935483871	5.792	5.093	3.31	1.557	1.038	0.267
0.129032258064516	3.668	3.277	2.164	1.217	0.8112	0.2112
0.161290322580645	3.5	3.028	2.158	1.008	0.6719	0.1837
0.193548387096774	3.26	2.869	2.06	0.9641	0.6427	0.1726
0.225806451612903	2.604	2.36	1.78	0.903	0.602	0.1679
0.258064516129032	2.575	2.281	1.592	0.8492	0.5661	0.1644
0.290322580645161	2.575	2.279	1.52	0.7114	0.4743	0.1531
0.32258064516129	2.575	2.271	1.51	0.7103	0.4735	0.1421
0.354838709677419	2.575	2.269	1.494	0.6818	0.4545	0.1409
0.387096774193548	2.575	2.267	1.49	0.6735	0.449	0.1386
0.419354838709677	2.575	2.261	1.453	0.668	0.4453	0.1309
0.451612903225806	2.575	2.26	1.428	0.6677	0.4451	0.1308
0.483870967741936	2.575	2.26	1.427	0.6543	0.4362	0.1295
0.516129032258065	2.575	2.253	1.419	0.6443	0.4295	0.1247
0.548387096774194	2.575	2.249	1.406	0.6316	0.421	0.1232
0.580645161290323	2.575	2.248	1.395	0.6315	0.421	0.1211
0.612903225806452	2.575	2.244	1.387	0.6311	0.4207	0.1202

0.645161290322581	2.575	2.241	1.386	0.6274	0.4182	0.1169
0.67741935483871	2.575	2.241	1.384	0.6179	0.4119	0.1169
0.709677419354839	2.575	2.239	1.355	0.6165	0.411	0.116
0.741935483870968	2.575	2.236	1.35	0.6088	0.4058	0.1159
0.774193548387097	2.575	2.234	1.342	0.5973	0.3982	0.1158
0.806451612903226	2.575	2.233	1.342	0.5822	0.3881	0.1153
0.838709677419355	2.575	2.233	1.333	0.5777	0.3851	0.1127
0.870967741935484	2.575	2.23	1.331	0.5773	0.3849	0.1113
0.903225806451613	2.575	2.218	1.306	0.5689	0.3793	0.1032
0.935483870967742	2.575	2.211	1.271	0.5356	0.3571	0.09767
0.967741935483871	2.575	2.186	1.238	0.5323	0.3549	0.09747
0.1	5.5796	4.9114	3.1954	1.523	1.01532	0.26142
					Average of yearly averages:	0.156668

Inputs generated by pe5.pl - Novemeber 2006

Data used for this run:

Output File: avocado

Metfile: w23188.dvf

PRZM scenario: CAAvocadoRLF_V2.txt

EXAMS environment file: pond298.exv

Chemical Name: Methomyl

Description	Variable Name	Value	Units	Comments
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Molecular weight	mwt	162.2	g/mol	
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Henry's Law Const.	henry	2.1e-11	atm-m ³ /mol	
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Vapor Pressure	vapr		torr	
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Solubility	sol	5.5e4	mg/L	
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Kd	Kd		mg/L	
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Koc	Koc	46	mg/L	
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Photolysis half-life	kdp	50	days	Half-life
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Aerobic Aquatic Metabolism	kbacw	5.5	days	Halfife
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Anaerobic Aquatic Metabolism	kbacs	28	days	Halfife
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Aerobic Soil Metabolism	asm	43	days	Halfife
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Hydrolysis:	pH 7	0	days	Half-life
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Method:	CAM	2	integer	See PRZM manual
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Incorporation Depth:	DEPI		cm	
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Application Rate:	TAPP	1.01	kg/ha	
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Application Efficiency:	APPEFF	0.95	fraction	
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Spray Drift	DRFT	0.051	fraction of application rate applied to pond	
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Application Date	Date	21-11	dd/mm or dd/mm or dd-mm or dd-mmm	
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Record 17: FILTRA

IPSCND 1

UPTKF

Record 18: PLVKRT

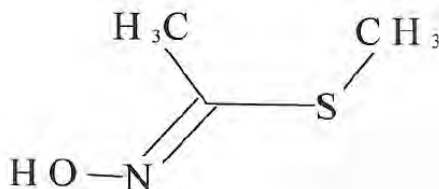
PLDKRT 0.309

FEXTRC 0.5

Flag for Index Res. Run	IR	EPA Pond
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Flag for runoff calc.	RUNOFF	none, monthly or total(average of entire run)
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ECOSAR example output:



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SMILES : ON=C(SC)C
CHEM :
CAS Num:
ChemID1:
MOL FOR: C3 H7 N1 O1 S1
MOL WT : 105.16
Log Kow: 1.102      (EPISuite Kowwin Estimate)
Log Kow:           (User Entered)
Log Kow: 1.12      (PhysProp DB exp value - for comparison only)
Melt Pt:           (User Entered for Wat Sol estimate)
Wat Sol: 1.247E+004 (mg/L, EPISuite WSKowwin Estimate)
Wat Sol:           (User Entered)
Wat Sol:           (PhysProp DB exp value)
  
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 Values used to Generate ECOSAR Profile

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Log Kow: 1.102      (EPISuite Kowwin Estimate)
Wat Sol: 1.247E+004 (mg/L, EPISuite WSKowwin Estimate)
  
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 Available Measured Data from ECOSAR Training Set

No Data Available

 ECOSAR v1.1 Class-specific Estimations

Aliphatic Amines

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
=====	=====	=====	=====	=====
Aliphatic Amines	: Fish	96-hr	LC50	76.219
Aliphatic Amines	: Daphnid	48-hr	LC50	8.436
Aliphatic Amines	: Green Algae	96-hr	EC50	8.557
Aliphatic Amines	: Fish		ChV	6.287
Aliphatic Amines	: Daphnid		ChV	0.626
Aliphatic Amines	: Green Algae		ChV	2.635
=====	=====	=====	=====	=====
Neutral Organic SAR	: Fish	96-hr	LC50	553.026
(Baseline Toxicity)	: Daphnid	48-hr	LC50	246.756
	: Green Algae	96-hr	EC50	227.679
	: Fish		ChV	49.021
	: Daphnid		ChV	22.379
	: Green Algae		ChV	33.275

NOTE: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect.

Class Specific LogKow Cut-Offs

Aliphatic Amines:

Maximum LogKow: 6.0 (Fish, Mysid LC50)
Maximum LogKow: 5.0 (Daphnid LC50)
Maximum LogKow: 7.0 (Green Algae EC50)
Maximum LogKow: 8.0 (Fish, Daphnid ChV)
Maximum LogKow: 7.0 (Green Algae ChV)

Baseline Toxicity SAR Limitations:

Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50)
Maximum LogKow: 6.4 (Green Algae EC50)
Maximum LogKow: 8.0 (ChV)