

Appendix C: KABAM Results – September 3, 2009. The program was run in default mode with Log K_{ow} = 4.7; K_{oc} = 6070 L/mg-OC; and surface water and pore water EECs of 5.36 and 3.31 ppb, respectively.

Table 1. Chemical characteristics of Chlorpyrifos.		
Characteristic	Value	Comments/Guidance
Pesticide Name	Chlorpyrifos	Required input
Log K _{ow}	4.7	Required input Enter value from acceptable or supplemental study submitted by registrant or available in scientific literature.
K _{ow}	50119	No input necessary. This value is calculated automatically from the Log K _{ow} value entered above.
K _{oc} (L/kg OC)	6070	Required input Input value used in PRZM/EXAMS to derive EECs. Follow input parameter guidance for deriving this parameter value (USEPA 2002).
Time to steady state (T _s ; days)	16	No input necessary. This value is calculated automatically from the Log K _{ow} value entered above.
Pore water EEC (µg/L)	3.31	Required input Enter value generated by PRZM/EXAMS benthic file. PRZM/EXAMS EEC represents the freely dissolved concentration of the pesticide in the pore water of the sediment. The appropriate averaging period of the EEC is dependent on the specific pesticide being modeled and is based on the time it takes for the chemical to reach steady state. Select the EEC generated by PRZM/EXAMS which has an averaging period closest to the time to steady state calculated above. In cases where the time to steady state exceeds 365 days, the user should select the EEC representing the average of yearly averages. The peak EEC should not be used.
Water Column EEC (µg/L)	5.36	Required input Enter value generated by PRZM/EXAMS water column file. PRZM/EXAMS EEC represents the freely dissolved concentration of the pesticide in the water column. The appropriate averaging period of the EEC is dependent on the specific pesticide being modeled and is based on the time it takes for the chemical to reach steady state. The averaging period used for the water column EEC should be the same as the one selected for the pore water EEC (discussed above).

Table 2. Input parameters for rate constants. "calculated" indicates that model will calculate rate constant.

Trophic level	k_1 (L/kg*d)	k_2 (d ⁻¹)	k_D (kg-food/kg-org/d)	k_E (d ⁻¹)	k_M^* (d ⁻¹)
phytoplankton	calculated	calculated	0*	0*	0
zooplankton	calculated	calculated	calculated	calculated	0
benthic invertebrates	calculated	calculated	calculated	calculated	0
filter feeders	calculated	calculated	calculated	calculated	0
small fish	calculated	calculated	calculated	calculated	0
medium fish	calculated	calculated	calculated	calculated	0
large fish	calculated	calculated	calculated	calculated	0

* Default value is 0.

k_1 and k_2 represent the uptake and elimination constants respectively, through respiration.

k_D and k_E represent the uptake and elimination constants, respectively, through diet.

k_M represents the metabolism rate constant.

Table 3. Mammalian and avian toxicity data for Chlorpyrifos. These are required inputs.

Animal	Measure of effect (units)	Value	Species	If selected species is "other," enter body weight (in kg) here.
Avian	LD ₅₀ (mg/kg-bw)	112	mallard duck	
	LC ₅₀ (mg/kg-diet)	423	Northern bobwhite quail	
	NOAEC (mg/kg-diet)	136	mallard duck	
	Mineau Scaling Factor	1.15	Default value for all species is 1.15 (for chemical specific values, see Mineau et al. 1996).	
Mammalian	LD ₅₀ (mg/kg-bw)	118	laboratory rat	
	LC ₅₀ (mg/kg-diet)	N/A	other	
	Chronic Endpoint	20	laboratory rat	
	units of chronic endpoint*	ppm		

Table 4. Abiotic characteristics of the model aquatic ecosystem.		
Characteristic	Value	Guidance*
Concentration of Particulate Organic Carbon (X_{POC} ; kg OC/ L)	0.00E+00	When using EECs generated by PRZM/EXAMS, use a value of "0" for both POC and DOC.
Concentration of Dissolved Organic Carbon (X_{DOC} ; kg OC/L)	0.00E+00	
Concentration of Dissolved Oxygen (C_{OX} ; mg O ₂ /L)	5.0	Default value is 5.0 mg O ₂ /L when using EECs generated by PRZM/EXAMS.
Water Temperature (T; °C)	15	Value is defined by the average water temperature of the EXAMS pond when using EECs generated by PRZM/EXAMS. Model user should consult output file of EXAMS to define this value.
Concentration of Suspended Solids (C_{SS} ; kg/L)	3.00E-05	Default value is 3.00x10 ⁻⁵ kg/L when using EECs generated by PRZM/EXAMS.
Sediment Organic Carbon (OC; %)	4.0%	Default value is 4.0% when using EECs generated by PRZM/EXAMS.
*When using pesticide concentrations from monitoring data or mesocosm studies, consult Appendix B of the User's Guide for specific guidance on selecting values for these parameters.		

Table 5. Characteristics of aquatic biota of the model ecosystem.					
Trophic Level	Wet Weight (kg)	% lipids	% NLOM	% Water	Do organisms in spire some pore water?
sediment*	N/A	0.0%	4.0%	96.0%	N/A
phytoplankton	N/A	2.0%	8.0%	90.0%	no
zooplankton	1.0E-07	3.0%	12.0%	85.0%	no
benthic invertebrates	1.0E-04	3.0%	21.0%	76.0%	yes
filter feeders	1.0E-03	2.0%	13.0%	85.0%	yes
small fish	1.0E-02	4.0%	23.0%	73.0%	yes
medium fish	1.0E-01	4.0%	23.0%	73.0%	yes
large fish	1.0E+00	4.0%	23.0%	73.0%	no
* N/A = not applicable Note that sediment is not a trophic level. It is included in this table because it is consumed by aquatic organisms of the KABAM foodweb.					

Table 6. Diets of aquatic biota of the model ecosystem.

Trophic level in diet	Diet for:					
	Zoo plankton	Benthic Invertebrates	Filter Feeder	Small Fish	Medium Fish	Large Fish
sediment*	0.0%	34.0%	34.0%	0.0%	0.0%	0.0%
phytoplankton	100.0%	33.0%	33.0%	0.0%	0.0%	0.0%
zooplankton		33.0%	33.0%	50.0%	0.0%	0.0%
benthic invertebrates			0.0%	50.0%	50.0%	0.0%
filter feeders				0.0%	0.0%	0.0%
small fish					50.0%	0.0%
medium fish						100.0%
Total	100.0%	100.0%	100.0%	100.0%	100.0%	100.0%
*Note that sediment is not a trophic level. It is included in this table because it is consumed by aquatic organisms of the KABAM foodweb.						

Table 7. Identification of mammals and birds feeding on aquatic biota of the model ecosystem.

Mammal/Bird #	Name	Body weight (kg)
Mammal 1	fog/water shrew	0.018
Mammal 2	rice rat/star-nosed mole	0.085
Mammal 3	small mink	0.45
Mammal 4	large mink	1.8
Mammal 5	small river otter	5
Mammal 6	large river otter	15
Bird 1	sandpipers	0.02
Bird 2	cranes	6.7
Bird 3	rails	0.07
Bird 4	herons	2.9
Bird 5	small osprey	1.25
Bird 6	white pelican	7.5

Table 8. Diets of mammals feeding on aquatic biota of the model ecosystem.

Trophic level in diet	Diet for:					
	fog/water shrew	rice rat/star-nosed mole	small mink	large mink	small river otter	large river otter
phytoplankton	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
zooplankton	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
benthic invertebrates	100.0%	34.0%	0.0%	0.0%	0.0%	0.0%
filter feeders	0.0%	33.0%	0.0%	0.0%	0.0%	0.0%
small fish	0.0%	33.0%	0.0%	0.0%	0.0%	0.0%
medium fish	0.0%	0.0%	100.0%	100.0%	100.0%	0.0%
large fish	0.0%	0.0%	0.0%	0.0%	0.0%	100.0%
Total	100.0%	100.0%	100.0%	100.0%	100.0%	100.0%

Table 9. Diets of birds feeding on aquatic biota of the model ecosystem.

Trophic level in diet	Diet for:					
	sandpipers	cranes	rails	herons	small osprey	white pelican
phytoplankton	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
zooplankton	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
benthic invertebrates	33.0%	33.0%	50.0%	50.0%	0.0%	0.0%
filter feeders	33.0%	33.0%	0.0%	0.0%	0.0%	0.0%
small fish	34.0%	0.0%	50.0%	0.0%	0.0%	0.0%
medium fish	0.0%	34.0%	0.0%	50.0%	100.0%	0.0%
large fish	0.0%	0.0%	0.0%	0.0%	0.0%	100.0%
Total	100.0%	100.0%	100.0%	100.0%	100.0%	100.0%

Table 10. Input parameters and calculations relevant to derivation of C_B .

Parameter	Phyto plankton	Zoo plankton	Benthic Invertebrates	Filter Feeders	Small Fish	Medium Fish	Large Fish
Equation A1							
C _B	0.012393	0.00931644	0.010153	0.006672	0.014033	0.015337	0.01828
C _{BD}	0.000000	0.00014996	0.000389	0.000251	0.001625	0.003145	0.006164
C _{BR}	0.01239312	0.00916649	0.00976385	0.00642116	0.01240764	0.01219249	0.01212096
C _S	0.000804						
C _{WDP}	0.00000331						
C _{WTO}	0.00000536						
k ₁	5891.383	42585.416	3795.429	1695.356	757.288	338.268	151.099
k ₂	2.448012	24.832445	2.026721	1.376922	0.314366	0.140422	0.062724
k _D	0.000000	0.301304	0.106907	0.046773	0.053580	0.037932	0.026854
k _E	0.000000	0.056334	0.013834	0.009205	0.005264	0.004649	0.003593
k _G	0.100000	0.012559	0.003155	0.001991	0.001256	0.000792	0.000500
k _M	0	0	0	0	0	0	0
m _o	1	1	0.95	0.95	0.95	0.95	1
m _p	0	0	0.05	0.05	0.05	0.05	0
Σ (P _i * C _{Di})	0	0.012393117	0.007437402	0.0074374	0.00973467	0.012093	0.01533728
Φ	1.00000000						
Equation A2							
X _{POC}	0.0000000						
X _{DOC}	0.0000000						
K _{OW}	50119						
Φ	1.00000000						
Equation A4							
C _S	0.0008						
C _{SOC}	0.0201						
C _{WDP}	0.00000						
K _{OC}	6070						
OC	4%						
Equation A5							
C _{ox}	N/A	5					
E _W	N/A	0.539638424					
G _V	N/A	0.007891472	0.703328201	3.14165167	14.0332425	62.6841919	280
k ₁	5891.383138	42585.41622	3795.429216	1695.35596	757.287688	338.267985	151.098759
K _{OW}	50119						
W _B	N/A	0.0000001	0.0001	0.001	0.01	0.1	1
Equation A6							
k ₁	5891.383138	42585.41622	3795.429216	1695.35596	757.287688	338.267985	151.098759

K_2	2.448012245	24.83244474	2.026721169	1.37692245	0.31436622	0.14042223	0.06272431
K_{BW}	2406.598721	1714.910339	1872.694318	1231.26466	2408.93466	2408.93466	2408.93466
K_{OW}	50119						
V_{LB}	0.02	0.03	0.03	0.02	0.04	0.04	0.04
V_{NB}	0.08	0.12	0.21	0.13	0.23	0.23	0.23
V_{WB}	0.9	0.85	0.76	0.85	0.73	0.73	0.73
β	0.35	0.035					
Equation A7							
K_G	0.1	0.012559432	0.003154787	0.00199054	0.00125594	0.00079245	0.0005
T	15						
W_B	N/A	0.0000001	0.0001	0.001	0.01	0.1	1
Equation A8							
C_{ox}	N/A	N/A	N/A	5	N/A	N/A	N/A
C_{SS}	N/A	N/A	N/A	3.00E-05	N/A	N/A	N/A
E_D	N/A	0.496269144					
G_D	N/A	6.07E-08	2.15E-05	9.42E-05	1.08E-03	7.64E-03	5.41E-02
G_V	N/A	N/A	N/A	3.14	N/A	N/A	N/A
K_D	0	3.01E-01	1.07E-01	4.68E-02	5.36E-02	3.79E-02	2.69E-02
K_{OW}	50119						
T	N/A	15					
W_B	N/A	0.0000001	0.0001	0.001	0.01	0.1	1
Equation A9							
C_{ox}	N/A	N/A	N/A	5	N/A	N/A	N/A
C_{SS}	N/A	N/A	N/A	3.00E-05	N/A	N/A	N/A
E_D	N/A	0.4963					
G_D	N/A	0.0000	0.0000	0.0000942	0.0011	0.0076	0.0541
G_F	N/A	0.000000	0.000015	0.000066	0.000726	0.004965	0.034777
G_V	N/A	N/A	N/A	3.1417	N/A	N/A	N/A
K_E	0	0.0563	0.0138	0.0092	0.0053	0.0046	0.0036
K_{GB}	N/A	0.2660	0.1843	0.2804	0.1462	0.1887	0.2082
K_{OW}	N/A	50119					
T	N/A	15					
V_{LB}	N/A	0.03	0.03	0.02	0.04	0.04	0.04
V_{LD}	N/A	0.02	0.01650	0.0165	0.03	0.035	0.04
V_{LG}	N/A	0.007966	0.005876	0.005876	0.003571	0.004311	0.004979
V_{NB}	N/A	0.12	0.21	0.13	0.23	0.23	0.23
V_{ND}	N/A	0.08	0.0796	0.0796	0.165	0.22	0.23
V_{NG}	N/A	0.03186	0.02835	0.02835	0.09819	0.13548	0.14315
V_{WB}	N/A	0.85	0.76	0.85	0.73	0.73	0.73
V_{WD}	N/A	0.9	0.9039	0.9039	0.805	0.745	0.73

V_{WG}	N/A	0.9602	0.9658	0.9658	0.8982	0.8602	0.8519
W_B	N/A	0.0000001	0.0001	0.001	0.01	0.1	1
β	N/A	0.035	0.035	0.035	0.035	0.035	0.035
ϵ_L	N/A	0.72	0.75	0.75	0.92	0.92	0.92
ϵ_N	N/A	0.72	0.75	0.75	0.6	0.6	0.6
ϵ_W	N/A	0.25	0.25	0.25	0.25	0.25	0.25
Calculation of BCF values							
C_{BCF}	0.012899369	0.009191919	0.00984569	0.00647337	0.01266497	0.01266497	0.01291189

Table 11. Estimated concentrations of Chlorpyrifos in ecosystem components.

Ecosystem Component	Total concentration ($\mu\text{g/kg-ww}$)	Lipid normalized concentration ($\mu\text{g/kg-lipid}$)	Contribution due to diet ($\mu\text{g/kg-ww}$)	Contribution due to respiration ($\mu\text{g/kg-ww}$)
Water (total)*	5	N/A	N/A	N/A
Water (freely dissolved)*	5	N/A	N/A	N/A
Sediment (pore water)*	3	N/A	N/A	N/A
Sediment (in solid)**	804	N/A	N/A	N/A
Phytoplankton	12,393	619656	N/A	12,393.12
Zooplankton	9,316	310548	149.96	9,166.49
Benthic Invertebrates	10,153	338430	389.05	9,763.85
Filter Feeders	6,672	333588	250.61	6,421.16
Small Fish	14,033	350827	1,625.46	12,407.64
Medium Fish	15,337	383432	3,144.79	12,192.49
Large Fish	18,285	457125	6,164.03	12,120.96
* Units: $\mu\text{g/L}$; **Units: $\mu\text{g/kg-dw}$				

Table 12. Total BCF and BAF values of Chlorpyrifos in aquatic trophic levels.

Trophic Level	Total BCF ($\mu\text{g/kg-ww}/(\mu\text{g/L})$)	Total BAF ($\mu\text{g/kg-ww}/(\mu\text{g/L})$)
Phytoplankton	2407	2312
Zooplankton	1715	1738
Benthic Invertebrates	1837	1894
Filter Feeders	1208	1245
Small Fish	2363	2618
Medium Fish	2363	2861
Large Fish	2409	3411

Table 13. Lipid-normalized BCF, BAF, BMF and BSAF values of Chlorpyrifos in aquatic trophic levels.

Trophic Level	BCF ($\mu\text{g/kg-lipid}$)/($\mu\text{g/L}$)	BAF ($\mu\text{g/kg-lipid}$)/($\mu\text{g/L}$)	BMF ($\mu\text{g/kg-lipid}$)/($\mu\text{g/kg-lipid}$)	BSAF ($\mu\text{g/kg-lipid}$)/($\mu\text{g/kg-OC}$)
Phytoplankton	120330	115607	N/A	31
Zooplankton	57164	57938	0.50	15
Benthic Invertebrates	61229	63140	1.10	17
Filter Feeders	60386	62237	1.09	17
Small Fish	59072	65453	1.08	17
Medium Fish	59072	71536	1.11	19
Large Fish	60223	85284	1.19	23

Table 14. Calculation of EECs for mammals and birds consuming fish contaminated by Chlorpyrifos.

Wildlife Species	Biological Parameters				EECs (pesticide intake)	
	Body Weight (kg)	Dry Food Ingestion Rate (kg-dry food/kg-bw/day)	Wet Food Ingestion Rate (kg-wet food/kg-bw/day)	Drinking Water Intake (L/d)	Dose Based (mg/kg-bw/d)	Dietary Based (ppm)
Mammalian						
fog/water shrew	0.02	0.140	0.585	0.003	5.942	10.15
rice rat/star-nosed mole	0.1	0.107	0.484	0.011	4.977	10.28
small mink	0.5	0.079	0.293	0.048	4.499	15.34
large mink	1.8	0.062	0.229	0.168	3.515	15.34
small river otter	5.0	0.052	0.191	0.421	2.931	15.34
large river otter	15.0	0.042	0.157	1.133	2.873	18.28
Avian						
sandpipers	0.0	0.228	1.034	0.004	10.6739	10.32
cranes	6.7	0.030	0.136	0.211	1.4634	10.77
rails	0.1	0.147	0.577	0.010	6.9827	12.09
herons	2.9	0.040	0.157	0.120	2.0063	12.75
small osprey	1.3	0.054	0.199	0.069	3.0586	15.34
white pelican	7.5	0.029	0.107	0.228	1.9512	18.28

Table 15. Calculation of toxicity values for mammals and birds consuming fish contaminated by Chlorpyrifos.

Wildlife Species	Toxicity Values			
	Acute		Chronic	
	Dose Based (mg/kg-bw)	Dietary Based (mg/kg-diet)	Dose Based (mg/kg-bw)	Dietary Based (mg/kg-diet)
Mammalian				
fog/water shrew	247.79	N/A	2.10	20
rice rat/star-nosed mole	168.09	N/A	1.42	20
small mink	110.81	N/A	0.94	20
large mink	78.36	N/A	0.66	20
small river otter	60.70	N/A	0.51	20
large river otter	46.12	N/A	0.39	20
Avian				
sandpipers	58.15	423.00	N/A	136
cranes	139.10	423.00	N/A	136
rails	70.18	423.00	N/A	136
herons	122.68	423.00	N/A	136
small osprey	108.13	423.00	N/A	136
white pelican	141.47	423.00	N/A	136

Table 16. Calculation of RQ values for mammals and birds consuming fish contaminated by Chlorpyrifos.

Wildlife Species	Acute		Chronic	
	Dose Based	Dietary Based	Dose Based	Dietary Based
Mammalian				
fog/water shrew	0.024	N/A	2.830	0.508
rice rat/star-nosed mole	0.030	N/A	3.494	0.514
small mink	0.041	N/A	4.791	0.767
large mink	0.045	N/A	5.294	0.767
small river otter	0.048	N/A	5.698	0.767
large river otter	0.062	N/A	7.352	0.914
Avian				
sandpipers	0.184	0.024	N/A	0.076
cranes	0.011	0.025	N/A	0.079
rails	0.100	0.029	N/A	0.089
herons	0.016	0.030	N/A	0.094
small osprey	0.028	0.036	N/A	0.113
white pelican	0.014	0.043	N/A	0.134