

Appendix G. Outputs from KABAM v.1.0

Tables G1-G16 contain the inputs and outputs generated by KABAM v.1.0 for parent dicofol. Parameters related to mammals consuming aquatic animals are not relevant to the CRLF assessment. KABAM was run in default mode, with the exception of body weights and diet compositions related to the CRLF. For more information on KABAM, see the user's guide.

Table G1. Chemical characteristics of dicofol.		
Characteristic	Value	Comments/Guidance
Pesticide Name	dicofol	Required input
Log K _{OW}	6.06	Required input Enter value from acceptable or supplemental study submitted by registrant or available in scientific literature.
K _{OW}	1148154	No input necessary. This value is calculated automatically from the Log K _{OW} value entered above.
K _{OC} (L/kg) OC)	7060	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)	315	No input necessary. This value is calculated automatically from the Log K _{OW} value entered above.
Pore water EEC (µg/L)	0.066	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)	0.22	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 G2. 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 G3. Mammalian and avian toxicity data for dicofol. 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)	265	other	1.135
	LC ₅₀ (mg/kg-diet)	903	Northern bobwhite quail	
	NOAEC (mg/kg-diet)	1	other	0.1
	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)		laboratory rat	
	LC ₅₀ (mg/kg-diet)	N/A	other	
	Chronic Endpoint		laboratory rat	
	units of chronic endpoint*	ppm		

*ppm = mg/kg-diet

Table G4. 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_{O_2} ; 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)	13	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 3.00×10^{-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 G5. Characteristics of aquatic biota of the model ecosystem.

Trophic Level	Wet Weight (kg)	% lipids	% NLOM	% Water	Do organisms in trophic level respire 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
*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. N/A = not applicable					

Table G6. 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 G7. 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	small CRLF 1	0.0014
Bird 2	small CRLF 2	0.0014
Bird 3	med CRLF 1	0.037
Bird 4	med CRLF 2	0.037
Bird 5	large CRLF 1	0.238
Bird 6	large CRLF 2	0.238

Table G8. 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 G9. Diets of birds feeding on aquatic biota of the model ecosystem.

Trophic level in diet	Diet for:					
	small CRLF 1	small CRLF 2	med CRLF 1	med CRLF 2	large CRLF 1	large CRLF 2
phytoplankton	100.0%	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	0.0%	100.0%	100.0%	0.0%	100.0%	0.0%
filter feeders	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
small fish	0.0%	0.0%	0.0%	100.0%	0.0%	0.0%
medium fish	0.0%	0.0%	0.0%	0.0%	0.0%	100.0%
large fish	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Total	100.0%	100.0%	100.0%	100.0%	100.0%	100.0%

Table G10. Input parameters and calculations relevant to derivation of C_B .

Parameter	Phytoplankton	Zooplankton	Benthic Invertebrates	Filter Feeders	Small Fish	Medium Fish	Large Fish
Equation A1							
C_B	0.008934	0.01001688	0.012874	0.008729	0.033064	0.070288	0.24624
C_{BD}	0.000000	0.00179747	0.004986	0.003589	0.024593	0.063420	0.240672
C_{BR}	0.00893444	0.00821941	0.00788747	0.00514064	0.00847142	0.00686845	0.00556914
C_S	0.000019						
C_{WDP}	0.00000007						
C_{WTO}	0.00000022						
k_1	15434.409	42653.494	3801.497	1698.066	758.498	338.809	151.340
k_2	0.280054	1.086223	0.088645	0.060241	0.013749	0.006141	0.002743

k _D	0.000000	0.229685	0.081495	0.040201	0.040844	0.028916	0.020471
k _E	0.000000	0.042878	0.010521	0.007896	0.004004	0.003539	0.002735
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	0.008934442	0.006260274	0.00626027	0.01144521	0.02296887	0.07028834
Φ	1.00000000						
Equation A2							
X _{POC}	0.0000000						
X _{DOC}	0.0000000						
K _{OW}	1148154						
Φ	1.00000000						
Equation A4							
C _S	0.0000						
C _{SOC}	0.0005						
C _{WDP}	0.00000						
K _{OC}	7060						
OC	4%						
Equation A5							
C _{ox}	N/A	5					
E _W	N/A	0.540501099					
G _V	N/A	0.007891472	0.703328201	3.14165167	14.0332425	62.6841919	280
k ₁	15434.40922	42653.49399	3801.496653	1698.06618	758.498301	338.808746	151.340308
K _{OW}	1148154						
W _B	N/A	0.0000001	0.0001	0.001	0.01	0.1	1
Equation A6							
k ₁	15434.40922	42653.49399	3801.496653	1698.06618	758.498301	338.808746	151.340308
k ₂	0.280053936	1.086223278	0.088645422	0.0602407	0.0137485	0.00614123	0.00274319
K _{BW}	55112.27383	39267.70386	42884.29776	28188.0214	55169.5115	55169.5115	55169.5115
K _{OW}	1148154						
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	13						
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	0.426539986					
G_D	N/A	5.38E-08	1.91E-05	9.42E-05	9.58E-04	6.78E-03	4.80E-02
G_V	N/A	N/A	N/A	3.14	N/A	N/A	N/A
k_D	0	2.30E-01	8.15E-02	4.02E-02	4.08E-02	2.89E-02	2.05E-02
K_{OW}	1148154						
T	N/A	13					
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	0.4265					
G_D	N/A	0.0000	0.0000	0.0000942	0.0010	0.0068	0.0480
G_F	N/A	0.000000	0.000013	0.000066	0.000644	0.004403	0.030845
G_V	N/A	N/A	N/A	3.1417	N/A	N/A	N/A
k_E	0	0.0429	0.0105	0.0079	0.0040	0.0035	0.0027
K_{GB}	N/A	0.2655	0.1839	0.2798	0.1458	0.1884	0.2079
K_{OW}	N/A	1148154					
T	N/A	13					
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}	0.0121247	0.008638895	0.009104336	0.00598432	0.01171249	0.01171249	0.01213729

See Appendix A of KABAM user's guide and technical documentation for equation details.

Table G11. Estimated concentrations of dicofol in ecosystem components.

Ecosystem Component	Total concentration (µg/kg-ww)	Lipid normalized concentration (µg/kg-lipid)	Contribution due to diet (µg/kg-ww)	Contribution due to respiration (µg/kg-ww)
Water (total)*	0	N/A	N/A	N/A
Water (freely dissolved)*	0	N/A	N/A	N/A
Sediment (pore water)*	0	N/A	N/A	N/A
Sediment (in solid)**	19	N/A	N/A	N/A
Phytoplankton	8,934	446722	N/A	8,934.44
Zooplankton	10,017	333896	1,797.47	8,219.41
Benthic Invertebrates	12,874	429118	4,986.07	7,887.47
Filter Feeders	8,729	436471	3,588.77	5,140.64
Small Fish	33,064	826605	24,592.77	8,471.42
Medium Fish	70,288	1757209	63,419.90	6,868.45
Large Fish	246,242	6156038	240,672.39	5,569.14

* Units: µg/L; **Units: µg/kg-dw

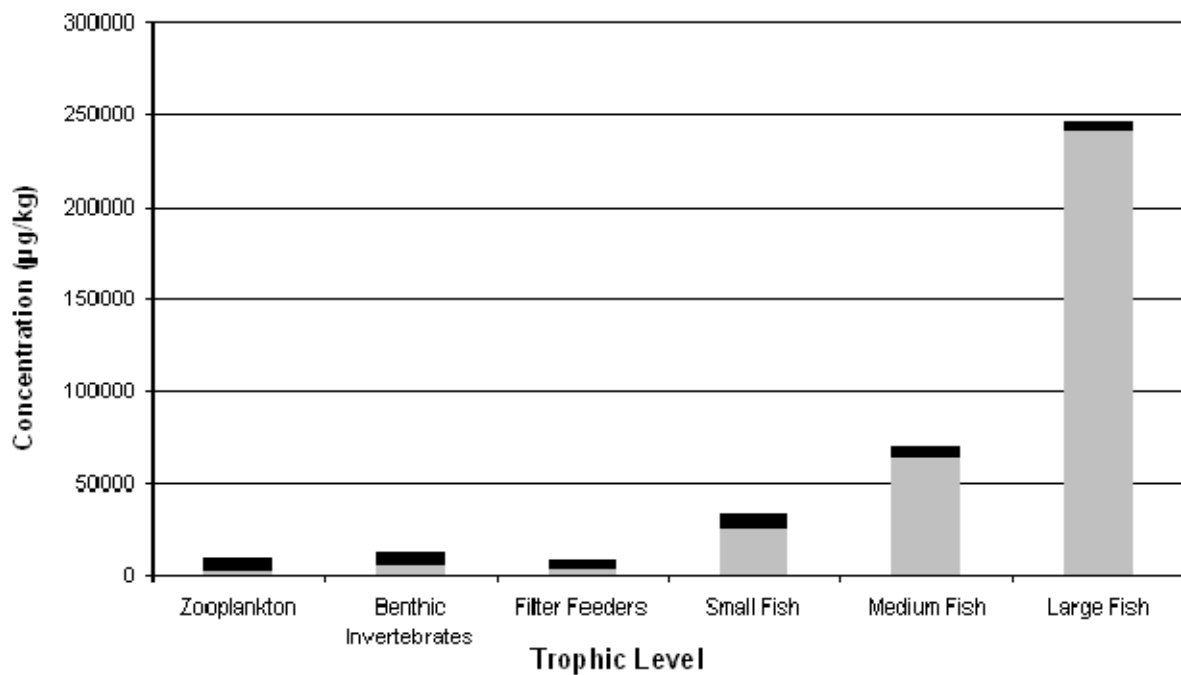


Figure 1. Total pesticide concentration per trophic level

■ Contribution due to respiration (µg/kg-ww)
 ■ Contribution due to diet (µg/kg-ww)

Table G12. Total BCF and BAF values of dicofol 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	55112	40611
Zooplankton	39268	45531
Benthic Invertebrates	41383	58516
Filter Feeders	27201	39679
Small Fish	53239	150292
Medium Fish	53239	319492
Large Fish	55170	1119280

Table G13. Lipid-normalized BCF, BAF, BMF and BSAF values of dicofol 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	2755614	2030555	N/A	959
Zooplankton	1308923	1517709	0.75	717
Benthic Invertebrates	1379445	1950537	1.67	921
Filter Feeders	1360072	1983957	1.69	937
Small Fish	1330964	3757295	2.17	1774
Medium Fish	1330964	7987312	2.80	3771
Large Fish	1379238	27981992	3.50	13212

Table G14. Calculation of EECs for mammals and birds consuming fish contaminated by dicofol.

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	7.534	12.87
rice rat/star-nosed mole	0.1	0.107	0.484	0.011	8.791	18.17
small mink	0.5	0.079	0.293	0.048	20.616	70.29
large mink	1.8	0.062	0.229	0.168	16.108	70.29
small river otter	5.0	0.052	0.191	0.421	13.430	70.29
large river otter	15.0	0.042	0.157	1.133	38.691	246.24
Avian						
small CRLF 1	0.0	0.577	5.767	0.001	51.5220	8.93
small CRLF 2	0.0	0.577	2.403	0.001	30.9323	12.87
med CRLF 1	0.0	0.184	0.766	0.006	9.8653	12.87
med CRLF 2	0.0	0.184	0.681	0.006	22.5224	33.06
large CRLF 1	0.2	0.096	0.400	0.023	5.1521	12.87
large CRLF 2	0.2	0.096	0.356	0.023	25.0045	70.29

Table G15. Calculation of toxicity values for mammals and birds consuming fish contaminated by dicofol.

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	0.00	N/A	0.00	0
rice rat/star-nosed mole	0.00	N/A	0.00	0
small mink	0.00	N/A	0.00	0
large mink	0.00	N/A	0.00	0
small river otter	0.00	N/A	0.00	0
large river otter	0.00	N/A	0.00	0
Avian				
small CRLF 1	97.03	903.00	N/A	1
small CRLF 2	97.03	903.00	N/A	1
med CRLF 1	158.57	903.00	N/A	1
med CRLF 2	158.57	903.00	N/A	1
large CRLF 1	209.64	903.00	N/A	1
large CRLF 2	209.64	903.00	N/A	1

Table G16. Calculation of RQ values for mammals and birds consuming fish contaminated by dicofol.

Wildlife Species	Acute		Chronic	
	Dose Based	Dietary Based	Dose Based	Dietary Based
Mammalian				
fog/water shrew	#DIV/0!	N/A	#DIV/0!	#DIV/0!
rice rat/star-nosed mole	#DIV/0!	N/A	#DIV/0!	#DIV/0!
small mink	#DIV/0!	N/A	#DIV/0!	#DIV/0!
large mink	#DIV/0!	N/A	#DIV/0!	#DIV/0!
small river otter	#DIV/0!	N/A	#DIV/0!	#DIV/0!
large river otter	#DIV/0!	N/A	#DIV/0!	#DIV/0!
Avian				
small CRLF 1	0.531	0.010	N/A	8.934
small CRLF 2	0.319	0.014	N/A	12.874
med CRLF 1	0.062	0.014	N/A	12.874
med CRLF 2	0.142	0.037	N/A	33.064
large CRLF 1	0.025	0.014	N/A	12.874
large CRLF 2	0.119	0.078	N/A	70.288