User's Guide and Technical Documentation

KABAM version 1.0

($\underline{K}_{OW}$ (based) $\underline{A}$quatic $\underline{B}$io$\underline{A}$ccumulation $\underline{M}$odel)

April 7, 2009

Environmental Fate and Effects Division (EFED)
Office of Pesticide Programs
U.S. Environmental Protection Agency
Washington, D.C.

Acknowledgements

Author

Kristina Garber

Technical Reviewers

Brian Anderson
Lawrence Burkhard
Paige Doelling
Keith Sappington
Thomas Steeger

Editorial Reviewer

Karen McCormack

QA/QC Officer

Nick Mastrota

QC Testers

Oak Ridge National Laboratories

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1. Introduction

1.1. Model Description

KABAM ($\underline{K}_{OW}$ (based) Aquatic BioAccumulation Model) is used to estimate potential bioaccumulation of hydrophobic organic pesticides in freshwater aquatic food webs and subsequent risks to mammals and birds via consumption of contaminated aquatic prey. This model can also be used to estimate pesticide concentrations in fish tissues consumed by humans. The model was designed for use by the U. S. Environmental Protection Agency Office of Pesticide Programs' Environmental Fate and Effects Division (EFED) scientists. KABAM is composed of two parts: 1) a bioaccumulation model estimating pesticide concentrations in aquatic organisms and 2) a risk component translating exposure and toxicological effects of a pesticide into risk estimates for mammals and birds consuming contaminated aquatic prey.

The bioaccumulation portion of KABAM is based on an aquatic food web bioaccumulation model published by Arnot and Gobas (2004). This model was originally published in 1993 by Gobas (Gobas 1993) and was modified by Arnot and Gobas (2004). The Arnot and Gobas (2004) model was selected for estimating pesticide bioaccumulation based on the following reasons: 1) the Gobas 1993 model underlying the Arnot and Gobas 2004 version is generally accepted by the scientific community as a reasonable approach for estimating bioaccumulation of persistent hydrophobic organic compounds in aquatic systems (Burkhard 1998); 2) the 1993 version of the model has been used by EPA for regulatory purposes (USEPA 1995, 2000, 2003); and 3) both Gobas 1993 and Arnot and Gobas 2004 have been published in peer-reviewed literature. Although originally developed and applied to the Great Lakes ecosystem for modeling PCBs and selected pesticides, this model has been applied and validated for other ecosystems, including the Hudson river, Fox river/Green Bay and Bayou D'Indie in Louisiana (USEPA 2003, Burkhard 2003). A detailed description of the Arnot and Gobas (2004) model is available in Appendix A.

The bioaccumulation portion of KABAM relies on a pesticide's octanol-water partition coefficient (K_{OW}) to estimate uptake and elimination constants through respiration and diet of aquatic organisms in different trophic levels. Pesticide tissue concentrations in aquatic organisms are calculated for different trophic levels of a food web through diet and respiration.

In the risk component of KABAM, pesticide concentrations in aquatic organisms are used to estimate dose- and dietary-based exposures and associated risk quotients for mammals and birds consuming aquatic organisms. The methods used in the risk component of KABAM are consistent with EFED's current modeling approach for assessing risks to terrestrial mammals and birds described in USEPA 2004a, as implemented in the T-REX model (version 1.4.1; USEPA 2008a).

1.2. When to Use this Model

KABAM should be used for pesticides having all of the following characteristics:

- The pesticide is a non-ionic, organic chemical.
- The Log K_{OW} value is between 4 and 8.
- The pesticide has the potential to reach aquatic habitats.

1.3. Conceptual Model

Conceptually, KABAM represents a freshwater aquatic ecosystem. This ecosystem receives runoff and spray drift containing pesticides from sites where pesticides are applied. The aquatic ecosystem incorporates seven food web components to describe the trophic transfer of a pesticide in an aquatic food web. These include, in increasing order of trophic level within the food web: phytoplankton, zooplankton, benthic invertebrates, filter feeders, small fish, medium fish and large fish. These components are referred to within this User's Guide as "trophic levels." They are not intended to represent discrete trophic levels, but rather generic levels of an aquatic food web (*e.g.,* primary producers, primary consumers, secondary consumers, and predators). KABAM also evaluates potential exposures and risks to mammals and birds that feed upon aquatic animals containing pesticide residues accumulated through the aquatic food web (Figure I).

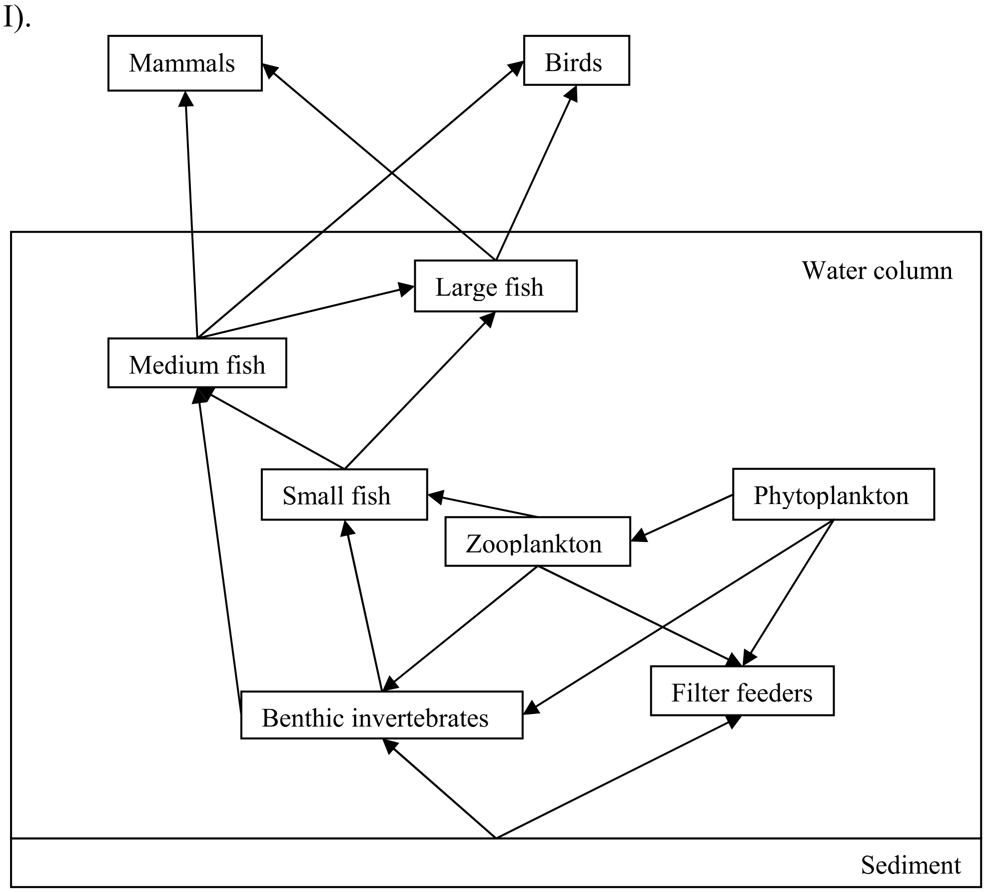

Figure I. Conceptual model depicting aquatic food web of KABAM. Arrows depict direction of trophic transfer of bioaccumulated pesticides from lower levels to higher levels of the food web.

KABAM can represent a specific ecosystem, as defined by the model user. The ecosystem can be defined by abiotic (*e.g.,* water temperature, % organic carbon in sediment) and biotic input parameters (*e.g.,* body weights of aquatic animals, feeding preferences of fish, birds, and mammals). The model user can modify these parameters to match the characteristics of ecosystems relevant to a specific mesocosm study or a field study.

For general use, the default model ecosystem for KABAM is defined as the EFED standard pond scenario for the Exposure Analysis Modeling System (EXAMS). The standard pond has two compartments: a water column and a benthic area. The water column is 20,000,000 liters in volume and the benthic area has a volume of 500,000 liters. The standard pond receives pesticides in runoff (dissolved in water and sorbed onto eroded soil) and spray drift from a 10-ha treatment field that is immediately adjacent to the pond. The treatment field is represented by various scenarios using the Pesticide Root Zone Model (PRZM). The meteorological data corresponding to the selected PRZM scenario can influence the runoff of a pesticide into the standard pond and also the water temperature of the pond environment.

The default biotic portions of KABAM are designed to be representative of organisms from the seven trophic levels defined above. Mammals and birds of concern are defined by considering species of mammals and birds relevant to the United States which rely upon aquatic ecosystems for their food sources.

1.4. Model Application

The application of KABAM is referred to in this User's Guide as the "KABAM tool." The KABAM tool is implemented in Microsoft® Excel 2003. This software program was chosen as an operating platform because it is available to EFED users and to the public. Excel is a commonly used spreadsheet program that most scientists are familiar with. Computers suitable for running the software programs necessary for this tool require no additional hardware.

Once the KABAM tool is opened, the "Model Description" worksheet is displayed. This worksheet contains the version information, a brief model description, and a list of references. Across the bottom of this Excel window are several worksheet tabs indicating the various portions of the KABAM tool, including "Chemical Specific Inputs," "Ecosystem Inputs," "Parameters & Calculations," and "Results." The requirements and functions of these worksheets are explained in more detail below.

The overall format of the KABAM tool was developed for ease of use. Tables embedded in the worksheets were designed for clarity of information and for eventual cut and paste from Excel into a Microsoft® Word document containing a risk assessment. Where necessary, comments are provided for guidance on selecting input parameters. For more detailed information than is contained in the spreadsheet concerning the model, input parameters, calculations, and results, this guidance document should be utilized.

2. Input Parameters

Two types of input parameters are required to run KABAM: those that are specific to the pesticide and those that define the aquatic ecosystem, including the mammals and birds of concern. These input parameters are distinguished by two worksheets that are titled "Chemical Specific Inputs" and "Ecosystem Inputs."

To run the model, the user is only required to input chemical specific values since default values are already inserted into the appropriate locations for ecosystem input parameters. These default values allow the user to run KABAM with reasonable and reliable parameters; however, the user can select other parameters to explore bioaccumulation of a chemical and associated potential risk to mammals and birds that consume aquatic animals. Guidance for altering input parameters from the default values is provided in this User's Guide.

2.1. Chemical Specific Inputs

The "Chemical Specific Inputs" worksheet contains three tables for the user to input data. Tables 1 and 3 **require** the user to input chemical-specific values. Table 2 contains default values that do not require user inputs, but are designed to allow the user flexibility in the case that chemical-specific data are available for uptake and depuration rate constants in aquatic organisms.

Table 1

Table 1 requires inputs related to the chemistry and estimated environmental concentrations (EECs) of the pesticide. Required inputs include: 1) pesticide name, 2) Log K_{OW}, 3) organic carbon partition coefficient (K_{OC}), 4) sediment pore water concentrations of pesticide residues (Pore water EEC), and 5) aqueous concentration of pesticide residues (water column EEC). This table contains no default values. The user should input values for each of these parameters in the "Value" column of Table 1.

The titles of several tables displayed in the KABAM tool are designed to automatically insert the pesticide name as entered in Table 1.

Of all parameters incorporated into KABAM, Log K_{OW} has the greatest influence on estimates of bioaccumulation in aquatic organisms (see section A.7 of Appendix A). As a result, this parameter is the most important for estimating potential exposures of mammals and birds to pesticides through consumption of contaminated aquatic organisms. Estimates of Log K_{OW} can be obtained for a pesticide from acceptable or supplemental registrant-submitted studies (OPPTS Guidelines 830.7550, 830.7560, 830.7570) and from scientific literature. One useful source for locating Log K_{OW} data in the scientific literature is Sangster (2007). Before using data from this database, the scientist should review the original citation and determine whether the data are acceptable or supplemental. If no measured values of Log K_{OW} are available, this value can be estimated using EPI Suite software that includes KOWIN (USEPA 2009), which considers contributions of the molecule's individual fragments to the overall Log K_{OW}. If a range of Log K_{OW} values is available, it is suggested that the model user input the high and low Log K_{OW} values separately in order to bracket the bioaccumulation potential and its associated risks.

Bioaccumulation potential increases as Log K_{OW} increases. General guidance for evaluating measured and estimated Log K_{OW} data is available in Appendix B of USEPA 2003.

In Table 1 of the KABAM tool (reproduced below), K_{OW} is automatically calculated as 10 to the power of the Log K_{OW} value that is entered by the model user. The K_{OW} is used to estimate uptake and clearance rate constants that define the concentrations of the pesticide in the tissues of the aquatic organisms.

K_{OC} data can be obtained from registrant-submitted studies (OPPTS Guidelines 835.1230, 835.1240) or from the scientific literature. As the K_{OC} value of a chemical increases, the estimated accumulation of a chemical also increases. The user should select the K_{OC} value input into PRZM/EXAMS for deriving aquatic and benthic EECs. Input parameter guidance for PRZM/EXAMS indicates that the K_{OC} parameter value should be calculated as “the average K_{OC} from batch experiments” (USEPA 2002). If no scientifically valid estimates of K_{OC} are available, this parameter value can be estimated as $0.35*K_{OW}$ (USEPA 2004b).

Table 1. Chemical characteristics of Pesticide X.

Characteristic	**Value**	**Guidance**
Pesticide Name	**Pesticide X**	**Required input**
Log K_{OW}	**5**	**Required input** Enter value from acceptable or supplemental study submitted by registrant or available in scientific literature.
K_{OW}	**100000**	No input necessary. This value is calculated automatically from the Log K_{OW} value entered above.
K_{OC} (L/kg OC)	**25000**	**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)	**30**	No input necessary. This value is calculated automatically from the Log K_{OW} value entered above.
Pore water EEC (µg/L)	**5**	**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 <u>not</u> be used.
Water Column EEC (µg/L)	**6**	**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).

Note: Table 1 of this User’s Guide contains example data for chemical specific characteristics.

The time to steady state (T_S; in days) is also calculated automatically by the KABAM tool according to Equation 1 (Hawker and Connell 1988). This equation is consistent with recommendations provided in USEPA and OECD guidelines for fish BCF studies for determining the time to reach steady state (USEPA 1996, OECD 1996). It should be noted that there is uncertainty in using this equation for chemicals with Log K_{OW} >6, since this falls outside of the range of data used to derive this relationship. Alternatively, the time to steady state can be defined using empirical data from available BCF studies that were sufficient to define steady state. This information can be used to supplement the calculated T_S value.

$$Equation\ 1.\quad T_S = \frac{(6.54x10^{-3}) * K_{OW} + 55.31}{24}$$

EECs from PRZM (v3.12.2, May 2005) and EXAMS (v2.98.4.6, April 2005) (coupled with the input shell pe5.pl, dated Aug 2007) are used in the KABAM tool. EECs generated by PRZM/EXAMS represent the freely dissolved concentration of the pesticide in the surface and pore water of the standard pond. The bioaccumulation portion of KABAM assumes that the aquatic environment is at steady state. Because the time to reach steady state is pesticide specific, the appropriate averaging period of the EEC should be determined on a chemical by chemical basis. Generally, the time to reach steady state can be related to the Log K_{OW} of a chemical, with increasing time required as the Log K_{OW} increases. Therefore, it is not relevant to use short-term (peak) estimates of pesticides in the aquatic environment. The EEC used to represent the concentration of the pesticide in the pore and surface waters of the aquatic habitat should be selected so that the averaging period (*i.e.,* 4-d, 21-d, 90-d, 1 year), is consistent with the time to steady state estimated for that chemical. For example, a chemical with a Log K_{OW} = 5 would have an estimated time to steady state value of 30 days. Since the standard output file from PRZM/EXAMS does not include a 30-d average, the next closest averaging period would be selected (either 21 or 60 days). Therefore, the EEC represented by the 21-day average would be selected for this chemical. In cases where the time to steady state exceeds 365 days, the user should select the EEC representing the yearly EEC.

In cases where multiple uses of a single pesticide are possible (*e.g.,* cotton, corn, apples), EECs from the different uses can be modeled to allow for an understanding of the bioaccumulation and associated risks associated with different uses.

Table 2

KABAM automatically calculates uptake and elimination constants through respiration (k_1 and k_2, respectively) and diet (k_D and k_E, respectively). In using the model with its default parameters in place, it is assumed that the elimination of the pesticide from aquatic organisms through metabolism does not occur (*i.e.,* metabolism rate constant k_M = 0).

In Table 2 (reproduced below) of the KABAM tool, the model user can enter measured rate constants for uptake and elimination constants. These data can be obtained from acceptable or supplemental studies submitted by the registrant or from the literature. For example, k_1 and k_2 rate constants for fish can be obtained from pesticide BCF studies submitted for the fish (OPPTS

Guideline 850.1730). However, caution should be used when altering rate constants. For example, the k_2 from a bioconcentration study typically represents a total elimination half life. However, the k_2 in KABAM represents elimination from the gills. Therefore, incorporation of a measured k_2 into KABAM without consideration of other elimination pathways may result in erroneous results. **In order to run the model, it is not necessary for the user to alter the default values inserted into Table 2.** If the model user alters the parameters in Table 2 of the KABAM tool, they will be highlighted yellow.

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.

The model user should exercise caution when using a value of k_M>0, as this approach will decrease predicted EECs and RQs for mammals and birds. Initially, k_M should be set to 0 as a screen. The assumption that there is no metabolism of the pesticide within aquatic organisms is conservative. If no metabolism is observed in available fish BCF studies, then k_M should not be altered. In cases where metabolism occurs, this assumption can result in overestimates of pesticide accumulation in tissues of aquatic organisms. In cases where the model user has evidence to indicate that metabolism may occur in fish (*i.e.,* from BCF studies) and RQ values exceed LOCs, then the user can estimate k_M using approaches described in Appendix H. This will allow the model user to characterize effects of metabolism on bioaccumulation in aquatic ecosystems and associated risks to mammals and birds consuming aquatic organisms.

Table 3

To calculate risk quotients, user-supplied avian and mammalian toxicity endpoints should be entered into Table 3 (reproduced below). Acceptable or supplemental registrant-submitted or open literature studies should be used to define the effects of the pesticide on birds and mammals. Required input data include: avian acute oral LD_{50} (OPPTS Guideline 850.2100), avian subacute dietary LC_{50} (OPPTS Guideline 850.2200), avian reproduction (expressed as a NOAEC or a NOAEL) (OPPTS Guideline 850.2300), mammalian acute oral LD_{50} (OPPTS Guideline 870.1100), or subacute dietary LC_{50} (if available), and mammalian reproduction NOAEC or NOAEL (OPPTS Guideline 870.3800).

Table 3. Mammalian and avian toxicity data for Pesticide X. 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)	50	mallard duck	
	LC_{50} (mg/kg-diet)	500	Northern bobwhite quail	
	NAOEC (mg/kg-diet)	10	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)	50	other	1.2
	LC_{50} (mg/kg-diet)	N/A	other	
	Chronic Endpoint	10	laboratory rat	
	units of chronic endpoint *	ppm		

*ppm = mg/kg-diet

Note: Table 3 of this User's Guide contains example data for chemical specific characteristics.

In the appropriate cell under the "value" column of Table 3, the user should input the lowest (most sensitive) available toxicity data for each toxicity endpoint. If an endpoint value is not discrete (*i.e.,* contains a ">" symbol), the whole number should be entered as a discrete value, keeping in mind that all resulting risk quotient (RQ) values derived using this endpoint are "<". For the chronic mammalian data, the user must also select the units of the value. The user should select units from the drop down menu as either "ppm" or "mg/kg-bw."

Under the "species" column, the user should use the drop down menu to select the appropriate test species associated with the toxicity value entered in the adjacent cell in the "value" column. If the test species is not one of the options available in the drop down list, the model user should select "other" as the test species. If "other" is selected, the user must enter the body weight (in kg) of the test species. In the case that "other" is selected as the test species, a message will appear in the spreadsheet below Table 3 to alert the user of the need to enter the body weight of the test species. These data should be obtained from the study report if possible (time weighted average of control animals). Alternatively, reference body weight values may be obtained from a variety of sources, including U.S. EPA 1993 and Dunning 1984. Failure to enter the body weight of the test species when it is entered as "other" will prevent calculation of risk quotients that correspond to that endpoint.

If available, the model user should enter chemical-specific data to represent the avian scaling factor (see Mineau et al. 1996). If no chemical specific data are available, the default value of 1.15 should be entered. This value is used to adjust avian dose-based toxicity values based on the weight of the species of concern (*e.g.,* herons) as described in the T-REX User's Guide (USEPA 2008a) and in Appendix G.

2.2. Ecosystem Inputs

In order to estimate pesticide concentrations in tissues of aquatic organisms, biotic and abiotic characteristics of the model aquatic ecosystem must be defined. In addition, the mammals and birds consuming aquatic organisms are also defined as ecosystem inputs.

To run KABAM, it is not necessary to alter any of the default parameters in the "Ecosystem Inputs" worksheet.

If the model user alters default parameter values, they will be highlighted yellow in the KABAM tool.

It may be necessary for the model user to incorporate alternate ecosystem input values if the modeling incorporates EECs from a source other than PRZM/EXAMS (*e.g.,* from a mesocosm study). In that case, the model user should enter parameter values that correspond to the specific water body used.

Table 4

Abiotic characteristics of the aquatic ecosystem that are necessary for KABAM are defined in Table 4 (reproduced below) of the model tool. These characteristics include: concentrations of particulate organic carbon (X_{POC}), dissolved organic carbon (X_{DOC}), dissolved oxygen (C_{OX}) and suspended solids (C_{SS}), water temperature (T), and % organic carbon (OC) content of the sediment. The model tool is populated with default values for these parameters, which can be altered based on the needs of the model user. Default values relevant to the abiotic characteristics of the aquatic ecosystem are designed to be consistent with the OPP standard pond scenario used in EXAMS. Brief explanations for these default values as well as guidance on selecting alternative values are provided in Appendix B.

Table 4. Abiotic characteristics of the model aquatic ecosystem.

Characteristic (symbol; units)	Value	Guidance*
Concentration of Particulate Organic Carbon (X_{POC}; kg OC/ L)	0	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	
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 3.00×10^{-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 5

Necessary biotic components of the aquatic ecosystem define characteristics of the sediment and water column biota. These include body weights and body compositions, specifically % lipids, % NLOM (non-lipid organic matter), and % water. These values are defined for the seven trophic levels of the aquatic ecosystem (phytoplankton, zooplankton, benthic invertebrates, filter feeders, small fish, medium fish and large fish) modeled by KABAM in Table 5 (reproduced below) of the tool. Default values for these biotic parameters are displayed in Table 5 below. A description of how these default parameters were selected is available in **Appendix C**. In addition, Table 5 allows the model user to define whether organisms within each trophic level respire pore water. If yes, it is assumed that 5% of the total respired water is from pore water. Default assumptions related to respiration of pore water for each trophic level are depicted in Table 5 below.

Table 5. 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 food web.
N/A = not applicable

Table 6

Table 6 (reproduced below) of the KABAM tool allows the model user to define the diet composition of each of the trophic levels of the aquatic ecosystem. The aquatic trophic levels are assigned a hierarchy, which is relevant to the assignment of diet composition. The order of the trophic levels, in increasing hierarchy, is as follows: phytoplankton, zooplankton, benthic invertebrates, filter feeders, small fish, medium fish, and large fish. The diet of each aquatic trophic level is composed of sediment or water column biota from lower trophic levels. The KABAM tool does not allow the model user to assign a portion of the diet of one organism to its own trophic level or to trophic levels that are higher. The default values defining the diet of each trophic level are in Table 6 below. An explanation of how these default parameters were determined is available in **Appendix C**.

Note that the total diet of each organism within the aquatic food web should equal 100%. If the total diet ≠ 100%, an error message will appear under Table 6.

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%
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 food web.

Table 7

Table 7 (reproduced below) of the KABAM tool allows the model user to define the mammalian and avian species of concern, as well as their body weights. Species are considered to be of concern for pesticide exposures through consumption of residues in freshwater aquatic animals that serve as prey.

For mammals, default species include the fog shrew (*Sorex sonomae*), the water shrew (*S. palustris*), the rice rat (*Oryzomys palustris*), the star-nosed mole (*Condylura cristata*), the American mink (*Neovison vison*), and the Northern river otter (*Lontra canadensis*). For birds, default species include sandpipers, rails, herons, kingfisher, ducks, grebes, ibis, rails, cormorants, osprey, cranes, bald eagles (*Haliaeetus leucocephalus*) and pelicans. Descriptions of how mammalian and avian species were selected, including their body weights, are provided in Appendices D and E, respectively. These appendices also provide descriptions of the species themselves as well as justifications for default parameters used to represent the species in KABAM (*i.e.,* body weight and diet).

The selected body weight value influences estimates of pesticide exposure through differential consumption of contaminated food items, as well as dose-based toxicity values. Therefore, the magnitude of the body weight parameter has an effect on the magnitude of the dose-based RQ. For mammals, higher body weight values result in higher dose-based RQs (keeping the diet constant). As a result, default body weight values for the fog shrew, water shrew, rice rat, and star-nosed mole were selected as higher values of relevant ranges in order to represent size classes that would be most vulnerable to exposures through bioaccumulation. In order to bound the risk of accumulated residues to mink and river otter, the lowest and highest body weights of these species were selected as defaults. For birds, higher body weight results in lower RQs. In order to bound the risk of accumulated residues to birds, the lowest and highest body weights of birds with the same diet were selected as defaults. The user can alter the assigned body weights to represent the low and high end of possible weights in order to bound the potential RQs for a particular species. Additional data on body weights of species of mammals and birds are provided in Appendices D and E, respectively.

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	0.450
Mammal 4	Large mink	1.800
Mammal 5	Small river otter	5.000
Mammal 6	Large river otter	15.000
Bird 1	Sandpipers	0.02
Bird 2	Cranes	6.7
Bird 3	Rails	0.07
Bird 4	Herons	2.90
Bird 5	Small osprey	1.25
Bird 6	White pelican	7.50

Tables 8 and 9

Tables 8 and 9 (reproduced below) of the KABAM tool allow the model user to define the diet composition of the mammals and birds of concern that are defined in Table 7. The animal names entered in Table 7 will appear at the heads of the columns of Tables 8 and 9. The diet of each mammal and bird species is attributed to a portion of each trophic level of the aquatic ecosystem. Justifications for the default diets for each mammal and bird species are provided in Appendices D and E, respectively. Note that the total diet of each mammal and bird should equal 100%. If not, an error message will appear under Table 8 or 9.

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.						
	Diet for:					
Trophic level in diet	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%

If the model user chooses to alter the default diet of a mammal or bird, the model user should consider the daily food intake for determining appropriate aquatic trophic levels to include within an animal's diet. The user should verify that the weight of an individual dietary item does not greatly exceed the daily food intake of the mammal or bird. This will prevent the user from simulating a bird or mammal that consumes prey that are much larger than could be reasonably consumed. This can be determined using allometric equations for estimating daily food intake, as described in Appendices D and E. In addition, these appendices contain data defining the daily food intake for several species of birds and mammals.

Pesticide exposures to mammals and birds through consumption of contaminated aquatic organisms are determined by weighing the exposure concentration by the contribution of each food item to the total diet. While this approach is reasonable for chronic exposures, it may underestimate acute exposures resulting from consumption of larger trophic level organisms within short periods of time. In order to explore high-end exposure concentrations and subsequent risks resulting from acute exposures, the model user can set the highest aquatic trophic level consumed by a bird or mammal to 100%. For example, high-end acute exposures of cranes (which consume benthic invertebrates, filter feeders, and medium fish) to a pesticide could be assessed by setting the crane diet to 100% of medium fish.

3. Parameters & Calculations

Also included in the KABAM tool is a tabularized summary of the relevant parameters for the bioaccumulation portion of KABAM. This summary is included in a separate worksheet, titled "Parameters & Calculations" (Table 10 of the KABAM tool) and represents values used to calculate pesticide tissue concentrations for the trophic levels of the aquatic ecosystem. This worksheet is locked (read only) in the KABAM tool and cannot be altered by the model user; however, this worksheet can be printed by the model user or copied into a risk assessment as a model output. A full description of the parameters contained in Table 10 of the KABAM tool as well as the equations used to calculate these parameters can be found in Appendix A.

4. Model Results

The final outputs of KABAM include Bioconcentration Factors (BCFs), Bioaccumulation Factors (BAFs), Biomagnification Factors (BMFs), Biota-Sediment Accumulation Factors (BSAFs), estimates of pesticide concentrations in tissues of aquatic organisms, and RQ values for mammals and birds consuming contaminated aquatic organisms.

Note that the "results" worksheet of KABAM is locked (read only) and cannot be altered by the model user, with the exception of format changes (*e.g.*, number of decimal places). Also, the KABAM tool does not automatically account for significant figures. The format of numerical values in the Tool can be altered by the user to increase or decrease the number of decimal places.

Table 11 and Figure 1

Table 11 (reproduced below**)** of the KABAM tool reports pesticide concentrations in tissues of aquatic organisms on both a total body weight and lipid normalized basis. The table also reports contributions of the pesticide concentration in tissue from respiration and from diet. These values are useful for understanding the dominant uptake route of the pesticide that influences bioaccumulation. Figure 1 (reproduced below) of the KABAM tool graphically represents the relative contributions of pesticide uptake through diet and through respiration to the overall concentrations of the pesticide in the tissues of the different aquatic animals.

Table 11. Estimated concentrations of Pesticide X 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)*	6	N/A	N/A	N/A
Water (freely dissolved)*	6	N/A	N/A	N/A
Sediment (pore water)*	5	N/A	N/A	N/A
Sediment (in solid)**	5,000	N/A	N/A	N/A
Phytoplankton	27,298	1364913	N/A	27,298.25
Zooplankton	21,065	702157	651.72	20,412.98
Benthic Invertebrates	23,678	789265	1,812.95	21,865.01
Filter Feeders	15,549	777440	1,167.92	14,380.88
Small Fish	34,713	867830	7,246.79	27,466.40
Medium Fish	41,050	1026242	14,492.66	26,557.01
Large Fish	56,332	1408297	30,795.48	25,536.39

* Units: µg/L; **Units: µg/kg-dw

Note: Table 11 of this User's Guide contains example results based on example chemical specific data entered in Tables 1 and 3.

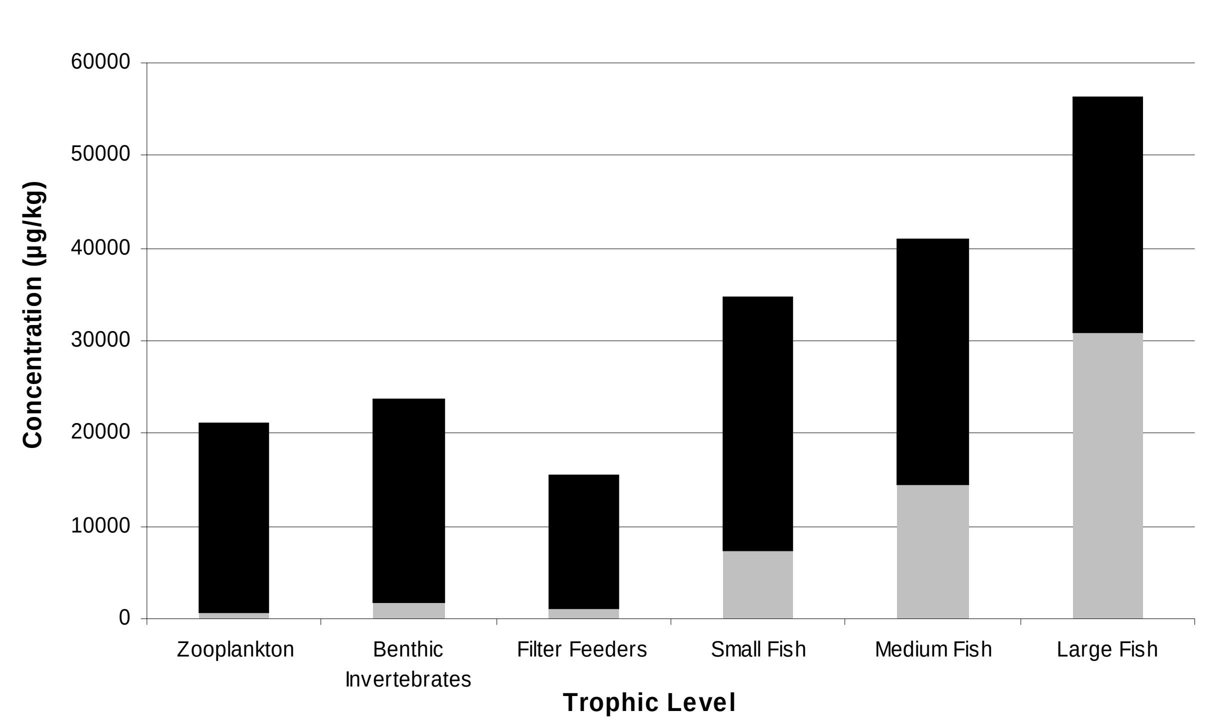

Figure 1. Total Pesticide Concentration per trophic level

Note: Figure 1 of this User's Guide contains example results based on example chemical-specific data entered in Tables 1 and 3.

Tables 12 and 13

BCF, BAF, BMF and BSAF are calculated by KABAM (**Tables 12 and 13**). These terms are intended to provide a relative measure of the pesticide concentration in an organism to the pesticide concentration in sources (*i.e.,* the environment and the diet) of that pesticide. Appendix F contains the equations used to calculate BCF, BAF, BMF and BSAF.

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

Trophic Level	**Total BCF (µg/kg-ww)/(µg/L)**	**Total BAF (µg/kg-ww)/(µg/L)**
Phytoplankton	4801	4550
Zooplankton	3421	3511
Benthic Invertebrates	3705	3946
Filter Feeders	2435	2591
Small Fish	4766	5786
Medium Fish	4766	6842
Large Fish	4806	9389

Note: Table 12 of this User's Guide contains example results based on example chemical specific data entered in Tables 1 and 3.

Table 13. Lipid-normalized BCF, BAF, BMF and BSAF values of Pesticide X in aquatic trophic levels.				
Trophic Level	**BCF (µg/kg-lipid)/(µg/L)**	**BAF (µg/kg-lipid)/(µg/L)**	**BMF (µg/kg-lipid)/(µg/kg-lipid)**	**BSAF (µg/kg-lipid)/(µg/kg-OC)**
Phytoplankton	240045	227485	N/A	11
Zooplankton	114028	117026	0.51	6
Benthic Invertebrates	123488	131544	1.16	6
Filter Feeders	121769	129573	1.14	6
Small Fish	119142	144638	1.16	7
Medium Fish	119142	171040	1.24	8
Large Fish	120143	234716	1.37	11

Note: Table 13 of this User's Guide contains example results based on example chemical specific data entered in Tables 1 and 3.

Tables 14, 15, and 16

Tables 14, 15, and 16 (reproduced below) of the KABAM tool summarize the estimated exposure values, mammal and bird toxicity values and resulting RQ values, respectively, used to estimate potential risks to mammals and birds that consume aquatic animals contaminated with pesticides accumulated through the aquatic food chain.

Table 14 uses the mammalian and avian body weights (entered by the model user) to calculate the dry food ingestion and drinking water intake rates according to allometric equations specific to mammals and birds. The wet food intake is calculated using the dry food intake and the % water of the diet. Dose-based EECs represent the sum of pesticide intake through diet and through drinking water, accounting for pesticide concentrations in diet items and in water and food and water intake rates. Dietary-based EECs represent the sum of pesticide intake through diet only, without consideration of species specific intake rates or body weights. Descriptions of the equations used to calculate food intake rates, water intake rates, dose-based EECs, and dietary-based EECs are available in Appendix G.

Table 14. Calculation of EECs for mammals and birds consuming fish contaminated by Pesticide X.						
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	13.857	23.68
Rice rat/star-nosed mole	0.1	0.107	0.484	0.011	11.921	24.64
Small mink	0.5	0.079	0.293	0.048	12.041	41.05
Large mink	1.8	0.062	0.229	0.168	9.408	41.05
Small river otter	5.0	0.052	0.191	0.421	7.844	41.05
Large river otter	15.0	0.042	0.157	1.133	8.852	56.33
Avian						
Sandpipers	0.0	0.228	1.034	0.004	25.5861	24.75
Cranes	6.7	0.030	0.136	0.211	3.6561	26.90
Rails	0.1	0.147	0.577	0.010	16.8571	29.20
Herons	2.9	0.040	0.157	0.120	5.0943	32.36
Small osprey	1.3	0.054	0.199	0.069	8.1859	41.05
White pelican	7.5	0.029	0.107	0.228	6.0108	56.33

Note: Table 14 of this User's Guide contains example results based on example chemical specific data entered in Tables 1 and 3.

Table 15 (reproduced below) of the KABAM tool summarizes the acute and chronic, dose-based and dietary-based toxicity values representing effects of a pesticide to mammals and birds. Dietary-based toxicity values are taken directly from user inputs in Table 3, without adjustment. Available dose-based toxicity values are adjusted for the weights of the animal tested (*e.g.,* laboratory rat, mallard duck) and of the animal for which the risks are being assessed (*e.g.,* mink, bald eagle). Methods for adjusting toxicity values are consistent with those used by T-REX (USEPA 2008a). A full description of the methodology for adjusting dose-based toxicity values is provided in Appendix G.

Table 15. Calculation of toxicity values for mammals and birds consuming fish contaminated by Pesticide X.				
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	142.87	N/A	1.05	10
Rice rat/star-nosed mole	96.92	N/A	0.71	10
Small mink	63.89	N/A	0.47	10
Large mink	45.18	N/A	0.33	10
Small river otter	35.00	N/A	0.26	10
Large river otter	26.59	N/A	0.20	10
Avian				
Sandpipers	25.96	500.00	N/A	100
Cranes	62.10	500.00	N/A	100
Rails	31.33	500.00	N/A	100
Herons	54.77	500.00	N/A	100
Small osprey	48.27	500.00	N/A	100
White pelican	63.16	500.00	N/A	100

Note: Table 15 of this User's Guide contains example results based on example chemical specific data entered in Tables 1 and 3.

Table 16 (reproduced below) of the KABAM tool presents RQs, which are the ratio of exposure concentrates to effects values. RQ values are then compared to Agency levels of concern (LOCs) for non-listed and listed mammals and birds. For acute exposures, the LOC is 0.5 for (non-listed) birds and mammals and 0.1 for federally-listed threatened and endangered (listed) species of mammals and birds. For chronic risk, the LOC is 1.0 for all species (non-listed and listed) mammals and birds (USEPA 2004). RQ values that exceed their respective LOC values appear in red and **bold** in Table 16.

Dose-based and dietary-based RQs are not equivalent. Dietary-based RQs are calculated by directly comparing the concentration of a pesticide administered to experimental animals in the diet in a toxicity study to the concentration estimated in selected food items. These RQs do not account for the fact that smaller-sized animals need to consume more food relative to their body weight than larger animals. The dose-based RQs account for these factors by incorporating the ingestion rate-adjusted exposure from the various food items to the different weight classes of assessed animals and the weight class-scaled toxicity endpoints.

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

Wildlife Species	Acute		Chronic	
	Dose Based	Dietary Based	Dose Based	Dietary Based
Mammalian				
Fog/water shrew	0.097	N/A	**13.198**	**2.368**
Rice rat/star-nosed mole	0.123	N/A	**16.737**	**2.464**
Small mink	0.188	N/A	**25.643**	**4.105**
Large mink	0.208	N/A	**28.335**	**4.105**
Small river otter	0.224	N/A	**30.498**	**4.105**
Large river otter	0.333	N/A	**45.296**	**5.633**
Avian				
Sandpipers	**0.986**	0.049	N/A	0.247
Cranes	0.059	0.054	N/A	0.269
Rails	**0.538**	0.058	N/A	0.292
Herons	0.093	0.065	N/A	0.324
Small osprey	0.170	0.082	N/A	0.410
White pelican	0.095	0.113	N/A	0.563

Note: Table 16 of this User's Guide contains example results based on example chemical specific data entered in Tables 1 and 3.

EECs and RQs for birds are based on the selected body weight of the bird as well as its diet. Default values for birds were designed to represent birds on the low and high end of weights with three different diets. Birds consuming benthic invertebrates, filter feeders, and fish include sandpipers, ducks and cranes (default birds 1 and 2, which are named sandpipers and cranes, respectively). Birds consuming benthic invertebrates and fish include belted kingfisher, rails, ibis, grebes, double-breasted cormorants, bitterns, egrets, and herons (default birds 3 and 4, which are named rails and herons, respectively). Birds consuming fish include osprey, bald eagles, and the white pelican (default birds 5 and 6, which are named small osprey and white pelican, respectively). In the case that RQs exceed the LOC for both birds within a feeding group, then it can be assumed that RQs would exceed the LOC for all of the birds within the feeding category since birds on the low and high end of the weight ranges have RQs of concern. In the case that RQs exceed the LOC for the default bird with the high body weight of a feeding category (*i.e.,* birds 2, 4, and 6), the model user can refine the EECs and RQs to be representative of specific bird species within a feeding category by entering specific body weights of individual species of concern. Appendix E contains species specific data on feeding habits and body weights of over 40 species of birds, including some listed species, which consume aquatic animals from freshwater habitats.

5. Assessing Pesticide Concentrations in Fish Tissues for Human Consumption

It is possible to use KABAM to derive pesticide concentrations in edible tissues of fish that are relevant to assessments of pesticide risks to human health. Current default values described above for % lipid content of fish applies to the whole fish; however, not all fish tissues are consumed by humans. Therefore, it is necessary to modify the output of the pesticide tissue concentration to account for a lower % lipid composition of edible tissues. This can be accomplished by entering in all the relevant default input parameters for KABAM as defined above. It may be necessary to explore different body weights of the large fish, based on those that would be expected to be consumed by humans.

The relevant output is the lipid normalized concentration of the pesticide in the large fish (Table 11). This value can be converted to the total pesticide concentration in edible tissues by multiplying by the % lipid content of the edible tissues. The default value for lipid content in edible tissue of the large fish is 3%, based on USEPA 2003. The resulting value represents the concentration of pesticide in fish tissue (in µg/kg-ww) potentially consumed by humans. This value can then be used in conjunction with fish consumption rates to characterize risks of a pesticide to humans consuming contaminated fish.

6. Model Assumptions, Limitations, and Uncertainties

There are several key assumptions and resulting uncertainties associated with modeling pesticide concentrations in tissues of aquatic organisms. The assumptions involve the equations of the model itself and the parameterization of those underlying equations. **Appendix A** describes the assumptions associated with the equations of the bioaccumulation model. In order to explore uncertainties associated with specific parameters and their influences on model outputs, a sensitivity analysis was conducted (see section A7 of Appendix A). This was used to define the parameters that have the greatest influence on model outputs (*e.g.*, K_{OW}, water column, and pore water EECs). Appendices B and C describe the parameterization of the model, including the associated assumptions.

In addition, the use of PRZM/EXAMS for deriving EECs in the surface and pore waters of the aquatic ecosystem introduces the assumptions and uncertainties associated with PRZM and EXAMS to KABAM.

One major assumption associated with KABAM concerns the model's assumed steady state. Given the episodic nature of pesticide applications, sporadic peak exposures to aquatic organisms would be expected. For a chemical with a Log K_{OW} of approximately 5, comparison of the fish tissue EECs predicted using the steady state and dynamic bioaccumulation modeling with PRZM/EXAMS/Arnot and Gobas indicates predictions are similar (USEPA 2008b) when a 60-d average was selected for water and sediment concentrations as input to the steady state model. This result suggests that steady-state bioaccumulation modeling can provide useful predictions of bioaccumulation potential even with highly dynamic exposures, provided proper consideration of the averaging period associated with water and sediment concentrations is made.

As discussed above, in using KABAM with default settings, it is assumed that the elimination of the pesticide from aquatic organisms through metabolism does not occur, *i.e.,* the metabolism rate constant (k_M) = 0. In cases where pesticide metabolism does occur, this could overestimate pesticide bioaccumulation. Appendix H of this guide provides methods for estimating k_M for fish using empirical data provided for specific chemicals (from BCF studies). This approach can be used to characterize effects of metabolism, but should be used with caution.

The Arnot and Gobas (2004) model is generally appropriate for chemicals with Log K_{OW} value $\geq$4 to $\leq$ 8. Uncertainty increases as the value increases above 8 because the model has generally been validated using chemicals with Log K_{OW} values within the range of 4 - 8. Making predictions for a chemical with a Log K_{OW} > 8 leads to uncertainty in model outputs because predictions are based upon extrapolations in its subroutines.

For chemicals with Log K_{ow} < 4, exposure from food becomes insignificant because uptake and depuration across the gills controls the residue in the organism. Thus, there is no need to run a food web model for these chemicals. In these cases, available BCF data are sufficient to predict residues in the aquatic species.

It is assumed that there is no predation within a trophic level of the aquatic food web (*e.g.,* medium fish cannot prey upon medium fish). It is also assumed that mammals and birds only consume organisms from the aquatic system.

Appendix A. Description of Bioaccumulation Model

The bioaccumulation portion of KABAM is based on the model published by Arnot and Gobas (2004). The purpose of this model is to estimate chemical concentrations (C_B) and BCF and BAF values for aquatic ecosystems. Conceptually, each aquatic organism is assumed to be a single compartment. Chemicals enter the organism through respiration and diet and leave the organism through respiration and fecal egestion. The chemical concentration in the organism can also be influenced by the growth of the organism as well as metabolism of the chemical within the organism. These processes that define uptake and loss of the chemical from aquatic organisms are described by rate constants and are incorporated into one equation that is used to define the concentration of the chemical in organism tissues (Equation A1, see Table A1). As uptake constants (*i.e.*, k_1 and k_D) increase, so does the estimated pesticide concentration in an organism. As elimination constants increase (*i.e.*, k_2, k_E, k_G and k_M), estimated pesticide concentrations in an organism decrease. However, for respiration and diet, processes of uptake and elimination are linked. Therefore, factors that would influence uptake constants would also influence elimination constants, so these cannot be considered independently. In addition, as the freely dissolved fraction of pesticide in the water (Φ) decreases, so do estimated pesticide concentrations in organisms. Rate constants defining the uptake of a chemical through respiration (k_1) and diet (k_D) and the elimination of a chemical through respiration (k_2) and fecal excretion (k_E) as well as growth dilution of a chemical (k_G) are estimated separately using equations A5-A9, which are described below. Parameter definitions and abbreviations are consistent with those published by Arnot and Gobas (2004) in order to ensure consistency with the publication and transparent methodology used in KABAM.

Use of Equation A1 involves several assumptions. The first assumption is that the organism is at steady state. The second assumption is that the pesticide is distributed homogenously throughout organisms. The third assumption is that the effects of chemical partitioning into egg and sperm cells on chemical mass in parents is not considered as a loss pathway. The fourth assumption is that when data are lacking to define the metabolism rate constant for a chemical, it is assumed that metabolism does not occur and that the elimination rate constant for metabolism (k_M) is 0.

Uptake and elimination of a chemical from an organism is influenced by the body composition of the model organism. Body composition includes lipid, non-lipid organic matter (NLOM; *e.g.*, carbohydrates and protein), and water. Chemicals are expected to partition differently to these components of an organism. Partitioning of a chemical into these components is related to the octanol-water partition coefficient (K_{OW}). It is assumed that octanol is a surrogate for the lipid fraction of an organism. It is also assumed that the partitioning of a chemical to NLOM is less than to octanol, but that there is a relationship between the partitioning of the chemical to NLOM and to octanol and that octanol serves as a reasonable surrogate for estimating this parameter.

Arnot and Gobas (2004) recommend that equation A1 be applied to an aquatic food web with seven trophic levels. In increasing order of hierarchy, these trophic levels include: 1) phytoplankton, 2) zooplankton, 3) benthic invertebrates, 4) filter feeders, 5) small (juvenile) fish, 6) medium sized fish, and 7) large fish. Concentrations in organisms are first calculated at the lowest level of the aquatic food chain (phytoplankton). Pesticide concentrations are then calculated for zooplankton, including consideration that the diet of zooplankton includes phytoplankton, which contain pesticide residues. Tissue residues are calculated for the next five trophic levels based on their diets of organisms from lower trophic levels.

Table A1. Equation A1, calculation of pesticide tissue residue (C_B) for single trophic levels and its associated parameters (Arnot and Gobas 2004).

$$Eq.\ A1 \quad C_B = \frac{k_1 * (m_0 * \Phi * C_{WTO} + m_P * C_{WDP}) + k_D * \Sigma(P_i * C_{Di})}{k_2 + k_E + k_G + k_M}$$

Parameters:

Symbol	Definition	Value	Units
C_B	pesticide concentration in the organism	calculated	g/kg (wet weight)
C_{BD}	pesticide concentration in the organism originating from uptake through diet; $C_{BD} = C_B$ when $k_1 = 0$	calculated	g/kg (wet weight)
C_{BR}	pesticide concentration in the organism originating from uptake through respiration; $C_{BR} = C_B$ when $k_D = 0$	calculated	g/kg (wet weight)
C_{Di}	concentration of pesticide in i (prey item)	calculated	g/kg (wet weight)
C_S	concentration of the chemical in sediment (dry weight of sediment)	Equation A4	g/(kg (dry) sediment)
C_{WDP}	freely dissolved pesticide concentration in pore water of sediment	input parameter (from PRZM/EXAMS)	g/L
C_{WTO}	total pesticide concentration in water column above the sediment	input parameter (from PRZM/EXAMS)	g/L
k_1	pesticide uptake rate constant through respiratory area (*i.e.*, gills, skin)	Equation A5	L/kg*d
k_2	rate constant for elimination of the pesticide through the respiratory area (*i.e.*, gills, skin)	Equation A6	d^{-1}
k_D	pesticide uptake rate constant for uptake through ingestion of food	Animals: Equation A8; Phytoplankton: 0	kg food/ (kg org*day)
k_E	rate constant for elimination of the pesticide through excretion of contaminated feces	Animals: Equation A9; Phytoplankton: 0	d^{-1}
k_G	organism growth rate constant	Animals: Equation A7; Phytoplankton: 0.1	d^{-1}
k_M	rate constant for pesticide metabolic transformation	0	d^{-1}
m_o	fraction of respiratory ventilation involving overlying water	$1 - m_p$	none
m_p	fraction of respiratory ventilation that involves pore-water of sediment	≤5%; 0 for organisms with no contact with pore water	none
P_i	fraction of diet containing i (prey item)	user defined	none
Φ	fraction of the overlying water concentration of the pesticide that is freely dissolved and can be absorbed via membrane diffusion	Equation A2	none

A.1. Calculation of Fraction of Chemical in the Water Column That Is Freely Dissolved (Φ)

Aquatic ecosystems contain organic matter suspended in the water column. This suspended organic matter is defined as dissolved organic carbon (DOC) and particulate organic carbon (POC). It is assumed that once chemicals partition to organic carbon, they are no longer bioavailable to aquatic organisms. The fraction of chemical in the water column that is freely dissolved (Φ), and thus bioavailable for uptake by aquatic animals is estimated according to Equation A2 (Table A2). This equation assumes that equilibrium exists between the pesticide concentration in the water and in the organic carbon in the water column. Equation A2 assumes that partitioning between POC and water and DOC and water can be related to partitioning of the chemical between octanol and water. These relationships are defined using proportionality constants (α_{POC} and α_{DOC}) that are defined from the scientific literature.

Table A2. Equation A2, derivation of available pesticide fraction in water (Φ) and its associated parameters (Arnot and Gobas 2004).

$$Eq.A2 \quad \Phi = \frac{1}{1+(X_{POC} * \alpha_{POC} * K_{OW}) + (X_{DOC} * \alpha_{DOC} * K_{OW})}$$

Parameters:

Symbol	Definition	Value	Units
X_{POC}	concentration of particulate organic carbon in water	user defined	kg/L
X_{DOC}	concentration of dissolved organic carbon in water	user defined	kg/L
K_{OW}	octanol water partition coefficient	user defined	none
Φ	fraction of the overlying water concentration of the pesticide that is freely dissolved and can be absorbed via membrane diffusion	calculated	none
α_{POC}	Proportionality constant to describe the similarity of phase partitioning of POC in relation to octanol	0.35	none
α_{DOC}	Proportionality constant to describe the similarity of phase partitioning of DOC in relation to octanol	0.08	none

The Arnot and Gobas (2004) approach for calculating the fraction of bioavailable pesticide in the water column (Equation A2) is different from the approach used in EPA's Exposure Analysis Modeling System (EXAMS) (Equation A3, Table A3). The major difference is that the approach employed by EXAMS accounts for decreases in bioavailable pesticide in the water column due to sorption to biota. The values for α_{DOC} for the two approaches are also slightly different. Despite these different approaches, for chemicals with Log K_{OW} values 4-8, the fractions of bioavailable pesticide in the water column estimated by the two approaches differ by <0.02 (Figure A1). Therefore, utilizing water column EECs generated by EXAMS is still consistent with the results that are generated using the approach described by Arnot and Gobas (2004).

Table A3. Equation A3, derivation of available pesticide fraction in water (F) by EXAMS and its associated parameters.			
$$Eq.A3 \quad F = \frac{1}{1 + (X_{POC} * \alpha_{POC} * K_{OW}) + (X_{DOC} * \alpha_{DOC} * K_{OW}) + \left(X_{biota} * 0.436 * K_{OW}^{0.907}\right)}$$			
Parameters:			
Symbol	**Definition**	**Value**	**Units**
F	fraction of the overlying water concentration of the pesticide that is freely dissolved and can be absorbed via membrane diffusion	calculated	none
K_{OW}	octanol water partition coefficient	user defined	none
OC_{SS}	percent organic carbon in suspended sediment	user defined	%
X_{SS}	concentration of suspended sediments in water column	user defined	kg/m^3
X_{POC}	concentration of particulate organic carbon in water	$X_{SS}*OC_{SS}$	kg/m^3
X_{DOC}	concentration of dissolved organic carbon in water	user defined	kg/m^3
X_{biota}	concentration of biota in water	user defined	kg/m^3
α_{POC}	Proportionality constant to describe the similarity of phase partitioning of POC in relation to octanol	0.35	none
α_{DOC}	Proportionality constant to describe the similarity of phase partitioning of DOC in relation to octanol	0.074	none

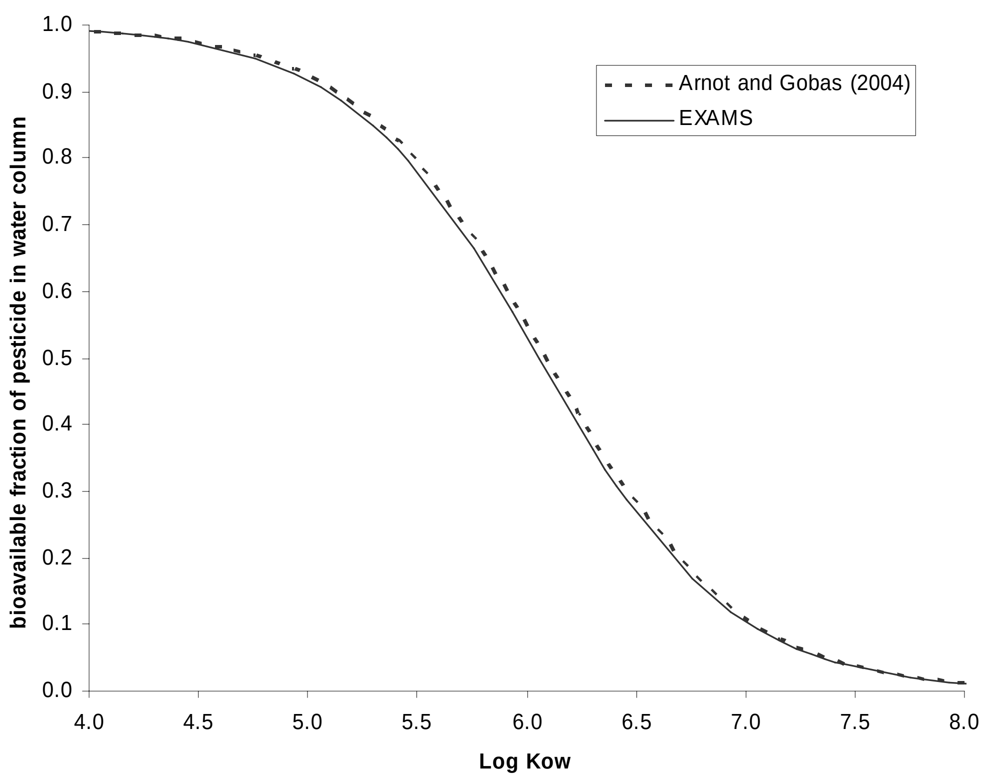

Figure A1. Fraction of bioavailable pesticide in water column estimated using approaches of Arnot and Gobas (2004) and EXAMS. Values for OC_{SS}, X_{SS}, X_{DOC} and X_{biota} are consistent with OPP standard pond scenario used in EXAMS.

A.2. Calculation of Chemical Concentration in Sediment

Since it is possible for aquatic organisms to be exposed to chemicals through consumption of contaminated sediment, it is necessary to estimate the concentration of the chemical of concern in the sediment. This is accomplished using Equation A4 (Table A4), which uses the concentration of the chemical in the pore water, the chemical $K_{OC,}$ and the organic carbon content of the sediment. This approach is consistent with EXAMS for calculating the fraction of pesticide sorbed to sediment in the benthic column.

Table A4. Derivation of pesticide concentration in the solid portion of the sediment (C_S) (Arnot and Gobas 2004).			
$$Eq.A4 \quad C_S = C_{SOC} * OC$$ $$Where: \quad C_{SOC} = C_{WDP} * K_{OC}$$			
Parameters:			
Symbol	**Definition**	**Value**	**Units**
C_S	concentration of the chemical in sediment (dry weight of sediment)	calculated	g/(kg (dry) sediment)
C_{SOC}	normalized (for OC content) pesticide concentration in sediment	calculated	g/(kg OC)
C_{WDP}	freely dissolved pesticide concentration in pore water	input parameter (from PRZM/EXAMS)	g/L
K_{OC}	organic carbon partition coefficient	user defined	L/kg OC
OC	percent organic carbon in sediment	user defined	%

A.3. Calculation of Respiration Uptake (k_1) and Elimination (k_2) Rate Constants

The respiratory uptake constant (k_1) is calculated differently for phytoplankton (Equation A5.1) and for animals (Equation A5.2). For phytoplankton, k_1 is dependent upon the K_{OW} of the chemical as well as 2 constants (A and B) that describe chemical uptake resistance through the aqueous and organic phases (respectively) of the plant. If A and B are kept constant at $6x10^{-5}$ and 5.5, respectively as recommended by Arnot and Gobas (2004), k_1 for phytoplankton increases with increasing K_{OW}, ranging by a factor of 10 from Log K_{OW} 4-8 (Figure A2).

For animals, k_1 is dependent upon the chemical uptake efficiency of the gills, the ventilation rate, and the body weight of the organism. The uptake efficiency of the gills is determined by the K_{OW} of the chemical, while the ventilation rate of the organism is determined by an allometric equation that is influenced by the body weight of that organism and the concentration of oxygen in the water column (C_{OX}) (Table A5). When C_{OX} and organism body weight are kept constant, Log K_{OW} has little effect on the k_1 for animals (0.8% change from Log K_{OW} 4-8). When Log K_{OW} and body weight are kept constant, C_{OX} strongly affects k_1. The value of k_1 decreases by 50%, as the C_{OX} value increases from 5 to 10 mg/L (Figure A3). The value of k_1 is also strongly influenced by the body weight of the organism, with decreasing k_1 observed with increasing body weight. As the body weight of the organism increases from $1x10^{-7}$ to 10 kg (a relevant range for aquatic organisms, see Appendix C), the k_1 value spans 3 orders of magnitude (Figure A3).

Table A5. Equations associated with the derivation of pesticide clearance through the respiratory (gill) system (k_1) and associated parameters (Arnot and Gobas 2004).

$$Eq.A5.1 \quad For\ phytoplankton: \quad k_1 = \frac{1}{A + B/K_{OW}}$$

$$Eq.A5.2 \quad For\ animals: \quad k_1 = \frac{E_W * G_V}{W_B}$$

$$Where: E_W = \left(1.85 + \frac{155}{K_{OW}}\right)^{-1}$$

$$G_V = 1400 * \left(\frac{W_B^{0.65}}{C_{OX}}\right)$$

Parameters

Symbol	Definition	Value	Units
A	constant related to the resistance to pesticide uptake through the aqueous phase of plant	$6.0x10^{-5}$ (default)	days
B	constant related to the resistance to pesticide uptake through the organic phase of plant	5.5 (default)	days
C_{ox}	concentration of dissolved oxygen	User input	(mg O_2)/L
E_W	pesticide uptake efficiency by gills (fraction)	calculated	none
G_V	ventilation rate of fish, invertebrates, zooplankton	calculated	L/d
k_1	pesticide uptake rate constant through respiratory area (*i.e.*, gills, skin)	calculated	L/kg*d
K_{OW}	octanol water partition coefficient	user defined	none
W_B	wet weight of the organism	user defined	kg

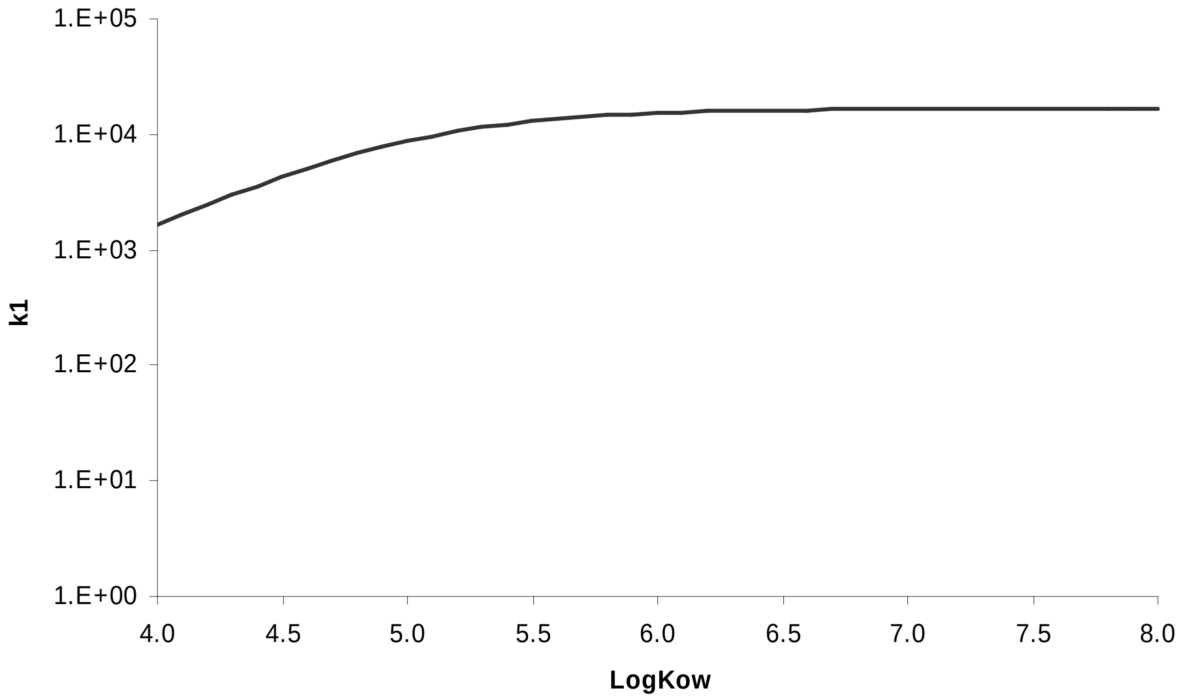

Figure A2. Relationship between Kow and k_1 for phytoplankton.

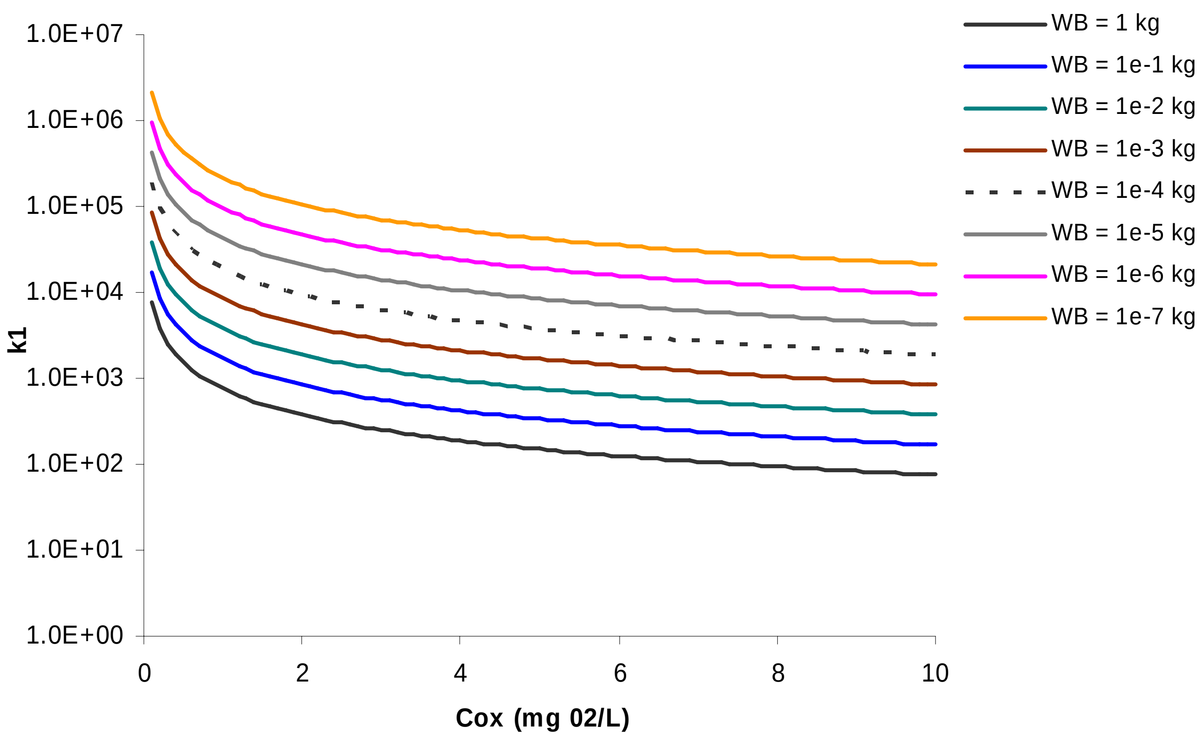

Figure A3. Relationship between C_{OX}, W_B and k_1 for aquatic animals.

The elimination rate constant for the respiratory system (k_2) is related to the respiratory uptake constants (k_1). This is because both constants are influenced by the same processes related to respiration. The value of k_2 is also influenced by the partitioning of the chemical between the organisms and the water. The organism-water partition coefficient (K_{BW}) is determined by the body composition of the organism (*i.e.*, lipid, NLOM, and water) and the K_{OW} of the chemical. It is assumed that the partitioning of the chemical between lipid and water is directly related to the octanol-water partition coefficient. It is also assumed that the chemical partitioning between NLOM and water can be related to the octanol-water partition coefficient using a proportionality constant (β) (Equation A6, Table A6).

Table A6. Equations involved in the derivation of the respiratory elimination rate constant (k_2) and associated parameters (Arnot and Gobas 2004).			
$$Eq.A6 \quad k_2 = \frac{k_1}{k_{BW}}$$ $$Where: \quad K_{BW} = V_{LB} * K_{OW} + V_{NB} * \beta * K_{OW} + V_{WB}$$			
Parameters:			
Symbol	**Definition**	**Value**	**Units**
k_1	pesticide uptake rate constant for chemical uptake through respiratory area (*i.e.*, gills, skin, membrane permeation)	calculated (Equation 5)	L/kg*d
k_2	rate constant for elimination of the pesticide through the respiratory area (*i.e.*, gills, skin, membrane permeation)	calculated	d^{-1}
K_{BW}	organism-water partition coefficient (based on wet weight)	calculated	none
K_{OW}	octanol water partition coefficient	user defined	none
V_{LB}	lipid fraction of organism	user defined	(kg lipid)/ (kg organism wet weight)
V_{NB}	NLOM (Non Lipid Organic Matter) fraction of animals, NLOC (Non Lipid Organic Carbon) of plants	user defined	kg NLOM/ (kg organism wet weight)
V_{WB}	water content of the organism	user defined	kg water/ (kg organism wet weight)
β	proportionality constant expressing the sorption capacity of NLOM or NLOC to that of octanol	Phytoplankton: 0.35; Animals:0.035	none

Elimination rate constants for phytoplankton (k_2) are calculated using seven parameters, including: K_{OW}, V_{LB}, V_{NB}, $V_{WB,}$ A, B, and β (defined above in Table A6). The parameters A, B and β are all constants. If the other parameters are considered in terms of ranges applicable to KABAM, K_{OW} has the greatest influence on the determination of k_2 for phytoplankton. When Log K_{OW} values are changed from 4 to 8, the k_2 value decreases by three orders of magnitude (Figure A4). The lipid fraction of the organism (V_{LB}) and the non-lipid organic carbon fraction (V_{NB}) influence k_2, with decreases in k_2 observed as V_{LB} and V_{NB} increase. These two parameters are related. As V_{LB} decreases, an increase in V_{NB} has a greater effect on k_2. Likewise, as V_{NB}

decreases, an increase in V_{LB} has a greater effect on k_2 (Figure A4). When the lipid fraction of organism (V_{LB}) is increased from 0.5 to 3%, the elimination rate constant through respiration, *i.e.*, k_2, decreases by >30% (Figure A5). A change in V_{NB} from 5% to 20% results in a decrease in the value of k_2 that is >50% (Figure A5). The water content (V_{WB}) of an organism has a negligible (<0.5%) effect on k_2.

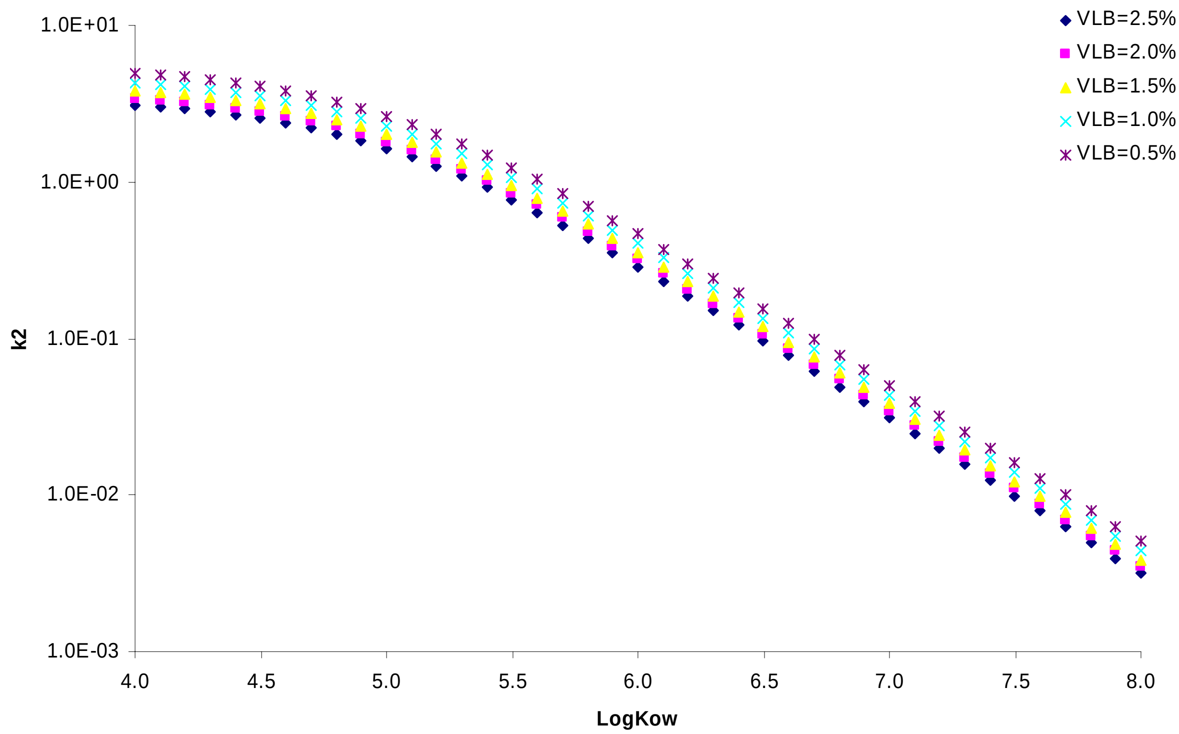

Figure A4. Influence of Log K_{OW} on k_2 (for phytoplankton) at different % lipid (V_{LB}) (with V_{NB} = 8%).

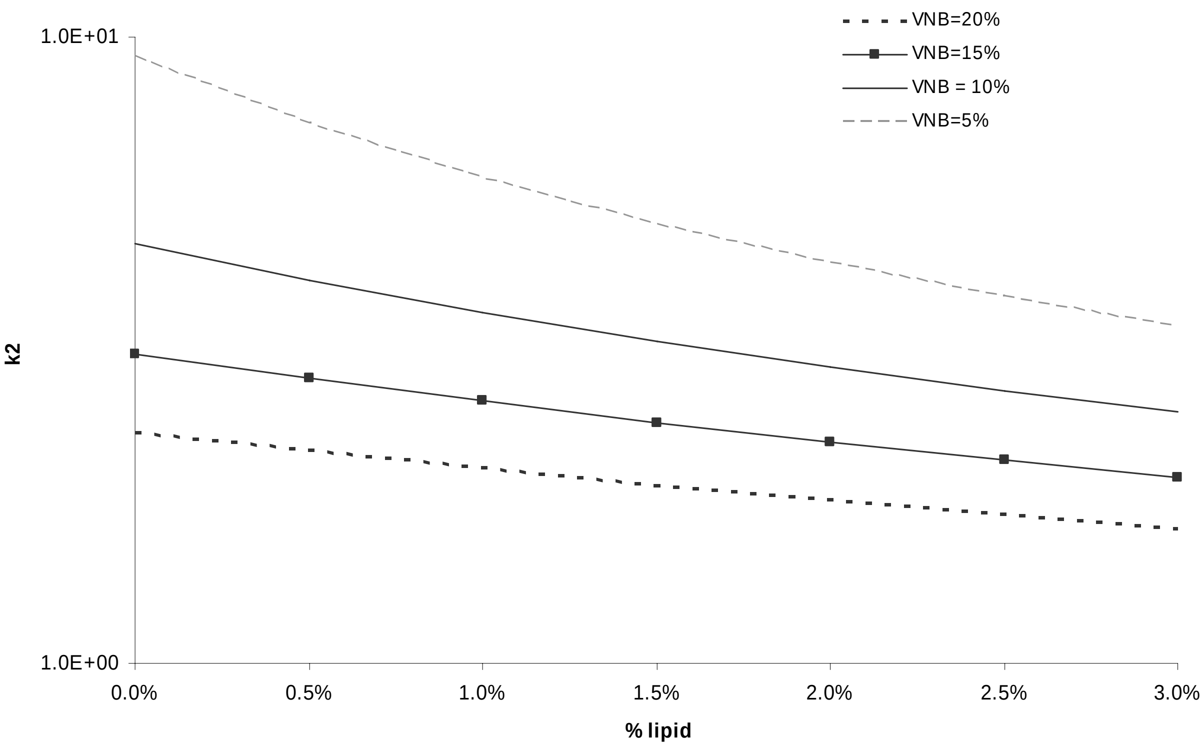

Figure A5. Influence of % lipid (V_{LB}) on k_2 (for phytoplankton) at different % NLOM (V_{NB}) at Log Kow 4. Note that for all Log Kow values from 4-8, the curves follow a similar trend for different V_{LB} and V_{NB}, but differ in magnitude of k_2.

To determine elimination constant from respiration (k_2) for animals, seven input parameters are required: K_{OW}, W_B, V_{LB}, V_{NB}, $V_{WB,}$ C_{OX}, and β (all of which are defined in Table A6). The parameter β is a constant representing the proportionality of the sorption of a chemical to NLOM to the K_{OW} of that chemical. If the other parameters are considered in terms of ranges applicable to KABAM, the octanol-water partition coefficient (K_{OW}) and the water content of the organism (V_{WB}) have the greatest influence on the determination of k_2. When Log K_{OW} values are changed from 4 to 8, the k_2 value decreases by 4 orders of magnitude (Figures A6 and A7). Body weight also influences k_2, with k_2 values decreasing by 2 orders of magnitude as the body weight is increased from $1x10^{-7}$ to 1 kg (this is a range considered relevant to aquatic animals, see Appendix C for more information) (Figure A6). The lipid fraction of the organism (V_{LB}) and the non-lipid organic matter fraction (V_{NB}) influence k_2, with decreases in k_2 observed as these two values increase. When V_{LB} is increased from 1 to 5%, k_2 decreases by 84% (Figure A7). When V_{NB} is increased from 15 to 40%, a 14% decrease in k_2 is observed. The water content (V_{WB}) of an organism has a negligible (<0.5%) effect on k_2. Increasing the concentration of the dissolved oxygen (C_{OX}) value from 5 to 10 mg/L results in a decrease of 50% in the value of k_2.

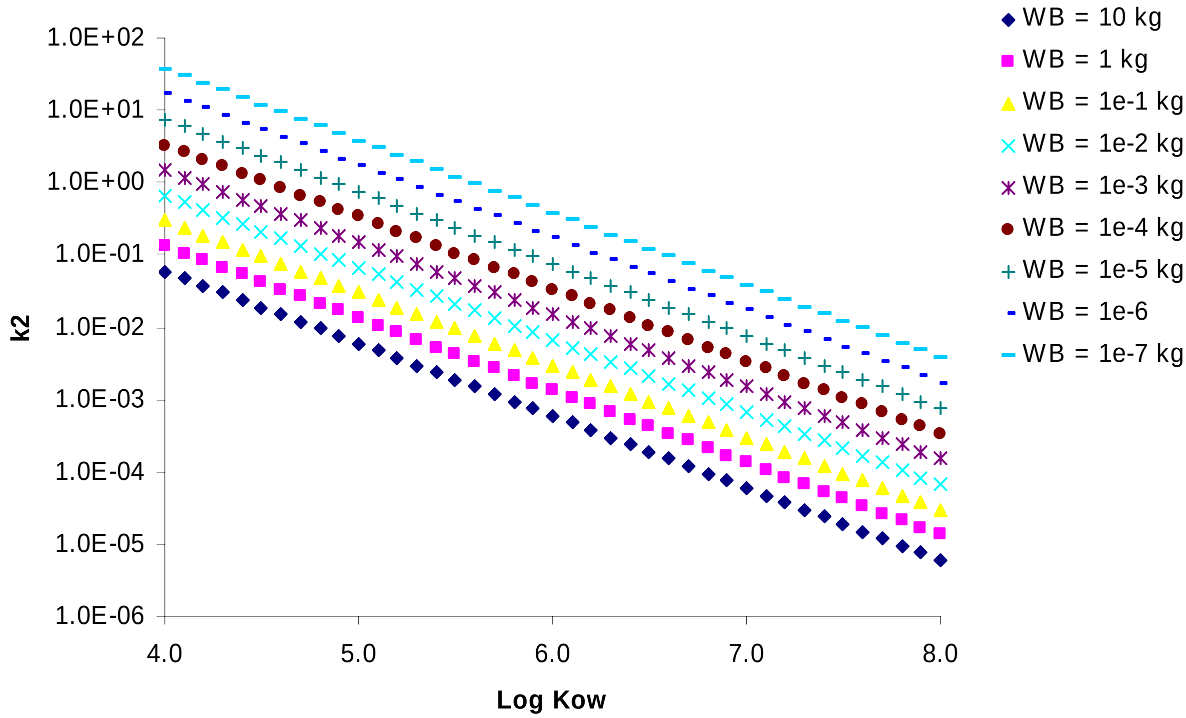

Figure A6. Influence of Log K_{OW} on k_2 (for animals) at different body weights (W_B) (with V_{LB} = 5%, V_{NB} = 20%, V_{WB} = 75% and C_{OX} = 10mg/L).

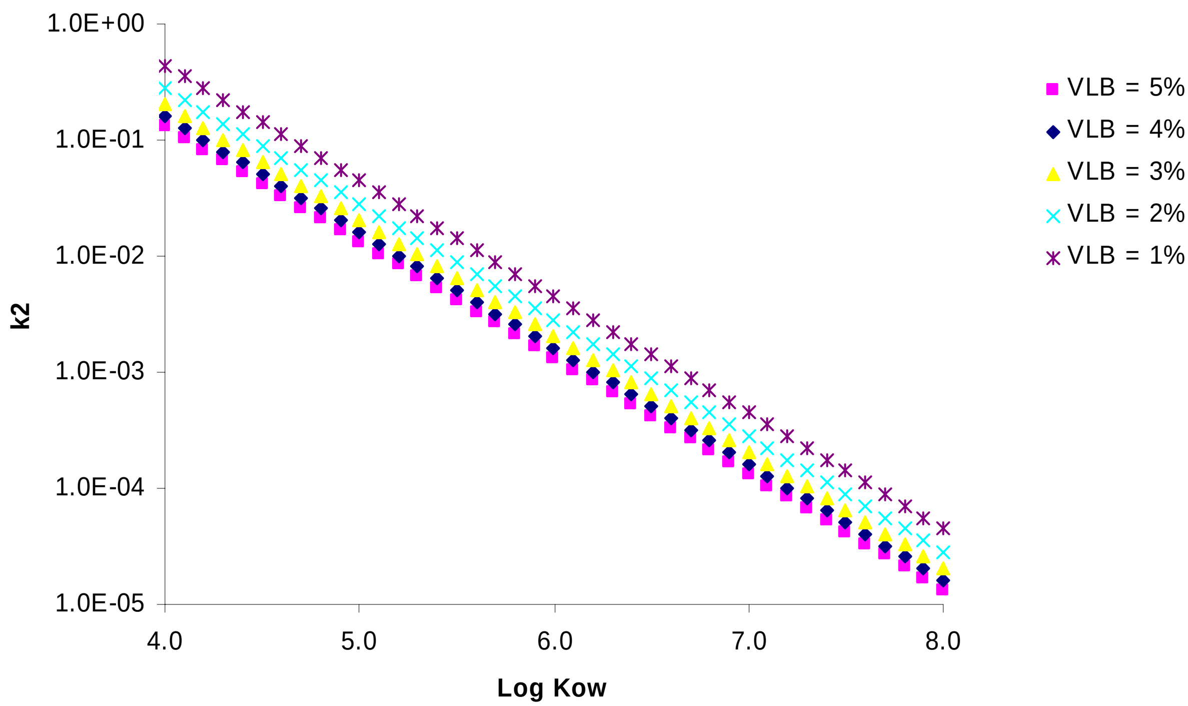

Figure A7. Influence of Log K_{OW} on k_2 (for animals) at different % lipid composition (V_{LB}) (with W_B = 1 kg, V_{NB} = 20%, V_{WB} = 75% and C_{OX} = 10 mg/L).

A.4. Calculation of Growth Rate Constant

Equations A7.1 and A7.2 provide an approximation of growth of aquatic organisms based on weight and temperature (Table A7). Comparing the results of the two equations indicates that higher temperatures result in higher growth rate constant (k_G) values (Figure A8). With both equations, as body weight increases, k_G decreases. There is some uncertainty associated with these equations, since growth rate can be influenced by additional factors, including species and prey availability. For KABAM, it is assumed that if the water temperature (T) < 17.5 ^oC (midpoint between 10 and 25^oC), equation A.7.1 is used and if T ≥ 17.5 ^oC, equation A.7.2 is used.

Table A7. Equations involving the derivation of the growth rate constant (k_G) and associated parameters (Arnot and Gobas 2004).

$$Eq.A7.1 \quad k_G = 0.0005 * W_B^{-0.2} \quad (T \approx 10\ ^oC)$$

$$Eq.A7.2 \quad k_G = 0.00251 * W_B^{-0.2} \quad (T \approx 25\ ^oC)$$

Parameters:

Symbol	Definition	Value	Units
k_G	organism growth rate constant	calculated	d^{-1}
T	temperature	user defined	^oC
W_B	wet weight of the organism	user defined	kg

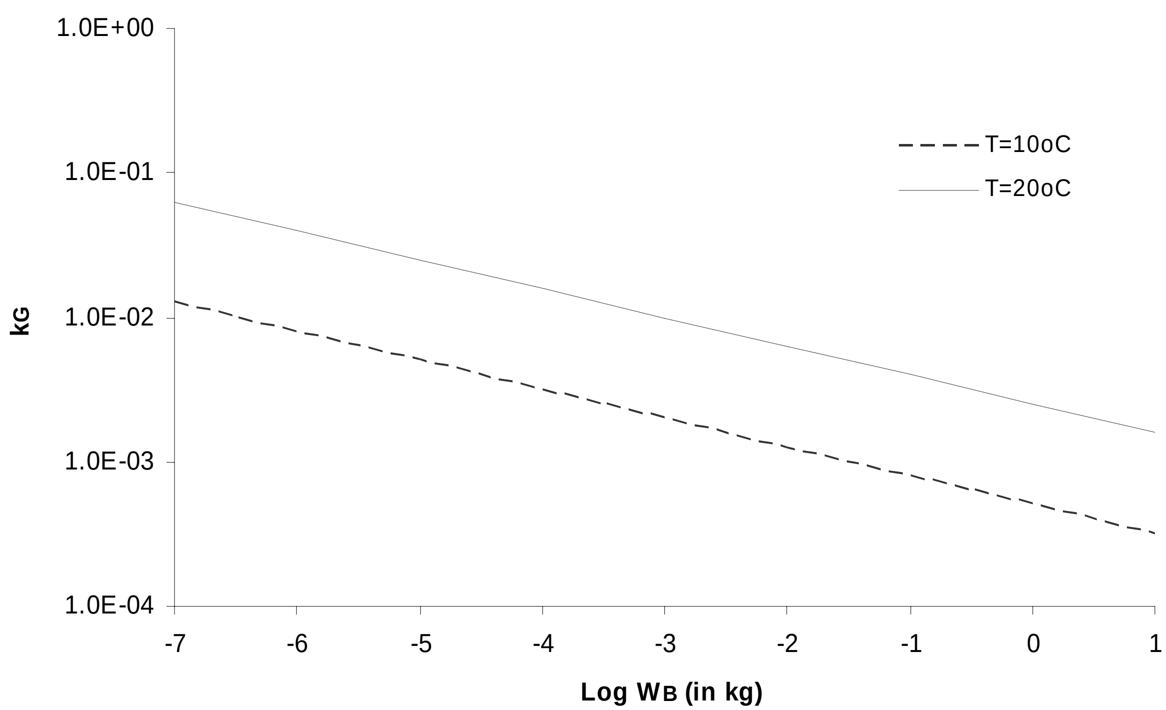

Figure A8. Relationship between body weight (W_B) and k_G at 2 different temperatures.

A.5. Calculation of Dietary Uptake (k_D) Rate Constant

In determining uptake and elimination rate constants related to dietary sources of chemicals (k_D and k_E, respectively), it is assumed that aquatic organisms are represented by a 2-phase model that includes the gastrointestinal tract (GIT) of the organisms and the organism itself. Since phytoplankton do not consume other organisms, a dietary uptake constant (k_D) is not a relevant rate constant, and the elimination rate constant due to fecal elimination (k_E) is considered insignificant in plants. Therefore, k_D and k_E are only calculated for animals.

The dietary uptake constant for a chemical in animals is influenced by the weight of the organism, the feeding rate of the organism (G_D), and the dietary pesticide transfer efficiency (E_D). The feeding rate is different for filter feeders compared to other aquatic organisms. Empirical dietary pesticide transfer efficiency (E_D) values vary from 0-100%. Variability in E_D has been attributed to various factors, including sorption coefficients of chemicals, composition of diet, and digestibility of diet. Based on several different observations, it is assumed by Arnot and Gobas (2004) that this value can be related to K_{OW} (Equation A8, Table A8).

Table A8. Equations involving the derivation of the pesticide clearance rate constant through diet (k_D) and associated parameters (Arnot and Gobas 2004).

$$Eq.A8 \quad k_D = E_D * \frac{G_D}{W_B}$$

$$Where: \quad E_D = (3.0x10^{-7} * K_{OW} + 2.0)^{-1}$$

$$For\ animals\ (except\ filter\ feeders): \quad G_D = 0.022 * W_B^{0.85} * \exp(0.06 * T)$$

$$For\ filter\ feeders: \quad G_D = G_V * C_{SS} * \sigma$$

$$G_V = 1400 * \left(\frac{W_B^{0.65}}{C_{OX}} \right)$$

Parameters:

Symbol	Definition	Value	Units
C_{ox}	concentration of dissolved oxygen	user defined	(mg O_2)/L
C_{SS}	concentration of suspended solids	user defined	kg/L
E_D	dietary pesticide transfer efficiency	calculated	%
G_D	feeding rate of organism	calculated	kg/d
G_V	ventilation rate of gills	calculated	L/d
k_D	pesticide uptake rate constant for uptake through ingestion of food	calculated	kg food/(kg org*day)
K_{OW}	octanol water partition coefficient	user defined	none
T	temperature	user defined	^oC
W_B	wet weight of the organism	user defined	kg
σ	efficiency of scavenging of particles absorbed from water	100	%

For aquatic organisms (non-filter feeders), the dietary uptake constant (k_D) is derived using 3 input parameters: octanol-water partition coefficient (K_{OW}), the weight of the organism (W_B), and temperature (T). For chemicals with Log K_{OW} ranging 4-5.5, changes in Log K_{OW} cause little (<4%) effects to the value of k_D; however, for chemicals with Log K_{OW} <5.5, increases in Log K_{OW} can result in decreases in this value up to an order of magnitude (Figure A9). Increases in W_B from $1x10^{-7}$ to 1 kg result in an order of magnitude decrease in k_D (Figure A9). Temperature also affects k_D, with an observed increase in k_D of 65% when the temperature is increased from 2.5 to 20^{o}C (Figure A10).

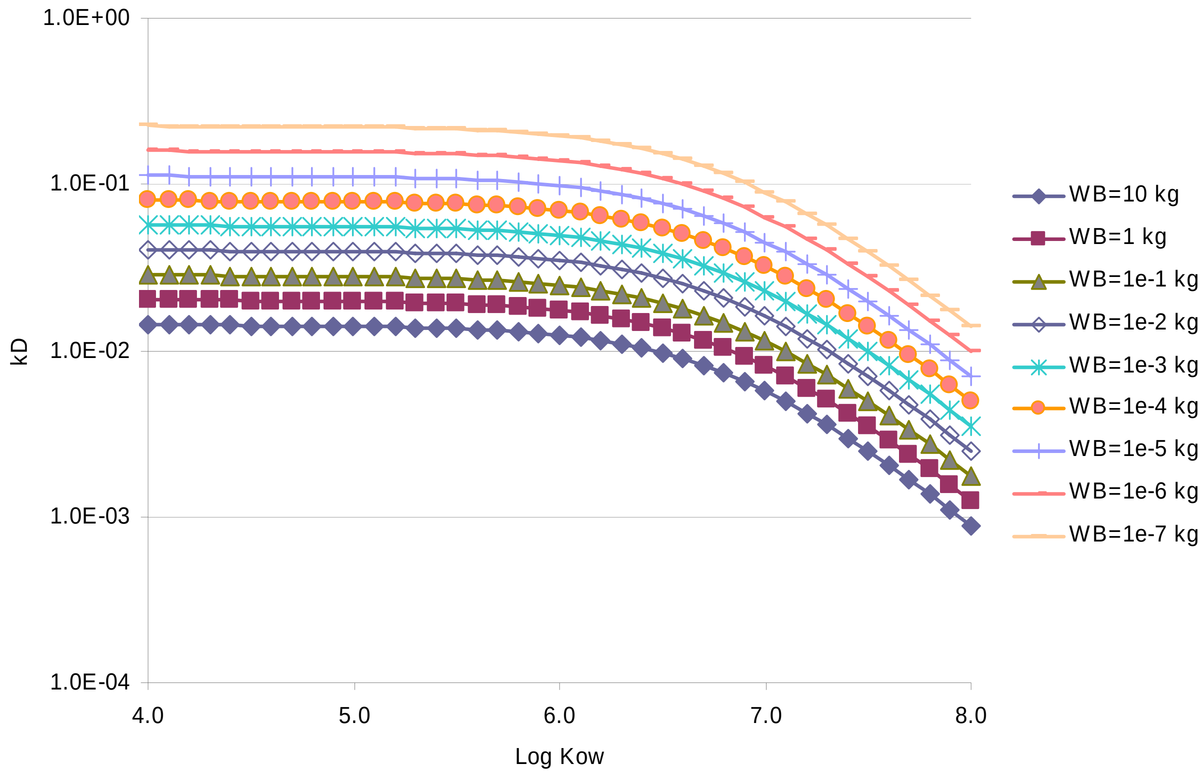

Figure A9. Relationship between Log K_{OW} and k_D (for non-filter feeders) at different body weights (W_B) (T=10^{o}C).

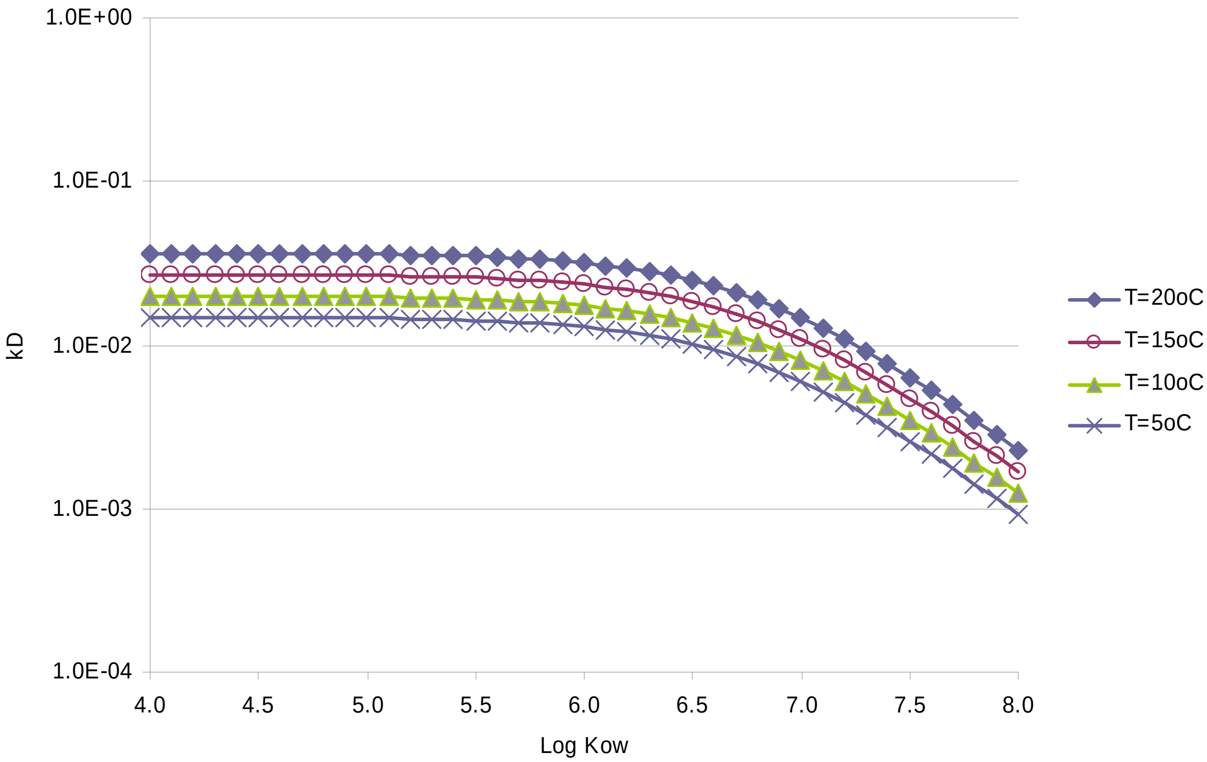

Figure A10. Relationship between Log K_{OW} and k_D (for non-filter feeders) at different water temperatures (W_B=1 kg).

For filter feeders, the dietary uptake constant (k_D) is derived using five input parameters: K_{OW}, W_B, C_{OX}, C_{SS} and σ (all of which are defined in Table A.8). For chemicals with Log K_{OW} values ranging 4-5.5, changes in Log K_{OW} cause little (<5%) effects to the value of k_D; however, as the Log K_{OW} increases from 6 to 8, the k_D for filter feeders decreases by an order of magnitude (Figure A11). Available National Water Quality Assessment (NAWQA) data for streams indicate that suspended sediment concentrations range 1-281 mg/L (USGS 2008b). If the concentration of suspended sediments (C_{SS}) is increased from $1x10^{-6}$ to $1x10^{-4}$ kg/L, k_D for filter feeders increases by 2 orders of magnitude (Figure A12). Increases in W_B from $1x10^{-4}$ to $1x10^{-2}$ kg (which is a reasonable range of weights for filter feeders; see Appendix C) result in an 80% decrease in k_D (Figure A11). Increases in oxygen concentration (C_{OX}) from 2 to 8 mg/L results in a decrease in k_D of 80% for filter feeders. Changes in the scavenging efficiency (σ) of filter feeders result in proportional changes to the k_D value. For example, a 25% decrease in σ results in a 25% decrease in k_D.

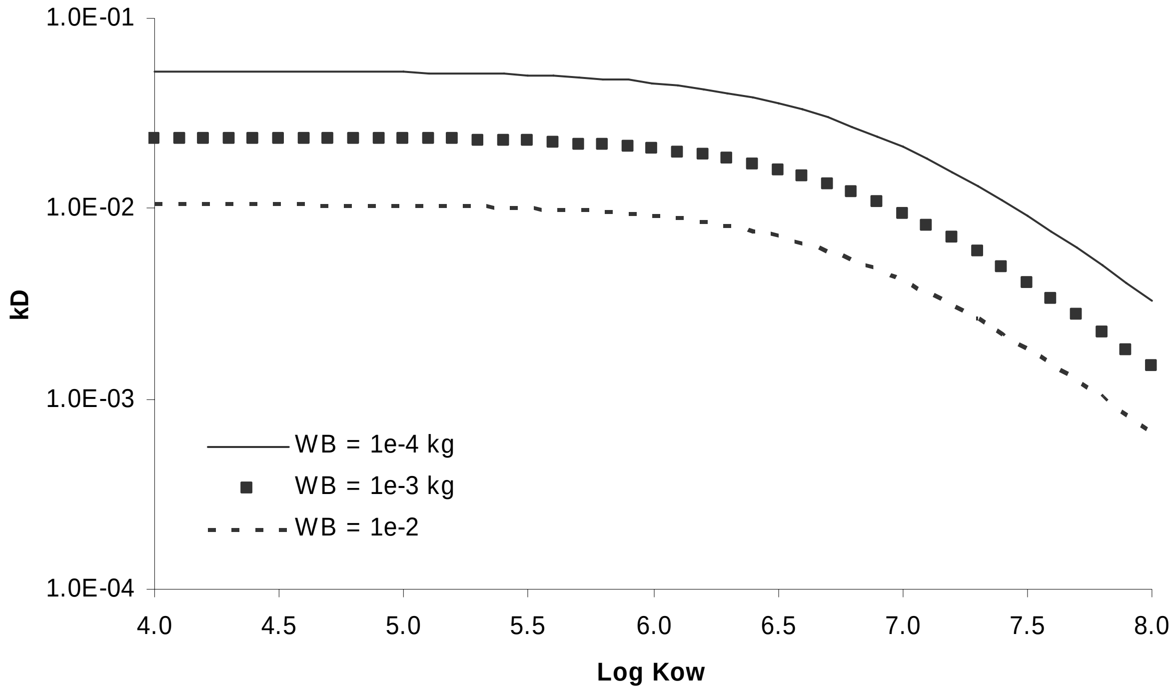

Figure A11. Relationship between Log K_{OW} and filter feeder k_D with different W_B values.

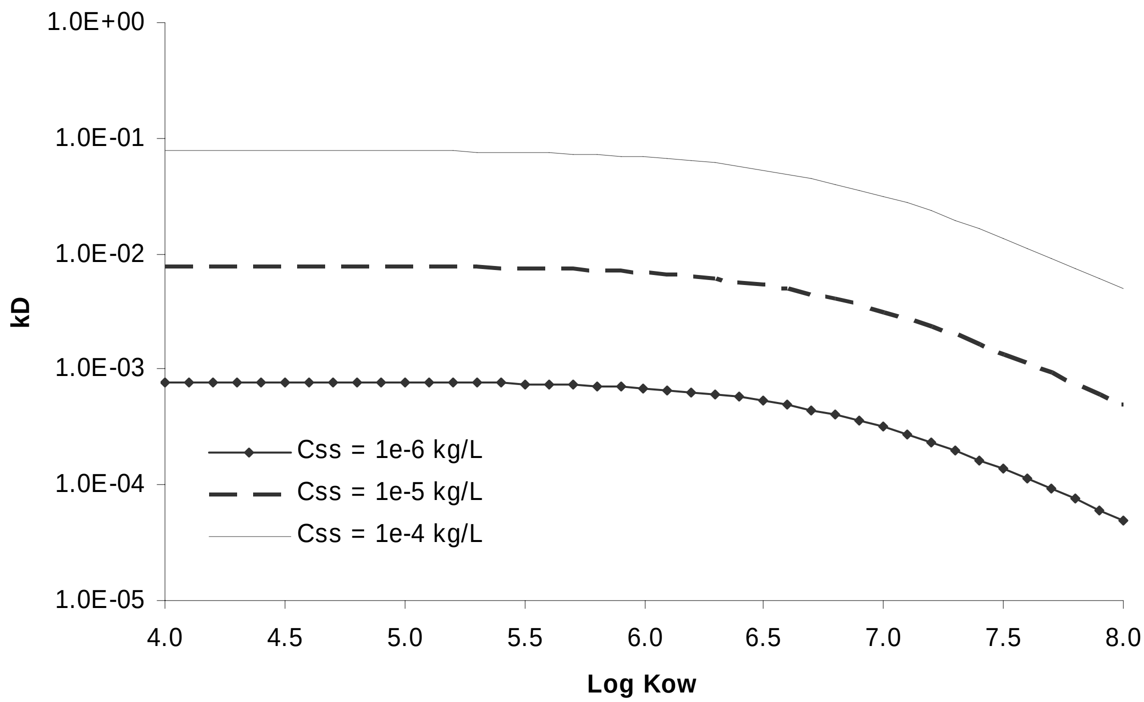

Figure A12. Relationship between Log K_{OW} and filter feeder k_D with different Css values.

A.6. Calculation of Dietary Elimination (k_E) Rate Constant

The rate constant for elimination of the pesticide through excretion of contaminated feces (k_E) is calculated using the fecal egestion rate (G_F), the dietary pesticide transfer efficiency (E_D), the partition coefficient of the pesticide between the gastro-intestinal tract and the organism (K_{GB}), and the body weight of the organism (W_B) (Equation A9, Table A9). For filter-feeding and non-filter feeding aquatic animals, k_E is calculated in a similar manner, with the exception of the method of calculating the feeding rate of an organism (G_D). An order of magnitude increase in either G_F, E_D, or K_{GB} results in an order of magnitude increase in fecal egestion rate constant (k_E). An order of magnitude increase in W_B results in an order of magnitude decrease in k_E. Effects of changes in individual input parameters used to derive G_F, E_D, and K_{GB} are explored below.

Table A9. Equations involving the derivation of the fecal elimination rate constant (k_E) and associated parameters (Arnot and Gobas 2004).

$$Eq.A9 \quad k_E = G_F * E_D * \frac{K_{GB}}{W_B}$$

$$Where: \quad E_D = (3.0x10^{-7} * K_{OW} + 2.0)^{-1}$$

$$K_{GB} = \frac{(V_{LG} * K_{OW} + V_{NG} * \beta * K_{OW} + V_{WG})}{(V_{LB} * K_{OW} + V_{NB} * \beta * K_{OW} + V_{WB})}$$

$$V_{LG} = \frac{(1-\varepsilon_L)*V_{LD}}{(1-\varepsilon_L)*V_{LD} + (1-\varepsilon_N)*V_{ND} + (1-\varepsilon_W)*V_{WD}}$$

$$V_{NG} = \frac{(1-\varepsilon_N)*V_{ND}}{(1-\varepsilon_L)*V_{LD} + (1-\varepsilon_N)*V_{ND} + (1-\varepsilon_W)*V_{WD}}$$

$$V_{WG} = \frac{(1-\varepsilon_W)*V_{WD}}{(1-\varepsilon_L)*V_{LD} + (1-\varepsilon_N)*V_{ND} + (1-\varepsilon_W)*V_{WD}}$$

$$G_F = [(1-\varepsilon_L)*V_{LD} + (1-\varepsilon_N)*V_{ND} + (1-\varepsilon_W)*V_{WD}] * G_D$$

$$For\ animals\ (except\ filter\ feeders): \quad G_D = 0.022 * W_B^{0.85} * \exp(0.06 * T)$$

$$For\ filter\ feeders: \quad G_D = G_V * C_{SS} * \sigma$$

$$G_V = 1400 * \left(\frac{W_B^{0.65}}{C_{OX}}\right)$$

Parameters:

Symbol	Definition	Value	Units
C_{ox}	concentration of dissolved oxygen	calculated	(mg O_2)/L
C_{SS}	concentration of suspended solids	user defined	kg/L

E_D	dietary pesticide transfer efficiency	calculated	%
G_D	feeding rate of organism	calculated	kg/d
G_F	egestion rate of fecal matter	calculated	(kg feces)/(kg organism)*d
G_V	ventilation rate of gills	calculated	L/d
k_E	rate constant for elimination of the pesticide through excretion of contaminated feces	for animals: calculated for plants: 0	d^{-1}
K_{GB}	partition coefficient of the pesticide between the gastro-intestinal tract and the organism	calculated	none
K_{OW}	octanol water partition coefficient	user defined	none
T	temperature	user defined	^oC
V_{LB}	lipid fraction of organism	user defined	(kg lipid)/ (kg organism wet weight)
V_{LD}	overall lipid content of diet	user defined	kg/kg
V_{LG}	lipid content in the gut	calculated	(kg lipid)/(kg digesta wet weight)
V_{NB}	NLOM (Non Lipid Organic Matter) fraction of animals, NLOC (Non Lipid Organic Carbon) of plants	user defined	kg NLOM/ (kg organism wet weight)
V_{ND}	overall NLOM content of diet	user defined	kg/kg
V_{NG}	NLOM content in the gut	calculated	(kg NLOM)/(kg digesta wet weight)
V_{WB}	water content of the organism	user defined	kg water/ (kg organism wet weight)
V_{WD}	overall water content of diet	user defined	kg/kg
V_{WG}	water content in the gut	calculated	(kg water)/(kg digesta wet weight)
W_B	wet weight of the organism	user defined	kg
β	proportionality constant expressing the sorption capacity of NLOM to that of octanol	0.035 for animals	none
ε_L	dietary assimilation rate of lipids	fish: 92%; aquatic inverts: 75%; zooplankton: 72%	%
ε_N	dietary assimilation rate of NLOM	fish: 60%; aquatic inverts: 75%; zooplankton: 72%	%
ε_W	dietary assimilation rate of water	freshwater organisms: 25%	%
σ	efficiency of scavenging of particles absorbed from water	100	%

A.6.1. Parameters Affecting G_F

The fecal egestion rate G_F is calculated using the feeding rate of the organism (G_D; kg/day), the dietary assimilation rates for lipids, NLOM, and water (ε_L, ε_N and ε_W, respectively) as well as the contents of the diet (V_{LD}, $V_{ND,}$ and V_{WD}).

For non-filter feeders, the feeding rate (G_D) is calculated using body weight and temperature. Generally, as body weight and temperature increase, so does the feeding rate of the aquatic animal (Figure A.13). An order of magnitude increase in body weight leads to an order of magnitude increase in the feeding rate of the organism. An order of magnitude increase in temperature leads to a 40% increase in the feeding rate of non-filter feeders.

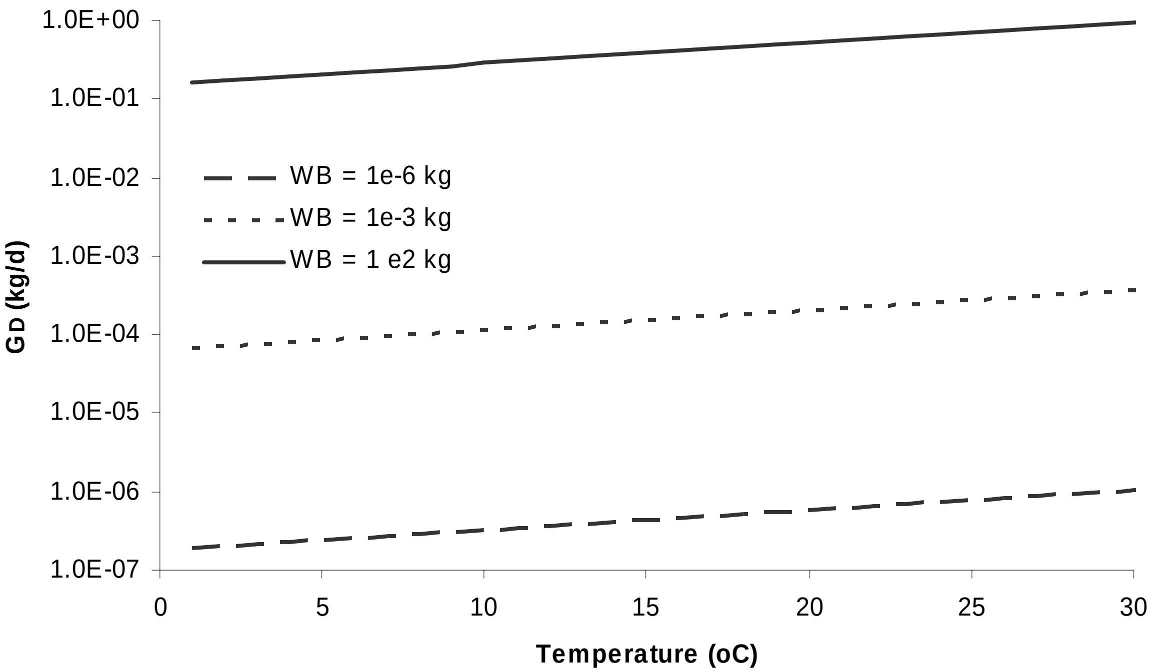

Figure A13. Relationship between temperature and G_D (non-filter feeders) with different W_B values.

For filter feeders, the feeding rate (G_D) is calculated using four parameters: the concentration of dissolved oxygen in the water (C_{OX}), body weight (W_B), the concentration of suspended solids (C_{SS}), and the scavenging efficiency of particles absorbed from water (σ). As with non-filter feeders, increases in body weight of filter feeders leads to increases in G_D (Figures A14-A16). An order of magnitude increase in body weight leads to an 80% increase in feeding rate (G_D). An increase in dissolved oxygen in the water (C_{OX}) from 2 to 10 mg/L results in a decrease in G_D of 80% (Figure A14). Decreases in scavenging efficiency lead to proportional decreases in G_D, with every 10% decrease in scavenging efficiency (σ), leading to a 10% decrease in G_D (Figure A15). An order of magnitude increase in the concentration of suspended solids (C_{SS}) leads to an order of magnitude increase in G_D (Figure A16).

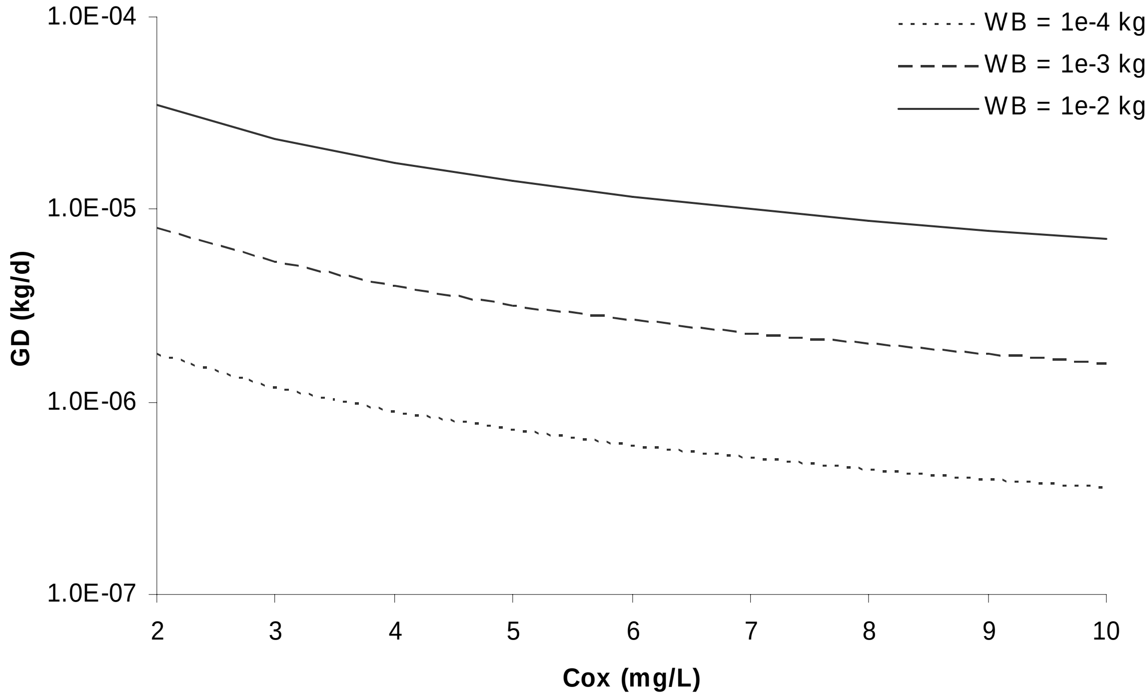

Figure A14. Relationship between Cox and G_D (filter feeders) with different W_B values.

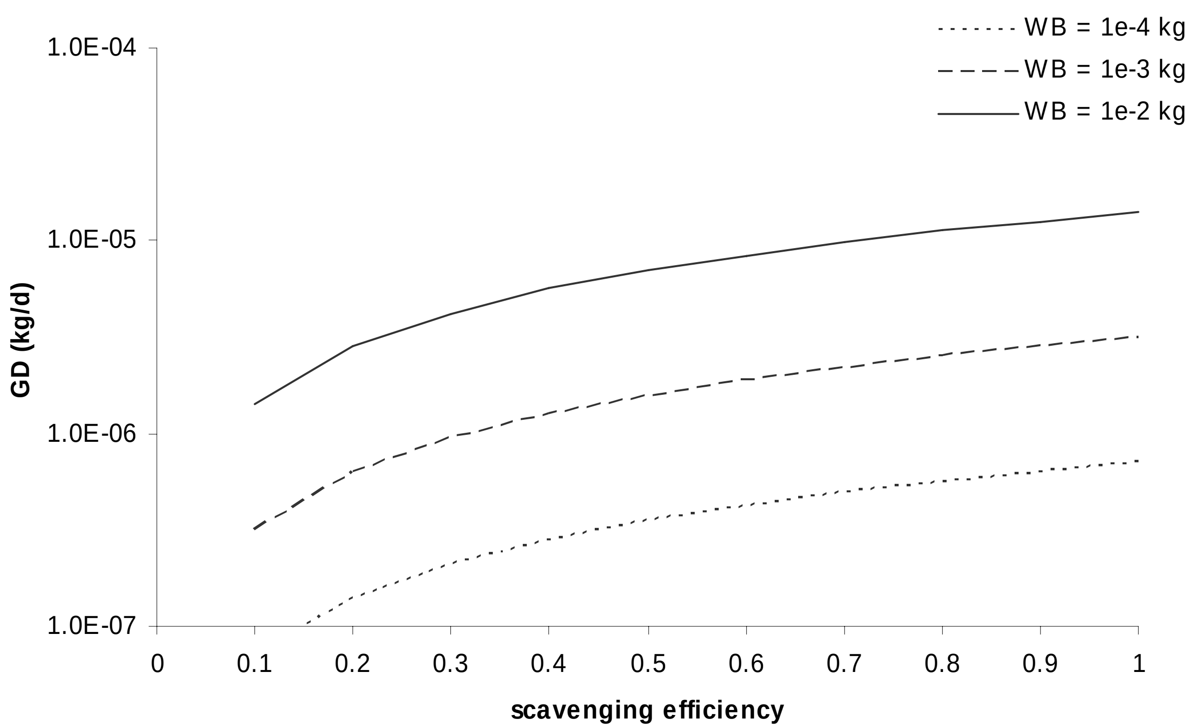

Figure A15. Relationship between scavenging efficiency and G_D (filter feeders) with different W_B values.

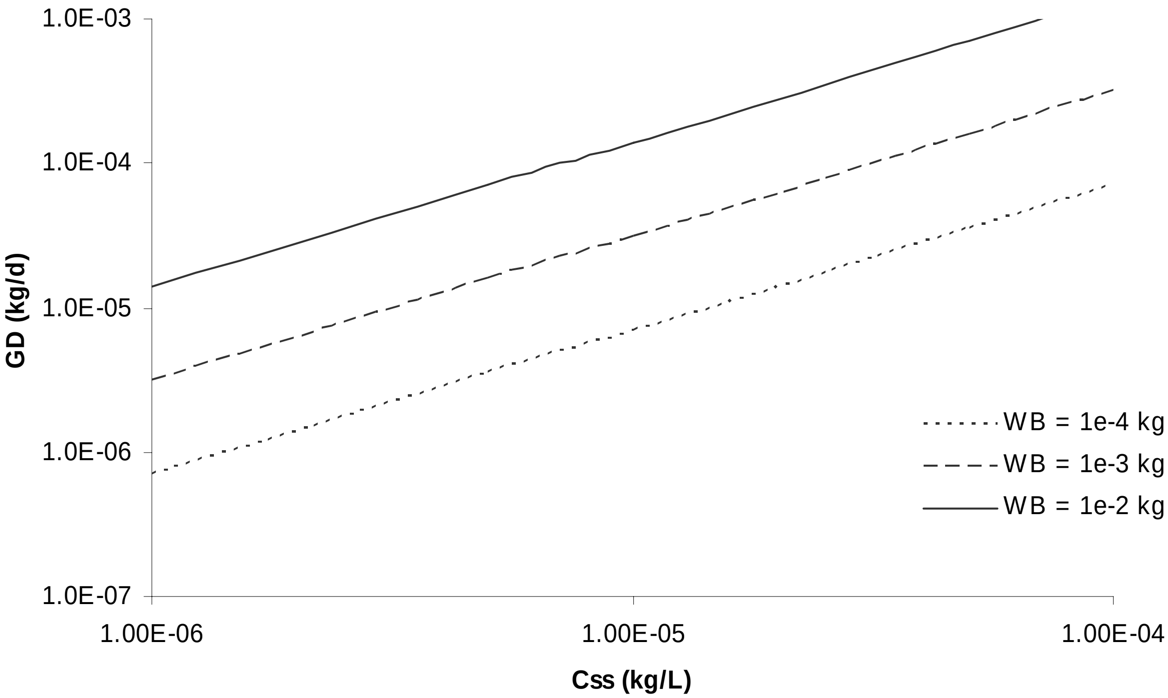

Figure A16. Relationship between concentration of suspended solids (Css) and G_D (filter feeders) with different W_B values.

The fecal egestion rate (G_F) is calculated using the following parameters: ε_L, ε_N, ε_W, V_{LD} , V_{ND}, V_{WD} as well as G_D, which is discussed above. When the default dietary assimilation rates for lipids, NLOM, and water (ε_L, ε_N, and ε_W, respectively) are used, changes in lipid, NLOM and water composition of the diet (V_{LD}, V_{ND} and V_{WD}, respectively) have little effect on G_F, when compared to effects of G_D on G_F (Figure A.17). This indicates that as the feeding rate of an animal (G_D) increases so does its fecal egestion rate (G_F), while the composition of the animal's diet has little effect on the fecal egestion rate.

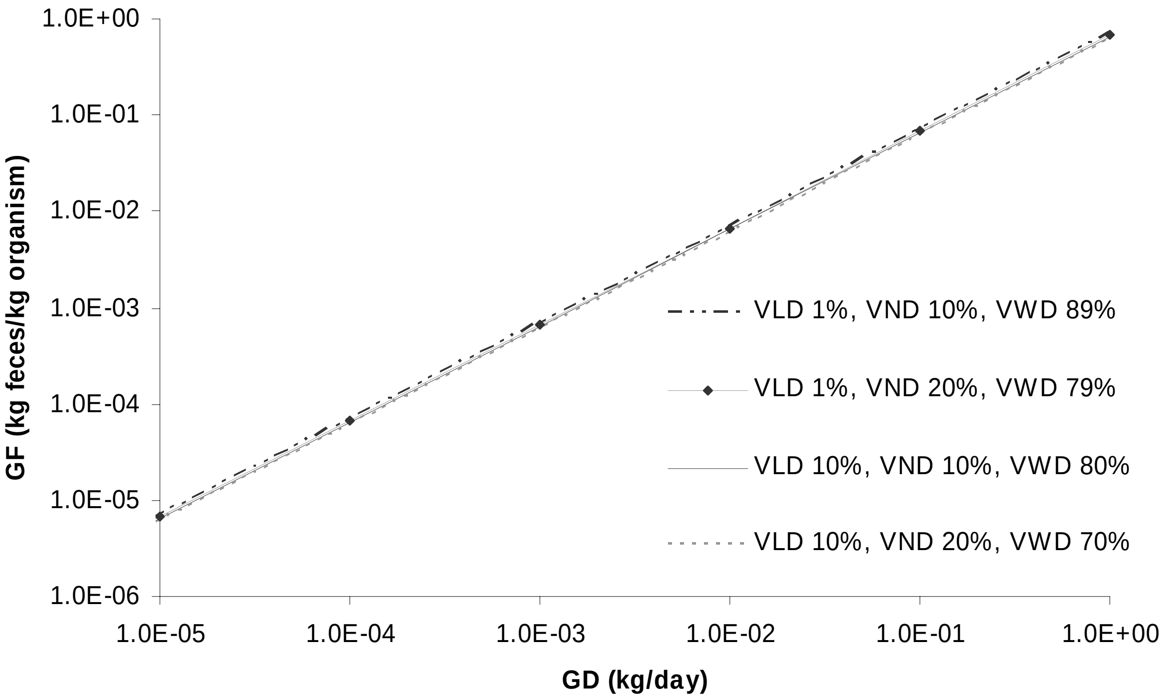

Figure A17. Relationship between G_D and G_F with different lipid, NLOM, and water compositions in the diet (V_{LD}, V_{ND}, and V_{WD}, respectively). Dietary assimilation rates for lipids, NLOM, and water are set to default values used to represent fish (see Table A9).

When setting the lipid, NLOM, and water composition (V_{LD}, V_{ND} and V_{WD}, respectively) of diet equal for fish, aquatic invertebrates, and zooplankton, the differences in dietary assimilation rates for lipids, NLOM, and water (ε_L, ε_N, and ε_W, respectively) of these three groups of animals have little effect on the fecal egestion rate (G_F), when compared to effects of the feeding rate (G_D) on G_F (Figure A.18). As with the composition of the diet, changes in G_D result in greater effects on G_F when compared to changes in the assimilation efficiencies of lipid, NLOM, and water.

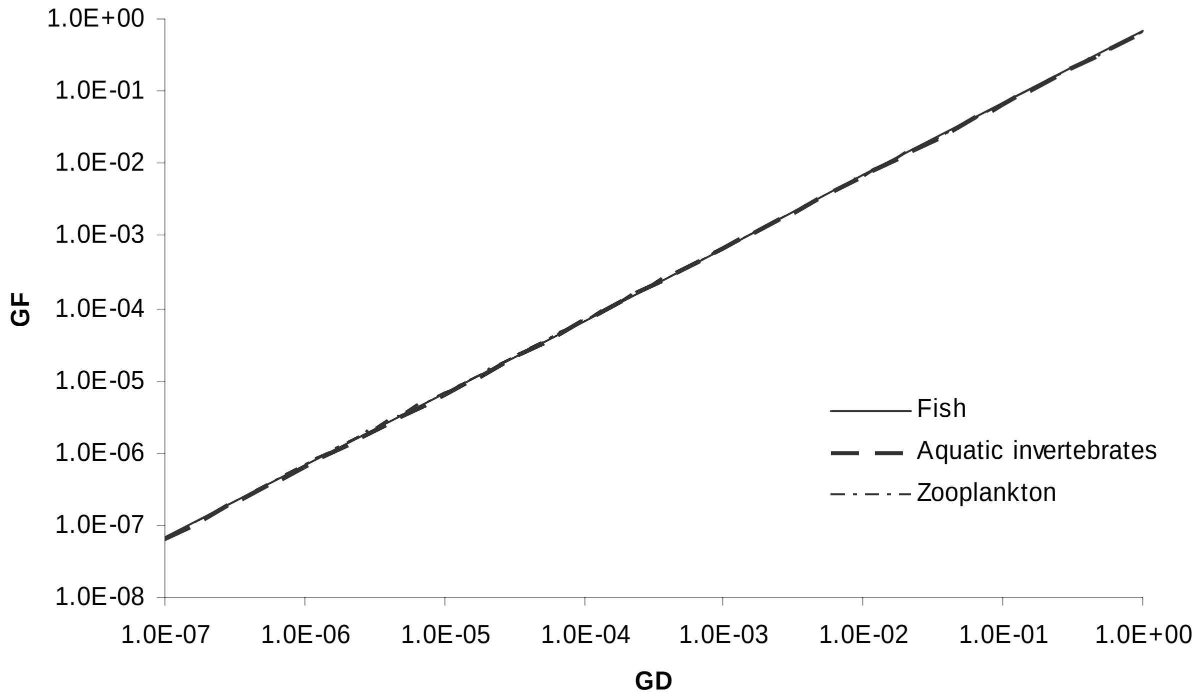

Figure A18. Relationship between G_D and G_F with dietary assimilation rates for lipids, NLOM, and water set to default values for fish, aquatic invertebrates, and zooplankton (see Table A9). Lipid, NLOM, and water compositions in the diet (V_{LD}, V_{ND}, and V_{WD}, respectively) are set to 1, 20, and 79%, respectively.

When $V_{LD,}$ $V_{ND,}$ V_{WD} are equal (*i.e.,* 33.33%) and when G_D is set to a constant number, variations of ε_L, $\varepsilon_{N,}$ and ε_W result in equivalent effects to G_F, with G_F decreasing as assimilation efficiency increases (*i.e.,* the organism eliminates less as its digestion [assimilation efficiency] becomes more efficient). If assimilation efficiency is set to 1 for lipid, NLOM, and water, the fecal elimination rate of the organism is 0 kg feces/kg org (Figure A.19).

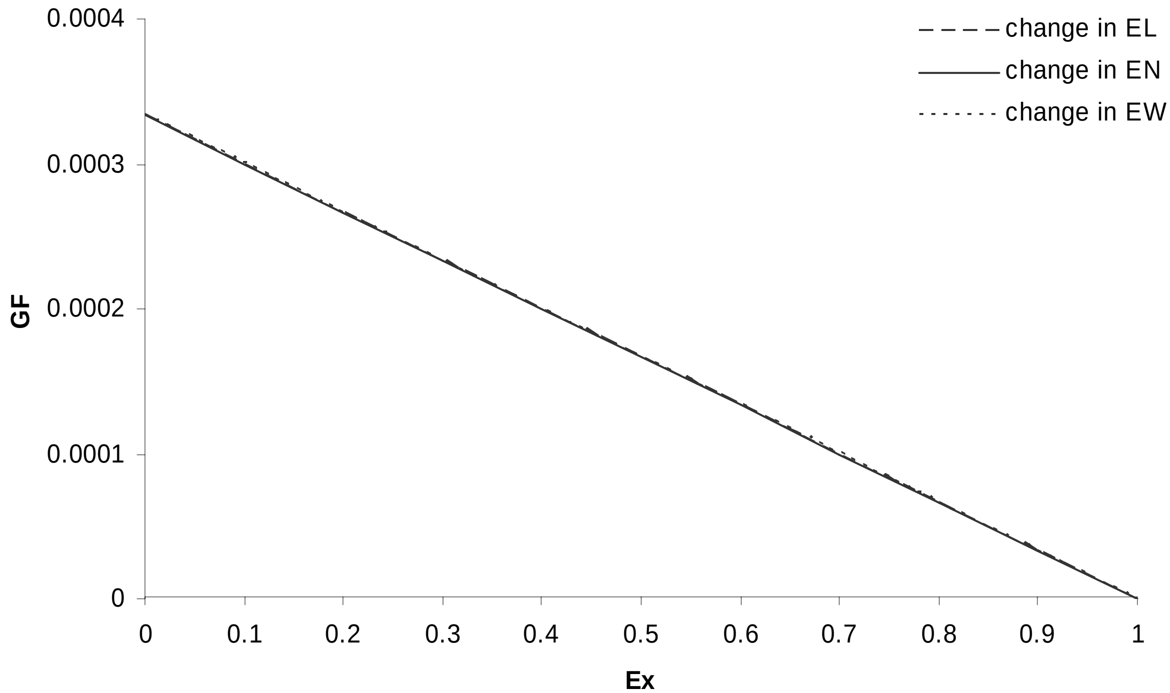

Figure A19. Relationship between dietary assimilation efficiencies (ε_L, ε_N, and ε_W) and G_F (V_{LD}=V_{ND}=V_{WD}=33.33%; G_D = 1.0x10^{-3} kg/day). Each dietary efficiency rate was altered independent of the others, with the others set to 1.

In summary, changes in the feeding rate of the organism (G_D) have the greatest effect on the fecal egestion rate of the organism (G_F). G_D is calculated for non-filter feeders using body weight and temperature. G_D is calculated for filter feeders, using the concentration of dissolved oxygen in the water (C_{OX}), body weight (W_B), the concentration of suspended solids (C_{SS}), and the efficiency of scavenging of particles absorbed from water (σ). Changes in these parameter values would be expected to have the greatest influence on G_F, which would result in influences on rate constant for pesticide elimination through excretion (k_E). Changes in the composition of the diet and the dietary assimilation rates are expected to have less of an influence on G_F when compared to G_D and the parameters used to derive G_D.

A.6.2. Parameters Affecting E_D

The efficiency of dietary pesticide transfer (E_D) is based only upon the K_{OW} of the pesticide. As K_{OW} increases, E_D decreases. For chemicals with Log K_{OW} 4-8, the efficiency of dietary pesticide transfer is 50-3% (Figure A.20).

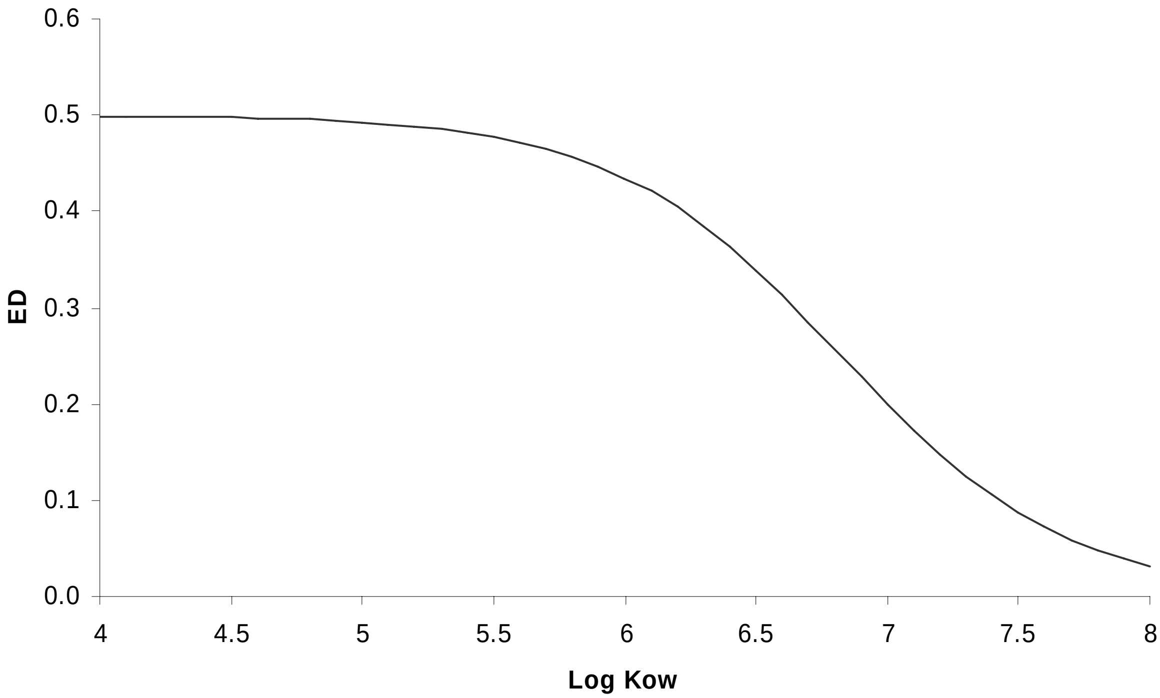

Figure A.20. Dietary transfer efficiency (E_D) vs. Log Kow.

A.6.3. Parameters Affecting K_{GB}

The equations used to calculate the contents of the gut (*i.e.,* $V_{LG,}$ $V_{NG,}$ and V_{WG}) listed in Table A.9 can be simplified as follows, using the equation for G_F:

$$V_{LG} = \frac{(1-\varepsilon_L)*V_{LD}*G_D}{G_F}$$

$$V_{NG} = \frac{(1-\varepsilon_N)*V_{ND}*G_D}{G_F}$$

$$V_{WG} = \frac{(1-\varepsilon_W)*V_{WD}*G_D}{G_F}$$

Using these simplified equations, changes in the feeding rate of the organism (G_D), the fecal egestion rate (G_F), diet composition, and dietary assimilation of lipid, NLOM, and water can be explored to understand effects on these parameters on estimations of the lipid composition of the gut. If ε_L, ε_N, and ε_W are all equal and V_{LD}, $V_{ND,}$ and V_{WD} are all equal, V_{LG}, $V_{NG,}$ and V_{WG} are equal. Changes in feeding rate (G_D) and fecal egestion rate (G_F) do not affect V_{LG}, V_{NG} or V_{WG} (Figure A.21). As would be expected, changes in V_{LD} result in effects to V_{LG}, with an order of magnitude increase in $V_{LD,}$ resulting in an order of magnitude increase in V_{LG} (Figure A.22). Also, changes in V_{ND} result in effects to V_{NG}, with an increase in V_{ND} from 10 to 20%, resulting in a 50% increase in V_{NG} (Figure A.23). An order of magnitude increase in V_{WD} (keeping V_{LD} and V_{ND} constant) results in slight (approximately 10%) decreases in V_{LG} and V_{NG} and slight (2%) increases in V_{WG} (Figure A.24). A decrease in ε_L from 0.9 to 0.1, results in an order of magnitude increase in the lipid content of the gut (V_{LG}) (Figure A.25), but only slight (<2%) changes to the NLOM and water contents of the gut (V_{NG} and V_{WG}, respectively). A decrease in ε_N from 0.9 to 0.1 results in an order of magnitude increase in the NLOM content of the gut (V_{NG}) (Figure A.26), as well as decreases in the gut composition attributed to lipid and water. A decrease in ε_W from 0.9 to 0.1 results in a 50% increase in the water content of the gut (V_{WG}), as well as an 80% decrease in the gut composition attributed to lipid and NLOM (Figure A.27). For invertebrates, dietary assimilation efficiencies vary significantly, leading to uncertainty in assigning one value to this parameter. Since hydrophobic chemicals are not likely to be stored in the water of organism tissues, it is assumed that this route is not significant to bioaccumulation.

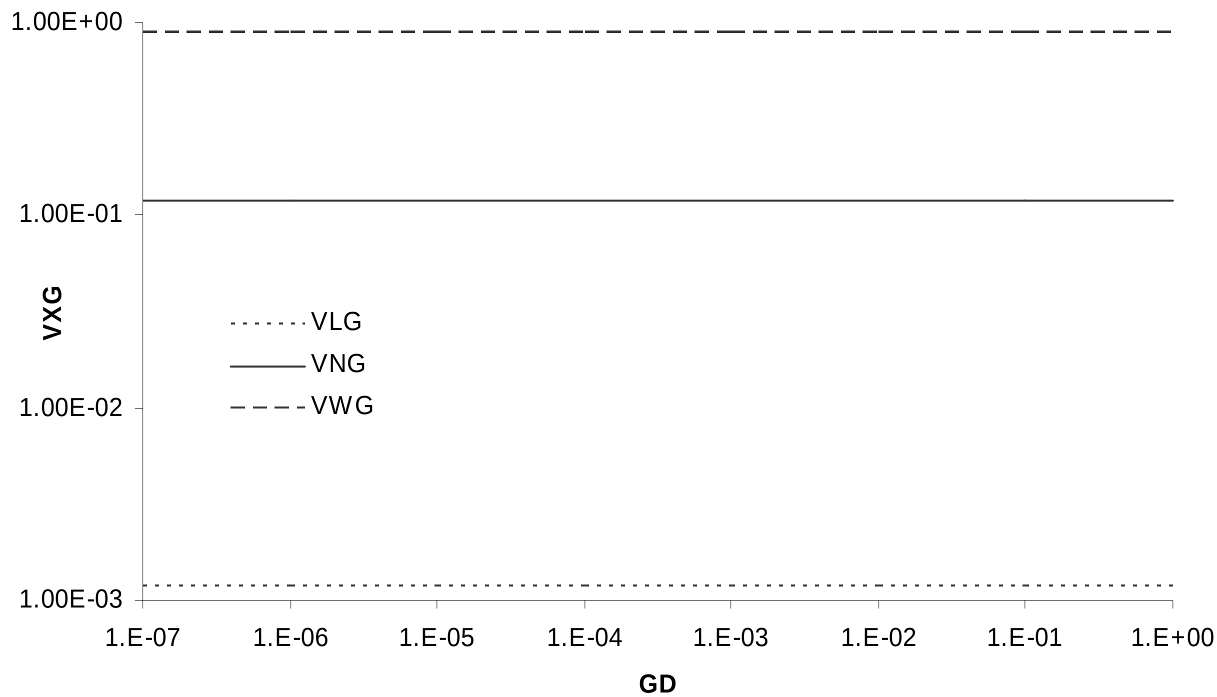

Figure A21. Relationship between gut contents (V_{LG}, V_{NG}, and V_{WG}) and G_D. ε_L, ε_N, and ε_W are set to defaults for fish (Table A9). V_{LD} = 1%, V_{ND} = 20%, and V_{WD} = 79%.

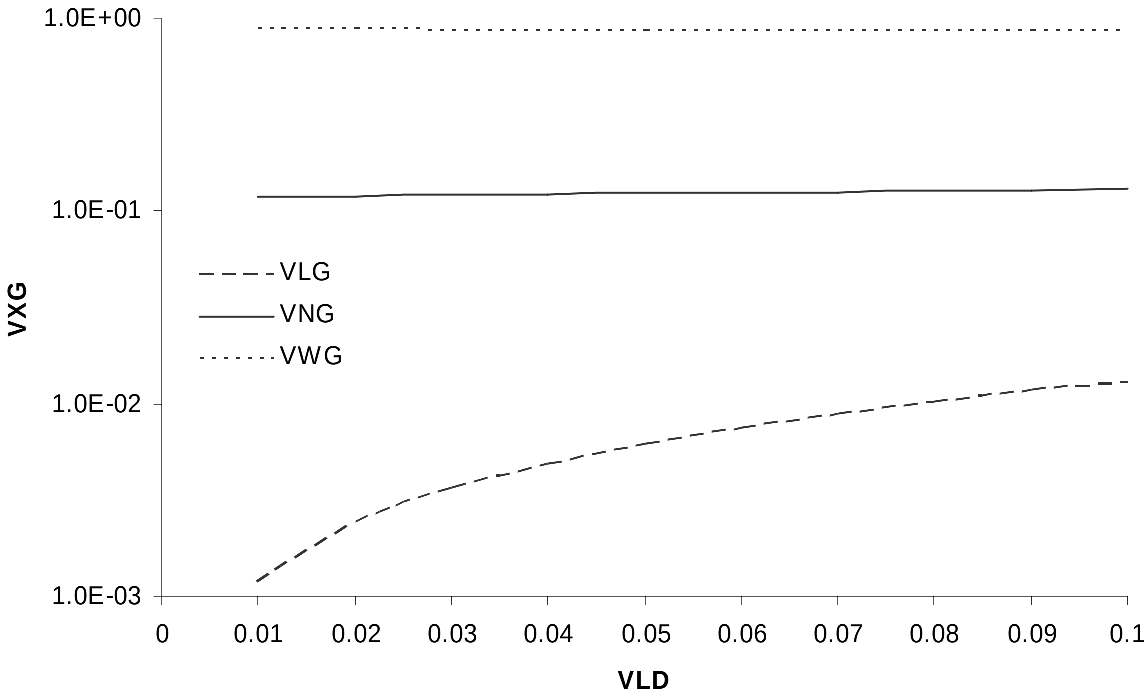

Figure A22. Relationship between gut contents (V_{LG}, V_{NG}, and V_{WG}) and V_{LD}. ε_L, ε_N, and ε_W are set to defaults for fish (Table A9). V_{ND} = 20%, $V_{WD} = 1-V_{ND}-V_{LD}$.

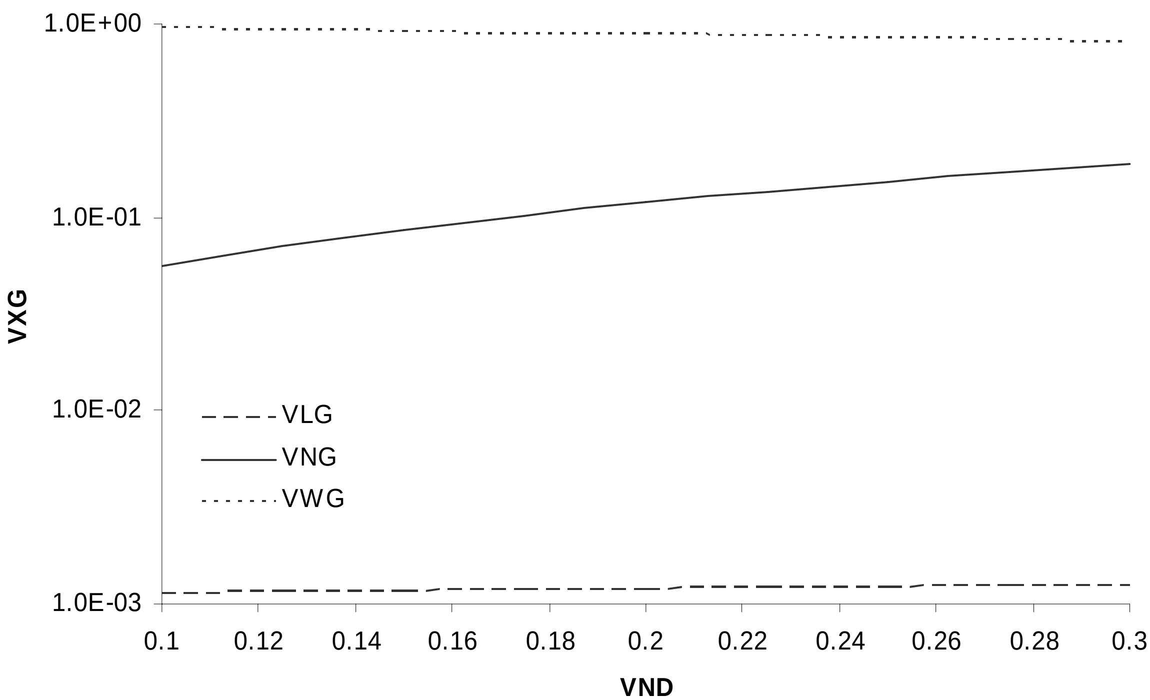

Figure A23. Relationship between gut contents (V_{LG}, V_{NG}, and V_{WG}) and V_{ND}. ε_L, ε_N, and ε_W are set to defaults for fish (Table A9). V_{LD} = 1%, $V_{WD} = 1-V_{ND}-V_{LD}$.

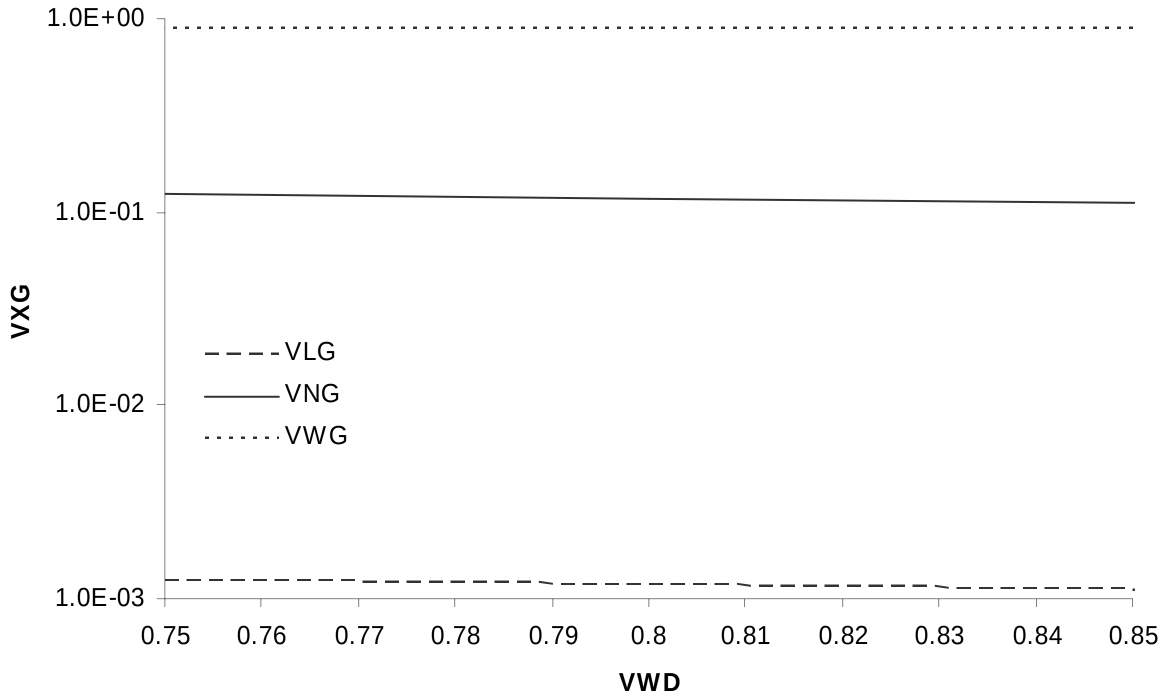

Figure A24. Relationship between gut contents (V_{LG}, V_{NG}, and V_{WG}) and V_{WD}. ε_L, ε_N, and ε_W are set to defaults for fish (Table A9). V_{LD} = 1%, V_{ND} = 20%. Note that V_{LD}+V_{ND}+V_{WD} does not equal 100%, except when V_{WD} = 0.79.

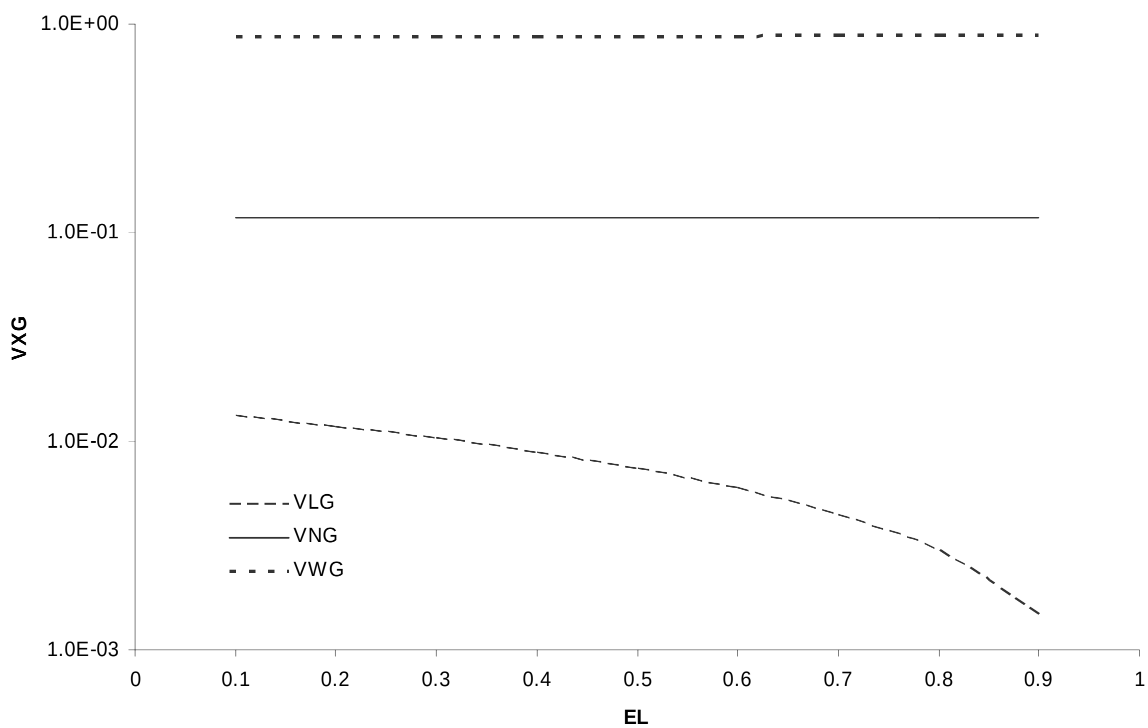

Figure A25. Relationship between gut contents (V_{LG}, V_{NG}, and V_{WG}) and ε_L. ε_N, and ε_W are set to defaults for fish (Table A9). V_{LD} = 1%, V_{ND} = 20%, V_{WD} = 79%.

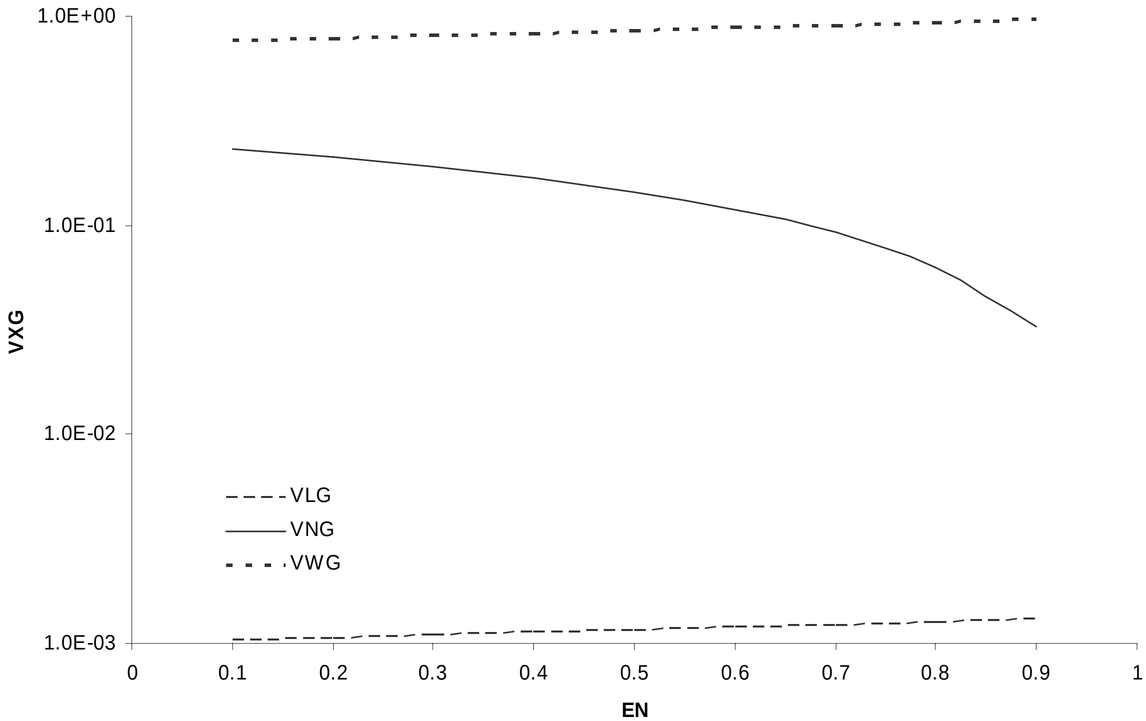

Figure A26. Relationship between gut contents (V_{LG}, V_{NG}, and V_{WG}) and ε_N. ε_L, and ε_W are set to defaults for fish (Table A9). V_{LD} = 1%, V_{ND} = 20%, V_{WD} = 79%.

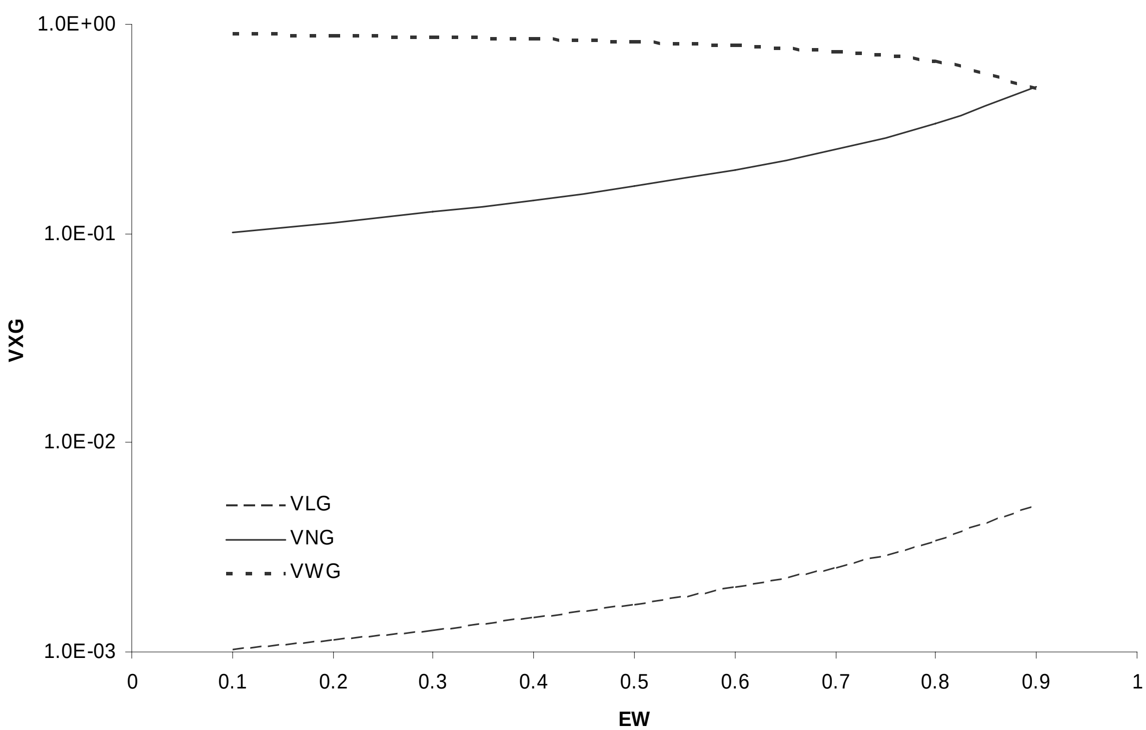

Figure A27. Relationship between gut contents (V_{LG}, V_{NG}, and V_{WG}) and ε_W. ε_L, and ε_N are set to defaults for fish (Table A9). V_{LD} = 1%, V_{ND} = 20%, V_{WD} = 79%.

The partitioning of a chemical between the gastrointestinal tract (GIT) and the organism is described by K_{GB}. This partition coefficient is determined using the contents of the gut (V_{LG}, $V_{NG,}$ and V_{WG}), the contents of the organism's body (V_{LB}, V_{NB} and V_{WB}) as well as the octanol water partition coefficient (K_{OW}) (Table A.9). An order of magnitude increase in the lipid content of the body (V_{LB}) results in an order of magnitude decrease in K_{GB} (Figures A.28 and A.29). An order of magnitude increase in the NLOM content of the body (V_{NB}) results in a decrease in K_{GB} of approximately 20%. An order of magnitude increase in the lipid content of the gut (V_{LG}) results in a 50% increase in K_{GB} (Figure A.28). An order of magnitude increase in the NLOM content of the gut (V_{NG}), results in an increase in K_{GB} of 70% (Figure A.29). Changes in the Log K_{OW} of a chemical from 4 to 8 do not alter K_{GB}.

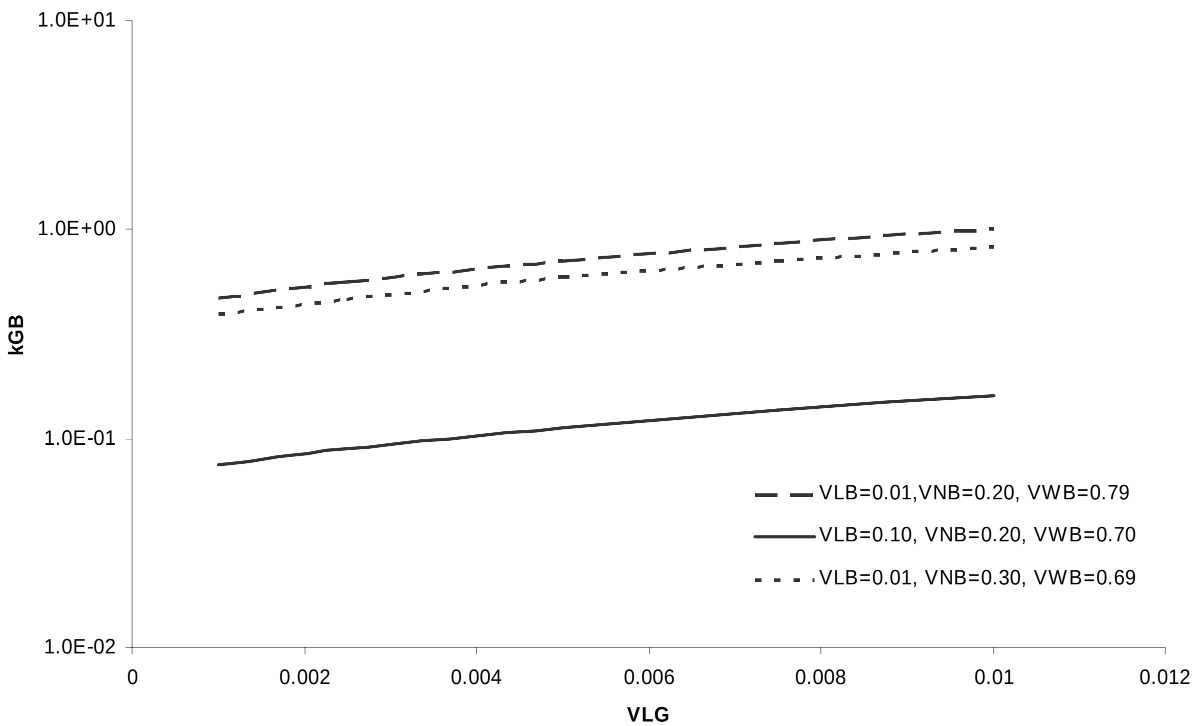

Figure A28. Relationship between lipid content of the gut (V_{LG}) and K_{GB}, with different body compositions (V_{LB}, V_{NB}, and V_{WB}).

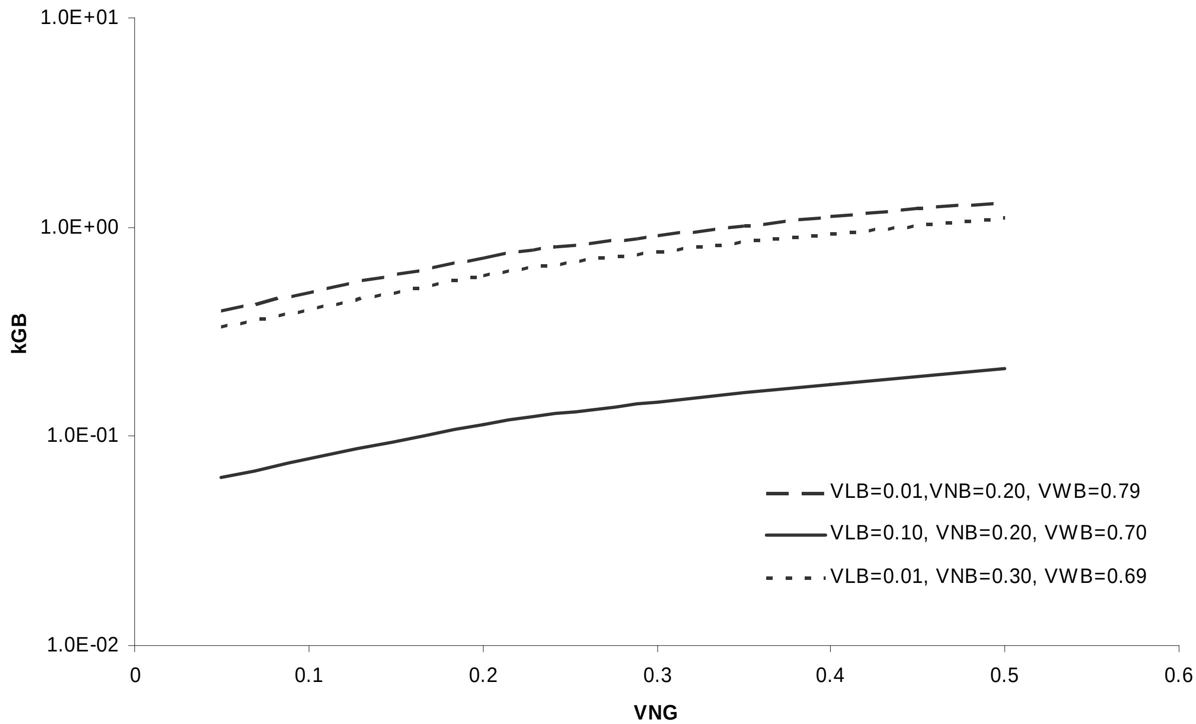

Figure A29. Relationship between NLOM content of the gut (V_{NG}) and K_{GB}, with different body compositions (V_{LB}, V_{NB}, and V_{WB}).

A.7. Overall Sensitivity of Body Concentration of Chemical (C_B) to Individual Input Parameters

A.7.1. First Sensitivity Analysis

In order to understand the influence of input parameters on model predictions of pesticide concentrations in tissue of aquatic organisms (C_B), a sensitivity analysis was conducted. Parameters were assigned uniform distributions and assumptions of ranges based on data in the scientific literature. The range for each parameter is defined in Table A10. Diets of each trophic level were varied according to the definitions in Table A11. Uniform distributions were used to allow unbiased selection of values from set ranges. Once parameter assumptions were assigned, a Monte Carlo simulation was carried out using Crystal Ball 2000. In this simulation, 10,000 trials were conducted with randomly selected parameter values resulting in predicted pesticide concentrations in each of the seven trophic levels. The sensitivity of the model to specific parameters was defined by the contribution of each parameter to the variance of the estimation of pesticide concentrations in each of the trophic levels.

The results of this analysis indicate that of all the variables in the model, the Log K_{OW} contributes the most to variability (<75% of total) in estimates of C_B for all animal trophic levels. For phytoplankton, the water column EEC, concentration of POC in the water column (X_{POC})

and Log K_{OW} contribute the greatest variability in the predicted C_B values (38, 28, and 22%, respectively).

A.7.2. Second Sensitivity Analysis

Based on the results of the first sensitivity analysis, a second analysis was conducted where the influence of individual parameters on variability in C_B was examined, with fixed Log K_{OW} values. In the second sensitivity analysis, the Log K_{OW} was set to values of 4, 5, 6, 7, and 8 and a Monte Carlo simulation (10,000 trials) was run for each Log K_{OW} value. Parameters were assigned uniform distributions and assumptions of ranges based on data in the scientific literature. The range for each parameter is defined in Table A10 (with the exception of Log K_{OW}). Diets of each trophic level were varied according to the definitions in Table A11.

The contributions of individual parameters at Log K_{OW} values of 4, 5, 6, 7 and 8 to the variability in the pesticide tissue concentration (C_B) of the seven aquatic trophic levels of KABAM are provided in Tables A12-A18. The results of this sensitivity analysis indicate that parameters have different relative importance in estimating C_B for the seven trophic levels (*e.g.,* the water column EEC contributes the most variability to the phytoplankton C_B, while the pore water EEC and fraction of respiratory ventilation that involves pore-water of sediment (m_P) value contribute the most variance to the zooplankton C_B). In addition, these tables indicate that the relative importance of individual parameters to estimates of C_B change with Log K_{OW}. It should be noted that several parameters in the Arnot and Gobas (2004) model are linked (*e.g.*, m_P and m_O, diet composition, V_{LB}, V_{NB}, and V_{WB}). Therefore, sensitivity of C_B predictions to one parameter implies sensitivity of the predictions to the linked parameters.

This sensitivity analysis also indicates that some parameters that are fixed in KABAM, including the constant related to the resistance to pesticide uptake through the aqueous phase of plant (A), proportionality constant expressing the sorption capacity of NLOM to that of octanol (β), and m_P (set to either 0 or 0.05), can contribute >10% of total variability in estimates of C_B.

Table A10. Parameters and associated assumptions used for first and second sensitivity analysis of KABAM.					
Para-meter	**Parameter Description**	**Trophic Level**	**Minimum of Range**	**Maximum of Range**	**Source/Comments**
A	Constant related to the resistance to pesticide uptake through the aqueous phase of plant	Phytoplankton	$1x10^{-5}$	$1x10^{-4}$	In Arnot and Gobas 2004, this value is set to a constant of $6.0x10^{-5}$ days. This value was varied by an order of magnitude around the reported constant value to understand the influence of this parameter on estimates of bioaccumulation. The reasonable range of values for this parameter is unknown.
B	Constant related to the resistance to pesticide uptake through the organic phase of plant	Phytoplankton	1	10	In Arnot and Gobas 2004, this value is set to a constant of 5.5 days. This value was varied by an order of magnitude around the reported constant value to understand the influence of this parameter on estimates of bioaccumulation. The reasonable range of values for this parameter is unknown.
C_{OX}	Concentration of dissolved oxygen (mg O_2/L)	All	4	12	Minimum is based on 60% of saturation of water with 6 mg/L as saturation (in 30°C water). Maximum is based on solubility limit of oxygen in cold water (5°C; see USGS 2008a).
C_{SS}	Concentration of suspended solids (kg/L)	All	$2.0x10^{-6}$	$5.0x10^{-4}$	Based on 5th and 95th percentiles of approximately 38,000 measurements of suspended sediment concentrations in surface waters of the US provided by NAWQA (USGS 2008b).
C_{WTO}	Total pesticide concentration in water column above the sediment	All	0.1	100	Assumed to be reasonable range for EECs expected from PRZM/EXAMS modeling.
C_{WTP}	Freely dissolved pesticide concentration in pore water of sediment	All	0.1	100	Assumed to be reasonable range for EECs expected from PRZM/EXAMS modeling.
Log Kow	Log of octanol-water partition coefficient	All	4	8	Assumption that bioaccumulation model can be used for chemicals with Log Kow 4-8.
Koc	Organic carbon partition coefficient	All	$3.5x10^3$	$3.5 x10^7$	Determined based on assumption that Koc can be estimated as 0.35*Kow. In sensitivity analysis, Koc is linked directly to K_{OW} in order to avoid error in selection of inconsistent values for these parameters.
m_p	Fraction of respiratory ventilation that involves pore-water of sediment	Zooplankton	0	1	Based on full range of parameter values.
		Benthic Inv.	0	1	Based on full range of parameter values.
		Filter Feeders	0	1	Based on full range of parameter values.
		Small Fish	0	1	Based on full range of parameter values.
		Medium Fish	0	1	Based on full range of parameter values.
		Large Fish	0	1	Based on full range of parameter values.
OC	Percent organic carbon in sediment	All	1%	10%	In the OPP standard pond used in EXAMS, the default value for this parameter is 4%. This parameter value is varied by 1 order of

Table A10. Parameters and associated assumptions used for first and second sensitivity analysis of KABAM.					
Para-meter	**Parameter Description**	**Trophic Level**	**Minimum of Range**	**Maximum of Range**	**Source/Comments**
					magnitude around the OPP standard pond value.
T	Temperature (^{o}C)	All	1	30	Reasonable range of values for this parameter in the environment.
V_{LB}	Lipid fraction of organism	Phytoplankton	0.5	2.0	See Table C1 of Appendix C.
		Zooplankton	1.0	4.0	See Table C2 of Appendix C.
		Benthic Inv.	0.5	12	See Tables C4-C9 of Appendix C.
		Filter Feeders	0.4	4	See Tables C13-C15 of Appendix C.
		Fish	0.5	8	See Table C19 of Appendix C.
V_{NB}	NLOM (Non Lipid Organic Matter) fraction of animals, NLOC (Non Lipid Organic Carbon) of plants	All	-	-	Set to equal 1-V_{LB}-V_{WB}
V_{WB}	Water content of the organism	Phytoplankton	0.85	0.95	Assume 5% deviation from mean (*i.e.*, 90%).
		Zooplankton	0.74	0.96	See Section C.2. of Appendix C.
		Benthic Inv.	0.69	0.83	See Table C3 of Appendix C.
		Filter Feeders	0.78	0.93	See Table C12 of Appendix C.
		Fish	0.71	0.80	See Table C18 of Appendix C.
W_B	Wet weight (kg) of the organism	Phytoplankton	-	-	Not a necessary parameter for phytoplankton.
		Zooplankton	$1x10^{-9}$	$1x10^{-7}$	See Section C.2. of Appendix C.
		Benthic Inv.	$5x10^{-6}$	$2x10^{-3}$	See Table C11 of Appendix C.
		Filter Feeders	$2x10^{-4}$	$1x10^{-2}$	See Section C.5 of Appendix C.
		Small Fish	$1x10^{-3}$	$5x10^{-2}$	See Table C16 of Appendix C.
		Medium Fish	$5x10^{-3}$	0.6	See Table C17 of Appendix C.
		Large Fish	0.25	3.6	See Section C.5 of Appendix C.
X_{POC}	Concentration of particulate organic carbon in water (kg/L)	All	$2.0x10^{-6}$	$5.0x10^{-4}$	Based on 5th and 95th percentiles of approximately 38,000 measurements of suspended sediment concentrations in surface waters of the US provided by NAWQA (USGS 2008b).
X_{DOC}	Concentration of dissolved organic carbon in water (kg/L)	All	$5.0x10^{-7}$	$5.0x10^{-5}$	In the OPP standard pond used in EXAMS, the default value for this parameter is $5.0x10^{-6}$. This parameter value is varied by 2 orders of magnitude around the OPP standard pond value.
β	Proportionality constant expressing the sorption capacity of NLOM or NLOC to that of octanol	All	0	1	Designed to represent all values equal to or less than the partitioning of a chemical between octanol and water.

Table A10. Parameters and associated assumptions used for first and second sensitivity analysis of KABAM.					
Para-meter	**Parameter Description**	**Trophic Level**	**Minimum of Range**	**Maximum of Range**	**Source/Comments**
ε_L	Dietary assimilation rate of lipids	Animals	0	1	Based on full range of parameter values.
ε_N	Dietary assimilation rate of NLOM	Animals	0	1	Based on full range of parameter values.
ε_W	Dietary assimilation rate of water	Animals	0	1	Based on full range of parameter values.
σ	Efficiency of scavenging of particles absorbed from water	Filter Feeders	0	1	Based on full range of parameter values.

Table A11. Dietary assumptions of aquatic trophic levels used for sensitivity analysis of KABAM.				
Trophic Level	**Organism in diet**	**Minimum Value**	**Maximum Value**	**Comments**
Zooplankton	Phytoplankton	100%	100%	-
Benthic Invertebrates	Sediment	0	50%	-
	Phytoplankton	0	50%	-
	Zooplankton	-	-	Set to 1- (% diet attributed to sediment + % diet attributed to phytoplankton)
Filter Feeder	Sediment	0	33%	-
	Phytoplankton	0	33%	-
	Zooplankton	0	33%	-
	Benthic invertebrates	-	-	Set to 1- (% diet attributed to sediment + % diet attributed to phytoplankton+% diet attributed to zooplankton)
Small Fish	Phytoplankton	0	50%	-
	Zooplankton	0	50%	-
	Benthic invertebrates	-	-	Set to 1- (% diet attributed to phytoplankton+% diet attributed to zooplankton)
Medium Fish	Zooplankton	0	50%	-
	Benthic invertebrates	0	50%	-
	Small fish	-	-	Set to 1- (% diet attributed to zooplankton + % diet attributed to benthic invertebrates)
Large Fish	Small fish	0	100%	It is assumed that large fish consume only smaller fish
	Medium Fish	-	-	Set to 1- (% diet attributed to small fish)

Table A12. Second sensitivity analysis results: Contribution to variance of specific variables to C_B values of phytoplankton at different Log Kow values.					
Variable	**4**	**5**	**6**	**7**	**8**
A	≤0.1%	≤0.1%	0.7%	9.3%	18.2%
V_{LB}	≤0.1%	≤0.1%	≤0.1%	0.2%	≤0.1%
V_{WB}	5.9%	3.4%	2.3%	0.2%	≤0.1%
Water Column EEC	59.6%	46.1%	44.9%	45.7%	43.0%
X_{POC}	7.0%	30.9%	39.1%	41.7%	38.0%
β	26.7%	18.6%	12.0%	2.1%	≤0.1%
Total	99.2%	99.0%	99.0%	99.2%	99.2%

Table A13. Second sensitivity analysis results: Contribution to variance of specific variables to C_B values of zooplankton at different Log Kow values.					
Variable	**4**	**5**	**6**	**7**	**8**
C_{OX}	≤0.1%	≤0.1%	0.2%	2.5%	4.3%
m_P	4.3%	23.0%	37.4%	39.5%	36.1%
Pore Water EEC	27.6%	37.2%	40.8%	40.6%	37.4%
T	≤0.1%	≤0.1%	1.3%	7.7%	19.6%
V_{LB}	1.2%	0.4%	0.6%	0.6%	≤0.1%
V_{WB}	20.8%	14.1%	8.8%	0.6%	0.8%
Water Column EEC	11.2%	2.2%	0.3%	≤0.1%	≤0.1%
W_B	≤0.1%	≤0.1%	≤0.1%	0.5%	0.6%
X_{POC}	1.7%	2.5%	0.8%	≤0.1%	≤0.1%
β	32.5%	20.2%	8.4%	1.7%	≤0.1%
ε_L	≤0.1%	≤0.1%	≤0.1%	0.2%	≤0.1%
ε_N	≤0.1%	≤0.1%	0.5%	1.1%	0.3%
Total	99.3%	99.6%	99.1%	95.0%	99.1%

Table A14. Second sensitivity analysis results: Contribution to variance of specific variables to C_B values of benthic invertebrates at different Log Kow values.					
Variable	**4**	**5**	**6**	**7**	**8**
Characteristics of prey*	≤0.1%	1.2%	12.0%	12.0%	6.0%
C_{OX}	≤0.1%	≤0.1%	≤0.1%	1.3%	1.6%
Diet composition	≤0.1%	0.2%	1.2%	1.0%	8.6%
m_P	4.9%	16.0%	5.3%	≤0.1%	≤0.1%
OC	≤0.1%	≤0.1%	0.9%	≤0.1%	≤0.1%
Pore Water EEC	37.2%	51.1%	61.4%	61.1%	59.4%
T	≤0.1%	≤0.1%	1.0%	8.2%	16.1%
V_{LB}	4.0%	2.5%	1.6%	1.0%	≤0.1%
V_{WB}	3.6%	1.5%	1.1%	0.6%	≤0.1%
Water Column EEC	14.4%	1.9%	≤0.1%	≤0.1%	≤0.1%
X_{POC}	2.5%	2.7%	0.5%	≤0.1%	≤0.1%
β	32.6%	21.5%	7.6%	0.4%	≤0.1%
ε_L	≤0.1%	≤0.1%	0.7%	1.2%	≤0.1%
ε_N	≤0.1%	0.5%	5.8%	5.6%	≤0.1%
Total	99.2%	99.1%	99.1%	92.4%	91.7%

*m_P, body composition, etc.

Table A15. Second sensitivity analysis results: Contribution to variance of specific variables to C_B values of filter feeders at different Log Kow values.					
Variable	**4**	**5**	**6**	**7**	**8**
Characteristics of prey*	≤0.1%	1.5%	11.8%	11.7%	2.5%
C_{OX}	≤0.1%	≤0.1%	≤0.1%	2.0%	3.8%
C_{SS}	0.2%	1.4%	2.4%	3.2%	8.1%
Diet composition	≤0.1%	≤0.1%	0.3%	0.6%	1.6%
m_P	3.1%	6.9%	≤0.1%	0.5%	0.7%
OC	≤0.1%	≤0.1%	0.9%	2.0%	4.1%
Pore Water EEC	28.6%	42.0%	52.2%	50.5%	42.3%
T	≤0.1%	≤0.1%	1.9%	13.0%	25.1%
V_{LB}	1.5%	1.5%	1.3%	0.4%	≤0.1%
V_{WB}	11.1%	7.0%	4.3%	2.8%	0.4%
Water Column EEC	10.6%	1.8%	≤0.1%	≤0.1%	≤0.1%
W_B	≤0.1%	≤0.1%	≤0.1%	≤0.1%	0.3%
X_{POC}	2.0%	2.2%	0.2%	≤0.1%	≤0.1%
β	42.0%	30.7%	13.7%	1.5%	≤0.1%
ε_L	≤0.1%	0.4%	2.6%	2.7%	0.5%
ε_N	≤0.1%	1.8%	5.3%	4.6%	1.2%
σ	≤0.1%	1.9%	2.1%	3.5%	7.8%
Total	99.1%	99.1%	99.0%	99.0%	98.4%

*m_P, body composition, etc.

Table A16. Second sensitivity analysis results: Contribution to variance of specific variables to C_B values of small fish at different Log Kow values.					
Variable	**4**	**5**	**6**	**7**	**8**
Characteristics of prey*	≤0.1%	3.3%	16.1%	18.2%	9.2%
C_{OX}	0.2%	0.2%	≤0.1%	1.3%	2.3%
Diet composition	≤0.1%	0.6%	2.2%	2.9%	2.7%
m_P	3.9%	4.4%	0.5%	≤0.1%	0.6%
OC	≤0.1%	≤0.1%	0.5%	1.5%	2.6%
Pore Water EEC	31.8%	45.3%	52.1%	53.0%	51.6%
T	≤0.1%	0.4%	0.8%	9.8%	27.7%
V_{LB}	2.5%	1.3%	1.3%	0.8%	0.3%
V_{WB}	1.5%	1.0%	0.3%	0.2%	≤0.1%
Water Column EEC	11.6%	1.5%	0.2%	≤0.1%	≤0.1%
X_{POC}	2.0%	2.6%	0.5%	≤0.1%	≤0.1%
β	45.7%	34.3%	13.8%	1.7%	0.2%
ε_L	≤0.1%	1.2%	4.4%	3.4%	0.9%
ε_N	≤0.1%	2.9%	6.8%	6.1%	0.8%
Total	99.2%	99.0%	99.5%	98.9%	98.9%

*m_P, body composition, etc.

Table A17. Second sensitivity analysis results: Contribution to variance of specific variables to C_B values of medium fish at different Log Kow values.					
Variable	**4**	**5**	**6**	**7**	**8**
Characteristics of prey*	≤0.1%	2.7%	17.3%	21.0%	10.0%
C_{OX}	0.3%	≤0.1%	≤0.1%	1.1%	2.4%
Diet composition	≤0.1%	0.2%	0.8%	0.6%	≤0.1%
m_P	1.5%	1.5%	≤0.1%	≤0.1%	0.2%
OC	≤0.1%	≤0.1%	0.4%	1.3%	1.9%
Pore Water EEC	20.5%	33.1%	43.3%	48.5%	49.0%
T	0.2%	≤0.1%	1.0%	11.1%	33.1%
V_{LB}	0.4%	0.2%	0.2%	0.4%	≤0.1%
V_{WB}	15.7%	9.1%	5.0%	4.2%	0.5%
Water Column EEC	7.7%	1.1%	0.2%	≤0.1%	≤0.1%
W_B	≤0.1%	0.2%	≤0.1%	≤0.1%	≤0.1%
X_{POC}	1.2%	1.7%	0.5%	≤0.1%	≤0.1%
β	51.2%	43.5%	20.9%	4.3%	0.5%
ε_L	0.2%	1.4%	2.2%	1.9%	0.3%
ε_N	0.6%	3.4%	7.4%	4.7%	0.7%
Total	99.5%	98.1%	99.2%	99.1%	98.6%

*m_P, body composition, etc.

Table A18. Second sensitivity analysis results: Contribution to variance of specific variables to C_B values of large fish at different Log Kow values.					
Variable	**4**	**5**	**6**	**7**	**8**
Characteristics of prey*	≤0.1%	5.8%	22.8%	23.1%	9.7%
C_{OX}	0.9%	0.9%	≤0.1%	0.9%	2.1%
Diet composition	0.3%	0.8%	0.9%	0.3%	≤0.1%
m_P	1.4%	0.3%	≤0.1%	≤0.1%	≤0.1%
OC	≤0.1%	≤0.1%	0.4%	1.1%	1.7%
Pore Water EEC	27.0%	35.1%	41.3%	45.1%	44.9%
T	1.4%	1.5%	0.7%	10.1%	35.1%
V_{LB}	1.8%	0.9%	1.3%	1.1%	≤0.1%
V_{WB}	1.1%	0.5%	0.5%	0.6%	0.2%
Water Column EEC	9.3%	1.2%	≤0.1%	≤0.1%	≤0.1%
X_{POC}	1.4%	1.7%	0.3%	≤0.1%	≤0.1%
β	52.0%	38.8%	13.8%	1.7%	≤0.1%
ε_L	≤0.1%	0.9%	1.7%	2.2%	0.4%
ε_N	2.0%	10.5%	15.3%	12.8%	4.3%
Total	98.6%	98.9%	99.0%	99.0%	98.4%

*mP, body composition, etc.

A.7.3. Third Sensitivity Analysis

A third sensitivity analysis was conducted to explore the influences of KABAM input parameters that are controlled by the user (including chemical specific inputs and ecosystem inputs), with the fixed parameters unchanged. In this sensitivity analysis, the Log K_{OW} was set to values of 4, 5, 6, 7, and 8, and a Monte Carlo simulation (10,000 trials) was run for each Log K_{OW} value. Parameters were assigned uniform distributions and assumptions of ranges based on data in the scientific literature. The range for each parameter is defined in Table A19. Diets of each trophic level were varied according to the definitions in Table A11.

The contributions of individual chemical specific and ecosystem input parameters at Log K_{OW} values of 4, 5, 6, 7, and 8 to the variability in the pesticide tissue concentration (C_B) of the seven aquatic trophic levels of KABAM are provided in Tables A20-A26. As with the second sensitivity analysis, the results of this analysis indicate that parameters have different relative importance in estimating C_B for the seven trophic levels. In addition, these tables indicate that the relative importance of individual parameters to estimates of C_B change with Log K_{OW}.

This sensitivity analysis indicates that several parameters contribute >10% of variance in C_B of one or more trophic levels. These include: water column EEC, pore water EEC, particulate organic carbon (X_{POC}), sediment organic carbon (OC), concentration of suspended solids (C_{SS}), water temperature (T), lipid composition (V_{LB}), diet composition, and characteristics of prey (including body composition, diet composition and m_P). Several of these parameters, including X_{POC}, OC, and C_{SS} have default values that were selected to be consistent with the standard pond used in EXAMS.

One notable observation resulting from this sensitivity analysis is that at Log K_{OW} 7 and 8, benthic invertebrate diet composed of sediment contributes ≥25% of the variance in C_B of all three size classes of fish. This indicates that the proportion of the benthic invertebrate diet attributed to sediment can influence the estimated pesticide concentrations in fish tissues.

As indicated above, several parameters in the Arnot and Gobas (2004) model are linked (*e.g.,* m_P and m_O, diet composition, V_{LB}, V_{NB} and V_{WB}). Therefore, sensitivity of C_B predictions to one parameter implies sensitivity of the predictions to the linked parameters.

Table A19. Parameters and associated assumptions used for third sensitivity analysis of KABAM.					
Para-meter	Parameter Description	Trophic Level	Minimum of Range	Maximum of Range	Source/Comments
C_{OX}	Concentration of dissolved oxygen (mg O_2/L)	All	4	12	Minimum is based on 60% of saturation of water with 6 mg/L as saturation (in 30°C water). Maximum is based on solubility limit of oxygen in cold water (5°C; see USGS 2008a).
C_{SS}	Concentration of suspended solids (kg/L)	All	$2.0x10^{-6}$	$5.0x10^{-4}$	Based on 5th and 95th percentiles of approximately 38,000 measurements of suspended sediment concentrations in surface waters of the US provided by NAWQA (USGS 2008b).
C_{WTO}	Total pesticide concentration in water column above the sediment	All	0.1	100	Assumed to be reasonable range for EECs expected from PRZM/EXAMS modeling.
C_{WTP}	Freely dissolved pesticide concentration in pore water of sediment	All	0.1	100	Assumed to be reasonable range for EECs expected from PRZM/EXAMS modeling.
Koc	Organic carbon partition coefficient	All	$3.5x10^3$	$3.5\ x10^7$	Determined based on assumption that Koc can be estimated as 0.35*Kow. In sensitivity analysis, Koc is linked directly to K_{OW} in order to avoid error in selection of inconsistent values for these parameters.
m_p	Fraction of respiratory ventilation that involves pore-water of sediment	Zooplankton	0	0.05	Based on default parameter values (0 or 0.05).
		Benthic Inv.	0	0.05	Based on default parameter values (0 or 0.05).
		Filter Feeders	0	0.05	Based on default parameter values (0 or 0.05).
		Small Fish	0	0.05	Based on default parameter values (0 or 0.05).
		Medium Fish	0	0.05	Based on default parameter values (0 or 0.05).
		Large Fish	0	0.05	Based on default parameter values (0 or 0.05).
OC	Percent organic carbon in sediment	All	1%	10%	In the OPP standard pond used in EXAMS, the default value for this parameter is 4%. This parameter value is varied by one order of magnitude around the OPP standard pond value.
T	Temperature (°C)	All	1	30	Reasonable range of values for this parameter in the environment.
V_{LB}	Lipid fraction of organism	Phytoplankton	0.5	2.0	See Table C1 of Appendix C.
		Zooplankton	1.0	4.0	See Table C2 of Appendix C.
		Benthic Inv.	0.5	12	See Tables C4-C9 of Appendix C.
		Filter Feeders	0.4	4	See Tables C13-C15 of Appendix C.
		Fish	0.5	8	See Table C19 of Appendix C.
V_{NB}	NLOM (Non Lipid Organic Matter) fraction of animals, NLOC (Non Lipid Organic Carbon) of plants	All	-	-	Set to equal $1-V_{LB}-V_{WB}$

Table A19. Parameters and associated assumptions used for third sensitivity analysis of KABAM.					
Para-meter	**Parameter Description**	**Trophic Level**	**Minimum of Range**	**Maximum of Range**	**Source/Comments**
V_{WB}	Water content of the organism	Phytoplankton	0.85	0.95	Assume 5% deviation from mean (*i.e.*, 90%).
		Zooplankton	0.74	0.96	See Section C.2. of Appendix C.
		Benthic Inv.	0.69	0.83	See Table C3 of Appendix C.
		Filter Feeders	0.78	0.93	See Table C12 of Appendix C.
		Fish	0.71	0.80	See Table C18 of Appendix C.
W_B	Wet weight (kg) of the organism at t	Phytoplankton	-	-	Not a necessary parameter for phytoplankton.
		Zooplankton	$1x10^{-9}$	$1x10^{-7}$	See Section C.2. of Appendix C.
		Benthic Inv.	$5x10^{-6}$	$2x10^{-3}$	See Table C11 of Appendix C.
		Filter Feeders	$2x10^{-4}$	$1x10^{-2}$	See Section C.5 of Appendix C.
		Small Fish	$1x10^{-3}$	$5x10^{-2}$	See Table C16 of Appendix C.
		Medium Fish	$5x10^{-3}$	0.6	See Table C17 of Appendix C.
		Large Fish	0.25	3.6	See Section C.5 of Appendix C.
X_{POC}	Concentration of particulate organic carbon in water (kg/L)	All	$2.0x10^{-6}$	$5.0x10^{-4}$	Based on 5th and 95th percentiles of approximately 38,000 measurements of suspended sediment concentrations in surface waters of the US provided by NAWQA (USGS 2008b).
X_{DOC}	Concentration of dissolved organic carbon in water (kg/L)	All	$5.0x10^{-7}$	$5.0x10^{-5}$	In the OPP standard pond used in EXAMS, the default value for this parameter is $5.0x10^{-6}$. This parameter value is varied by two orders of magnitude around the OPP standard pond value.

Table A20. Third sensitivity analysis results: Contributions to variance of specific variables to C_B values of phytoplankton at different Log Kow values.					
Variable	**4**	**5**	**6**	**7**	**8**
V_{LB}	0.7%	0.4%	0.3%	<0.1%	<0.1%
V_{WB}	7.6%	5.1%	3.3%	0.5%	<0.1%
Water Column EEC	80.1%	55.9%	51.8%	52.9%	52.8%
X_{POC}	11.3%	38.0%	44.2%	46.1%	46.8%
Total	99.7%	99.4%	99.6%	99.5%	99.6%

Table A21. Third sensitivity analysis results: Contributions to variance of specific variables to C_B values of zooplankton at different Log Kow values.					
Variable	**4**	**5**	**6**	**7**	**8**
C_{OX}	<0.1%	<0.1%	<0.1%	0.6%	3.1%
m_P	<0.1%	2.2%	22.2%	44.0%	40.2%
Pore Water EEC	<0.1%	2.2%	22.8%	42.0%	38.8%
T	<0.1%	<0.1%	<0.1%	3.0%	15.5%
V_{LB}	12.3%	12.7%	13.3%	7.2%	1.1%
V_{WB}	1.3%	0.8%	0.9%	0.4%	<0.1%
Water Column EEC	75.0%	48.0%	16.0%	0.9%	<0.1%
W_B	<0.1%	<0.1%	<0.1%	<0.1%	0.6%
X_{POC}	10.7%	33.5%	24.2%	1.5%	<0.1%
Total	99.3%	99.4%	99.4%	99.6%	99.3%

Table A22. Third sensitivity analysis results: Contributions to variance of specific variables to C_B values of benthic invertebrates at different Log Kow values.					
Variable	**4**	**5**	**6**	**7**	**8**
Characteristics of prey*	<0.1%	<0.1%	<0.1%	0.2%	<0.1%
C_{OX}	<0.1%	0.5%	2.2%	0.2%	<0.1%
Diet composition	<0.1%	1.2%	21.1%	34.4%	36.5%
m_P	<0.1%	0.8%	0.3%	<0.1%	<0.1%
OC	<0.1%	0.8%	11.6%	16.6%	18.6%
Pore Water EEC	0.2%	6.0%	35.1%	41.8%	42.0%
T	<0.1%	1.3%	4.0%	<0.1%	1.7%
V_{LB}	31.1%	38.5%	20.0%	6.3%	0.8%
V_{WB}	<0.1%	<0.1%	0.5%	0.2%	<0.1%
Water Column EEC	57.8%	27.9%	1.7%	<0.1%	<0.1%
X_{POC}	7.4%	22.3%	3.0%	<0.1%	<0.1%
Total	96.5%	99.3%	99.5%	99.7%	99.6%

*m_P, body composition, etc.

Table A23. Third sensitivity analysis results: Contributions to variance of specific variables to C_B values of filter feeders at different Log Kow values.

Variable	4	5	6	7	8
Characteristics of prey*	<0.1%	2.1%	7.7%	14.8%	5.3%
C_{OX}	<0.1%	<0.1%	0.5%	<0.1%	1.3%
C_{SS}	0.3%	12.6%	12.5%	6.3%	13.0%
Diet composition	<0.1%	0.8%	2.9%	2.5%	7.6%
m_P	0.2%	0.3%	<0.1%	<0.1%	<0.1%
OC	<0.1%	1.9%	15.6%	19.7%	18.4%
Pore Water EEC	0.2%	8.2%	39.5%	45.4%	39.2%
T	<0.1%	<0.1%	0.9%	1.0%	10.8%
V_{LB}	24.2%	24.0%	16.5%	9.5%	4.0%
V_{WB}	0.6%	<0.1%	0.4%	0.4%	<0.1%
Water Column EEC	64.8%	26.7%	1.4%	<0.1%	<0.1%
W_B	<0.1%	<0.1%	<0.1%	0.2%	<0.1%
X_{POC}	9.2%	22.6%	1.6%	<0.1%	<0.1%
Total	99.5%	99.2%	99.5%	99.8%	99.6%

*m_P, body composition, etc.

Table A24. Third sensitivity analysis results: Contributions to variance of specific variables to C_B values of small fish at different Log Kow values.

Variable	4	5	6	7	8
Characteristics of prey*	<0.1%	3.1%	21.0%	32.6%	28.6%
C_{OX}	<0.1%	2.1%	5.6%	0.6%	<0.1%
Diet composition	<0.1%	1.1%	6.8%	9.4%	10.0%
m_P	<0.1%	0.7%	<0.1%	<0.1%	<0.1%
OC	<0.1%	<0.1%	6.6%	13.3%	14.5%
Pore Water EEC	<0.1%	2.4%	27.4%	38.6%	39.4%
T	<0.1%	4.2%	11.2%	<0.1%	6.5%
V_{LB}	28.7%	25.3%	13.4%	4.8%	0.5%
V_{WB}	<0.1%	0.2%	<0.1%	<0.1%	<0.1%
Water Column EEC	61.8%	34.4%	2.7%	<0.1%	<0.1%
W_B	<0.1%	0.4%	0.7%	0.2%	<0.1%
X_{POC}	8.7%	25.4%	4.3%	<0.1%	<0.1%
Total	99.2%	99.3%	99.7%	99.5%	99.5%

*m_P, body composition, etc.

Table A25. Third sensitivity analysis results: Contributions to variance of specific variables to C_B values of medium fish at different Log Kow values.					
Variable	**4**	**5**	**6**	**7**	**8**
Characteristics of prey*	<0.1%	4.9%	25.2%	38.4%	30.7%
C_{OX}	<0.1%	3.9%	8.6%	0.9%	<0.1%
Diet composition	<0.1%	0.3%	2.7%	2.6%	1.4%
m_P	<0.1%	0.2%	<0.1%	<0.1%	<0.1%
OC	<0.1%	<0.1%	6.7%	14.0%	14.6%
Pore Water EEC	0.2%	3.0%	27.0%	39.7%	41.2%
T	0.2%	9.7%	14.8%	0.2%	11.1%
V_{LB}	19.3%	14.0%	6.6%	3.0%	0.3%
V_{WB}	2.4%	1.8%	1.4%	0.4%	<0.1%
Water Column EEC	68.4%	35.5%	2.4%	<0.1%	<0.1%
W_B	<0.1%	0.4%	0.4%	<0.1%	<0.1%
X_{POC}	8.8%	25.8%	3.8%	<0.1%	<0.1%
Total	99.3%	99.5%	99.6%	99.2%	99.3%

*m_P, body composition, etc.

Table A26. Third sensitivity analysis results: Contribution to variance of specific variables to C_B values of large fish at different Log Kow values.					
Variable	**4**	**5**	**6**	**7**	**8**
Characteristics of prey*	0.2%	5.3%	24.5%	38.0%	30.7%
C_{OX}	<0.1%	6.6%	9.7%	1.1%	<0.1%
Diet composition	<0.1%	0.4%	2.4%	2.4%	<0.1%
OC	<0.1%	<0.1%	5.5%	13.3%	13.0%
Pore Water EEC	<0.1%	2.3%	22.7%	36.4%	38.1%
T	0.2%	15.9%	17.2%	0.3%	16.0%
V_{LB}	27.5%	19.3%	11.6%	8.0%	1.5%
V_{WB}	<0.1%	0.2%	<0.1%	<0.1%	<0.1%
Water Column EEC	62.6%	28.8%	2.2%	<0.1%	<0.1%
W_B	<0.1%	0.4%	<0.1%	<0.1%	<0.1%
X_{POC}	7.9%	19.9%	3.6%	<0.1%	<0.1%
Total	98.4%	99.1%	99.4%	99.5%	99.3%

*m_P, body composition, etc.

Appendix B. Explanation of Defaults and Alternative Values Representing Abiotic Characteristics of Aquatic Ecosystem

Abiotic characteristics of the aquatic ecosystem that are necessary for KABAM are defined in Table 4 of the model tool. These characteristics include concentrations of particulate organic carbon (X_{POC}), dissolved organic carbon (X_{DOC}), dissolved oxygen (C_{OX}), suspended solids (C_{SS}), water temperature (T), and % organic carbon (OC) content of the sediment. The model tool is populated with default values for these parameters, which can be altered based on the needs of the model user. Default values are based on the abiotic characteristics of the aquatic ecosystem and are designed to be consistent with the OPP standard pond scenario used in EXAMS. Brief explanations for these default values as well as guidance on selecting alternative values are provided below for each parameter.

B.1. Particulate Organic Carbon (X_{POC}) and Dissolved Organic Carbon (X_{DOC})

X_{POC} and X_{DOC} are entered by the model user in units of kg OC/L. These parameters are relevant to estimating the available pesticide fraction in water (Φ). The greater the value of either of these parameters, the less pesticide is available in water. Less available pesticide results in lower concentrations of pesticide in tissues of aquatic organisms.

The estimated environmental concentrations (EECs) generated by PRZM/EXAMS in the water column and pore water represent the available concentration of the pesticide in water. Therefore, a default value of "0" is assumed for both X_{POC} and X_{DOC}. As a result, the pesticide concentration available in the water is equal to the PRZM/EXAMS EEC input in Table 1.

It may be necessary for the model user to incorporate alternate values for the X_{POC} and X_{DOC} parameters if the modeling incorporates EECs from a source other than PRZM/EXAMS. For example, if the exposure concentrations are available from monitoring data or mesocosm studies, X_{POC} and X_{DOC} specific to the monitoring study may be used. In that case, if the empirical exposure concentrations correspond to the total water column (*i.e.,* unfiltered), the model user would want to enter X_{POC} and X_{DOC} values that correspond to the specific water body used. If given a range of available values, the user should consider that use of lower X_{POC} and X_{DOC} values will result in more conservative estimates of pesticide accumulation in the aquatic food web.

B.2. Concentration of Dissolved Oxygen (C_{OX})

The C_{OX} parameter influences the ventilation rate of aquatic animals. As C_{OX} decreases, the gill ventilation rate of aquatic animals increases (because animals need to take in more water to acquire the amount of oxygen they require). With an increase in the gill ventilation rate, the rate constants for pesticide uptake (k_1) and elimination (k_2) through respiration both increase. Although the increase in k_1 leads to an increase in pesticide uptake, the increase in k_2 also leads to an increase in pesticide elimination. The net effect is a decrease in pesticide concentration in aquatic organism tissues. Therefore, a decrease in the value of C_{OX} results in a decrease in pesticide concentrations in tissues of aquatic organisms.

C_{OX} is entered by the model user in units of mg O_2/L. The default value for this parameter is 5.0 mg O_2/L, based on the OPP standard pond. This concentration does not represent the highest possible value for C_{OX} (*i.e.,* the limit of solubility of oxygen) and is not expected to result in the most conservative estimates of pesticide in aquatic animal tissues. However, it is consistent with the OPP standard pond which is used to derive EECs.

The model user could explore the influence of C_{OX} on the predictions of pesticide tissue concentrations in aquatic organisms by selecting a higher value, for example the solubility of oxygen (potential range: 6-12 mg O_2/L). To determine the solubility of oxygen in water at specific temperatures and pressures, see USGS 2008a.

It may be necessary for the model user to incorporate an alternate C_{OX} value if the modeling incorporates EECs from a source other than PRZM/EXAMS. In that case, the model user should enter a C_{OX} value that corresponds to the specific water body used.

B.3. Water Temperature (T)

The water temperature parameter influences calculation of the growth dilution rate constant (k_G), the pesticide uptake rate constant through diet (k_D), and the pesticide elimination rate constant through excretion of feces (k_E). The growth dilution rate constant (k_G) is dependent on whether the temperature is above or below 17.5^{o}C. The growth dilution rate constant is higher when the temperature is above 17.5^{o}C compared to when the temperature is below 17.5^{o}C (Figure A.8). Temperature affects the pesticide uptake rate through the dietary uptake rate constant (k_D) by changing the feeding rate of the animal (G_D). An increase in temperature results in an increase in the feeding rate, and with that, an increase in the pesticide uptake constant for the diet (Figure A.10). The fecal egestion rate constant (k_E) is affected by temperature by changing the feeding rate (G_D) as well as the fecal egestion rate (G_F) of the animal. An increase in temperature results in an increase in the feeding rate (Figure A.13), and with that, an increase in the fecal egestion rate. The increase in the fecal egestion rate results in an increase in the pesticide rate constant for pesticide elimination through excretion. In summary, increase in temperature results in an increase in k_D, k_E, and k_G. Although k_G and k_E represent processes (*i.e.,* pesticide elimination/dilution) that compete with k_D (*i.e.,* pesticide uptake), the net increase in the two processes (uptake and elimination/dilution) does not cancel each other out.

The water temperature of the EXAMS' pond varies based on the selected PRZM scenario. Therefore, the model user should select the water temperature based on the PRZM scenario used for deriving EECs. If the modeling incorporates EECs from a source other than PRZM/EXAMS, the water temperature relevant to the other EECs should be utilized.

B.4. Concentration of Suspended Solids (C_{SS})

The concentration of suspended solids (C_{SS}) is relevant to filter feeders only. C_{SS} influences the calculation of the rate constants for pesticide uptake through diet (k_D) and pesticide elimination through excretion of feces (k_E). An increase in C_{SS} leads to an increase in the feeding rate of filter feeders (G_D) which in turn results in an increase in the pesticide uptake through diet (k_D). An increase in C_{SS} also leads to an increase in the fecal egestion rate of filter feeders (G_F) and an increase in the pesticide elimination through excretion of fecal matter (k_E). Although k_D and k_E represent competing processes, the net increase in the two does not cancel each other out.

C_{SS} is entered by the model user in units of kg/L. The default value for this parameter is 3.00×10^{-5} kg/L, based on the OPP standard pond. If the modeling incorporates EECs from a source other than PRZM/EXAMS, a C_{SS} value relevant to the other EECs should be utilized.

B.5. Sediment Organic Carbon (OC)

Sediment organic carbon (OC) is a parameter that influences organisms that consume sediment. As OC increases, the concentration of the pesticide in the solid component of the sediment increases to the extent that the pesticide sorbs to organic matter. As the pesticide concentration in sediment increases, the pesticide concentration in organisms that consume sediment also increases.

OC is entered by the model user as % of the dry weight of the sediment. The default value for this parameter is 4.0%, based on the OPP standard pond. If the modeling incorporates EECs from a source other than PRZM/EXAMS, an OC value relevant to the other EECs should be utilized.

Appendix C. Explanation of Default Values Representing Biotic Characteristics of the Aquatic Ecosystem, Including Food Web Structure

The seven trophic levels of the aquatic ecosystem of KABAM are phytoplankton, zooplankton, benthic invertebrates, filter feeders, small fish, medium fish, and large fish. In KABAM, each trophic level is defined by its % lipid, % Non Lipid Organic Matter (NLOM), % water, body weight, and diet. Each of these trophic levels is described within this Appendix, with emphasis on the information relevant to KABAM and explanations of default parameters used to define these trophic levels (in Tables 5 and 6 of the KABAM tool). If the model user wishes to explore the influences of changes in parameter values representing the aquatic food web on EECs and RQs for birds and mammals, this can be accomplished by altering parameter values within the range of reported values for a specific parameter.

Although the % water composition of an aquatic organism does not influence the bioaccumulation of a chemical in that organism (see Appendix A), it is an important consideration for the definition of % lipid and the percent non-lipid organic matter (% NLOM). Often, tissue analysis results and body weight data in the scientific literature are reported on a dry weight basis. For KABAM, input parameters for body composition are entered on a wet weight basis. Therefore, % water composition is discussed in the sections below since it is necessary to understand the water composition of an organism in order to translate the reported data into input parameters for KABAM.

Lipid composition of an organism can influence the bioaccumulation of a chemical (See Appendix A), with higher lipid composition leading to higher accumulation. Since KABAM is intended for use in ecological risk assessments of pesticides with the potential to bioaccumulate in aquatic ecosystems, it is necessary for this tool to serve as a conservative representation of bioaccumulation. Default parameter values for % lipid were selected from the open literature and are intended to represent the high-end of available data (75th-90th percentiles).

C.1. Phytoplankton

Phytoplankton are microscopic autotrophic aquatic organisms that derive their nutrition from photosynthesis. Groups of freshwater phytoplankton include algae (green, yellow-green and golden-brown), cyanobacteria (blue-green algae), diatoms and dinoflagellates. Phytoplankton can be unicellular, colonial, or filamentous. These organisms have limited mobility that is based on water movements; however, some are able to move via flagella. An aquatic habitat will generally contain an assemblage of phytoplanktonic species that vary in proportion over time and space (Wetzel 1983).

For parameterization of KABAM, it is necessary to define the % water, % lipid and % NLOM contents of phytoplankton. The body weight is not a necessary input for phytoplankton, nor is the diet composition since these organisms do not consume other organisms.

Since it is assumed that phytoplankton are present in the water column of the aquatic ecosystem where photosynthesis can occur, it is assumed that phytoplankton do not reside in benthic sediment and do not respire pore water. This should be indicated in Table 5 of the KABAM tool (*i.e.,* "no" should be entered in the column titled: "Do organisms in trophic level respire some pore water?").

Aquatic plant tissues are composed of approximately 90% water by weight (Hannan and Dorris 1970; Raven et al. 1999, Sladecek and Sladeckova 1963). **The default parameter for the water composition of phytoplankton is 90%.**

Reported % lipid values for phytoplankton vary from 2-27% of dry weight. If it is assumed that phytoplankton are composed of 90% water, then this range of lipid compositions is equivalent to 0.2-2.7% on a wet weight basis (Table C1). For KABAM, **the default parameter for % lipid of phytoplankton was selected as 2% to represent a high-end estimate (75th to 90th percentile of data in Table C1) of this parameter.**

The wet weight of an organism is the sum of the water, lipid, and NLOM content. If the water content of phytoplankton is 90% of the wet weight, and the % lipid is known (2%), the NLOM content of phytoplankton is the % remaining after subtracting the water and lipid content from 100%. **Therefore, the default parameter for the NLOM composition of phytoplankton is 8%.**

Table C1. Percent lipid composition of freshwater phytoplankton (under culture conditions) reported in the scientific literature.

Species	Mean% Lipid (dry weight basis)	Mean% Lipid (wet weight basis)	Source
Not stated	Not stated	0.5	Oliver and Niimi 1988
Anabaena sp.	6.8 (±0.4)	0.68*	Stange and Swackhamer 1994
Anabaena sp.	5.3 (±2.4)	0.53*	Stange and Swackhamer 1994
Anabaena sp.	2.2 (±0.2)	0.22*	Stange and Swackhamer 1994
Chamydomonas reinhardtii	10.8 (±6.2)	1.08*	Lürling and Van Donk 1997
Chlamydomonas applanata	18.2	1.82*	Shifrin and Chisholm 1981
Chlamydomonas applanata	16	1.60*	Shifrin and Chisholm 1981
Chlorella ellipsoidea	13.5	1.35*	Shifrin and Chisholm 1981
Chlorella pyrenoidosa	13.4	1.34*	Shifrin and Chisholm 1981
Chlorella pyrenoidosa	14.4	1.44*	Shifrin and Chisholm 1981
Chlorella pyrenoidosa	16.4	1.64*	Shifrin and Chisholm 1981
Chlorella pyrenoidosa	16	1.60*	Shifrin and Chisholm 1981
Chlorella vulgaris	12.5	1.25*	Shifrin and Chisholm 1981
Chlorella vulgaris	13	1.30*	Shifrin and Chisholm 1981
Cryptomonas pyrenoidifera	8.5 (±5.1)	0.85*	Lürling and Van Donk 1997
Microcystis aeruginosa	5.8 (±2.3)	0.58*	Lürling and Van Donk 1997
Nannochloris sp.	20.2	2.02*	Shifrin and Chisholm 1981
Nitzschia palea	22.2	2.22*	Shifrin and Chisholm 1981
Oocystis polymorpha	12.6	1.26*	Shifrin and Chisholm 1981
Ourococcus sp.	27	2.70*	Shifrin and Chisholm 1981
Scenedesmus acutus	6.4 (±2.5)	0.64*	Lürling and Van Donk 1997
Scenedesmus obliquus	19	1.90*	Shifrin and Chisholm 1981
Selanastrum gracile	20.8	2.08*	Shifrin and Chisholm 1981
Selenasrum capricornutum	19.5 (±0.2)	1.95*	Stange and Swackhamer 1994
Selenasrum capricornutum	16.0 (±0.3)	1.60*	Stange and Swackhamer 1994
Selenasrum capricornutum	8.0 (±0.9)	0.80*	Stange and Swackhamer 1994
Synedra sp.	7.5 (±1.6)	0.75*	Stange and Swackhamer 1994
Synedra sp.	13.7 (±0.7)	1.37*	Stange and Swackhamer 1994
Synedra sp.	11.7 (±4.5)	1.17*	Stange and Swackhamer 1994
Synedra ulna	23	2.30*	Shifrin and Chisholm 1981
Average		1.4	
75th percentile		1.8	
90th percentile		2.1	

*Calculated from reported % lipid based on dry weight and assumption that algae wet weight is 90% water.

C.2. Zooplankton

Zooplankton are aquatic animals that are suspended in water. This group is primarily composed of rotifers, cladocera and copepods, but also includes protozoa and insects at immature life stages. Species of zooplankton primarily consume phytoplankton but also consume detritus, bacteria, yeast, and other (smaller) zooplankton (Wetzel 1983). **For parameterization of KABAM, zooplankton is represented by herbivorous species that have a diet composed 100% of phytoplankton.**

Since it is assumed that zooplankton are present in the water column of the aquatic ecosystem and do not reside in the benthic sediment, it is assumed that zooplankton do not respire pore water. This should be indicated in Table 5 of the KABAM tool (*i.e.,* "no" should be entered in the column titled: "Do organisms in trophic level respire some pore water?").

Beers (1966) reported water compositions of several groups of marine zooplankton inhabiting the Atlantic Ocean. Average % water composition of these groups ranged 74-96%, with an average % water composition of 86% corresponding to copepods. Based on this information, **the default % water composition of zooplankton is 85%.** This value is used to translate dry weight data into equivalent wet weight values.

Reported mean % lipid values for zooplankton vary from 6.4-24.3% of dry weight. If it is assumed that zooplankton are composed of 85% water, then this range of lipid compositions is equivalent to 0.96-3.6% on a wet weight basis (Table C2). Based on this information, **the default % lipid for zooplankton is set to 3% to represent a high-end (75th to 90th percentile) estimate of this parameter.**

The wet weight of an organism is the sum of the water, lipid, and NLOM content. If the water content of zooplankton is 85% of the wet weight, and the % lipid is known (3%), then NLOM content of zooplankton is the % remaining after subtracting the water and lipid content from 100%. **Therefore, the default parameter for the NLOM composition of zooplankton is 12%.**

Wright (1958) provided biomass data for two species of zooplankton (*Daphnia longispina* and *D. pulex*) in a reservoir in Montana, where the average body weight of zooplankton was $1.3x10^{-7}$ kg-wet weight (assuming 85% water content; range $0.9\text{-}1.6x10^{-7}$ kg-wet weight). Acharya et al. (2005) provided dry body weights for *Bosmina freyi* that translate to approximately $0.3\text{-}3x10^{-8}$ kg-wet weight (assuming 85% water content). Jeppesen et al. (2004) provided body weight data for *Daphnia sp.* that translate to approximately $0.67\text{-}3.3x10^{-7}$ kg-wet weight (assuming 85% water content). Based on this information, **the default weight for zooplankton is set to $1x10^{-7}$ kg-wet weight,** with the intention of being a representative weight of species of zooplankton.

Table C2. Percent lipid composition of freshwater zooplankton reported in the scientific literature.

Zooplankton identification	Mean% Lipid (dry weight basis)	Mean% Lipid (wet weight basis)	Source
Daphnia magna (cladoceran)	6.4-19.7	0.96-3.0*	McKee and Knowles 1987
Unspecified	6.7*	1.0±0.33	Morrison et al. 1997
Mostly cladocerans, also copepods and rotifers	10.8 (±3.6)	1.6*	Mitra et al. 2007
Mostly cladocerans, also copepods and rotifers	12.1 (±3.0)	1.8*	Mitra et al. 2007
Mostly cladocerans, also copepods and rotifers	12.2 (±2.4)	1.8*	Mitra et al. 2007
Leptodora kindtii	13.1 (±1.0) **	2.0	Vijverberg and Frank 1976
Mostly cladocerans, also copepods and rotifers	13.7 (±1.9)	2.1*	Mitra et al. 2007
Mostly cladocerans, also copepods and rotifers	13.9 (±1.9)	2.1*	Mitra et al. 2007
Mostly cladocerans, also copepods and rotifers	14.6 (±1.0)	2.2*	Mitra et al. 2007
Cyclopodia	15.9 (±1.8) **	2.4	Vijverberg and Frank 1976
Chydorus sphaericus	18.5 (±2.8) **	2.8	Vijverberg and Frank 1976
Bosmina coregoni	20.5 (±1.9) **	3.1	Vijverberg and Frank 1976
Eurytemora affinus	23.6 (±2.7) **	3.5	Vijverberg and Frank 1976
Daphnia hyalina	24.3 (±5.3)**	3.6	Vijverberg and Frank 1976
Average		2.3	
75th percentile		2.9	
90th percentile		3.3	

*Calculated from reported % lipid based on dry weight and assumption that zooplankton wet weight is 85% water.
**Expressed as % of total organic matter attributed to lipid. It is assumed that this is equivalent to a dry weight basis.

C.3. Benthic invertebrates

The benthic invertebrate trophic level includes animals that inhabit the sediments of aquatic habitats. Benthic invertebrates include a diverse group of animals, including crustaceans (*e.g.,* crayfish, amphipods), aquatic worms (*e.g.,* oligochaetes), aquatic insect larvae (*e.g.,* Diptera, caddisflies, beetles, mayflies and dragonflies), protozoa, snails, and nematodes. Different species of benthic invertebrates have a variety of feeding strategies, including herbiovory, detritivory, and predation upon other benthic invertebrates (Covich et al. 1999). In order to represent all of these feeding strategies with the benthic invertebrate trophic level of KABAM, it is assumed that benthic invertebrates consume organic matter from sediment, phytoplankton, and zooplankton in equal quantities. **Therefore, the default diet composition of benthic invertebrates is 34% sediment, 33% phytoplankton, and 33% zooplankton.**

Since it is assumed that benthic invertebrates are present in the benthic compartment of the aquatic ecosystem, it is assumed that benthic invertebrates respire sediment pore water. This should be indicated in Table 5 of the KABAM tool (*i.e.*, "yes" should be entered in the column titled: "Do organisms in trophic level respire some pore water?").

Available water composition data for benthic invertebrates include a range of 69-83% water (Table C3). The average value of the available data is 76%. **Based on this average, the default value for KABAM representing the % water of benthic invertebrates is 76%.**

Table C3. Water composition (%) of benthic invertebrates reported in the scientific literature.

Organism	Mean% Water	Source
Crayfish (*Orconectus propinquus*)	69	Gewurtz et al. 2000
Hyalella azteca	72.5	Lotufo et al. 2001
Mayfly larvae	73	Gewurtz et al. 2000
Diporeia sp.,	73.1	Lotufo et al. 2001
Crayfish *(Astacus fluviatilis)*	80.0	Sidwell 1981
*Lumbriculus variegatus (*oligochaete)	81	Liebig et al. 2005
Crayfish *(Astacus, Orconectus* and *Procambarus)*	82.5*	USDA 2005

*excluding the shell

Lipid data are available for various freshwater crustaceans, oligochaetes, and insect larvae. These values indicate a wide range (approximately 1 to 10% of wet weight) of lipid composition of benthic invertebrates (Tables C4-C9). **The default lipid composition for benthic invertebrates is 3%.** This value was selected to be representative of a high-end value (75^{th} percentile) of available lipid compositions for freshwater benthic invertebrates (Table C10).

Table C4. Lipid composition (%) of *Hyalella azteca* (a freshwater crustacean) reported in the scientific literature.

Source	Mean% Lipid (dry weight basis)	Mean% Lipid (wet weight basis)
Lotufo et al. 2001	2.4*	0.66±0.03
Lotufo et al. 2001	3.2*	0.88±0.04
Lotufo et al. 2001	6.3*	1.73±0.25
Lotufo et al. 2001	6.5*	1.79±0.41
Lotufo et al. 2000	6.9 (±0.9)	1.9*
Lotufo et al. 2000	7.0 (±1.1)	1.9*
Lotufo et al. 2000	7.2 (±0.8)	2.0*
Kane Driscoll and Landrum 1997	7.5 (±1.5)	2.1*
Lotufo et al. 2000	7.5 (±0.9)	2.1*
Lotufo et al. 2000	7.7 (±1.5)	2.1*
Kane Driscoll et al. 1997	8.2 (±0.7)	2.3*
Kane Driscoll et al. 1997	8.4(±0.7)	2.3*
Average	6.6	1.8
75^{th} percentile	7.6	2.1
90^{th} percentile	8.2	2.3

*Calculated from reported % lipid and assumption that dry:wet weight ratio for *H. azteca* is 0.275 (based on Lotufo et al. 2001).

Table C5. Lipid composition (%) of freshwater crayfish (crustaceans) reported in the scientific literature.

Genus	Mean% Lipid (wet weight basis)	Source
Astacus fluviatilis	0.5	Sidwell 1981
Orconectus	0.86 (±0.11)	White et al. 1998
Astacus, Orconectus and *Procambarus*	1.0	USDA 2005
Undefined	1.9 (±0.47)	Morrison et al. 1997
Orconectes propinquus	2.4 (±0.26)	Morrison et al. 2000
Orconectes	2.52 (±0.16)	Gewurtz et al. 2000
Procambarus	2.95 (±1.25)	Lin et al. 2004
Procambarus	3.02 (±1.29)	Lin et al. 2004
Average	1.9	
75th percentile	2.6	
90th percentile	3.0	

Table C6. Lipid composition (%) of *Diporeia sp.* (freshwater crustaceans) reported in the scientific literature.

Source	Mean% Lipid (dry weight basis)	Mean% Lipid (wet weight basis)
Landrum et al. 2007	10.78 (±1.5)	2.9*
Landrum et al. 2007	11.97 (±0.38)	3.2*
Landrum et al. 2007	17.1 (±0.64)	4.6*
Kane Driscoll et al. 1997	20.1 (±4.6)	5.4*
Kukkonen et al. 2004	20.4*	5.5±0.7
Kane Driscoll et al. 1997	21.3 (±6.7)	5.7*
Lotufo et al. 2001	22.2*	5.97±0.75
Kukkonen et al. 2004	23.0*	6.2±1.4
Lotufo et al. 2001	23.3*	6.27±1.21
Lotufo et al. 2000	23.7 (±8.5)	6.4*
Lotufo et al. 2000	23.9 (±6.3)	6.4*
Kane Driscoll and Landrum 1997	27.2 (±1.3)	7.3*
Lotufo et al. 2001	40.3*	10.85±0.62
Lotufo et al. 2001	43.1*	11.59±1.18
Average	23.5	6.3
75th percentile	23.9	6.4
90th percentile	36.4	9.8

*Calculated from reported % lipid and assumption that dry:wet weight ratio for *Diporeia sp.* is 0.269 (based on Lotufo et al. 2001).

Table C7. Lipid composition (%) of *Lumbriculus variegatus* (a freshwater oligochaete) reported in the scientific literature.

Source	Mean% Lipid (dry weight basis)	Mean% Lipid (wet weight basis)
Croce et al. 2005	5.8*	1.1±0.1
Kukkonen et al. 2004	6.3*	1.2±0.13
Liebig et al. 2005	8 (±0.4)	1.5*
Kukkonen et al. 2004	7.9	1.5±0.19
Kukkonen and Landrum 1994	9.2 (±0.9)	1.7*
Fisk et al. 1998	10.5*	2.0±0.2
Kukkonen and Landrum 1994	11.1 (±1.4)	2.1*
Fisk et al. 1998	12.1*	2.3±0.2
Fisk et al. 1998	13.2*	2.5±0.3
Kukkonen and Landrum 1994	13.2 (±4.3)	2.5*
Fisk et al. 1998	15.3*	2.9±0.3
Fisk et al. 1998	17.9*	3.4±0.8
Fisk et al. 1998	18.9*	3.6±0.8
Fisk et al. 1998	19.5*	3.7±0.6
Average	12.1	2.3
75th percentile	14.8	2.8
90th percentile	18.6	3.5

*Calculated from reported % lipid and assumption that water composition of *L. variegatus* is 81% (Liebig et al. 2005).

Table C8. Lipid composition (%) of other freshwater oligochaetes reported in the scientific literature.

Organism Identification	Mean% Lipid (dry weight basis)	Mean% Lipid (wet weight basis)	Source
Tubifex tubifex and *Limnodrilus hoffmeisteri*	5.3*	1*	Oliver and Niimi 1988
*Ilyodrilus templetoni***	5.85 (±2.28)	1.1*	Lu et al. 2003
*Ilyodrilus templetoni***	6.11 (±0.55)	1.2*	Lu et al. 2003
*Ilyodrilus templetoni***	6.72 (±1.59)	1.3*	Lu et al. 2003
*Ilyodrilus templetoni***	7.44 (±1.33)	1.4*	Lu et al. 2003
*Ilyodrilus templetoni***	7.35 (±1.26)	1.4*	Lu et al. 2003
*Ilyodrilus templetoni***	8.82 (±1.60)	1.7*	Lu et al. 2003
Oligochaete	9.5 (±1.0)	1.8*	Landrum et al. 2007
Limnodrilus sp.	11.93 (±0.16)	2.3*	Jonker et al. 2004
Oligochaete	12.8 (±1.8)	2.4*	Landrum et al. 2007
Average	8.2	1.6	
75th percentile	9.3	1.8	
90th percentile	12.0	2.3	

*Calculated from reported % lipid and assumption that water composition of *L. variegatus* is 81% (Liebig et al. 2005).

**Mean of values for *I. templetoni* is 1.4% (wet weight). When this value is used in calculating the mean and percentile values for the group of oligochaetes, the mean is 1.8% (wet weight). The 75th and 90th percentiles are 2.2 and 2.4, respectively.

Table C9. Lipid composition (%) of freshwater insect larvae reported in the scientific literature.

Organism Identification	Mean% Lipid (wet weight basis)	Source
Chironomus riparius	0.6	Leonards et al. 1997
Hexagenia limbata (mayfly larvae)	1.5 (±0.05)	Morrison et al. 2000
H. limbata and *H. rigida*	1.50 (±0.052)	Gewurtz et al. 2000
Caddisfly larvae	1.7	Morrison et al. 1997
Mayfly larvae	2.0 (±0.25)	Morrison et al. 1997
Average	1.5	
75th percentile	1.7	
90th percentile	1.9	

Table C10. Mean lipid composition (%, wet weight basis) of freshwater benthic invertebrates from data in Tables C4-C9.

Benthic Invertebrate	Mean	75th Percentile	90th Percentile
Insect Larvae	1.5	1.7	1.9
Hyalella azteca (a freshwater crustacean)	1.8	2.1	2.3
Freshwater oligochaetes (excluding *L. variegatus*)	1.8	2.2	2.4
Crayfish (freshwater crustaceans)	1.9	2.6	3.0
Lumbriculus variegatus (a freshwater oligochaete)	2.3	2.8	3.5
Diporeia sp. (freshwater crustaceans)	6.3	6.4	9.8
Mean	2.6	3.0	3.8

The wet weight of an organism is the sum of the water, lipid, and NLOM content. By default, if the water content of benthic invertebrates is 76% of the wet weight, and the % lipid is known (default = 3%), the NLOM content of benthic invertebrates is the % remaining after subtracting the water and lipid content from 100%. **Therefore, the default parameter for the NLOM composition of benthic invertebrates is 21%.**

The benthic invertebrate trophic level is composed of a wide variety of taxonomic groups. The body weights of organisms within this group can vary by orders of magnitude (Table C11). **The default weight for benthic invertebrates is set to 1x10^{-4} kg-wet weight,** with the intention of being representative of a midpoint weight of species of benthic invertebrates.

Table C11. Body weights (wet) of freshwater benthic invertebrates reported in the scientific literature.

Benthic Invertebrate	Weight (kg)	Source
Amphipods	0.05x10^{-4}	Leonards et al. 1997
Mayfly larvae	0.16x10^{-4} *	Morrison et al. 1997
Chironomids	0.24x10^{-4}	Leonards et al. 1997
Caddisfly larvae	0.32x10^{-4} *	Morrison et al. 1997
Snails	0.82x10^{-4}	Leonards et al. 1997
Crayfish	18.0x10^{-4}	Morrison et al. 1997

*converted from reported dry weight to wet weight assuming 75% water content.

C.4. Filter Feeders

Filter feeders are benthic invertebrates that are distinguished by their feeding habits. These organisms feed by straining water and extracting organic material such as detritus and plankton. Examples of freshwater filter feeders include mollusks. For KABAM, it is assumed that filter feeders consume materials suspended in the water column, including phytoplankton, zooplankton, and detritus. It is also assumed that filter feeders consume suspended sediment incidentally. **The default composition of the diet of this trophic level is 34% sediment, 33% phytoplankton, and 33% zooplankton.**

Since it is assumed that filter feeders are present in the benthic sediment compartment of the aquatic ecosystem, it is also assumed that filter feeders respire sediment pore water. This should be indicated in Table 5 of the KABAM tool (*i.e.,* "yes" should be entered in the column titled: "Do organisms in trophic level respire some pore water?").

According to available data, water composition of freshwater mollusks ranges 78-93% (Table C12). **The default water content of filter feeders is set to 85%,** based on the midpoint of the range of available data.

Table C12. Water composition (%) of freshwater mollusks reported in the scientific literature.

Identification	Mean % water*	Source
Corbicula strata (freshwater clam)	77.6	Sidwell 1981
Corbicula japonica (freshwater clam)	79.8	Sidwell 1981
Corbicula sandai (freshwater clam)	80.0	Sidwell 1981
Corbicula fluminea (freshwater clam)	81.4	Sidwell 1981
lamellibrancha clams (subclass)	82	USDA 2005
Corbicula leana (freshwater clam)	82.1	Sidwell 1981
Dreissena polymorpha (zebra mussel)	87	Bervoets et al. 2005
D. polymorpha	88-93	Hendriks et al. 1998
Anodonta anatine (mussels)	90.6-92.8	Hyötyläinen et al. 2002

*It is assumed that this does not include the shell.

Data on lipid content are available for several species of freshwater mollusks. These values range 0.4-4% of wet weight (Tables C13 - C15). **The default lipid composition for filter feeders is 2%.** This value was selected to be representative of a high end (75^{th} percentile of *Dreissena sp.* and *Corbicula sp.*) value of available lipid compositions for freshwater mollusks.

Table C13. Percent lipid composition of *Dreissena sp.* (freshwater mollusks) reported in the scientific literature.

Species	Mean % Lipid (dry weight basis)	Mean % Lipid (wet weight basis)	Source
D. polymorpha	4.3*	0.55	Bervoets et al. 2005
D. polymorpha	14	1	Hendriks et al. 1998
D. polymorpha	8.5*	1.1	Kwon et al. 2006
D. polymorpha	9.1	1.2*	Becker van Slooten and Tarradellas 1994
D. bugensis	9.0 (±1.4)	1.2*	Marvin et al. 2002
D. bugensis	10 (±0.5)	1.3	Marvin et al. 2002
D. polymorpha	11 (±0.6)	1.4*	Marvin et al. 2002
D. polymorpha	10.8*	1.4 (±0.1)	Kwon et al. 2006
D. polymorpha	11.5*	1.5 (±0.1)	Kwon et al. 2006
D. polymorpha	12.3*	1.6 (±0.1)	Kwon et al. 2006
D. polymorpha	12 (±4.4)	1.6*	Marvin et al. 2002
D. polymorpha	17	2	Hendriks et al. 1998
D. polymorpha	18	2	Hendriks et al. 1998
Average	11.3	1.4	
75th percentile	12.3	1.6	
90th percentile	16.4	1.9	

* Calculated from reported % lipid and assumption that water composition of *D. polymorpha* is 87% (Bervoets et al. 2005).

Table C14. Percent lipid composition of *Corbicula sp.* (freshwater clams) reported in the scientific literature.

Species	Mean % Lipid (wet weight basis)	Source
C. leana	1.1	Sidwell 1981
C. japonica	1.2*	Kang et al. 2002
C. japonica	1.2	Sidwell 1981
C. fluminea	1.5	Sidwell 1981
C. sandai	2.4	Sidwell 1981
C. strata	4.0	Sidwell 1981
Average	1.9	
75th percentile	2.2	
90th percentile	3.2	

*Based on reported mean lipid content of 5.8% dry weight and 80% moisture content reported for this species by Sidwell 1981.

Table C15. Percent lipid composition of other freshwater filter feeders reported in the scientific literature.

Identification	Mean % Lipid (dry weight basis)	Mean % Lipid (wet weight basis)	Source
Sphaerium striantium (fingernail clam)	8.7	0.36	Rice and White 1987
Elliptio complanata	3.2 (±1.2)	0.48*	Marvin et al. 2002
Anodonta anatine (mussels)	11.2 (±0.8)	0.81	Hyötyläinen et al. 2002
Anodonta anatine (mussels)	12.2 (±0.7)	0.98	Hyötyläinen et al. 2002
Lamellibrancha (clams)	5.5	1.0	USDA 2005
Anodonta anatine (mussels)	10.9 (±0.6)	1.02	Hyötyläinen et al. 2002
Anodonta anatine (mussels)	11.3 (±0.9)	1.05	Hyötyläinen et al. 2002

*Calculated using assumption that filter feeders are 85% water.

The wet weight of an organism is the sum of the water, lipid, and NLOM content. By default, if the water content of filter feeders is 85% of the wet weight and the % lipid is known (default = 2%), the NLOM content of filter feeders is the % remaining after subtracting the water and lipid content from 100%. **Therefore, the default parameter for the NLOM composition of filter feeders is 13%.**

Reported wet weights of various species of mollusks range 0.2-12 x10^{-3} kg. Mean wet weights of *Dreissena polymorpha* have been reported as 0.41 ± 0.26 x10^{-3} kg (Van Haelst et al. 1996). Wet weights of *C. fluminea* ranged approximately 0.2-2 x10^{-3} kg (Andrès et al. 1999, Vidal et al. 2002). Hyötyläinen et al. (2002) reported wet weights of *Anodonta anatine* tissue as ranging 4.5-12.1 x10^{-3} kg. Based on this information, **the default weight of filter feeders is set to 1 x10^{-3} kg,** with the intention of being a representative weight of mollusks.

C.5. Fish (Small, Medium and Large Sizes)

There are hundreds of species of fish inhabiting fresh waters of the United States and Canada, including ponds, lakes, streams, and rivers. Species of bluegill and other sunfish (*Lepomis spp.*), bass (*Micropterus spp.*), and crappie (*Pomoxis spp.*) are common inhabitants of fresh warm water ponds, lakes, and streams distributed throughout the continental United States (Page and Burr 1991, Carlander 1977). As described below, these species were used to define default parameters for the small, medium, and large fish in KABAM. Although there are many other species of fish in ponds of the U.S. (*e.g.,* perch, minnows), sunfish, crappie, and bass were considered representative of fish that are found in freshwaters of the U.S., and thus suitable for models for defining input parameters for use in KABAM.

Several bird and mammal species (*e.g.,* belted kingfisher [*Megaceryle alcyon*], northern river otter) consume amphibians, in addition to fish. For KABAM, it is assumed that the default fish also represent, *i.e.*, serve as surrogates for, aquatic-phase amphibians, such as salamanders and frogs. This assumption is consistent with OPP's policy in which exposure and effects data for fish are assumed to be representative of aquatic-phase amphibians (USEPA 2004).

Default parameters for small fish in KABAM are designed to represent the young-of-year (YOY), *i.e.,* fish that have hatched within the year, before January 1 of the next year, of sunfish, bass and crappie. YOY of these species consume copepods, cladocerans, rotifers (*i.e.,* zooplankton), chironomid larvae, and mayfly larvae (*i.e.,* benthic invertebrates) (Carlander 1977). Average body weights of YOY of sunfish, bass, and crappie are provided in Table C16. **For KABAM, it is assumed that the small fish weighs 0.01 kg and its diet is 50% zooplankton and 50% benthic invertebrates.**

Table C16. Average body weights for young of the year fish (Source: Carlander 1977).

Species (scientific name)	Average body weight (kg)
Green sunfish (*Lepomis cyanellus*)	0.001-0.01
Pumpkinseed (*L. gibbosus*)	0.002
Warmouth (*L. gulosus*)	<0.011
Bluegill (*L. macrochirus*)	0.0001-0.05
Redear sunfish (*L. microlophus*)	0.0006-0.04
Largemouth bass (*Micropterus salmoides*)	0.0002-0.02
White crappie (*Pomoxis annularis*)	0.0002-0.01
Black crappie (*P. nigromaculatus*)	0.0005-0.02

The medium fish in KABAM is designed to represent adult sunfish and crappie. These fish reach sexual maturity between ages 1 and 3, with lifespans ≥6 years. Their diets include insects, insect larvae, crustaceans, snails, and other fish (Carlander 1977). Mature fish range in weight, 0.005-0.579 kg, depending upon their age (Table C17; data from Carlander 1977). Although mature fish display a wide range of weights, most species weigh approximately 0.1 kg as adults. **For KABAM, it is assumed that the medium-sized fish weighs 0.1 kg and its diet is 50% benthic invertebrates and 50% small fish.**

Table C17. Average body weights (in kg) of medium fish at different ages.

Species (scientific name)	1 yr	2 yr	3 yr	4 yr	5 yr	6 yr	7 yr	8 yr
Green sunfish (*Lepomis cyanellus*)	0.01	0.024	0.048	0.086	0.086	0.132	-	-
Pumpkinseed (*L. gibbosus*)	0.005	0.034	0.034	0.063	0.099	0.157	0.157	0.157
Warmouth (*L. gulosus*)	0.011	0.046	0.046	0.085	0.163	0.163	-	-
Bluegill (*L. macrochirus*)	0.014	0.052	0.052	0.090	0.141	0.141	0.208	0.208
Redear sunfish (*L. microlophus*)	0.026	0.081	0.125	0.187	0.187	0.265	-	-
White crappie (*Pomoxis annularis*)	0.031	0.085	0.123	0.181	0.346	0.346	0.579	0.579
Black crappie (*P. nigromaculatus*)	0.037	0.097	0.143	0.210	0.289	0.363	0.468	0.468

- Indicates data were not available

The large fish in KABAM is designed to represent the largemouth bass (*Micropterus salmoides*), which is a predatory fish commonly found in warm waters throughout the continental United States. It is also designed to be representative of large predatory fish that are consumed by mammals and birds. The diet of largemouth bass is composed primarily of fish, including sunfish, crappie, perch, shad and smaller-sized largemouth bass. Largemouth bass will also consume crayfish, especially when no other fish are available. Largemouth bass become sexually mature between ages 2-5, with a lifespan reaching beyond 10 years. Adult largemouth bass weigh 0.25-3.6 kg, depending upon their age (Carlander 1977). **For KABAM, it is assumed that the large fish weighs 1 kg, and consumes 100% medium-sized fish.**

Since small and medium fish consume benthic invertebrates, it is assumed that these fish are sometimes present in the benthic compartment of the aquatic ecosystem. Therefore, it is assumed that small and medium fish respire some pore water. It is assumed that medium fish are predominantly present in the water column of the aquatic ecosystem, where they are consumed by large fish. It is assumed that large fish do not respire pore water. This should be indicated in Table 5 of the KABAM tool (*i.e.,* "yes" should be entered for small and medium fish and "no" should be entered for large fish in the column titled: "Do organisms in trophic level respire some pore water?").

Available water composition data for *Lepomis sp., Pomoxis sp.,* and *Micropterus sp*. include a range of 71-80% water (Table C18). Although water composition data were not available for largemouth bass, data do exist for smallmouth bass (*M. dolomieu*) and are used as a surrogate for largemouth bass. The average value of the available data is 73%. **Based on this average, the default value for KABAM representing the % water of all fish is 73%.**

Table C18. Water composition data for fish relevant to small, medium, and large default fish of KABAM.

Species (scientific name)	Reported Body Weight (kg)	Corresponding Default fish	% water	Source
Black crappie (*Pomoxis nigromaculatus*)	0.102 (±0.007)	Medium	70.7 (±0.29)	Sethajintanin et al. 2004
Smallmouth bass (*Micropterus dolomieu*)	0.277 (±0.0901)	Medium-Large	71.1 (±1.26)	Sethajintanin et al. 2004
Smallmouth bass (*Micropterus dolomieu*)	0.870 (±0.0685)	Medium-Large	71.3 (±1.76)	Sethajintanin et al. 2004
Smallmouth bass (*Micropterus dolomieu*)	0.326 (±0.177)	Medium-Large	71.9 (±1.44)	Sethajintanin et al. 2004
Black crappie (*Pomoxis nigromaculatus*)	0.148 (±0.021)	Medium	71.9 (±0.84)	Sethajintanin et al. 2004
Smallmouth bass (*Micropterus dolomieu*)	0.395 (±0.222)	Medium-Large	72.0 (±0.99)	Sethajintanin et al. 2004
Black crappie (*Pomoxis nigromaculatus*)	0.114 (±0.016)	Medium	72.1 (±0.87)	Sethajintanin et al. 2004
Black crappie (*Pomoxis nigromaculatus*)	0.111 (±0.015)	Medium	72.6 (±0.38)	Sethajintanin et al. 2004
Black crappie (*Pomoxis nigromaculatus*)	0.0798 (±0.012)	Medium	73.2 (±0.59)	Sethajintanin et al. 2004
Smallmouth bass (*Micropterus dolomieu*)	0.154 (±0.0647)	Medium	73.4 (±2.11)	Sethajintanin et al. 2004
Bluegill (*L. macrochirus*)	Not reported	unknown	79.5	Sidwell 1981

Lipid content of fish reported in the literature varies widely for *Lepomis sp., Pomoxis sp., and Micropterus sp.* from 0.5-8% on a wet weight basis, with an average value of 2.9% and a 75th percentile of 4.0% (Table C19). Table C19 includes lipid composition data for wild-caught and laboratory-reared *Lepomis sp., Pomoxis sp., and Micropterus sp.* Several lipid content values available in the literature cannot be related to the weights of the fish analyzed due to a lack of information included in the individual studies. Thus, these lipid contents cannot be related to one of KABAM's default fish. Based on this and the data in Table C19, **the default lipid composition for all three fish is set to 4%, to be representative of a high-end value.**

Table C19. Lipid composition data for fish relevant to small, medium, and large default fish of KABAM.

Species (scientific name)	Reported Body Weight (kg)	Corresponding Default fish	% Lipid (wet weight)	Source
Green sunfish (*Lepomis cyanellus*)	Not reported	Unknown	0.5-2	Price and Birge 2006
Bluegill (*L. macrochirus*)	0.012 (±0.0012)	Small	0.72 (±0.46)	Liber et al. 1999
Largemouth bass (*Micropterus salmoides*)	Not reported	Small (defined based on length data)	0.89 (±0.19)*	Miranda and Hubbard 1994
Largemouth bass (*Micropterus salmoides*)	Not reported	Small (defined based on length data)	0.95(±0.26)*	Miranda and Hubbard 1994
Largemouth bass (*Micropterus salmoides*)	Not reported	Small (defined based on length data)	0.97 (±0.18)*	Miranda and Hubbard 1994
White crappie (*Pomoxis annularis*)	Not Reported	Assume medium (spawning fish)	1	Neuman and Murphy 1992
Longear sunfish (*L. megalotis*)	Not reported	Unknown	1-2	Price and Birge 2006
Bluegill (*L. macrochirus*)	Not reported	Unknown	1-3	Price and Birge 2006
Largemouth bass (*Micropterus salmoides*)	Not reported	Unknown	1-5	Price and Birge 2006
Largemouth bass (*Micropterus salmoides*)	Not reported	Small (defined based on length data)	1.3 (±0.29)*	Miranda and Hubbard 1994
Largemouth bass (*Micropterus salmoides*)	Not reported	Small (defined based on length data)	1.3 (±0.24)*	Miranda and Hubbard 1994
Largemouth bass (*Micropterus salmoides*)	Not reported	Small (defined based on length data)	1.6 (±0.47)*	Miranda and Hubbard 1994
Bluegill (*L. macrochirus*)	Not reported (juveniles)	Presume small	1.7*	Fischer et al. 1998
Bluegill (*L. macrochirus*)	Not reported (adult males)	Presume medium	1.8*	Fischer et al. 1998
Smallmouth bass (*Micropterus dolomieu*)	Not reported	Unknown	1.90	Kay et al. 2005
White crappie (*Pomoxis annularis*)	Not Reported	Assume medium (spawning fish)	2	Neuman and Murphy 1992
Bluegill (*L. macrochirus*)	Not reported (adult females)	Presume medium	2.1*	Fischer et al. 1998
Black crappie (*Pomoxis nigromaculatus*)	0.114 (±0.016)	Medium	2.19 (±0.51)	Sethajintanin et al. 2004
Bluegill (*L. macrochirus*)	Not reported	Unknown	2.3	Sidwell 1981
Black crappie (*Pomoxis nigromaculatus*)	0.111 (±0.015)	Medium	2.54 (±1.85)	Sethajintanin et al. 2004
Smallmouth bass (*Micropterus dolomieu*)	Not reported	Unknown	2.70	Kay et al. 2005
Black crappie (*Pomoxis nigromaculatus*)	0.148 (±0.021)	Medium	2.82 (±0.36)	Sethajintanin et al. 2004
White crappie (*Pomoxis annularis*)	Not Reported	Assume medium (spawning fish)	3	Neuman and Murphy 1992
Smallmouth bass (*Micropterus dolomieu*)	0.395 (±0.222)	Medium-Large	3.09 (±1.08)	Sethajintanin et al. 2004

Black crappie (*Pomoxis nigromaculatus*)	0.0798 (±0.012)	Medium	3.11 (±1.63)	Sethajintanin et al. 2004
Black crappie (*Pomoxis nigromaculatus*)	0.102 (±0.007)	Medium	3.15 (±0.40)	Sethajintanin et al. 2004
Smallmouth bass (*Micropterus dolomieu*)	Not reported	Medium-Large (defined based on length data)	3.3 (±0.3)	Kwon et al. 2006
Smallmouth bass (*Micropterus dolomieu*)	0.154 (±0.0647)	Medium	3.33 (±1.8)	Sethajintanin et al. 2004
Smallmouth bass (*Micropterus dolomieu*)	0.326 (±0.177)	Medium-Large	4.17 (±1.34)	Sethajintanin et al. 2004
Smallmouth bass (*Micropterus dolomieu*)	0.870 (±0.0685)	Medium-Large	4.93 (±0.33)	Sethajintanin et al. 2004
White crappie (*Pomoxis annularis*)	Not Reported	Assume medium (spawning fish)	5	Neuman and Murphy 1992
White crappie (*Pomoxis annularis*)	Not Reported	Assume medium (spawning fish)	5	Neuman and Murphy 1992
Smallmouth bass (*Micropterus dolomieu*)	0.277 (±0.0901)	Medium-Large	5.03 (±0.358)	Sethajintanin et al. 2004
Smallmouth bass (*Micropterus dolomieu*)	Not reported	Medium-Large (defined based on length data)	5.5 (±0.4)	Kwon et al. 2006
Smallmouth bass (*Micropterus dolomieu*)	Not reported	Medium-Large (defined based on length data)	5.6 (±0.2)	Kwon et al. 2006
Smallmouth bass (*Micropterus dolomieu*)	Not reported	Medium-Large (defined based on length data)	5.8 (±0.4)	Kwon et al. 2006
White crappie (*Pomoxis annularis*)	Not Reported	Assume medium (spawning fish)	6	Neuman and Murphy 1992
Bluegill (*L. macrochirus*)	0.00972 (±0.00276)	Small	7.9 (±0.14)	Carr et al. 1997
			Average	2.9
			75th percentile	4.0
			90th percentile	5.5

*Calculated from reported dry weight assuming that fish = 73% water (Table C18).

The wet weight of an organism is the sum of the water, lipid, and NLOM content. By default, if the water content of fish is 73% of the wet weight, and the % lipid is known (default = 4%), the NLOM content of fish is the % remaining after subtracting the water and lipid content from 100%. **Therefore, the default parameter for NLOM composition is 23%.**

Appendix D. Selection of Mammal Species of Concern and Corresponding Biological Parameters

Mammal species of concern were defined for use as default species in KABAM. Mammals were considered to be of concern for pesticide exposures through aquatic bioaccumulation if their diets incorporated freshwater aquatic animals. Specific species were identified using a *Field Guide to Mammals of North America* (Reid 2006). This guide contains information on the ranges, taxonomy, habits, feeding preferences, and habitats of mammals located in the continental United States, Canada, and Alaska.

A review of this source identified six species of mammals that consume aquatic animals. These include the American water shrew (*Sorex palustris*), the fog shrew (*Sorex sonomae*), the star-nosed mole (*Condylura cristata*), the marsh rice rat (*Oryzomys palustris*), the American mink (*Mustela vison*), and the Northern river otter (*Lontra canadensis*). Additional references were sought to obtain data on the body weights and feeding preferences of these mammals. These species are used in KABAM to represent mammals of concern for risks of pesticide exposures through aquatic bioaccumulation. Descriptions of these species are provided below. Information from these species descriptions were used to define the default parameters used to represent mammals in the KABAM tool.

D.1. Descriptions of Mammal Species

D.1.1. American Water Shrew (*Sorex palustris*)

The distribution of the American water shrew includes Canada, Alaska, and areas of the continental United States, including the West Coast, Rocky Mountains, Great Lakes, Appalachian, and New England areas. These shrews inhabit areas boarding fast and slow moving streams, marshes, creeks, and ponds. This species is primarily insectivorous, consuming aquatic invertebrates, such as stonefly nymphs, mayflies, caddisflies, and diptera. The American water shrew is also known to consume other animals, including fish, salamanders, leaches, and dead mice. Documented body weights range 0.008-0.018 kg, with males weighing more than females (Beneski and Stinson 1987).

D.1.2. Fog Shrew (*Sorex sonomae*)

Fog shrews inhabit parts of Oregon and California on the Pacific Coast in the “fog belt.” This species is found in marshes, near streams, and in forests. Their diet includes insects, earthworms, centipedes, slugs, snails, and amphibians. Their weight ranges 0.0055-0.015 kg (Reid 2006, Smithsonian 2008).

D.1.3. Marsh Rice Rat (*Oryzomys palustris*)

Marsh rice rats are distributed in states along the Gulf of Mexico and East Coast of the United States. This species inhabits wetlands, marshes, swamps, meadows, and areas along streams. Its diet includes insects, fiddler crabs, snails, fish, clams, arthropods, wetland plants, seeds, fungus, baby turtles, bird eggs, and carrion (of mammals and birds). Their weight ranges 0.045-0.080 kg (Wolfe 1982).

Six subspecies of *O. palustris* have been recognized (Wolfe 1982). One of these subspecies, *Oryzomys palustris natator* has been federally listed as endangered since 1991. This subspecies is known to occur in Florida and has a designated critical habitat (USFWS 1993).

D.1.4. Star-nosed Mole (*Condylura cristata*)

The star-nosed mole is distributed throughout the Eastern and Great Lakes regions of the United States and Canada. It inhabits marshy areas and streams. The diet of this species includes aquatic annelids, aquatic insects, small fish, mollusks, crustaceans, grubs, and earthworms. Reported body weights range 0.034-0.085 kg. The weights of these animals do not differ by sex but by location within their geographic distribution range, with smaller animals being observed in the southern parts of the range (*e.g.,* Tennessee) (Petersen and Yates 1980, Reid 2006, Smithsonian 2008).

D.1.5. American Mink (*Mustela vison*)

The American mink is distributed throughout the United States and Canada, except in the dry areas of Arizona, Nevada, California, Utah, and Texas. Mink inhabit wetlands and marshes. Their diet is composed mostly of fish, amphibians (frogs), crustaceans (crayfish and crabs), muskrats, and other small mammals. They will also consume squirrels, birds, bird eggs, reptiles, aquatic insects, earthworms, and snails if given the opportunity. Individual body weights vary based on range and sex, with females weighing less than males. Documented body weights of this species range 0.45-1.8 kg (Larivière 1999, USEPA 1993).

D.1.6. Northern River Otter (*Lontra canadensis*)

The historical distribution of the Northern river otter includes most of the United States and Canada. The current distribution of this species in the United States includes states bordering the Gulf of Mexico and Great Lakes, the East Coast, New England, the West Coast and Alaska, as well as Canada (Larivière and Walton 1998, Reid 2006). Northern river otters inhabit lakes, swamps, marshes, streams, and ponds. The diet of this species is primarily fish, but also includes frogs, crayfish, small mollusks, reptiles, birds, and fruits. Body weights range 5-15 kg, with males weighing more than females (USEPA 1993, Larivière and Walton 1998).

D.2. Determination of Mammalian Default Parameters for KABAM

Tables 7 and 8 of the KABAM tool allow the user to identify six mammal species of concern, their body weights and their diets. For the purpose of KABAM, mammalian species of concern include those that consume aquatic animals. Based on the information above, relevant species in the United States include the American water shrew, the fog shrew, the star-nosed mole, the marsh rice rat, the American mink, and the Northern river otter. A detailed version (with specific mammals identified) of the conceptual model of the aquatic ecosystem depicted in Figure I of the

User's Guide is provided in Figure D1. Default values representing the body weights and diets of these mammals are described below.

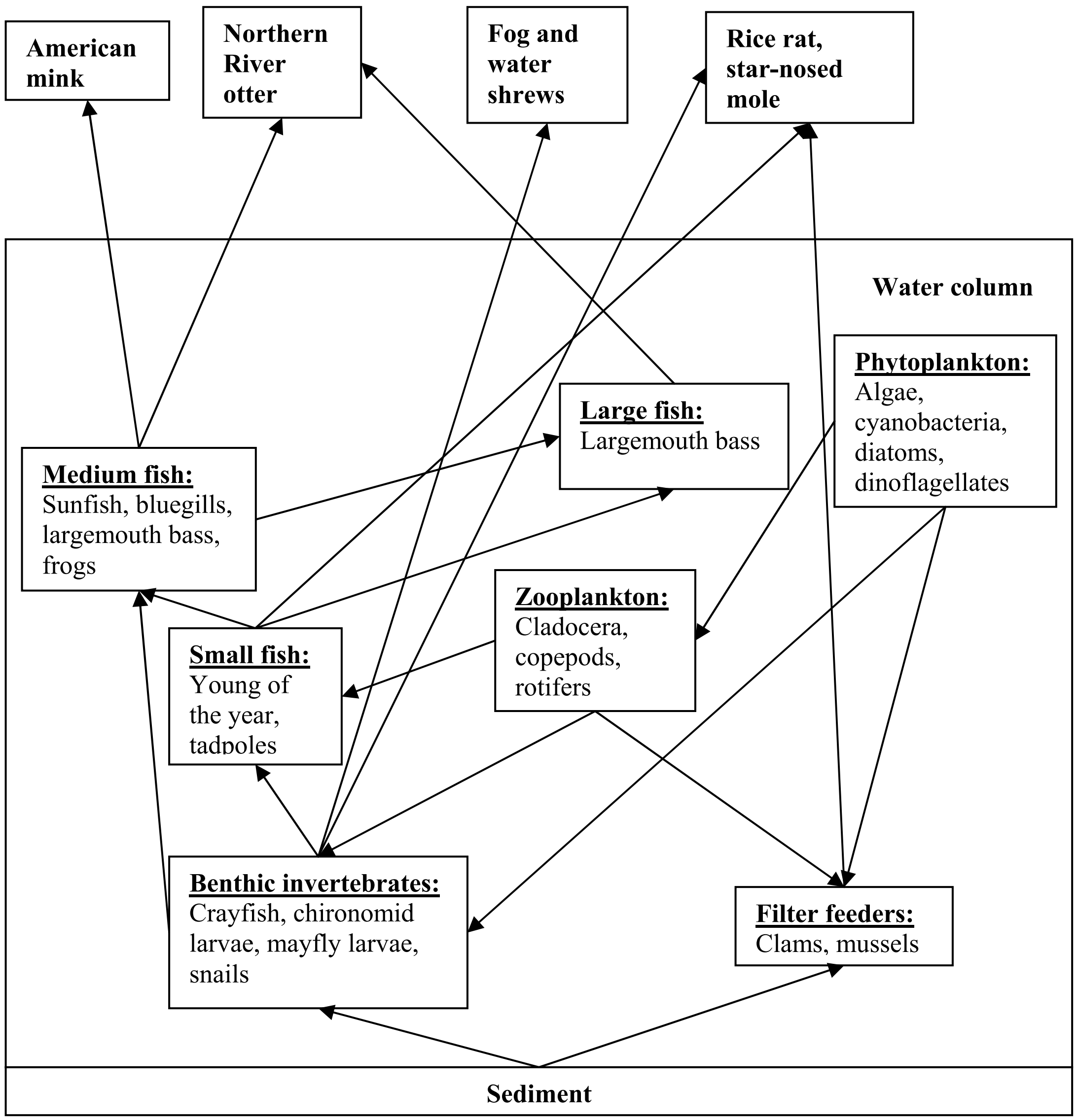

Figure D1. Detailed conceptual model depicting aquatic food web, with mammals included. Arrows depict direction of trophic transfer of bioaccumulated pesticides from lower levels to higher levels of the food web.

D.2.1. Identification of Default Body Weights for Mammalian Species

Body weight and diet are the parameters that distinguish one mammalian species from another within KABAM. Two pairs of species have similar body weights and diets, such that they can be grouped together. These pairs are 1) the American water shrew and the fog shrew; and 2) the star-nosed mole and the marsh rice rat. The American mink and the northern river otter are sufficiently different in body weights to distinguish them as separate default species in the model.

The selected body weight value influences the estimates of pesticide exposure through consumption of contaminated food items, as well as dose-adjusted toxicity values. Therefore, the magnitude of the body weight parameter has an effect on the magnitude of the RQ. Since higher body weight values result in higher dose-based RQs, the higher body weight values were selected to represent the four groups of mammals used in KABAM. In order to bound risk estimates for the two heaviest species of mammals (*i.e.*, American mink and Northern river otter), default parameters are set to the minimum and maximum body weights. The following values are suggested for inclusion in Table 7 of the KABAM tool to represent mammals 1-6:

Mammal #	Name	Body weight (kg)
Mammal 1	Fog/Water Shrew	0.018
Mammal 2	Rice Rat/Star-nosed mole	0.085
Mammal 3	Small Mink	0.450
Mammal 4	Large Mink	1.800
Mammal 5	Small River Otter	5.000
Mammal 6	Large River Otter	15.000

D.2.2. Determination of Daily Food Intake

If the weight of a food item (*i.e.,* aquatic trophic level) is less than that of the amount of food consumed by the mammal in one day, then the food item is a reasonable assignment. In order to determine whether or not a particular trophic level is relevant to a mammal, the daily food intake is estimated.

The dry food intake per day (F_{dry}, kg/day) for a mammal can be calculated according to Equation D1 (USEPA 1993). This value can be converted to represent food intake per day on a wet weight basis (F_{wet}, kg/day) by assuming that the diet of an organism is 75% water (Equation D2, see Appendix C for % water of aquatic organisms).

$$Equation\ D1.\quad F_{dry} = 0.0687 * BW^{0.822}$$

$$Equation\ D2.\quad F_{wet} = \frac{F_{dry}}{1-(\%\ water\ of\ diet)}$$

The resulting wet food intakes per day for the mammalian species of concern for KABAM are provided in Table D1. This table presents food intake per day for each species based on the low and high ranges of the body weights. These wet food intakes can be used to assign appropriate aquatic animals to the default diets of these mammals.

Table D1. Low- and high-end body weights and estimated food intake per day of mammals which consume aquatic animals.

Species	Body Weight (kg)	Dry Food Intake per day (kg)	Wet Food Intake per day (kg)	Percent Body Weight Consumed Daily
Shrew (Water and Fog)	0.006	0.001	0.004	67%
Shrew (Water and Fog)	0.018	0.003	0.010	56%
Rice Rat, Star-nosed mole	0.034	0.004	0.017	50%
Rice Rat, Star-nosed mole	0.085	0.009	0.036	42%
Mink	0.450	0.036	0.143	31%
Mink	1.800	0.111	0.446	25%
River Otter	5.000	0.258	1.032	20%
River Otter	15.000	0.636	2.545	17%

D.2.3. Definition of Default Diets of Mammals for use in KABAM

Water/fog shrew

The diets of the American water and fog shrews (see section D.1) include species that would be classified as benthic invertebrates (*e.g.,* stonefly nymphs, mayflies, and snails) and fish (*e.g.,* fish and amphibians) according to the trophic levels of KABAM. **However, since these species are primarily insectivorous, the default diet is assigned as 100% benthic invertebrates.**

Based on the daily food intake for these two species (Table E.1), it is reasonable to assume that these shrews can consume organisms in the small fish category. If interested in the potential acute risk to water/fog shrews from pesticides through consumption of fish/amphibians, the model user could define the diet of these mammals as 100% small fish. Since this represents a higher trophic level in the aquatic ecosystem than the benthic invertebrates, this assumption may result in a higher RQ.

Rice rat/star-nosed mole

The diets of the rice rat and the star-nosed mole (see section D.1) include species that would be classified as benthic invertebrates (*e.g.,* arthropods, snails), filter feeders (*e.g.,* clams) and fish according to the trophic levels of KABAM. Based on the daily food intake for these two species (Table E.1), it is reasonable to assume that individuals of these species could consume organisms in the small fish category. **Since no data are available to define feeding preferences of these two species, for the purpose of KABAM, the default diet composition of these mammals is equally distributed among these three trophic levels (*i.e.,* 34% benthic invertebrates, 33% filter feeders, and 33% small fish).**

American mink

The diet of the American mink (see section D.1) includes species that would be classified as benthic invertebrates (*e.g.,* crayfish) and small/medium-sized fish according to the trophic levels of KABAM. Based on the daily food intake for this species (Table E.1), it is reasonable to assume that these mammals could consume organisms in the small and medium fish category. **The default diet for this mammal is 100% medium fish.**

Northern river otter

The diet of the Northern river otter (see section D.1) is primarily fish, but also includes species that would be classified as benthic invertebrates (*e.g.,* crayfish) according to the trophic levels of KABAM. Based on the daily food intake for this species (Table D.1), it is reasonable to assume that these mammals may consume organisms in the small, medium, and large fish categories. According to USEPA 1993, river otters have been documented as including various fish that would be classified in different trophic levels of KABAM, including sunfish and bass. **Therefore, the default diet for this mammal is 100% medium fish for the small otter and 100% large fish for the large otter.**

Appendix E. Selection of Bird Species of Concern and Corresponding Biological Parameters

Bird species of concern were identified in order to define default parameters (for body weight and diet composition) to represent birds in KABAM. Bird species were considered to be of concern for pesticide exposures through aquatic bioaccumulation if their diets incorporated freshwater aquatic animals. Specific species were identified using the Smithsonian handbooks' *Birds of North America (Eastern and Western Regions)* (Alsop 2001a and 2001b). These handbooks contain information on the ranges, taxonomy, habits, feeding preferences, and habitats of birds located in the continental United States, Canada, and Alaska.

A review of this source identified over 40 bird species of concern that fall into 11 families. These families include: Accipitridae (eagles, hawks and kites), Alcedinidae (kingfisher), Anatidae (ducks), Ardeidae (herons, egrets and bitterns), Gruidae (cranes), Pelecanidae (pelicans), Phalacrocoracidae (cormorants), Podicipedidae (grebes), Rallidae (rails), Scolopacidae (sandpiper) and Threskiornithidae (ibis). Descriptions of these families are provided below.

It should be noted that this review was not intended to be inclusive of every relevant species or family of birds inhabiting North America. Rather, the intention of this review was to identify birds that may consume aquatic animals containing pesticides that bioaccumulate in aquatic ecosystems. Information from identified bird species and families was used to define the default parameters representing birds in the KABAM tool. These default parameters are described below.

E.1. Bird Family Descriptions

E.1.1. Accipitridae (Eagles, Hawks and Kites)

Most species of this family prey upon terrestrial rodents; however, several rely upon aquatic animals for their diet (Table E1). These species include the osprey (*Pandion haliaetus*) and the bald eagle (*Haliaeetus leucocephalus*) (Alsop 2001a and 2001b). Ospreys fly over freshwater and saltwater areas and catch fish from the surface of the water using their feet. Body weights of osprey range from 1.25 to 2.0 kg (USEPA 1993). Bald eagles eat fish, rodents, birds, and carrion. Body weights of adult bald eagles range 3.0 – 5.8 kg (USEPA 1993). An additional member of this family, the snail kite (*Rostrhamus sociabilis*), has a subspecies that is federally listed as endangered (USFWS 2008). This species is known to occur in wetlands of Florida, where the bird eats snails (Alsop 2001a). The average body weight of this bird is 0.38 kg (Dunning 1984).

Table E1. Body weights and diets of species of Accipitridae that prey upon aquatic animals.

Species (scientific name)	Body weight (kg)	Diet
Snail kite (*Rostrhamus sociabilis*)	0.38[1]	snails[2]
Osprey (*Pandion haliaetus*)	1.25-2.00[3]	fish[3]
Bald eagle (*Haliaeetus leucocephalus*)	3.00 – 5.80[3]	fish, rodents, birds, and carrion[3]

[1]Dunning 1984; [2]Alsop 2001a and 2001b; [3]USEPA 1993

E.1.2. Alcedinidae (kingfisher)

One species of this family, the belted kingfisher (*Ceryle alcyon*) is widely distributed throughout North America, inhabiting freshwater areas such as lakes, rivers, and ponds, as well as marine coastal areas. This species feeds primarily upon fish, but its diet also includes amphibians, insects, and crayfish. Body weights of this species range 0.13-0.22 kg (USEPA 1993; Table E2).

Table E2. Body weights and diets of species of Alcedinidae that prey upon aquatic animals.

Species (scientific name)	Body weight (kg)	Diet
Belted kingfisher (*Ceryle alcyon*)	0.13-0.22[1]	primarily fish, but also amphibians, insects and crayfish[1]

[1]USEPA 1993

E.1.3. Anatidae (Ducks)

There are many species of ducks that are widely distributed in North America (Table E3). Ducks predominantly inhabit freshwater areas such as lakes, rivers, wetlands, and ponds. Their diets include a wide variety of aquatic organisms, such as aquatic insects, insect larvae, snails, amphibians, fish, crayfish, mollusks, plankton, and aquatic plants (Alsop 2001a and 2001b). Body weights of ducks vary based on the species, with a range of 0.3-2.0 kg for ducks inhabiting freshwater areas (Dunning 1984).

Table E3. Body weights and diets of species of Anatidae that prey upon aquatic animals.

Species (scientific name)	Body weight (kg)[1]	Diet[2]
Cinnamon teal (*Anas cyanoptera)*	0.36-0.41	seeds, aquatic insects, rice, algae, snails, crustaceans
Bufflehead (*Bucephala alboela)*	0.30-0.55	aquatic insects and insect larvae, snails, small fish, seeds
Wood duck (*Aix sponsa)*	0.64-0.91	plants, animals, snails, tadpoles, salamanders
Hooded merganser (*Lophodytes cuculatus)*	0.54-0.91	fish, crustaceans, aquatic insects, aquatic animals
Lesser scaup (*Aythya affinis)*	0.54-1.05	plants and animals
Common goldeneye (*Bucephala clangula)*	0.80-1.40	mollusks, crustaceans, insects, aquatic plants
Mallard (*Anas platyrhynchos)*	0.72-1.58	plants, insects, mollusks, crustaceans
Red-breasted merganser (*Mergus serrator)*	0.91-1.31	fish
Common merganser (*Mergus merganser)*	1.05-2.05	small fish, mollusks, crustaceans, aquatic insects, some plants

[1]Dunning 1984; [2]Alsop 2001a and 2001b

E.1.4. Ardeidae (Herons, Egrets and Bitterns)

This family includes species of herons, bitterns and egrets, several of which inhabit waters of North America (Table E4). Their habitats include freshwater areas such as lakes, rivers, ponds, wetlands, and streams, as well as marine coastal areas. These birds wade through water to spear their food with their beaks. Their diets include fish, crustaceans, amphibians, snakes, crayfish, and insects (Alsop 2001a and 2001b, USEPA 1993). Individuals of this family range in weight from 0.08 to 2.9 kg, depending upon the species (Dunning 1984, USEPA 1993).

Table E4. Body weights and diets of species of Ardeidae that prey upon aquatic animals.

Species (scientific name)	Body weight (kg)[1]	Diet[2]
Least bittern (*Ixobrychus exilis)*	0.08-0.09	fish, insects
Green heron (*Butorides virescens)*	0.21[2]	fish, aquatic invertebrates
Snowy egret (*Egretta thula)*	0.35-0.40	crustaceans, insects, fish
Little blue heron (*Egretta caerulea)*	0.32-0.45	small vertebrates, crustaceans, large insects
American bittern (*Botaurus lentiginosus)*	0.52-1.07	frogs, small eels, small fish, snakes, salamanders, crayfish, small rodents, water bugs
Yellow-crowned night heron (*Nyctanassa violacea)*	0.72-0.85	crustaceans, fish, shellfish
Black crowned night heron (*Nycticorax nycticorax)*	0.73-1.01	fish, mollusks, small rodents, frogs, snakes, crustaceans, plants, eggs, birds
Great egret (*Ardea alba)*	0.80-1.07	fish, frogs, snakes, crayfish, large insects
Great blue heron (*Ardea herodias)*	1.87-2.88	fish, other aquatic animals

[1]Dunning 1984; [2]Alsop 2001a and 2001b

E.1.5. Gruidae (Cranes)

Cranes inhabit freshwater wetlands and marshes. These birds eat fish, frogs, small mammals, mollusks, crustaceans, and plants (Alsop 2001a and 2001b). Two species of cranes, *i.e.*, the whooping crane (*Grus americana*) and the Mississippi sandhill crane (*Grus canadensis pulla*), are federally listed as endangered (USFWS 2008). Body weights of the whooping crane and sandhill crane range 2.5-6.7 kg (Dunning 1984) (Table E5).

Table E5. Body weights and diets of species of Gruidae that prey upon aquatic animals.

Species (scientific name)	Body weight (kg)[1]	Diet[2]
Whooping crane (*Grus americana*)	5.44-6.36	fish, frogs, small mammals, mollusks, crustaceans, and plants
Sandhill crane (*Grus canadensis*)	2.45-6.70	plants and animals

[1]Dunning 1984; [2]Alsop 2001a and 2001b

E.1.6. Pelecanidae (Pelicans)

There is one species of pelican that inhabits freshwater aquatic habitats of North America: the American white pelican (*Pelecanus erythrorhynchos*). Their habitats include freshwater areas such as lakes, rivers, ponds, wetlands and streams, as well as marine coastal areas. The diet of these birds includes fish (Alsop 2001a and 2001b). The average weight of the American white pelican is 7.5 kg (Dunning 1984) (Table E6).

Table E6. Body weights and diets of species of Pelecanidae that prey upon aquatic animals.

Species (scientific name)	Body weight (kg)	Diet
American white pelican (*Pelecanus erythrorhynchos*)	7.5[1]	fish[2]

[1]Dunning 1984; [2]Alsop 2001a and 2001b

E.1.7. Phalacrocoracidae (Cormorants)

Of the species of cormorants inhabiting North America, the double-breasted cormorant (*Phalacrocorax auritus*) is the most widespread, inhabiting freshwater areas such as lakes, rivers, ponds, as well as marine coastal areas. Cormorants dive for their prey, which includes fish, crustaceans, and amphibians (Alsop 2001a and 2001b). The average weight of the double-breasted cormorant is 1.8 kg (Dunning 1984).

Table E7. Body weights and diets of species of Phalacrocoracidae that prey upon aquatic animals.

Species (scientific name)	Body weight (kg)	Diet
Double-breasted cormorant (*Phalacrocorax auritus*)	1.60-2.04[1]	fish, crustaceans and amphibians[2]

[1]Dunning 1984; [2]Alsop 2001a and 2001b

E.1.8. Podicipedidae (Grebes)

Several species of grebes reside in the continental United States (Table E8). Their habitats include freshwater areas such as lakes, rivers, ponds, wetlands, and streams, as well as marine areas. These birds forage for aquatic insects, crustaceans, and fish by diving underwater (Alsop 2001a and 2001b). They range in weight 0.2-1.8 kg (Alsop 2001a and 2001b, Dunning 1984).

Table E8. Body weights and diets of species of Podicipedidae that prey upon aquatic animals.

Species (scientific name)	Body weight (kg)[1]	Diet[2]
Eared grebe (*Podiceps nigricollis)*	0.22-0.37	aquatic insects
Pied-billed grebe (*Podilymbus podiceps)*	0.34-0.55	aquatic insects, small fish, crustaceans
Horned grebe (*Podiceps auritus)*	0.33-0.53	fish, crustaceans, aquatic insects
Western grebe (*Aechmorphorus occidentalis)*	0.80-1.82	fish
Clark's grebe (*Aechmophorus clarkia)*	1.50[2]	fish

[1]Dunning 1984; [2]Alsop 2001a and 2001b

E.1.9. Rallidae (Rails)

Rail species inhabit freshwater areas such as lakes, rivers, ponds, wetlands and streams as well as saltwater marshes of North America. These species feed upon crustaceans, aquatic insects, snails, fish, and plants (Alsop 2001a and 2001b). Individuals of this family range in weight from 0.07 to 0.49 kg (Dunning 1984) (Table E9). One species from this family, the clapper rail (*Rallus longirostris*) is federally listed as an endangered species and is known to occur in Arizona, California, Nevada, and Utah (USFWS 2008).

Table E9. Body weights and diets of species of Rallidae that prey upon aquatic animals.

Species (scientific name)	Body weight (kg)[1]	Diet[2]
Sora (*Porzana carolina)*	0.08	plants, insects, spiders, small crustaceans, snails
Virginia rail (*Rallus limicola)*	0.07-0.12	insects (primarily), worms, crustaceans, small fish
King rail (*Rallus elegans)*	0.25-0.49	plants, aquatic invertebrates, aquatic vertebrates
Clapper rail (*Rallus longirostris*)	0.25-0.35	crabs, crustaceans, worms, amphibians, reptiles, mollusks, small fish, aquatic insects

[1]Dunning 1984; [2]Alsop 2001a and 2001b

E.1.10. Scolopacidae (Sandpipers)

Many species of sandpipers inhabit freshwater aquatic habitats of North America (Table E10). These habitats include lakes, rivers, ponds, wetlands, and streams. Their diets include aquatic invertebrates, insects, crustaceans, small fish, amphibians, and mollusks (Alsop 2001a and 2001b). Body weights of sandpipers range 0.02- 0.70 kg (Dunning 1984).

Table E10. Body weights and diets of species of Scolopacidae that prey upon aquatic animals.

Species (scientific name)	Body weight (kg)[1]	Diet[2]
Least sandpiper (*Calidris minutilla)*	0.02[2]	insects and larvae, crustaceans
Spotted sandpiper (*Actitis macularia)*	0.03-0.06	invertebrates, small fish
Wilson's phalarope (*Phalaropus tricolor)*	0.07[2]	larvae, crustaceans, seeds
Greater yellow legs (*Tringa melanoleca)*	0.12-0.22	small fish, insects and larvae, crabs, snails
Willet (*Catoptrophorus semipalmatus)*	0.22	aquatic insects, mollusks, small fish
Long-billed curlew (*Numenius americanus)*	0.57-0.70	aquatic insects, larvae, mollusks, crustaceans, small amphibians

[1]Dunning 1984; [2]Alsop 2001a and 2001b

E.1.11. Threskiornithidae (Ibis)

Ibis inhabit freshwater areas such as lakes, rivers, ponds, wetlands, and streams, as well as marine coastal areas of North America. These species are wading birds that feed upon crayfish, aquatic invertebrates, fish, and frogs (Alsop 2001a and 2001b). Individuals of this family range in weight from 0.4 to 1.3 kg (Dunning 1984) (Table E11).

Table E11. Body weights and diets of species of Threskiornithidae that prey upon aquatic animals.

Species (scientific name)	Body weight (kg)[1]	Diet[2]
White-faced ibis (*Plegadis chihi)*	0.43-0.81	crayfish, aquatic invertebrates, fish, frogs
White ibis (*Eudocimus albus*)	0.59-1.28	not stated

[1]Dunning 1984; [2]Alsop 2001a and 2001b

E.2. Detailed Conceptual Model

A detailed version of the conceptual model of the aquatic ecosystem depicted in Figure I of the User's Guide, with specific birds identified, is provided in Figure E1.

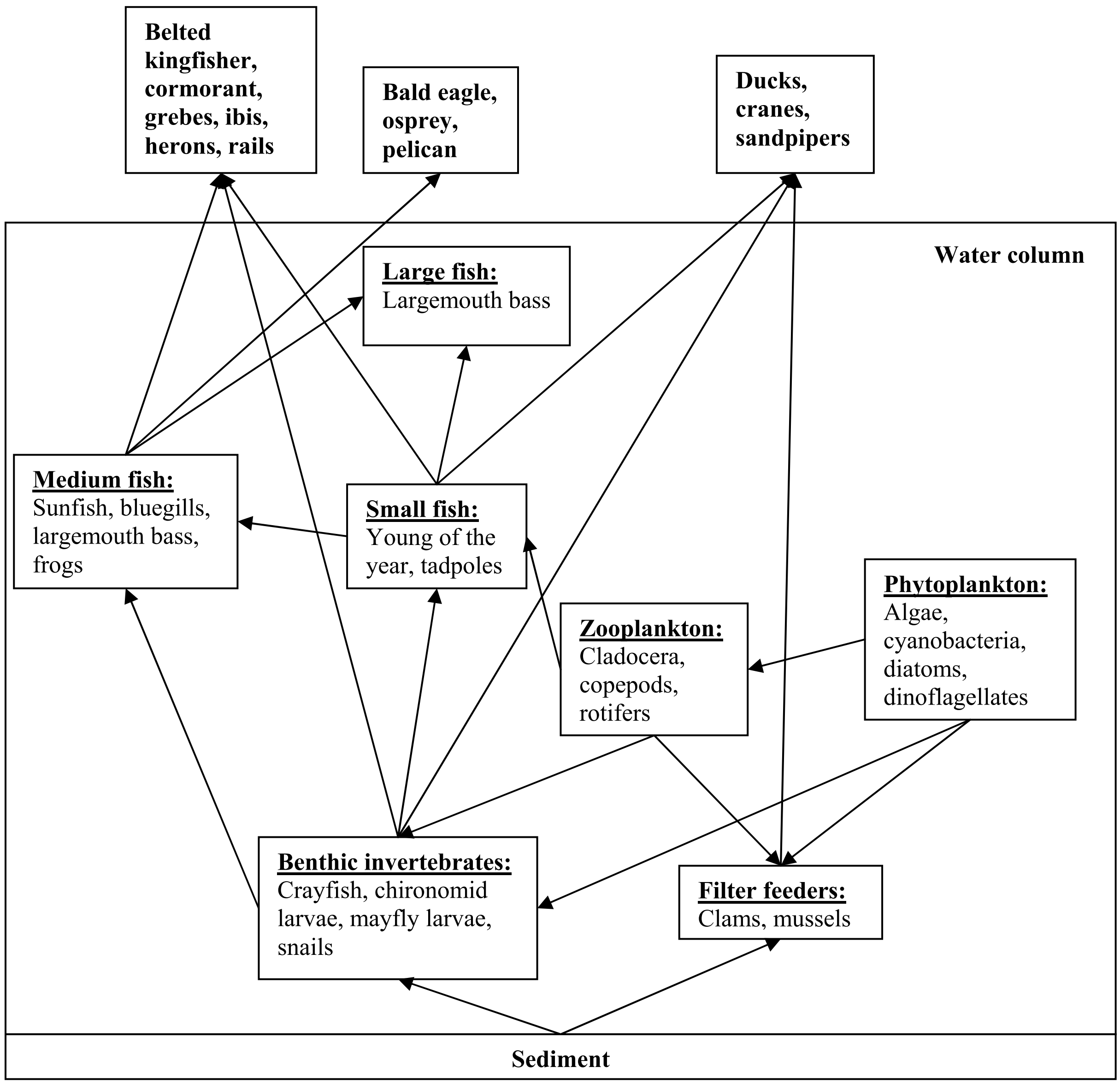

Figure E1. Detailed conceptual model depicting aquatic food web of KABAM. Arrows depict direction of trophic transfer of bioaccumulated pesticides from lower levels to higher levels of the food web.

E.3. Determination of Daily Food Intake

If the weight of a food item (*i.e.,* aquatic trophic level) is less than that of the amount of food consumed by the bird in one day, then the food item is a reasonable assignment. In order to determine whether or not a particular trophic level is relevant to a bird, the daily food intake is estimated.

The dry food intake per day (F_{dry}, kg/day) for a bird can be calculated according to Equation E1 (USEPA 1993). This value can be converted to represent food intake per day on a wet weight basis (F_{wet}, kg/day) by assuming that the diet of an organism is 75% water (Equation E2, see Appendix C for % water of aquatic organisms).

$$Equation \quad E1. \quad F_{dry} = 0.0582 * BW^{0.651}$$

$$Equation\ E2. \quad F_{wet} = \frac{F_{dry}}{1-(\%\ water\ of\ \ diet)}$$

Of the bird families described above, body weights range 0.02-7.5 kg. The resulting wet food intakes per day for birds of concern for KABAM are provided in Table E12. This table presents food intake values per day for each species based on body weight. These wet food intakes can be used to assign appropriate aquatic animals to the default diets of these birds.

Table E12. Body weights representative of birds that consume aquatic animals and corresponding daily dry and wet food intakes.

Family or species	Body weight range (kg)	Dry Food Intake per day (kg)	Wet Food Intake per day (kg)
Sandpipers	0.02- 0.70	0.005-0.046	0.018-0.185
ducks	0.30-2.00	0.027-0.091	0.106-0.366
cranes	2.45-6.70	0.104-0.201	0.417-0.803
belted kingfisher	0.13-0.22	0.015-0.022	0.062-0.087
rails	0.07-0.49	0.010-0.037	0.041-0.146
ibis	0.43-1.28	0.034-0.068	0.134-0.273
grebes	0.22-1.82	0.022-0.086	0.087-0.344
Double-breasted cormorant	1.8	0.085	0.341
Bitterns, egrets, herons	0.08-2.90	0.011-0.116	0.045-0.466
osprey	1.25-2.00	0.067-0.091	0.269-0.366
Bald eagle	3.00 – 5.80	0.119-0.183	0.476-0.731
white pelican	7.5	0.216	0.864

E.4. Definition of Default Parameters to Represent Birds in KABAM

Based on the species descriptions above, birds can be divided into three groups based on their diets. The three diets include: 1) filter feeders, benthic invertebrates and fish, 2) benthic invertebrates and fish and 3) fish. (Table E13). These three diets were used to define the default parameters representing birds in KABAM (Table E14), which are described below.

Table E13. Summary of diets and body weights of families of birds defined as consuming aquatic animals.

Diet	Family or species	Body weight range (kg)
Filter feeders, benthic invertebrates, fish	Sandpipers	0.02- 0.70
	Ducks	0.30-2.00
	Cranes	2.45-6.70
Benthic invertebrates and fish	Belted kingfisher	0.13-0.22
	Rails	0.07-0.49
	Ibis	0.43-1.28
	Grebes	0.22-1.82
	Double-breasted cormorant	1.80
	Bitterns, egrets, herons	0.08-2.90
Fish	Osprey	1.25-2.00
	Bald eagle	3.00 – 5.80
	White pelican	7.50

Table E14. Default body weights and diet parameters for use in KABAM to represent birds.

Bird #	Bird Name	Relevant Families/species	Default weight (kg)	Default diet
1	Sandpipers	Sandpipers, ducks, cranes	0.02	33% benthic invertebrates 33% filter feeders 34% small fish
2	Cranes	Sandpipers, ducks, cranes	6.70	33% benthic invertebrates 33% filter feeders 34% medium fish
3	Rails	Belted kingfisher, rails, ibis, grebes, double-breasted cormorant, bitterns, egrets, herons	0.07	50% benthic invertebrates 50% small fish
4	Herons	Belted kingfisher, rails, ibis, grebes, double-breasted cormorant, bitterns, egrets, herons	2.90	50% benthic invertebrates 50% medium fish
5	Small Osprey	Osprey, bald eagle, white pelican	1.25	100% medium fish
6	White pelican	Osprey, bald eagle, white pelican	7.50	100% large fish

E.4.1. Birds Consuming Benthic Invertebrates, Filter Feeders, and Fish

Because sandpipers, ducks, and cranes share similar diets (*i.e.,* benthic invertebrates, filter feeders, and fish), they are considered as a group for defining input parameters for KABAM. Two of the default birds in KABAM (# 1 and 2) represent birds with a similar diet.

Comparison of the daily wet food consumption for sandpipers (Table E12) to the weight of small and medium fish in KABAM (0.01 and 0.1 kg, respectively) indicates that not all of these species would be expected to consume medium-sized fish. Therefore, it is assumed that sandpipers consume small fish. All species of cranes are expected to be able to consume a medium-sized (0.1 kg) fish in one day. Therefore, it is assumed that the diet of cranes is composed of medium-sized fish. Since the relative proportion of benthic invertebrates, filter feeders and fish within the diets of these species is unknown, it is assumed that these prey items compose an equal share of the diet of these birds.

The 1st default bird in KABAM has a diet of 33% benthic invertebrates, 33% filter feeders and 34% small fish. This bird is intended to represent the low end of birds that consume benthic invertebrates, filter feeders, and small fish. Therefore, the default body weight of 0.02 kg was selected because it is consistent with the lowest body weight of birds that have this diet (Table E13).

The 2nd default bird in KABAM has a diet of 33% benthic invertebrates, 33% filter feeders, and 34% medium fish. This bird is intended to represent the high end of birds that consume benthic invertebrates, filter feeders, and medium-sized fish. Therefore, the default body weight of 6.7 kg was selected (Table E14).

It should be noted that pesticide EECs and subsequent RQs for sandpipers, ducks, and cranes are bound by KABAM's default birds 1 and 2. RQs for these two default birds are intended to represent birds with similar size and feeding habits as sandpipers, ducks, and cranes. These EECs and RQs can be refined by the model user to represent a specific bird species by entering specific body weights of individual species of concern and the appropriate species composition of their diet.

E.4.2. Birds Consuming Benthic Invertebrates and Fish

Because belted kingfisher, rails, ibis, grebes, double-breasted cormorants, bitterns, egrets, and herons share similar diets (*i.e.,* benthic invertebrates and fish), they are considered as a group for defining input parameters for KABAM. Two of the default birds in KABAM (# 3 and 4) represent birds with a similar diet.

Comparison of the daily wet food consumption for small rails, small grebes, and the belted kingfisher (Table E12) to the weight of small and medium-sized fish in KABAM (0.01 and 0.1 kg, respectively) indicates that not all of these species would be expected to consume medium fish. Therefore, it is assumed that some of these species consume small fish. Species of rails, ibis, grebes, bitterns, egrets, herons and the double-breasted cormorant are expected to be able to consume a 0.1 kg fish per day. Therefore, it is assumed that the diet of these species is composed of medium-sized fish. Since the relative proportion of benthic invertebrates and fish within the diets of these species is unknown, it is assumed that these prey items compose an equal share of the diet of these birds.

The 3rd default bird in KABAM has a diet of 50% benthic invertebrates and 50% small fish. This bird is intended to represent the low end of birds that consume benthic invertebrates and small-sized fish. Therefore, the default body weight of 0.07 kg was selected because it is consistent with the lowest body weight of birds that have this diet (Table E13).

The 4th default bird in KABAM has a diet of 50% benthic invertebrates and 50% medium fish. This bird is intended to represent the high end of birds that consume benthic invertebrates and medium-sized fish. Therefore, the default body weight of 2.9 kg was selected (Table E14).

It should be noted that pesticide EECs and subsequent RQs for belted kingfisher, rails, ibis, grebes, double-breasted cormorants, bitterns, egrets, and herons are bounded for KABAM's default birds 3 and 4. RQs for these two default birds are intended to represent birds with similar sizes and feeding habits. These EECs and RQs can be refined for specific bird species by entering specific body weights of individual species of concern and entering the appropriate diet.

E.4.3. Birds Consuming Fish

Because osprey, bald eagles, and white pelicans share similar diets (*i.e.,* fish), they are considered as a group for defining input parameters for KABAM. Two of the default birds in KABAM (# 5 and 6) represent birds with a similar diet.

Comparison of the daily wet food consumption for the lower end body weight (1.25 kg) of these birds to the weight of medium and large fish in KABAM (0.1 and 1.0 kg, respectively) indicates that the lower weight individuals of these bird species are able to consume medium fish, but unlikely to consume large fish. Therefore, it is assumed that the diet of default bird #5 (named osprey), can be represented by 100% medium-sized fish. Comparison of the daily wet food consumption (0.86 kg/day) for the higher end body weight (7.5 kg) of these birds to the weight of large fish in KABAM (1.0 kg) indicates that the higher weight individuals of these bird species are likely to consume large fish. Therefore, it is assumed that the diet of default bird #6 (named white pelican), can be represented by 100% large-sized fish.

In order to bound EECs and RQs for these three birds, the lowest and highest body weights were selected to represent KABAM's default birds 5 and 6, respectively, in KABAM. These EECs and RQs can be refined for specific bird species by entering specific body weights of individual species of concern.

Appendix F. Description of Equations Used to Calculate the BCF, BAF, BMF, and BSAF Values

Bioconcentration, bioaccumulation, and biomagnification factors are calculated in the "results" worksheet of the KABAM tool using data from the "parameters & calculations" worksheet. The equations for these calculations are described below.

F.1. Bioconcentration

Bioconcentration is a measure of the amount of pesticide residue in an organism's tissue relative to the concentration in the organism's environment (USEPA 2008c). This includes pesticide uptake through respiration and contact, not through dietary sources. Bioconcentration factors (BCFs) are calculated by considering pesticide tissue concentrations with respect to environmental pesticide concentrations. BCF values >1 indicate that the concentration in the organism is greater than that of the medium (*e.g.*, soil or water) from which the pesticide was taken. BCFs can be calculated on a total organism basis or normalized to the lipid content of the organism.

KABAM calculates the total (body weight) BCFs of a chemical for each aquatic organism according to **Equation F1** (USEPA 2003). C_{BCF} is calculated using equation A1 (see Table A.1 of Appendix A for a full description) where $C_B = C_{BCF}$, when $k_D = k_E = k_M = k_G = 0$. The units of total BCF values are expressed as: (µg pesticide/kg wet weight)/(µg pesticide/L water). Total BCF values account for the total amount of the pesticide in the water (*i.e.,* C_{WTO}).

$$Equation\ F1. \quad Total\ BCF = \frac{C_{BCF}}{C_{WTO}}$$

$$Eq.\ A1 \quad C_B = \frac{k_1 * (m_0 * \Phi * C_{WTO} + m_P * C_{WDP}) + k_D * \Sigma(P_i * C_{Di})}{k_2 + k_E + k_G + k_M}$$

KABAM also calculates the lipid-normalized BCFs of a chemical for each aquatic organism according to **Equation F2** (USEPA 2003). The units of lipid normalized BCF values are expressed as: (µg pesticide/kg lipid)/(µg pesticide/L water). V_{LB} represents the fraction of lipid in the body of the organism for which the BCF is being derived. Lipid normalized BCF values account for the pesticide concentration that is freely dissolved in the water (*i.e.,* C_{WTO}*Φ).

$$Equation\ \ F2. \quad Lipid\ normalized\ BCF = \frac{\left({C_{BCF}}/{V_{LB}} \right)}{C_{WTO} * \Phi}$$

F.2. Bioaccumulation

Bioaccumulation is the net uptake of a pesticide from the environment by all possible routes (*e.g.,* respiration, diet, dermal) from any source (*e.g.,* water, sediment, and other organisms) (Spacie *et al*. 1995). Bioaccumulation factors (BAF) are calculated by considering pesticide tissue concentrations with respect to environmental pesticide concentrations. BAF values >1 indicate that the accumulation in the organism is greater than that of the medium (*e.g.*, soil or water) from which the pesticide was taken. These factors can be calculated on a total organism basis or normalized to the lipid content of the organism.

KABAM calculates the total BAFs of a chemical for each aquatic organism according to **Equation F3** (USEPA 2003). The units of total BAF values are expressed as: (µg pesticide/kg wet weight)/(µg pesticide/L water). C_B is calculated according to **Equation A1**. Total BAF values account for the total amount of the pesticide in the water (*i.e.,* C_{WTO}).

$$Equation\ \ F3.\quad Total\ BAF = \frac{C_B}{C_{WTO}}$$

Lipid-normalized BAFs of a chemical are calculated for each aquatic organism according to **Equation F4** (USEPA 2003). The units of lipid normalized BAF values are expressed as: (µg pesticide/kg lipid)/(µg pesticide/L water). The variable C_B is calculated according to **Equation A1**. The variable V_{LB} represents the fraction of lipid in the body of the organism for which the BCF is being derived. Lipid normalized BAF values account for the pesticide concentration that is freely dissolved in the water (*i.e.,* C_{WTO}*Φ).

$$Equation\ \ F4.\quad Lipid\ normalized\ BAF = \frac{\left({C_B}/{V_{LB}} \right)}{C_{WTO} * \Phi}$$

Accumulation factors are also derived by considering pesticide tissue concentrations with respect to pesticide concentrations in sediment. Biota-sediment accumulation factors (BSAFs) are calculated by dividing the lipid normalized concentration of a chemical in an organism by the chemical concentration in the sediment (dry weight), normalized to the organic carbon content of the sediment (**Equation F5**) (USEPA 2003). The variable C_{SOC} represents the pesticide concentration in the sediment, normalized to the organic carbon content of the sediment (units of g/kg OC).

$$Equation\ \ F5.\quad BSAF = \frac{\left({C_B}/{V_{LB}} \right)}{C_{SOC}}$$

F.3. Biomagnification

Biomagnification is the increase of a pesticide concentration in the tissue of an organism compared to the tissue concentrations of its prey (USEPA 2008b). Biomagnification factors (BMFs) are calculated by considering lipid normalized pesticide tissue concentrations within an organism with respect to the lipid normalized concentrations of that pesticide in the prey of the organism. Factors >1 indicate the occurrence of biomagnification.

KABAM calculates the BMFs of a chemical for each aquatic organism according to **Equation F6** (USEPA 2003). The units of BMF values are expressed as: (µg pesticide/kg lipid)/(µg pesticide/kg lipid). The variable C_B is calculated according to **Equation A1**. V_{LB} represents the fraction of lipid in the body of the organism for which the BMF is being derived. P_i represents the fraction of diet containing prey item i. C_{Di} represents the concentration of the pesticide in prey item i and V_{LBi} represents the fraction of lipid in the body of the prey item i. It should be noted that although KABAM allows aquatic organisms to consume sediment, uptake of pesticide through consumption of sediment is not considered in the calculation of BMFs in the model tool.

$$Equation\ \ F6. \quad BMF = \frac{\left({C_B}/{V_{LB}} \right)}{\sum \left(P_i * {C_{Di}}/{V_{LBi}} \right)}$$

Appendix G. Description of Equations Used to Calculate Dietary-Based and Dose-Based EECs, Toxicity Values, and RQs for Mammals and Birds Consuming Contaminated Aquatic Organisms

Exposures of birds and mammals to pesticides accumulated in tissues of aquatic organisms are calculated by the KABAM tool. Relevant toxicity data are also calculated by KABAM based on input data from toxicity studies for birds and mammals. The equations used to estimate exposure and to adjust toxicity values and to calculate RQs depicted in Tables 14-15 of the KABAM tool are described below.

G.1. Food Ingestion Rates

Dry food ingestion rates (FI_{dry}) are estimated for mammals and birds using allometric equations that relate food intake with body weight (**Equations G1 and G2**, respectively). FI is calculated in kg dry food/kg-bw day and BW is animal body weight in kg.

$$Equation\ G1. \quad FI_{dry} = \frac{0.0687 * BW^{0.822}}{BW} \quad (mammals)$$

$$Equation\ G2. \quad FI_{dry} = \frac{0.0582 * BW^{0.651}}{BW} \quad (birds)$$

Food intake (FI) values are converted from food dry weight/kg-bw day to food wet weight/day using the wet weight of the assigned diet of each mammal and bird (**Equation G3**). The variable P_i represents the fraction of diet of the mammal or bird containing prey item i (an aquatic organism). The variable V_{WBi} represents the fraction of water in the body of the prey item i.

$$Equation\ \ G3. \quad FI_{wet} = \frac{FI_{dry}}{1 - \sum\left(P_i * V_{WBi}\right)}$$

G.2. Drinking Water Intake Rates

Drinking water intake rates (DW) for mammals and birds are calculated based on **Equations G4 and G5** (USEPA 1993); where BW represents the body weight (in kg) of the animal for which the drinking water intake is being assessed. Resulting units of DW are L/day.

$$Equation\ G4. \quad DW = \left(0.099 * BW^{0.90}\right) \quad (mammals)$$

$$Equation\ G5. \quad DW = \left(0.059 * BW^{0.67}\right) \quad (birds)$$

G.3. Dose-based EECs

Dose-based EECs are estimated assuming that pesticide intake is a function of the amount of pesticide contained in the food and drinking water of an animal. The dose-based EEC is derived according to **Equation G6**. In this equation, pesticide intake through food is calculated as the sum of the products of the fraction of each prey item in the diet (P_i) and the pesticide tissue residue concentration for each prey item (C_{Bi}; μg/kg-ww). The sum of the pesticide residues ingested through food is converted into units of mg pesticide/kg food. This value is then multiplied by the intake rate for wet food (kg food/kg-bw day). The resulting value is in units of mg pesticide/kg-bw day. Pesticide intake through drinking water is calculated by multiplying the concentration of the pesticide in water (C_{WTO}, mg/L) by the water intake (DW in units of L/d) and dividing by the bodyweight of the mammal or bird of concern. This results in units of mg pesticide/kg-bw day. The sum of pesticide intake through diet and through drinking water is the dose-based EEC.

$$Equation\,G6. \quad Dose-based \quad EEC = \sum \left(P_i * C_{Bi}\right) * FI_{wet} + \frac{C_{WTO} * DW}{BW}$$

G.4. Dietary-based EECs

Dietary-based EECs are estimated assuming that pesticide intake is a function of the amount of pesticide contained in the food of an animal. This differs from the dose-based EECs in that pesticide exposure through drinking water is not considered. In addition, the dietary-based exposure value is not adjusted for the relative amount of food consumed per day by animals of different sizes. The dietary-based EEC is derived according to **Equation G7**. In this equation, the pesticide intake through food is calculated as the sum of the products of the fraction of each prey item in the diet (P_i) and the pesticide tissue residue concentration for each prey item ($C_{Bi;}$ μg/kg-ww).

$$Equation\ G7. \quad Dietary-based \quad EEC = \sum \left(P_i * C_{Bi}\right)$$

G.5. Adjusted Dose-based Toxicity Values

Available dose-based toxicity values are adjusted for the weights of the animal tested (*e.g.,* laboratory rat, mallard duck) and of the animal for which the risks are being assessed (*e.g.,* mink, bald eagle). These adjustments are made for mammals and birds according to **Equations G8 and G9**, respectively (USEPA 2006). In these equations, AT = adjusted toxicity value; LD_{50} or NOAEL = endpoint reported by toxicity study; TW = body weight of tested animal (350g rat; 1580g mallard, 178 g Northern bobwhite quail or weight defined by the model user for an alternative species); AW = body weight of assessed animal; x = Mineau scaling factor. Chemical specific values for x may be located in Mineau et al. 1996). If no chemical specific data are available, the default value of 1.15 should be used for this parameter. Methods for adjusting toxicity values are consistent with those used by T-REX (USEPA 2008a).

$$Equation\ G8.\quad AT = \left(LD_{50}\ or\ NOAEL\right)\left(\frac{TW}{AW}\right)^{0.25}\quad (mammals)$$

$$Equation\ G9.\quad AT = LD_{50}\left(\frac{AW}{TW}\right)^{(x-1)}\quad (birds)$$

Appendix H. Methods for Estimating Metabolism Rate Constant (k_M)

Generally, chemical-specific data are not available to determine the metabolism rate constant (k_M) for aquatic organisms. However, this parameter can be estimated using data from available bioconcentration factor (BCF) studies, in combination with estimated rate constants. Two separate approaches can be employed to estimate k_M. The first utilizes Equation A1 from Arnot and Gobas 2004. The second utilizes a method described by Arnot et al. 2008. These approaches are described below.

H.1. Use of Equation A1

In this approach, Equation A1 (see Table A1 of Appendix A) is rearranged to solve for k_M (Equation H1). In a BCF study, fish are fed uncontaminated food; therefore, uptake through the dietary pathway is assumed to be negligible. As a result, it is assumed that $k_D = 0$. BCF studies with fish involve water-only exposures, so fish do not respire pore water. As a result, $m_O = 1$ and $m_P = 0$. To calculate k_M, the model user should use the measured concentration of pesticide in the test water. In this case, it is assumed that this value represents the freely dissolved pesticide in the water, and therefore, $\Phi = 1$. Based on these assumptions, Equation H1 can be restated as Equation H2.

$$Eq.\,A1 \quad C_B = \frac{k_1 * (m_0 * \Phi * C_{WTO} + m_P * C_{WDP}) + k_D * \Sigma(P_i * C_{Di})}{k_2 + k_E + k_G + k_M} \quad \text{(From Appendix A)}$$

$$Eq.\,H1 \quad k_M = \frac{k_1 * (m_0 * \Phi * C_{WTO} + m_P * C_{WDP}) + k_D * \Sigma(P_i * C_{Di})}{C_B} - (k_2 + k_E + k_G)$$

$$Eq.\,H2 \quad k_M = \frac{k_1 * (C_{WTO})}{C_B} - k_2 - k_E - k_G$$

Equation H2 can be used to estimate k_M from available data from a BCF study.

- Empirical estimates of k_1 (L/kg*d), total pesticide concentration in fish tissues (C_B; g/kg-ww) and C_{WTO} (g/L) from the BCF study should be entered into this equation.
- k_2 (d^{-1}) is calculated as $k_{1(empirical)}/K_{BW}$ (see Table A6 of Appendix A). To calculate K_{BW}, it is necessary to have estimates of % lipid, % non-lipid organic matter (NLOM), and % water of the test fish (V_{LB}, V_{NB} and V_{WB}, respectively).
    - **If % lipid data are not available for the test fish, this approach should not be used and it should be assumed that $k_M = 0$.**
    - If % lipid data are available, but % NLOM and % water are not available, it can be assumed that the fish are 73% water and that % NLOM is equal to 100-73-% lipid.
- k_E (d^{-1}) can be estimated using the KABAM tool. The model user should use the large fish of KABAM to calculate k_E.

- Body weight of the fish and water temperature should be set to mean reported values from the study. **If body weight data are not available for the test fish, this approach should not be used and it should be assumed that $k_M = 0$.**
- This constant is influenced by the % lipid, % NLOM, and % water of the diet (V_{LD}, V_{ND} and V_{WD}, respectively). Calculation of this constant requires input of diet of the large fish to be 100% medium fish (Table 6 of KABAM tool). If data are available from the BCF study report to define the % lipid, % NLOM, and % water of the feed of the test fish, the data should be entered in the appropriate columns of Table 5 of the KABAM tool for the medium fish. Otherwise, if these data are not available, the % lipid, % NLOM, and % water of the medium fish can be set to the default values of 4, 23, and 73%, respectively.

- k_G (d^{-1}) can be estimated from empirical data on body weight over the study period. If k_G cannot be estimated, the model user can use k_G from the large fish.

H.2. Use of Arnot et al. 2008

In this approach, it is assumed that the elimination rate constant measured during the BCF study (k_T) is the sum of elimination through respiration, fecal elimination and metabolism of the pesticide by the fish as well as growth dilution (Equation H3, Arnot et al. 2008). Equation H3 can be rearranged into Equation H4, to solve for k_M.

$$Eq. H3 \quad k_T = k_2 + k_E + k_G + k_M$$

$$Eq. H4 \quad k_M = k_T - k_2 - k_E - k_G$$

Equation H4 can be used to estimate k_M from available data from a BCF study.

- k_T (d^{-1}) is the total elimination rate constant estimated from the depuration period of the BCF study.
- As with the first approach, k_2 (d^{-1}) can be calculated as $k_{1(empirical)}/K_{BW}$ (see table A6 of Appendix A).
- k_E (d^{-1}) can be estimated using the KABAM tool. See discussion above on how to derive this constant value.
- k_G (d^{-1}) can be estimated from empirical data on body weight over the study period. If k_G cannot be estimated, the model user can use k_G from the large fish.

H.3. Assumptions and Uncertainties

If k_M is calculated as a negative value, it should be assumed that no biotransformation of the chemical occurs and k_M should be set to 0 in Table 2 of the KABAM tool. Since a negative biotransformation rate would indicate that the organism is creating the pesticide, it is assumed that this is not possible for a pesticide.

There is some uncertainty in using the model estimated k_G value (using Equation A7), as it may differ from the growth rate of the test species of the BCF study.

The first approach involves use of total pesticide concentration in fish tissues (C_B; g/kg-ww) and C_{WTO} (g/L). It would be appropriate to enter mean values for these parameters into equation H2. However, variability in these parameters can influence predictions of k_M. Therefore, the model user should explore variability associated with these values by considering standard deviation, as well as minimum and maximum values for these parameters. This will result in a range of relevant k_M values.

Both approaches involve use of fish body composition data (V_{LB}, V_{NB}, and V_{WB}). It would be appropriate to use mean values to calculate K_{BW} (and ultimately k_2). However, variability in these parameters can influence predictions of k_M. Therefore, the model user should explore variability associated with these values by considering standard deviation, as well as minimum and maximum values for these parameters. This approach will result in a range of relevant k_M values.

Both approaches involve using the KABAM tool to calculate k_E. This involves the use of diet composition data (V_{LD}, V_{ND}, and V_{WD}). In the case that data are not available from the study report to define the % lipid, % NLOM, and % water of the diet of the test fish, there is uncertainty in using default values for these parameters, as they may differ from the diet of the test species of the BCF study.

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