

APPENDIX B. CHANGES TO MODEL CODE

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1 Introduction

This appendix to the bioaccumulation modeling report presents details regarding changes to the Lower Passaic River Study Area (LPRSA) bioaccumulation model code based on discussions with the US Environmental Protection Agency (USEPA). These changes include the following:

- ◆ Changing the method for calculating chemical concentrations in phytoplankton (Section 2)
- ◆ Changing the dietary chemical transfer efficiency (E_D) parameter from a calculated value (based on the octanol-water partition coefficient [K_{OW}]) to a model input (Section 3)
- ◆ Developing species-specific growth and consumption rates (Section 4)

The sections that follow describe the rationale for these changes, the implementation of these changes in the model, and a discussion of the impact of these changes on the bioaccumulation model output.

2 Phytoplankton Calculations

As discussed with USEPA during the March 28, 2018, bioaccumulation modeling meeting, the approach for calculating the chemical concentration in the phytoplankton/algae model compartment was updated. The initial approach was to use the Arnot and Gobas (2004a) model equation, which was based on uptake and elimination rates for phytoplankton. The revised approach was to use the concentration in suspended algal particulates calculated in the chemical fate and transport (CFT) model to estimate the concentration. Because there are no plankton data available for the LPRSA, it is not possible to evaluate these two options relative to empirical data. Furthermore, as discussed at the March 28 meeting, all parties agreed that if available, plankton data would likely be highly variable, making it difficult to determine the correct approach. Thus, the site-specific suspended algal particulate data from the CFT model were selected for use in the LPRSA bioaccumulation model, because they allow for the incorporation of site-specific model predictions (i.e., rather than the use of a generic equation).

2.1 UPDATED MODEL EQUATION

The suspended algal particulate value provided in the CFT model is presented as a carbon-normalized concentration (i.e., ng of chemical per g of carbon). Conversely, the bioaccumulation model needs chemical concentrations for biota in terms of wet weight (i.e., ng/g wet weight [ww]). To un-carbon normalize the concentration in suspended algal particulate for use in the bioaccumulation model, the fractions of lipids and non-lipid organic carbon (NLOC) for the algae/plankton compartment were used (see Section 3.3.3 of the main report). Equation 2-1 shows this conversion:

$$C_{ww} = CAC \times (F_{lipid} + F_{NLOC}) \quad \text{Equation 2-1}$$

Where:

C_{ww}	=	chemical concentration in wet weight
CAC	=	carbon-normalized chemical concentration in suspended algal particulates
F_{lipid}	=	fraction of lipid in plankton/algae (equal to 0.0012)
F_{NLOC}	=	fraction of NLOC in plankton/algae (equal to 0.0388)

2.2 EVALUATION OF CHANGE

To evaluate the impact of this change on the LPRSA bioaccumulation model, chemical concentrations for the phytoplankton/algae compartment were compared using the two approaches (i.e., the Arnot and Gobas (2004a) equation and the suspended algal particulate approach). As shown in Table 2-1, concentrations increased for all chemicals (by an average factor of about 3.7 for 2,3,7,8-tetrachlorodibenzo-*p*-dioxin [TCDD], 4.6 for tetrachlorobiphenyl (tetraCB), and 95 for 1,2,3,4,6,7,8-

heptachlorodibenzofuran [HpCDF]) when the suspended algal particulate approach was used. Chemical concentrations for the zooplankton compartment also increased significantly (because zooplankton are assumed to consume 100% phytoplankton/algae), but the impact on the overall model was low.

Table 2-1. Calculated concentration in phytoplankton

Chemical	Calculation Method	Model-predicted Concentration in Phytoplankton (µg/kg ww)		
		RM 0–RM 6	RM 6–RM 14.7	RM 14.7–Dundee Dam
2378-TCDD	Arnot and Gobas (2004a) equation ^a	0.0043	0.0025	0.00011
	calculated from suspended algal particulate concentration provided in CFT model	0.017	0.0091	0.00040
TetraCB	Arnot and Gobas (2004a) equation ^a	7.9	7.4	5.5
	calculated from suspended algal particulate concentration provided in CFT model	40	32	24
1,2,3,4,6,7,8-HpCDF	Arnot and Gobas (2004a) equation ^a	0.0013	0.00024	0.000018
	calculated from suspended algal particulate concentration provided in CFT model	0.14	0.022	0.0016

^a The growth rate constant used for these calculations is the default value of 0.08 per day, as provided in Arnot and Gobas (2004).

CFT – contaminant fate and transport

HPCDF – heptachlorodibenzofuran

RM – river mile

TCDD – tetrachlorodibenzo-*p*-dioxin

ww – wet weight

3 Addition of E_D Parameter as Model Input

As discussed with USEPA during the June 5, 2018, bioaccumulation modeling meeting, the approach for determining the chemical-specific E_D parameter was updated. Previously the Arnot and Gobas (2004a) model equation, which was based on the K_{OW} , was used to define the E_D parameter. The revised approach is to alter the model structure so that the E_D parameter is a separate input parameter from the K_{OW} . This approach was selected because, as described later in this appendix, the K_{OW} is not necessarily a good predictor of the E_D (Section 3.2), and because this poor relationship impacted the ability to achieve a good model calibration. This section describes support for that decision and the development of E_D values for the LPRSA bioaccumulation model.

3.1 BACKGROUND ON E_D PARAMETER

Arnot and Gobas (2004b) expressed the bioaccumulation of chemicals from diet through the dietary uptake rate constant, k_D (kg food/kg organism/day), the calculation of which is shown in Equation 3-1 (Arnot and Gobas 2004b):

$$k_D = E_D \times G_D / W_B \quad \text{Equation 3-1}$$

Where: E_D = chemical transfer efficiency (fraction)
 k_D = function of the dietary chemical transfer efficiency
 G_D = feeding rate (kg/day)
 W_B = weight of the organism (kg)

The unitless dietary chemical transfer efficiency parameter, E_D , is defined as the amount of chemical transferred from food to the organism divided by the amount of chemical consumed (Arnot and Gobas 2004b; Clark and Mackay 1991). While E_D is assumed to be constant for a particular species and specific compound (Clark and Mackay 1991), observed variances in E_D can be attributed to various factors, including differences in compound K_{OW} , the composition and digestibility of food, compound steric hinderance in gut membrane permeation, experimental artifacts, differences in gut morphology between species, and differences in food digestion between species (Arnot and Gobas 2004b).

Arnot and Gobas (2004b) explored the relationship between E_D and $\log K_{OW}$ as a way to calculate an E_D value for use in bioaccumulation modeling. They found several studies that observed a reduction in E_D with increasing K_{OW} for high- K_{OW} chemicals in invertebrates and fish. Furthermore, the authors found that the average E_D for chemicals with a $\log K_{OW}$ between 4 and 6 was approximately 50%. They noted that these trends are consistent with a two-phase resistance model and developed an equation to represent the relationship between E_D and K_{OW} :

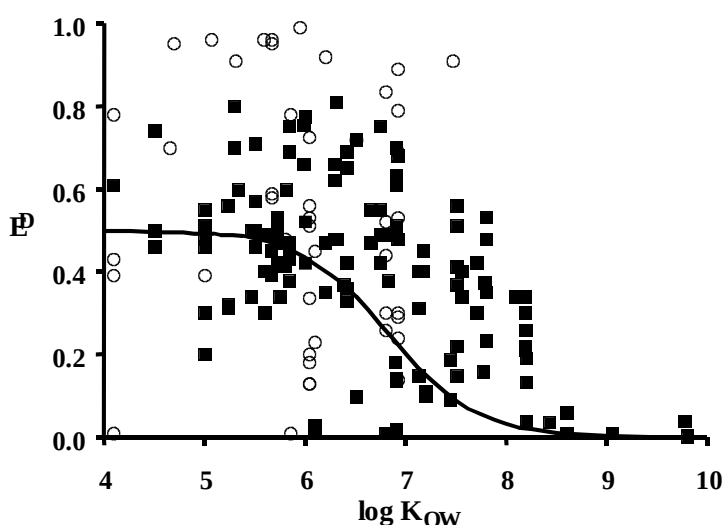
$$E_D = ((3.0 \times 10^{-7}) \times K_{OW} + 2.0)^{-1} \quad \text{Equation 3-2}$$

Where: E_D = chemical transfer efficiency
 K_{OW} = octanol-water partition coefficient

This relationship was previously used to calculate E_D values for the bioaccumulation model for the LPRSA.

3.2 RATIONALE FOR CHANGE TO MODEL STRUCTURE

Initial runs of the model for 2,3,7,8-TCDD determined that optimal calibrations occurred at low log K_{OW} (~5.5) and high log K_{OW} (~7.5) relative to the best estimate for log K_{OW} (~6.4). USEPA wanted to understand the reason for this model behavior, as communicated in a memorandum (dated June 1, 2018) and again during the June 2018 bioaccumulation modeling meeting. USEPA found that when K_{OW} values were increased from 5.5 to 7.5, the predicted dietary uptake (k_D) declined by an order of magnitude, while the contamination in the food increased by an order of magnitude. The combination of these two effects creates a parabolic relationship. This parabolic relationship is driven by the prediction of k_D as a function of log K_{OW} . The prediction of k_D is governed by the Arnot and Gobas (2004b) model fit to data for E_D , as seen in Figure 3-1.



Note: Figure taken from Arnot and Gobas (2004b); fish data indicated by closed squares ($n = 128$) and invertebrate data indicated by open circles ($n = 45$)

Figure 3-1. Relationship between E_D and K_{OW}

USEPA concluded that the E_D parameter value resulting from the relationship between log K_{OW} and E_D (as shown in Figure 3-1) was highly uncertain. In response, a literature search was conducted for experimentally derived E_D values for 2,3,7,8-TCDD. USEPA's preliminary literature search identified a possible range of E_D

values for 2,3,7,8-TCDD of 0.12 to 0.45. Based on the uncertain relationship between log K_{OW} and E_D , and the possible literature values identified, it was agreed that further investigation into this parameter was needed.

3.3 LITERATURE REVIEW

A literature review was conducted to better understand chemical characteristics that influence E_D and to compile experimentally derived E_D values.

3.1.1 Correlation with other parameters

Research suggests that various chemical parameters may have a relationship with E_D , such as chlorination (Clark and Mackay 1991; Tanabe et al. 1982). Tanabe et al. (1982) found that the absorption efficiencies of polychlorinated biphenyls (PCBs) decreased as the number of chlorine atoms increased. However, the relationship between compound chlorination and E_D did not prove strong enough to use as a predictor for E_D . Similarly, other researchers have noted similar trends with E_D values. For example, Loonen et al. (1991) noted that the absorption efficiencies of polychlorinated dibenzo-*p*-dioxin (PCDD) and polychlorinated dibenzofuran (PCDFs) are much lower than those for PCBs with similar log K_{OW} values (Table 3-1). These data support USEPA's conclusion that K_{OW} values are poor predictors of E_D between log K_{OW} 5.5 and 7.5.

Table 3-1. Absorption efficiencies for PCBs and PCDDs/PCDFs

Group	Chemical	E_D	Log K_{OW}
PCBs	2,2,5,5-tetraCB	0.42	6.1
	2,2,4,4,5,5-hexaCB	0.61	6.9
	2,2,3,3,4,4,5,5-octaCB	0.40	7.1
	decaCB	26	8.3
PCDDs/ PCDFs	2,3,4,7,8-penta-CDF	0.22	6.9
	1,2,3,4,6,7,9-pepta-CDF	0.05	7.9
	1,2,3,4,6,7,8-hepta-CDD	0.08	8.0
	octa-CDD	0.02	8.2

Source: Loonen et al. (1991)

E_D – dietary chemical transfer efficiency

K_{OW} – octanol-water partition coefficient

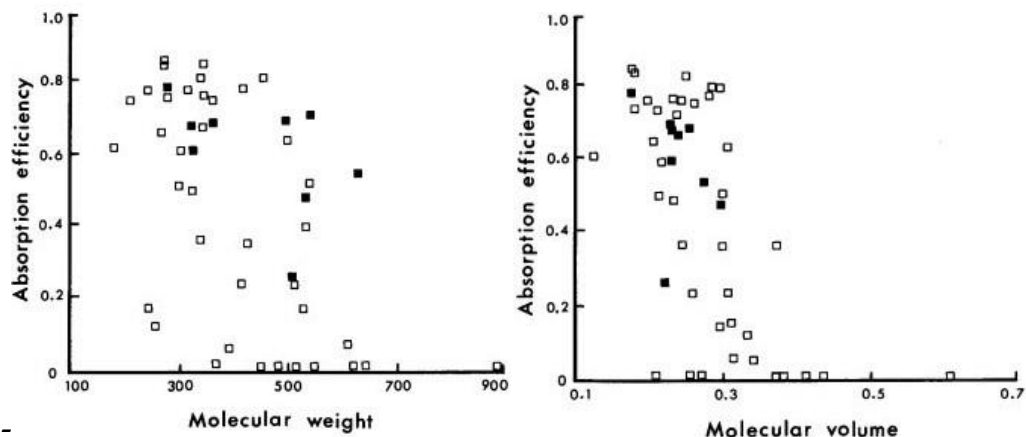
PCB – polychlorinated biphenyl

PCDD – polychlorinated dibenzo-*p*-dioxin

PCDF – polychlorinated dibenzofuran

tetraCB – tetrachlorobiphenyl

Niimi and Oliver (1988) investigated the relationship between E_D values and molecular weight and volume. They observed a loose relationship between molecular weight and E_D , and while the relationship between molecular volume and E_D was more convincing, it was not adequate to use to predict E_D (Figure 3-2). Neither of these chemical parameters, nor K_{OW} , proved useful to predict E_D values.



Source: Niimi and Oliver (1988)

Figure 3-2. E_D values (absorption efficiency) vs molecular weight and molecular volume

3.1.2 Compilation of literature values

To capture accurate E_D values for 2,3,7,8-TCDD, tetraCBs, and 1,2,3,4,6,7,8-HpCDF, empirically derived values were obtained from the literature. Data from the literature included E_D values from chronic toxicity tests with five different fish species fed two different diets (Attachment B-1). This dataset, which is summarized in Table 3-2, provided a range of E_D values for 2,3,7,8-TCDD and tetraCBs and a single value for HpCDF. Due to the limited data available for HpCDF, E_D values for other CDF compounds were compiled to assess a range of values that could be used in place of specific hepta-CDF values.

Table 3-2. Range of empirically derived E_D values for 2,3,7,8-TCDD, tetraCB, and PCDFs.

Compound	Species	No. of Studies	E_D Range	References
2,3,7,8-TCDD	rainbow trout	7	0.1–0.58	Jones et al. (2001); Hawkes and Norris (1977); Gobas (1988); Fisk et al. (1997); Morrison et al. (1999)
	guppies	1	0.51	Bruggeman et al. (1984)
	lake whitefish	3	0.66–0.76	Fisk et al. (1998)
TetraCB	rainbow trout	6	0.34–0.83	Clark et al. (1990); Fisk et al. (1998); Niimi and Oliver (1983)
	goldfish	5	0.47–0.53	Bruggeman et al. (1981); Clark et al. (1990); Gobas (1993)
Di-CDF	rainbow trout	2	0.12–0.25	Morrison et al. (1999)
Tetra-CDF	rainbow trout	5	0.1–0.59	Morrison et al. (1999)
Penta-CDF	rainbow trout	5	0.1–0.44	Morrison et al. (1999); Muir et al. (1990)
	guppies	1	0.22	Loonen et al. (1991)

Compound	Species	No. of Studies	E_D Range	References
Hexa-CDF	rainbow trout	6	0.25–0.31	Morrison et al. (1999)
	fathead minnow	4	0.31	Morrison et al. (1999)
Hepta-CDF	guppies	1	0.05	Loonen et al. (1991)
Octa-CDF	guppies	1	0.001	Clark and Mackay (1991)
	rainbow trout	2	0.05–0.18	Morrison et al. (1999)

E_D – dietary chemical transfer efficiency

PCDF – polychlorinated dibenzofuran

TCDD – tetrachlorodibenzo-*p*-dioxin

tetraCB – tetrachlorobiphenyl

Arnot and Gobas (2004b) suggest that there may be differences in E_D values between species, and that some experimental factors may influence empirically derived E_D values. The E_D values obtained from the literature for tetraCBs offer the largest dataset to evaluate the potential for species differences or experimental artifacts that can influence E_D derivation. Table 3-3 presents summary statistics to evaluate several of these factors, including the type of diet used and the differences across species (note that these are the same studies presented in Table 3-2). Although samples sizes are limited, Table 3-3 shows the following:

- ◆ **Comparison across species** – The E_D values for different species exposed to tetraCB using similar commercial diets were all within the same range. In contrast, the E_D values from difference species exposed to tetra-CDDs (again using similar commercial diets) suggest that there may be differences among species and dioxin compounds; however, the data is limited.
- ◆ **Comparison across diet types** – The available data indicate that diet type (i.e., commercial diets or fish oil capsules) may have an impact on E_D values. It is uncertain which diet type is more environmentally relevant: The fish oil capsule is likely more similar to the lipid content of prey consumed by the test species, while the commercial flake food may be more similar to detrital sources of food. Considering many fish species are omnivorous, eating different food items at different life stages, a reasonable E_D value representative of all food types is likely to be between these values.

Table 3-3. Evaluation of the impact of diet type and species on E_D values

Chemical	Species	Diet Type	Count Studies	E _D (fraction)		
				Mean	Minimum	Maximum
Comparison across species for tetraCBs						
TetraCBs	rainbow trout	commercial diet	6	0.40	0.34	0.47
	gold fish	commercial diet	5	0.5	0.47	0.53
	guppies	commercial diet	1	0.51	0.51	0.51
Comparison across species for 2,3,7,8-TCDD						
2,3,7,8-TCDD	rainbow trout	commercial diet	3	0.49	0.43	0.58
2,3,7,8-TCDD	lake whitefish	commercial diet	3	0.70	0.66	0.76

Chemical	Species	Diet Type	Count Studies	E _D (fraction)		
				Mean	Minimum	Maximum
1,2,3,7-TCDD	rainbow trout	commercial diet	1	0.14	0.14	0.14
1,2,3,7-TCDD	fathead minnow	commercial diet	1	0.11	0.11	0.11
Comparison of diets for tetraCBs						
TetraCBs	rainbow trout	commercial diet	6	0.40	0.34	0.47
	rainbow trout	fish oil capsule	9	0.75	0.66	0.83

E_D – dietary chemical transfer efficiency

TCDD – tetrachlorodibenzo-*p*-dioxin

tetraCB – tetrachlorobiphenyl

3.4 SELECTION OF E_D VALUES FOR USE IN THE LPRSA BIOACCUMULATION MODEL

The compilation of empirically derived E_D values from the literature represents a realistic range of values for different fish species consuming different diets. For the purposes of bioaccumulation modeling, the arithmetic mean was calculated using all diet types and species for 2,3,7,8-TCDD and tetraCBs (Table 3-4). Only one 1,2,3,4,6,7,8-HpCDF-specific value was available. This value was used as the nominal value, and the range of values for hexa-, hepta-, and octa-CDF were used to provide a distribution range for hepta-CDF (Table 3-4). The values for hexa- and octa-CDF are assumed to provide a reasonable range of possible values for hepta-CDF due to their degree of chlorination and can be used in lieu of the limited data.

Table 3-4. Selected E_D values for use in the LPRSA bioaccumulation model

Bioaccumulation Model Chemical	E _D Values		Description / Notes
	Nominal Value	Distribution Range (Literature)	
2,3,7,8-TCDD	0.49	0.10–0.76	Nominal value and range are based on the mean and range, respectively, of the available data for 2,3,7,8-TCDD (Table 3-2).
TetraCBs	0.57	0.34–0.83	Nominal value and range are based on the mean and range, respectively, of the available data for various tetraCB congeners (Table 3-2).
1,2,3,4,6,7,8-HpCDF	0.05	0.001–0.31	Nominal value is equal to the single value available for 1,2,3,4,6,7,8-HpCDF; range is equal to the range for hexa-CDF and octa-CDF (Table 3-2).

E_D – dietary chemical transfer efficiency

TCDD – tetrachlorodibenzo-*p*-dioxin

HpCDF – heptachlorodibenzofuran

tetraCB – tetrachlorobiphenyl

LPRSA – Lower Passaic River Study Area

The nominal value and distribution range presented in Table 3-4 provide a reasonable range of E_D values that can be used in the bioaccumulation model. While the species represented in this dataset do not necessarily reside in the LPRSA, they are standard test species that have been used as surrogates to provide data for many fish in freshwater communities.

4 Development of Species-specific Growth and Consumption Rate

Based on comments from USEPA regarding the discrepancies in the model-calculated growth and consumption rates (first discussed during the August 28, 2018, bioaccumulation modeling meeting), it was determined that a different approach than the default equations in the Arnot and Gobas (2004a) model should be used to calculate these rates. This decision was based on the fact that the growth rates predicted by the default equations were not consistent with observations from the literature, possibly, in part, because the default equations from Arnot and Gobas (2004a) are based on cold-water fish species (i.e., species that live in water of less than 12°C), which are not appropriate for the LPRSA.

As discussed with USEPA during subsequent meetings, various approaches were considered for developing species-specific growth and consumption rates. Ultimately, the Fish Bioenergetics Model 4.0 (hereafter referred to as the FB4 model (Fish Bioenergetics 2021)) was agreed upon because it a) provides a reasonable approach for estimating growth and consumption rates that could be adapted for use in the LPRSA bioaccumulation model and b) produces results consistent with literature observations.

4.1 SELECTION OF FB4 SPECIES AND INPUT PARAMETERS

This section presents an overview of the FB4 model (Section 4.1.1), the selected representative species for the LPRSA model (Section 4.1.2), and the required input parameters needed in the FB4 model (Section 4.1.3 to 4.1.6).

4.1.1 FB4 model overview

The FB4 model uses taxon-specific physiological estimates of energy consumption and energy expenditure to represent the energy balance equation. Each of the physiological processes is described by a set of functions that are regulated primarily by water temperature and body size. The model uses a linear equation to provide a reasonable estimated consumption rate given an assumed growth rate. The FB4 is a compilation of 105 published bioenergetics models, but not all LPRSA species are represented, meaning that identifying a representative or surrogate species was necessary when implementing the FB4 model.

The FB4 model requires a species from the database that is either in the bioaccumulation model or a surrogate for a species in the bioaccumulation model, as well as user-identified initial body weight, end body weight, temperature, oxycaloric coefficient, and diet proportions.

4.1.2 Selection of representative species

The FB4 database did not have species models for all species in the LPRSA bioaccumulation model, so surrogate species were selected as needed. The surrogate species considered and the species selected for use in the FB4 portion of the LPRSA bioaccumulation model are summarized in Table 4-1.

Table 4-1. Selected species for FB4 model

Model Compartment	Selected FB4 Species	Rationale
Bass	largemouth bass	Possible representative species for the freshwater bass compartment in the LPRSA model were largemouth bass and smallmouth bass (striped bass were also available but are ecologically less similar). The FB4 model for smallmouth bass appears to be for young-of-year fish; thus, the largemouth bass (adult fish) model was selected to best represent bass in the LPRSA.
Carp	bighead and silver carp	Bighead carp and silver carp were both potential surrogates. Since the FB4 models for these species were similar, both were used as surrogates.
Catfish	brown bullhead	No catfish were available in the FB4 database; brown bullhead was selected as the most representative species.
White perch	yellow perch	Options for a representative species in the FB4 dataset included Eurasian perch, Nile perch, Sacramento perch, and yellow perch. Yellow perch was selected as the most suitable to represent white perch.
Small forage fish	bluegill	This group of fish could be represented by bluegill sunfish or California killifish. The FB4 model results for the two species were different, so both could not be used. Since only juvenile lifestage data were available for California killifish, bluegill was selected as the surrogate for modeling.
Small filter-feeding fish	na	No suitable representative species were available; therefore, the same model used for small forage fish was applied.
Blue crab	blue crab	Although not in the main FB4 database, an FB4 blue crab model was developed by Brylawski and Miller (2003). That model was updated with respiration data from Booth and McMahon (1992) to reflect adult crab respiration rates, and the updated model was used to develop the regression models for blue crab.
American eel	na	No suitable representative species were available; therefore, the same model used for catfish was applied. Although the growth rates for these species are similar (Table 4-3), catfish and eel are very different species, and thus the extent of this uncertainty is unknown.

LPRSA – Lower Passaic River Study Area

na – not applicable

While multiple lifestages were available for some of the species, the adult lifestage was used in the final linear regression. The use of other lifestages was examined as part of the sensitivity analysis. More detail is provided in Section 4.2 of this appendix.

4.1.3 Initial and end body weights

Initial weights were set equal to the weights used to parameterize the bioaccumulation model (i.e., the average weight of LPRSA fish/crab included in analytical samples from the 2009/2010 sampling efforts) (see Section 3.3.3 of the main report).

End weights were determined by estimating annual growth rate, then applying it to the starting weight for each species. Since the fish collected in the LPRSA 2009/2010

sampling efforts were not aged, a weight of evidence approach was used to estimate LPRSA species-specific growth rates. Three lines of evidence were considered:

- ◆ **Approach 1** – Gewurtz equation (Section 4.1.3.1)
- ◆ **Approach 2** – von Bertalanffy growth function (VBGF) and LPRSA data (Section 4.1.3.2)
- ◆ **Approach 3:** The use of available generic species lifespan information and LPRSA data (Section 4.1.3.3)

Selected species-specific body weights (initial and end body weights), along with the growth rates used to develop these weights, are presented in Section 4.1.3.4.

4.1.3.1 Approach 1 – Gewurtz equation

A standard growth equation, originally developed by Thomann (1981) and Thomann et al. (1992) but commonly cited from Gewurtz et al. (2006), was initially applied across species in the bioaccumulation model (Equation 4-1):

$$k_g = 0.00586(1.113)^{T-20} * (W_i * 1000)^{-0.2} \quad \text{Equation 4-1}$$

Where: k_g = growth
 T = temperature in Celsius
 W_i initial weight

While this equation is frequently used in bioaccumulation models and is simple to apply, it does not incorporate LPRSA data and does not constrain growth rate. Thus, this approach was not used to derive growth rates for the LPRSA bioaccumulation model.

4.1.3.2 Approach 2 – von Bertalanffy growth function and LPRSA data

To use the length and weight data from the LPRSA, and therefore make the estimated end weights as LPRSA-specific as possible, VBGF parameters were used in combination with LPRSA field data to estimate annual growth rates. The following data were compiled for each species:

- ◆ **Step 1** – FishBase (FishBase 2021) was queried for VBGF parameters by species; parameters were available for all species except blue crab and American eel. Species-specific growth information was available under the “growth” hyperlink at the bottom of each species-specific webpage.
 - ◆ Values were available for each VBGF parameter (L_{∞} [cm] and K); parameters were available for all species except blue crab and American eel. Parameter values were included (Step 2) if they met the following criteria:
 - The study was identified as “not questionable” by FishBase.

- The water temperature range of the study fell within the range of Passaic River temperatures (0.4 to 27°C). Studies that did not list water temperature were not included.
- ◆ When more than one value was reported for each parameter, the geomean of those values was calculated. These calculated species-specific VBGF parameter values were used in Step 2.
- ◆ **Step 2** – The age of each fish from the 2009/2010 LPRSA sampling was calculated using the species-specific VBGF growth model calculated in Step 1. Following the calculation of the estimated age of each fish, the fish were sorted by age and binned into age classes. For shorter-lived species (such as bluegill), fish were binned by 0.5-year increments; for longer-lived species (such as carp), fish were binned by 1-year increments.
- ◆ **Step 3** – Length (cm) vs. weight (kg ww) was plotted for each species, and a power trendline was fit to the data.
- ◆ **Step 4** – The median length was calculated by age class bin as described in Step 2. The length-to-weight relationship derived in Step 3 was used to estimate weight for each age class based on median length. Annual growth was calculated for each age class based on percent increase in weight by age class.
- ◆ **Step 5** – The geomean of the annual growth rate was calculated (Table 4-2).

Following this approach, annual growth rates were calculated for all LPRSA model species (Table 4-2).

Table 4-2. Estimated age and growth rates using VBGF approach

Species	Estimated Age Range of LPRSA data (years)	Count of FishBase Studies ^a	Annual Growth Rate Range	Annual Growth Rate GeoMean	Notes
Small forage fish	0–3.5	7	44–505%	232%	bluegill FishBase VBGF values and LPRSA data used to represent all small forage fish
Blue crab	na	0	na	na	no studies available on FishBase
Carp	3–9	15	9–35%	20%	na
Catfish	1–2; 4–16	1	4–77%	14%	na
White perch	0–10	2	4–512%	31%	na
Bass	0–4	54	na	73%	LPRSA dataset appears to be skewed toward younger fish (81% of samples were estimated to be < 3 years of age); thus, the annual growth rate for fish 3–4 years of age was selected. ^b

Source of growth rate information: FishBase (2021).

^a VBGF parameters from studies that were noted as "not questionable" by FishBase and were conducted in waters that had temperatures between 0 and 27°C (i.e., inclusive of the water temperatures measured during the LPRSA study) were included in the analysis. If a study entry in FishBase did not report the water temperature, it was excluded.

- ^b The lifespan of bass is approximately 10 to 12 years and the oldest age class of fish from the 2009/2010 LPRSA sampling was estimated to be 3 to 4 years. Growth rate is higher in younger fish, so using the geomean of bass ages 0.5 to 4.0 years old resulted in a much higher growth rate than that reported in the literature. The annual growth rate of fish ages 3 to 4 is similar to literature values and was used to calculate an end weight for bass in the FB4 model.

na – not applicable

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VBGF – von Bertalanffy growth function

4.1.3.3 Approach 3 – generic life history approach using LPRSA data

A third approach, which was conducted by USEPA, estimated annual average growth rates using available information regarding the lifespans of modeled organisms, available literature regarding age and length data, and LPRSA fish/crab data from 2009/2010 (Table 4-3). A range of ages was estimated for LPRSA fish/crab, and then each individual was assigned to an age class. The age-to-weight trend line was then used to calculate an annual growth rate. This estimate was bounded by adjusting the assumptions regarding the maximum and minimum ages for LPRSA fish.

Table 4-3. Estimated growth rates using the generic life history approach

Species	Annual Growth Rate			Estimated Age Range of LPRSA Fish (Years)			Notes and Citations
	Min.	Best Estimate	Max.	Min.	Best Estimate	Max.	
Small forage fish	90%	164%	212%	1 to 5	1 to 3	1 to 2	A maximum age of 4 years was reported for mummichog (FishBase 2021), and a maximum of 6 years was reported for striped killifish (Clemmer and Schwartz 1964). Growth rate is much higher and more variable for young-of-the-year fish than for older fish.
Blue crab	62%	69%	76%	1 to 2	1 to 3	1 to 4	Crab lifespan was based on Darnell et al. (2009) and Hines et al. (2003).
Carp	14%	19%	29%	1 to 14	2 to 12	2 to 8	Carp lifespan was based on information from FishBase (2021).
Catfish	10%	15%	21%	1 to 18	1 to 12	1 to 9	Catfish lifespan was based on information from FishBase (2021)
White perch	25%	43%	59%	1 to 11	1 to 11	1 to 8	Age estimates were developed based on Bath and O'Connor (1982). The two largest white perch were excluded for the minimum growth estimate.
Large American eel	7%	13%	26%	1 to 40	1 to 20	1 to 10	Age estimates are from Machut et al. (2007); values are based on growth rate of 590-g eel in this age range.
Small American eel	11%	17%	33%	1 to 40	1 to 20	1 to 10	Age estimates are from Machut et al. (2007); values are based on growth rate for 280-g eel in this age range.
Bass	19%	29%	40%	1 to 14	1 to 9	1 to 5	Uncertainty exists in age vs size. LPRSA bass are either all young (< 4 years of age as suggested by VBGF evaluation) or slower growing than average.

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VBGF – von Bertalanffy growth function

4.1.3.4 Selected growth rate and model end weights

Annual growth rates (which were used to calculate end body weights for use in the FB4 model) were selected based on either Approach 2 or Approach 3 (Table 4-4). In general, rates were based on the VGBF approach (Approach 2), which was considered the most robust since it included growth data from multiple studies across various conditions that were comparable to growth rates from the literature review. Growth rates from both approaches were compared to one another as well as to growth rates calculated using the 2019 aging data from the LRPSA (Windward 2020) to evaluate potential uncertainty in the selected rates.

Table 4-4. Selected annual growth rate and comparison with 2019 LPRSA data

Species	Annual Growth Rate		Discussion of Uncertainty Associated with Selected Growth Rates
	Approach 2 (VBGF)	Approach 3 (Life History)	
Small forage fish	232% (44–505%)	164% (90–212%)	Growth rates for small forage fish are highly variable (both approaches), and rates are much higher for young-of-the-year fish. Growth rates calculated using the 2019 aging data ranged from 11 to 28% (sunfish were estimated to be 1 to 4 years of age). These rates are not applicable for the model because they are based on much larger fish (fish collected in 2019 were > 18 g; modeled fish were 2.7 g). While there is some uncertainty because of the wide range of growth rates derived using both Approaches 2 and 3, the modeled fish are likely young-of-year fish, and thus a higher growth rate than that for older fish is expected.
Blue crab	na	69% (62–76%)	na (blue crab aging not conducted)
Carp	20% (9–35%)	19% (14–29%)	Similar average growth rates were derived using Approaches 2 and 3. In addition, growth rates calculated using the 2019 aging data were similar, providing increased confidence in the selected growth rate. Growth rates calculated using the 2019 aging data ranged from < 0 to 27% (carp were estimated to be 4 to 11 years of age).
Catfish	14% (4–77%)	15% (10–21%)	Similar average growth rates were derived using Approaches 2 and 3. In addition, growth rates calculated using the 2019 aging data were similar, providing increased confidence in the selected growth rate. Growth rates calculated using the 2019 aging data ranged from < 0% to 22% (catfish were estimated to be 4 to 11 years of age).
White perch	31% (4–512%)	43% (25–59%)	Similar average growth rates were derived using Approaches 2 and 3. In addition, growth rates calculated using the 2019 aging data were similar (average of 28%), providing increased confidence in the selected growth rate. Growth rates calculated using the 2019 aging ranged from 7 to 60% (perch were estimated to be 0 to 3 years of age), with the rate appearing to decrease with age.
American eel ^a	na	17% (11–33%) 13% (7–26%)	na (no model selected). Growth rates calculated using the 2019 aging data ranged from 14 to 54% (eel were estimated to be 6 to 13 years of age).
Bass	73% (na) ^b	29% (19–40%)	The growth rate derived using Approach 2 was higher than that for Approach 3. Growth rates calculated using the 2019 aging data ranged from 33 to 37% (bass were estimated to be 2 to 5 years of age), rates similar to the high-end rate derived from Approach 3 (which assumed an age range of 1 to 5 years). There is considerable variability across bass growth rates, indicating a high level of uncertainty. LPRSA bass appear to be younger than a typical bass population (e.g., based on bass aged from the Housatonic River that were up to 14 years of age), so a higher-than-typical growth rate may be realistic. However, the selected growth rate may overestimate the end weight used in the FB4 model. This uncertainty is evaluated in Section 4.2 of this appendix.

Note: Selected annual growth rates are indicated with green shading.

^a No growth rate was selected for American eel. Instead, the growth and consumption rate for eel was based on that for catfish, because among the LPRSA species, catfish life history traits were determined to be the most similar to those of eel.

^b For bass, the end weight was calculated using the VBGF-derived annual growth rate for fish ages 3 to 4 years, instead of the geomean of annual growth across age classes (see Table 4-2).

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VBGF – von Bertalanffy growth function

The selected annual growth rates (presented in Table 4-4) were used to calculate end weights for use in the FB4 model (Table 4-5).

Table 4-5. Start and end weight used for FB4 model

Species	Selected Annual Growth Rate (Table 4-4)	Start Weight (kg)	End Weight (kg)
Small forage fish	232%	0.0027	0.0090
Blue crab	69%	0.14	0.24
Carp	20%	3.1	3.7
Catfish	14%	0.88	1.0
White perch	31%	0.094	0.12
American eel	na	na	na
Bass	73%	0.29	0.50

4.1.4 Temperature

Another input required for the FB4 model is water temperature throughout the year in the LPRSA. The average monthly temperature calculated and used in the CFT model was used in the FB4 model (Table 4-6). Minimum and maximum temperature years were also calculated for use in the sensitivity analysis.

Table 4-6. Average and range of temperatures in the LPRSA by month

Day	Month	Water Temperature (degrees C)		
		Mean	Range of Temperatures for Sensitivity Analysis ^a	
			Low	High
1	January	3.0	0.5	5.5
31	February	1.6	-0.9	4.1
60	March	1.93	-0.6	4.4
90	April	6.47	4.0	9.0
120	May	12.5	10.0	15.0
151	June	16.8	14.3	19.3
181	July	22.4	19.9	24.9
212	August	25.0	22.6	27.6
243	September	24.2	21.7	26.7
273	October	20.3	17.8	22.8
304	November	14.2	11.7	16.7
334	December	8.1	5.6	10.6

^a Range for sensitivity analysis was calculated as +/- 2.5°C from the mean value.

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4.1.5 Oxycaloric coefficient

The oxycaloric coefficient calculates the mass of oxygen consumed converted to energy and varies based on diet. With the absence of species-specific oxycaloric coefficients, the default value (13,560 J/g O₂) was used in all final models.

4.1.6 Diet proportions

The final FB4 input explored was diet proportion (a much simpler diet is required for the FB4 model than for the bioaccumulation model). By default, the FB4 model assumes that fish/crab exclusively eat invertebrates for the first 91 days of the modeled year, undergo a linear diet transition between day 91 and day 183, and consume a fish-only diet from day 183 through the end of the modeled year.

Alternative values were tested as part of the sensitivity analysis and were found to have little impact on the FB4 model output. Thus, the default diet proportions for the FB4 model were used to develop the final models.

4.2 EVALUATION OF FB4 MODEL SENSITIVITY

An analysis of the FB4 model sensitivity was conducted to evaluate the impact of the key input parameters (i.e., initial weight, end weight, temperature, oxycaloric coefficient, diet proportion, and lifestage) on the FB4 model output.

Catfish and bass were used for the sensitivity analyses for initial weight, end weight, temperature, oxycaloric coefficient, diet proportion, and lifestage. These species were selected because they represented the two different shapes of consumption and growth rate relationships seen among all modeled organisms. Effects of changes in the parameters on the results of the FB4 model can be seen in the figures presented in Attachment B-2. Key results are summarized as follows:

- ◆ **Initial and end weights** – Adjusting the initial weight or end weight is unlikely to impact the final coefficients of the regression equations at a magnitude that will affect the performance of the bioaccumulation model, especially in the portion of the regression equations that will be used in the bioaccumulation model (i.e., excluding data with high consumption rates).
- ◆ **Water temperature** – Temperature profiles that represented a warm and cool year (i.e., the mean monthly temperatures $\pm 2.5^{\circ}\text{C}$) were used to evaluate model sensitivity. Although there were small differences in the relationship between temperature and consumption rate for bass, the resulting impacts on the consumption rate equation were small.
- ◆ **Oxycaloric coefficient** – Changes to this parameter resulted in only minor changes to the FB4 model output and thus had limited impacts on the growth and consumption rate equations for the two species evaluated (i.e., bass and catfish).

- ◆ **Diet proportion** – The FB4 model output for bass changed by less than 1% when comparing the FB4 default diet and a diet based on that developed for the LPRSA bioaccumulation model. While there was a slightly greater impact for catfish than for bass, the differences were minor with regard to their impact on the growth and consumption rate equations.
- ◆ **Lifestage** – The effect of lifestage was examined for yellow perch and bluegill. Lifestage had the greatest impact on the model results of any of the parameters evaluated. Consumption rates for adult perch were approximately double that for juvenile perch. Similarly, the relationship between growth and consumption rate for both perch and bluegill was drastically different between the two lifestages.

Ultimately, the sensitivity analyses indicated that selecting the correct lifestage for the surrogate species in the FB4 model was the most influential input to shape the model. The initial weight, end weight, temperature profile, and diet proportions may somewhat impact the temperature-to-consumption rate relationship, but these parameters had less of an impact on the consumption rate-to-growth rate relationship.

4.3 DEVELOPMENT OF EQUATIONS FOR USE IN THE LPRSA BIOACCUMULATION MODEL

Ultimately, the FB4 model output was used to develop species-specific growth and consumption rate equations for use in the LPRSA bioaccumulation model. For each species, an equation was developed to estimate the species-specific consumption rate as a factor of water temperature, and growth rates were then estimated from the consumption rate.

4.3.1 Method for equation development

For each species, the appropriate FB4 model (or two models for species in cases when multiple appropriate surrogates were identified) was selected and used to develop regression equations. The data were truncated when needed for the purposes of fitting the regression model to ensure that the fit was not skewed by data at the extremes of the model that did not follow the trend. Based on the shape of the curves, it was determined that consumption and growth rates exceeding those directly observed in the FB4 results were not reliable or realistic. The maximum allowable value of the regression equations ($C_{\max}$ or $KG_{\max}$) was determined as the maximum consumption rate or growth rate, respectively, of the FB4 model results.

Temperature was related to the log of the species-specific consumption rate ($C = e^{((a+b)*T)}$). The upper limits of the consumption rate for developing the consumption rate vs temperature equations were set to 90% of the maximum consumption rate. This approach was selected, rather than using a user-specified maximum value, because the curve tended to form a plateau at high temperatures

such that there was no increase in consumption rate with increasing temperatures. Using 90% of the maximum consumption rate excluded these plateaus.

Consumption rate and growth rate were related in linear space ($G = (a + b) * C$). The upper limits of the consumption rate for the growth rate vs consumption rate equations were 0.01 g/g/day for catfish, 0.02 g/g/day for perch, and 0.008 g/g/day for blue crab. Above these limits, the model shape turned downward (i.e., slope changed from positive to negative), a phenomenon that occurred in the simulated summer months due to thermal stress. Setting upper limits was not necessary for the other species. This approach (i.e., manually setting the upper limit for some species) was used, rather than 90% of the maximum growth rate (as was done for the consumption rate vs temperature relationship), to avoid over- or under-limiting this maximum value.

4.3.2 Final Growth and Consumption Rate Equations

The species-specific growth and consumption rate equation parameters used in the LPRSA bioaccumulation model are presented in Table 4-7. The equations for the consumption rate (Equation 4-2) and growth rate (Equation 4-3) are as follows:

$$C = e^{(CvTa + CvTb * T)} \quad (\text{up to } C_{max}) \quad \text{Equation 4-2}$$

$$KG = KGvCa + KGvCb * C \quad (\text{up to } KG_{max}) \quad \text{Equation 4-3}$$

Where:	C	=	species-specific consumption rate
	CvTa	=	species-specific intercept for consumption rate equation (Table 4-7)
	CvTb	=	species-specific slope for consumption rate equation (Table 4-7)
	T	=	water temperature (degrees Celsius)
	C _{max}	=	species-specific maximum consumption rate (Table 4-7)
	KG	=	species-specific growth rate
	KGvCa	=	species-specific intercept for growth rate equation (Table 4-7)
	KGvCb	=	species-specific slope for growth rate equation (Table 4-7)
	KG _{max}	=	species-specific maximum growth rate (Table 4-7)

Table 4-7. Growth and consumption rate parameters for the LPRSA bioaccumulation model

LPRSA Model Compartment	FB4 Surrogate Organism(s)	Consumption Rate Equation			Growth Rate Equation		
		Intercept (CvTa)	Slope (CvTb)	Maximum (C _{max})	Intercept (KGvCa)	Slope (KGvCb)	Maximum (KG _{max})
Small forage fish, small filter-feeding fish	bluegill sunfish	-5.24	0.0975	0.0501	-0.00208	0.240	0.0101
Catfish, small American eel, large American eel ^a	brown bullhead	-10.9	0.366	0.0108	-0.00107	0.357	0.00242
Blue crab	blue crab	-6.15	0.0827	0.0155	0.000451	0.171	0.00292
Carp	bighead and silver carp	-7.00	0.121	0.0176	-0.00172	0.321	0.00309
White perch ^a	yellow perch (adult)	-5.57	0.0886	0.0218	-0.000704	0.158	0.00242
Bass	largemouth bass (adult)	-6.59	0.130	0.0278	-0.00520	0.566	0.0105

^a For the development of the consumption rate equations for catfish and perch, the low end of the FB4 model output was truncated (to consumption rates of less than 0.01 and 0.02 g/g/day for catfish and perch, respectively) in order to eliminate a non-linear “hook” at the high-consumption-rate end of the output. The models were fit, and adjusted r^2 values were calculated for only the sections below these values.

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The final models for LPRSA organisms are presented in Figure 4-1. The fits of these models were determined to be acceptable for use in the bioaccumulation model for all species, both for growth and consumption equations. With one exception, the equations fit the FB4 model output with an adjusted r^2 of 0.94 or greater. The one exception (the growth rate equation for white perch) had an adjusted r^2 of 0.76. The consumption rate and growth rate equations developed and discussed above reasonably replicated the FB4 relationship. The use of the maximum values presented in Table 4-7 is important to prevent over-prediction of the consumption rate and growth rate. Since the consumption rate is estimated using an exponential relationship, a lower bound is not necessary. While a lower bound could be set for the growth rate equation, it is not unreasonable for negative growth rate to occur, and a lower bound would not improve the accuracy of the regression equation; therefore, no lower bound is used for the LPRSA bioaccumulation model.

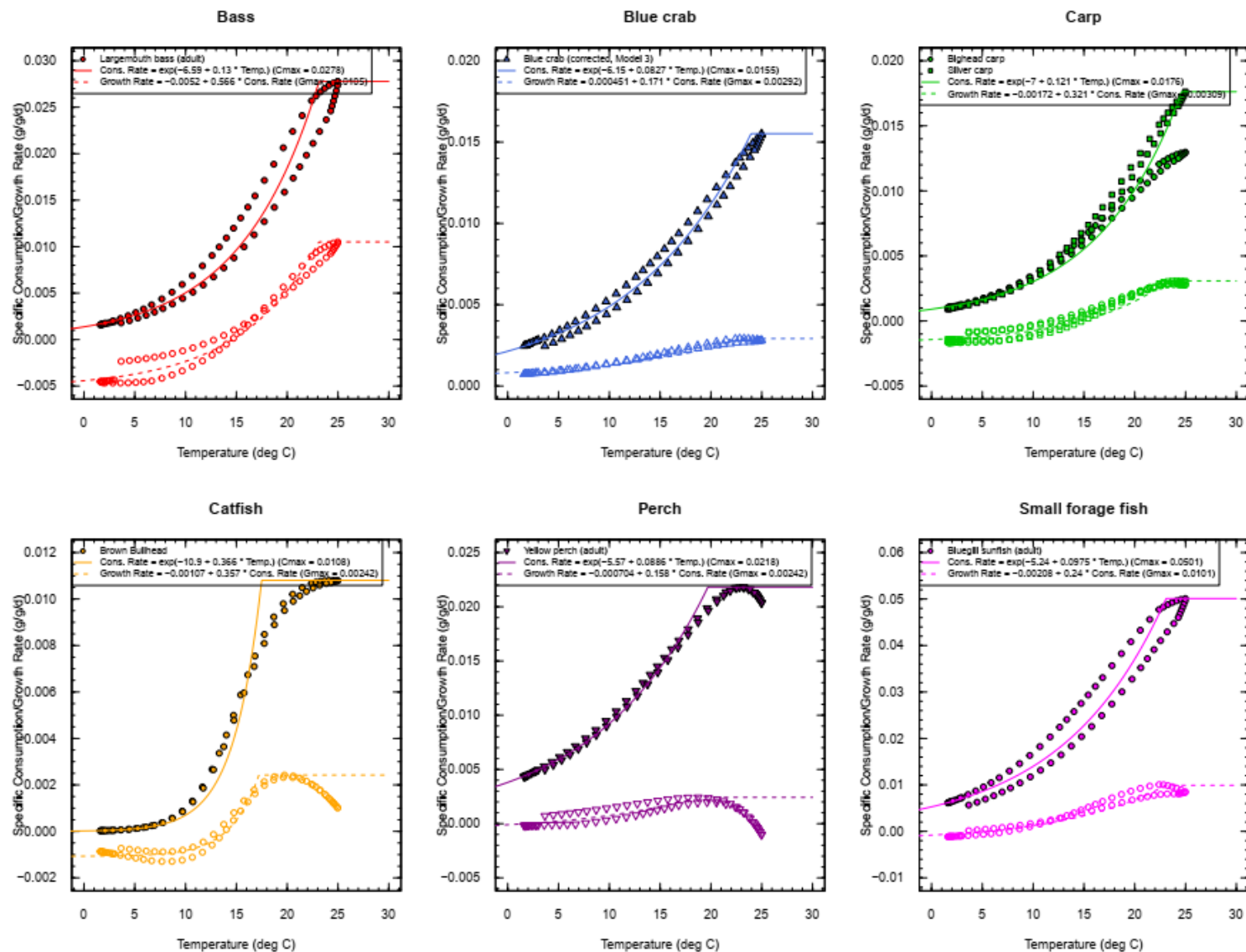


Figure 4-1. Final growth and consumption rate equations

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