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Bioaccumulation and Aquatic System Simulator (BASS) User's Manual Version 2.3

by

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Notice

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Foreword

This report describes the theoretical development, parameterization, and application software of the BASS **B**ioaccumulation and **A**quatic **S**ystem **S**imulator. This generalized, community-based simulation model is designed to predict the population and bioaccumulation dynamics of age-structured fish communities exposed to hydrophobic organic chemicals and class B and borderline metals that complex with sulfhydryl groups (e.g., cadmium, copper, lead, mercury, nickel, silver, and zinc). This report is not a case study on the application of BASS but a reference and user's guide. The intended audience of this report includes EPA Program and Regional environmental engineers and scientists, technical staff in other state and federal agencies, and fisheries ecologists who routinely analyze and estimate the bioaccumulation of chemicals in fish for ecological or human health exposure assessments.

Process-based models like BASS enable users to observe quantitatively the results of a particular abstraction of the real world. Moreover, such models can be argued to be the only objective method to make extrapolations to unobserved or unobservable conditions such as in the case of analyzing alternative management options for new or existing chemicals.

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Abstract

BASS (**B**ioaccumulation and **A**quatic **S**ystem **S**imulator) is a Fortran 95 simulation program that predicts growth, population, and bioaccumulation dynamics of age-structured fish assemblages exposed to hydrophobic organic pollutants and class B or borderline metals that complex with sulfhydryl groups (e.g., cadmium, copper, lead, mercury, nickel, silver, and zinc). The model's bioaccumulation algorithms are based on diffusion kinetics and are coupled to a process-based model for the growth of individual fish. These algorithms consider both biological attributes of fishes and physico-chemical properties of the chemicals that together determine diffusive exchange across gill membranes and intestinal mucosa. Biological characteristics used by the model include the fish's gill morphometry, feeding and growth rate, and proximate composition (i.e., its fractional aqueous, lipid, and structural organic content). Relevant physico-chemical properties include the chemical's aqueous diffusivity, n-octanol / water partition coefficient (K_{ow}), and, for metals, binding coefficients to proteins and other organic matter. BASS simulates the growth of individual fish using a standard mass balance, bioenergetic model (i.e., growth = ingestion - egestion - respiration - specific dynamic action - excretion). A fish's realized ingestion is calculated from its maximum consumption rate adjusted for the availability of prey of the appropriate size and taxonomy. The community's food web is delineated by defining one or more foraging classes for each fish species based on body weight, body length, or age. The dietary composition of each of these foraging classes is specified as a combination of benthos, incidental terrestrial insects, periphyton / attached algae, phytoplankton, zooplankton, and one or more fish species. Population dynamics are generated by predatory mortalities defined by the community's food web and standing stocks, physiological mortality rates, maximum longevity of species, toxicological responses to chemical exposures, and dispersal. The model's temporal and spatial scales are that of a day and of a hectare, respectively.

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1. Introduction

Fish health can be defined from ecological and human health / value perspectives in many ways. Questions relating to an ecological perspective include:

1. Are individual fish growth and condition sufficient to enable them to survive periods of natural (e.g., overwintering) and man-induced stress?
2. Are individual fish species able to maintain sustainable populations? For example, is individual growth adequate to attain the minimum body size required for reproduction? Is there adequate physical environment for successful spawning? Is there adequate physical habitat for the survival of the young-of-year?
3. Do regional fish assemblages exhibit their expected biodiversity or community structure based on biogeographical and physical habitat considerations?
4. Are regional fish assemblages maintaining their expected level of productivity based on biogeographical and physical habitat considerations?
5. Are appropriately sized fish abundant enough to maintain piscivorous wildlife (e.g., birds, mammals, and reptiles) during breeding and non-breeding conditions?
6. Are potential fish prey sufficiently free of contaminants (endocrine disruptors, heavy metals, etc.) so as not to interfere with the growth and reproduction of piscivorous wildlife?
7. How will native fishes respond to the introduction of nonnative fish species, including those stocked for recreational fishing?

From a human health or use perspective, another important question related to fish health is:

8. Is the fish community / assemblage of concern fishable? That is, are target fish species sufficiently abundant and of the desired quality? Fish quality in this context can be defined by desired body sizes (e.g., legal or trophy length) and the absence of chemical contaminants.

Some important indicators that have been used often to assess such questions include: (1) physical habitat dimensions (e.g., bottom type and cover, occurrence of structural elements such as woody debris or sand bars, mean and peak current velocities, water temperature, and sediment loads); (2) community species and functional diversity; (3) total community biomass (kg/ha or kg/km); (4) population density (fish/ha or fish/km) and biomass (kg/ha or kg/km) of dominant or valued species; (5) age and size class structure of dominant or valued species; (6) annual productivity of the community and its dominant species; (7) individual growth rates and condition factors (i.e., the ratio of a fish's current body weight to its expected body weight based on its length); and (8) levels of chemical contaminants in muscle or whole fish.

To evaluate alternative management options or to forecast expected future consequences of existing conditions, however, simulation models that can predict individual and population growth of fish and their patterns of chemical bioaccumulation are also important tools for assessing several of the aforementioned dimensions of fish health.

Although the growth of individual fish has often been described using empirical models such as the von Bertalanffy, logistic, Gompertz, or Richards models [see for example Ricker (1979) and Schnute (1981)], process-based bioenergetic models such as those described by Kitchell et al. (1977), Minton and McLean (1982), Stewart et al. (1983), Cuenco et al. (1985), Stewart and Binkowski (1986), Beauchamp et al. (1989), Stewart and Ibarra (1991), Lantry and Stewart (1993), Rand et al. (1993), Roell and Orth (1993), Hartman and Brandt (1995a), Petersen and Ward (1999), Rose et al. (1999), Schaeffer et al. (1999), and van Nes (2002) have become important tools for predicting fish growth. Because these process-based models predict fish growth based on the mass or energy balance of ingestion, egestion, respiration, specific dynamic action, and excretion, they can generally be parameterized independently of their current application. Moreover, because of the inherent difficulties in obtaining reliable field-based measurements of fish population dynamics and productivity, researchers are increasingly using such bioenergetic models to characterize these population and community level endpoints. See for example Stewart and Ibarra (1991) and Roell and Orth (1993).

The ability to predict accurately the bioaccumulation of chemicals in fish has become an essential component of ecological and human health risk assessments for chemical pollutants. Not only are accurate estimates needed to predict realistic dietary exposures to humans and piscivorous wildlife, but they are also needed to assess potential ecological risks to fish assemblages themselves more accurately. Although exposure-referenced benchmarks such as LC_{50} and EC_{50} have been widely used for hazard assessments, most deleterious effects of chemical pollutants are caused by the internal accumulation of those compounds, rather than their environmental concentrations per se. Many authors (Neely 1984, Friant and Henry 1985, McCarty et al. 1985, McCarty 1986, Connell and Markwell 1992, McCarty and Mackay 1993, Verhaar et al. 1995, van Loon et al. 1997) have discussed the benefits of explicitly considering chemical bioaccumulation when assessing expected ecological consequences of chemical

pollutants in aquatic and marine ecosystems. Residue-based toxicity studies confirm this supposition (Opperhuizen and Schrap 1988, van Hoogen and Opperhuizen 1988, Donkin et al. 1989, Tas et al. 1991, van Wezel et al. 1995, Driscoll and Landrum 1997).

Although concentrations of moderately hydrophobic chemicals in fish can often be predicted accurately by assuming equilibrium partitioning of the chemicals between the fish's organic constituents and the aqueous environment, this approach frequently fails to predict observed concentrations of extremely hydrophobic chemicals and metals that are often the chemicals of greatest concern. Observed deviations can be either considerably above or below those predicted by equilibrium partitioning. Several factors can be identified to explain these discrepancies.

Lower than expected contamination levels can result when the length of exposure is insufficient to allow chemicals to equilibrate. Because bioconcentration and bioaccumulation are generally treated as first-order linear processes, the time needed for chemicals to equilibrate between fish and their exposure media is an increasing function of the elimination half-lives of those chemicals in fish. For example, the time required for chemicals to achieve 95% of their equilibrium concentrations is approximately 4.3 times their elimination half-lives. Because the elimination half-lives of chemicals generally increase as their hydrophobicities increase, the time needed for chemicals to reach equilibrium concentrations in fish also increases as a function of chemical hydrophobicity. Consequently, for extremely hydrophobic chemicals such as polychlorinated biphenyls (PCBs) and dioxins that have elimination half-lives ranging from months to over a year, the time to equilibrium can be on the order of years. If the fish species of concern is short lived, the time needed for equilibrium can exceed the species' expected life span. Even when time is sufficient for equilibration, whole-body concentrations of fish can be much lower than those expected from thermodynamic partitioning due to physical dilution of the chemical that accompanies body growth or due to *in situ* biotransformation of the parent compound.

One of two possible assumptions is implicitly made whenever equilibrium-based estimators are used. The first of these is that only the selected reference route of exposure is significant in determining the total chemical accumulation in fish. The alternative assumption is that there are multiple routes of exposure that all covary with the chosen reference pathway in a constant manner. For bioconcentration factors (BCFs), the implicit assumption is that virtually the entire burden is exchanged directly with the water across the fish's gills or possibly across its skin. Although direct aqueous uptake is certainly the most significant route of exchange for moderately hydrophobic chemicals, dietary uptake accounts for most of a fish's body burden for extremely hydrophobic chemicals. This shift in the relative significance of the direct aqueous and dietary pathways is determined by the relative rates of exposure via these media and by a fundamental difference in the nature of chemical exchange from food and water. Consider, for example, the relative absolute exposures to a fish via food and water. The fish's direct aqueous exposure, AE (µg/d), is the product of its ventilation volume, Q (ml/d), and the chemical's aqueous concentration, C_w (µg/ml). Similarly, the fish's dietary exposure, DE (µg/d), is the product of its feeding rate, F_w (g wet wt/d), and the chemical's concentration in the fish's prey, C_p (µg/g wet wt). If the fish feeds only on one type of prey that has equilibrated with the water, one can calculate when the fish's aqueous and dietary exposures are equal using the equations

$$\begin{aligned} AE &= DE \\ Q\,C_w &= F_w\,C_p \\ Q/F_w &= BCF \end{aligned} \qquad (1.1)$$

Using data from Stewart et al. (1983) and Erickson and McKim (1990), the ventilation-to-feeding ratio for a 1 kg trout would be on the order of $10^{4.3}$ ml/g. Assuming that the quantitative structure activity relationship (QSAR) for the trout's prey is $BCF = 0.048\,K_{ow}$ (Mackay 1982), one would conclude that food is the trout's predominant route of exposure for any chemical whose octanol / water partition coefficient is greater than $10^{5.6}$. Although chemical exchange from both food and water occur by passive diffusion, uptake from food, unlike direct uptake from water, does not necessarily relax the diffusion gradient into the fish. This fundamental difference results from the digestion and assimilation of food that can actually cause chemical concentrations of the fish's gut contents to increase (Connolly and Pedersen 1988, Gobas et al. 1988). Predicting residue levels of chemicals, whose principal route of exchange is dietary, is further complicated since most fish species demonstrate well-defined size-dependent, taxonomic, and temporal trends regarding the prey they consume. Consequently, one would not expect a single BAF to be sufficiently accurate for risk assessments for all fish species or even different sizes of the same species.

Process-based models that describe a fish's chemical exchanges from food and water in concert with its growth, provide objective and scientifically sound frameworks that can overcome many of the aforementioned limitations of equilibrium-based BAFs and BCFs. Although numerous models have been developed toward this end (Norstrom et al. 1976, Thomann 1981, Jensen et al. 1982, Thomann and Connolly 1984, Barber et al. 1987, Gobas et al. 1988, Barber et al. 1991, Borgmann and Whittle 1992, Thomann et al. 1992, Gobas 1993, Madenjian et al. 1993, Jackson 1996, Luk and Brockway 1997, Morrison et al. 1999,

Arnot and Gobas 2004, Gewurtz et al. 2006, Park et al. 2008, Lopes et al. 2012), they differ significantly regarding how food web structure and dietary exposures are represented.

This report describes the theoretical framework, parameterization, and use of BASS (**B**ioaccumulation and **A**quatic **S**ystem **S**imulator). This generalized, process-based, Fortran 95 simulation model is designed to predict the growth of individuals and populations within an age-structured fish community and the bioaccumulation dynamics of those fish when exposed to mixtures of metals and organic chemicals. The model is formulated so that its parameterization does not rely upon calibration data sets from specific toxicokinetic and population field studies, but rather upon physical and chemical properties that can be estimated using chemical property calculators such as CLOGP (http://www.biobyte.com/bb/prod/clogp40.html) or the Chemical Transformation Simulator (CTS) (Wolfe et al. 2016) and on ecological, morphological, and physiological parameters that can be obtained from the published literature or computerized databases.

2. Model Formulation

To model the chemical bioaccumulation and growth of individuals and populations within an age-structured fish community, BASS solves the following system of differential equations for each age class or cohort of fish:

$$\frac{dB_f}{dt} = J_g + J_i - J_{bt} \tag{2.1}$$

$$\frac{dW_d}{dt} = F_d - E_d - R - EX - SDA \tag{2.2}$$

$$\frac{dN}{dt} = - EM - NM - PM \tag{2.3}$$

where B_f and W_d are the chemical body burden (µg/fish) and dry body weight (g dry wt/fish), respectively, of the average individual within the cohort; and N is the cohort's population density (fish/ha). In Equation (2.1), J_g is the net chemical exchange (µg/d) across the fish's gills from the water; J_i is the net chemical exchange (µg/d) across the fish's intestine from food; and J_{bt} is the chemical's biotransformation rate (µg/d). In Equation (2.2), F_d, E_d, R, EX, and SDA are the fish's feeding, egestion, routine respiration, excretion, and specific dynamic action (i.e., the respiratory expenditure in excess of R required to assimilate food), respectively, in units of g dry wt/d. Although many physiologically based models for fish growth are formulated in terms of energy content and flow (e.g., kcal/fish and kcal/d), Equation (2.2) is fundamentally identical to these bioenergetic models since energy densities of fish depend on their dry weight (Kushlan et al. 1986, Hartman and Brandt 1995b, Schreckenbach et al. 2001). Finally, in Equation (2.3) EM, NM and PM are the cohort's rates (fish/ha/d) of emigration/dispersal, non-predatory, and predatory mortality, respectively. Although immigration can be a significant determinant of population sizes, this process is not modeled in BASS. Because cohort recruitment is treated as a boundary condition, the right-hand side of Equation (2.3) does not require a term for recruitment. Although it may not be immediately apparent from the notation used, these equations are tightly coupled. For example, the realized feeding of fish depends on the availability (i.e., density and biomass) of suitable prey. The fish's predatory mortality, in turn, is determined by individual feeding levels and population densities of its predators. Finally, the fish's dietary exposure is determined by its rate of feeding and the levels of chemical contamination in its prey.

The following sections describe how each mass flux in the above system of equations is formulated in BASS. **Table 2.1** summarizes the definitions of the variables used to develop these equations. Because the system of units used to formulate chemical exchanges is essentially the CGS-system (centimeter, gram, second) and the system of units used to formulate a fish's growth is the CGD-system (centimeter, gram, day), some unit conversion is necessary to make the coupled system of equations dimensionally consistent. Readers should also note that while the growth of fish is modeled in terms of dry weight, a fish's chemical bioaccumulation is formulated in terms of its wet body weight since BASS models the chemical uptake and excretion by fish as chemical diffusion between aqueous phases.

2.1. Modeling Internal Distribution of Chemicals

Chemical exchanges across gills of fish and from their food are generally considered to occur by passive diffusion of chemicals between a fish's internal aqueous phase and its external aqueous environment, whether the latter is the surrounding ambient water or the aqueous phase of the fish's own intestinal contents. Consequently, to model these exchanges one must first consider how chemicals distribute within the bodies of fish. If a fish is conceptualized as a three-phase solvent consisting of water, lipid, and non-lipid organic matter, then its whole-body chemical concentration can be expressed as

$$\begin{aligned} C_f = \frac{B_f}{W_w} &= P_a C_a + P_l C_l + P_o C_o \\ &= \left(P_a + P_l \frac{C_l}{C_a} + P_o \frac{C_o}{C_a} \right) C_a \end{aligned} \tag{2.4}$$

where W_w is the fish's wet weight (g wet wt/fish); P_a, P_l, and P_o are the fractions of the whole fish that are water, lipid, and non-lipid organic material, respectively; and C_a, C_l, and C_o are the chemical's concentrations in those respective phases. Because the depuration rates of chemicals from different fish tissues often do not differ significantly (Grzenda et al. 1970, van Veld et al. 1984, Branson et al. 1985, Norheim and Roald 1985, Kleeman et al. 1986a, b), internal equilibration between these three phases can be assumed to be rapid in comparison to external exchanges. For organic chemicals, this assumption means that Equation (2.4) simplifies to

$$C_f = \left(P_a + P_l K_l + P_o K_o \right) C_a \tag{2.5}$$

where K_l and K_o are the chemical's partition coefficients between lipid and water and between organic carbon and water, respectively.

For metals, however, Equation (2.4) is more complicated. Although metals do partition into lipids (Simkiss 1983), their accumulation within most other organic media occurs by complexation reactions with specific binding sites. Consequently,

for metals the term $P_o C_d / C_a$ in Equation (2.4) could be formulated as a function of an appropriate stability coefficient and the availability of binding sites. Appendix A summarizes an equilibrium complexation model that was initially formulated for BASS. Despite its apparent correctness, however, this algorithm greatly overestimated metal (particularly mercury) bioaccumulation in fish. Although this overestimation can be attributed to several factors, the most likely explanation for the algorithm's unsatisfactory performance is that kinetics limits the complexation of metal in fish. Because kinetic modeling was considered incongruent with the time scales of most other major processes represented elsewhere in BASS, a much simpler algorithm was adopted.

Because many fate and transport models (e.g., EXAMS and WASP) have successfully used operationally defined distribution coefficients K_d to model the accumulation of metals in organic media, a similar approach was adopted for BASS. Thus, for a metal

$$C_f = \left(P_a + P_l K_l + P_o K_d\right) C_a \qquad (2.6)$$

where K_l is again an appropriate partition coefficient between lipid and water; and K_d is an appropriate metal-specific distribution coefficient. Although this equation appears identical to Equation (2.5) for organic contaminants, the relative values of K_d and K_o in relation to K_l can be remarkably different. See Section 3.1.

Because C_a equals the chemical's ambient environmental water concentration C_w at equilibrium, it follows from Equations (2.4) and (2.6) that a fish's thermodynamic bioconcentration factor ($K_f = C_f / C_w$ at equilibrium) for a chemical pollutant of concern is

$$K_f = \begin{cases} P_a + P_l K_l + P_o K_o & \text{for organics} \\ P_a + P_l K_l + P_o K_d & \text{for metalics} \end{cases} \qquad (2.7)$$

2.2. Modeling Exchange from Water

Because chemical exchange (J_g) across the gills of fish occurs by simple diffusion, it can be modeled by Fick's first law of diffusion as

$$J_g = S_g k_g \left(C_w - C_a\right) \qquad (2.8)$$

where S_g is the fish's total gill area (cm^2); k_g is the chemical's conductance (cm/s) across the gills from the interlamellar water; and C_w is the chemical's concentration (µg/ml) in the environmental water (Yalkowsky et al. 1973, Mackay 1982, Mackay and Hughes 1984, Gobas et al. 1986, Gobas and Mackay 1987, Barber et al. 1988, Erickson and McKim 1990). When Equations (2.5), (2.6), and (2.7) are substituted into this equation, one obtains

$$J_g = S_g k_g \left(C_w - \frac{C_f}{K_f} \right) \qquad (2.9)$$

Although the chemical's conductance k_g could be specified as a ratio of the chemical's diffusivity to the thickness of an associated boundary layer, implementation of this definition can be problematic since the boundary layer thickness is a function of the gill's ventilation velocity and varies along the length of the gill's secondary lamellae. To avoid this problem, a fish's net chemical exchange rate coefficient, $S_g k_g$, can be estimated by reformulating the gill's net chemical exchange as

$$J_g = Q\left(C_w - C_B\right) \qquad (2.10)$$

where Q is the fish's ventilation volume (cm^3/s); and C_B is the chemical's bulk concentration in the expired gill water. When Equations (2.8) and (2.10) are equated, it follows that

$$S_g k_g = Q \left(\frac{C_w - C_B}{C_w - C_a} \right) \qquad (2.11)$$

Despite its appearance, the right-hand side of this equation can be readily quantified. In particular, the ventilation volume of fish can be estimated by

$$Q = \frac{R_{O2}}{\alpha_{O2} C_{w,O2}} \qquad (2.12)$$

where R_{O2} is the fish's rate of oxygen consumption (µg/s); α_{O2} is the fish's oxygen assimilation efficiency; and $C_{w,O2}$ is the environmental water's dissolved oxygen concentration (µg/ml). If one makes certain assumptions concerning the geometry of the interlamellar spaces and the nature of mass transport between the gill's secondary lamellae, the chemical's normalized bulk concentration in the expired gill water ($(C_w - C_B)/(C_w - C_a)$) can also be calculated as outlined below.

Because the gill's secondary lamellae form flat channels having high aspect ratios (i.e., mean lamellar height / interlamellar distance), they can be treated as parallel plates, and the flow of water between them can be treated as Poiseuille slit flow (Hills and Hughes 1970, Stevens and Lightfoot 1986). Under this assumption, an expression for a chemical's concentration in the bulk expired gill water can be obtained using the solutions of the partial differential equation (PDE) that describes steady-state, convective mass transport between parallel plates, i.e.,

$$\frac{3}{2}\left(1 - \frac{x^2}{r^2}\right) V \frac{\partial C}{\partial y} = D \frac{\partial^2 C}{\partial x^2} \qquad (2.13)$$

where V is the gill's mean interlamellar flow velocity (cm/s); D is the chemical's aqueous diffusivity (cm^2/s); and x and y are the lateral and longitudinal coordinates of the channel along which

diffusion and convection occurs, respectively. In this equation, $C = C(x, y)$ is the chemical's interlamellar concentration at the distances x from the surface of the lamellae and y along its length. The surfaces of adjacent lamellae are located at $x = \pm r$ where r is the hydraulic radius of the lamellar channel that equals half the interlamellar distance d (cm). The midline between adjacent lamellae is therefore denoted by x=0. The gill's mean interlamellar flow velocity can be readily formulated as the ratio of the fish's ventilation volume to the gill's cross-sectional pore area, X_g (cm^2). Because the gill's pore area is related to its lamellar surface area by

$$X_g = \frac{S_g d}{l} \tag{2.14}$$

where d is the mean interlamellar distance (cm); and l is the mean lamellar length (cm) (Hills and Hughes 1970), a fish's mean interlamellar flow velocity is given by

$$V = \frac{Q l}{S_g d} \tag{2.15}$$

To solve Equation (2.13), two boundary conditions must be specified. Because adjacent lamellae presumably exchange the chemical equally well, the solutions should be symmetrical about the channel's midline. To insure this characteristic, the boundary condition

$$\left.\frac{\partial C}{\partial x}\right|_{x=0} = 0 \tag{2.16}$$

is assumed. The second necessary boundary condition must describe how chemical exchange across the secondary lamellae actually occurs. Assuming steady state diffusion from the interlamellar water to the fish's aqueous blood, this boundary condition can be formulated as

$$D\left.\frac{\partial C}{\partial x}\right|_{x=r} = -k_m\left[C(r,y) - C_a\right] \tag{2.17}$$

where k_m is the permeability (cm/s) of the gill membrane. Although this boundary condition has been used as is (Barber et al. 1991), it can also be modified to address potential perfusion limitations on gill uptake. To accomplish the latter task, a formulation patterned after Erickson and McKim (1990) is used. In particular, consider the following reformulation

$$D\left.\frac{\partial C}{\partial x}\right|_{x=r} = -k_m\left\{C(r,y) - \left[C_a(l) + \frac{J_s(y,l)}{q_p}\right]\right\} \tag{2.18}$$

where $C_a(y)$ is the chemical's aqueous phase concentration at point y along the length of a secondary lamella; $C_a(l) = C_a$ is the chemical's concentration in the afferent lamellar blood; $J_s(y, l)$ is the chemical's accumulated uptake (µg/s) along the lamellar segment $[y, l]$; and q_p is the lamellar perfusion rate (cm^3/s). If both sides of the lamella uptake chemical, then $J_s(y, l)$ can be formulated as

$$\begin{aligned} J_s(y,l) &= 2\int_y^l\int_0^h D\left.\frac{\partial C}{\partial x}\right|_{x=r} du\,dv \\ &= 2\,h\,D\int_y^l \left.\frac{\partial C}{\partial x}\right|_{x=r} dv \end{aligned} \tag{2.19}$$

where h is the height (cm) of the secondary lamella. Using this expression, the boundary condition (2.18) can now be written as

$$D\left.\frac{\partial C}{\partial x}\right|_{x=r} = -k_m\left[C(r,y) - C_a - \frac{2\,h\,D}{q_p}\int_y^l \left.\frac{\partial C}{\partial x}\right|_{x=r} dv\right] \tag{2.20}$$

Once the solution of Equation (2.13) for these boundary conditions has been obtained, the chemical's bulk concentration in the expired gill water can be evaluated using the weighted average

$$C_B = \frac{\int_0^r C(x,l)\left(1 - \frac{x^2}{r^2}\right) dx}{\int_0^r 1 - \frac{x^2}{r^2}\,dx} \tag{2.21}$$

that scales each concentration profile $C(x, l)$ by its relative velocity.

A canonical solution to Equation (2.13) can be obtained by non-dimensioning $C(x, y)$, x, and y as follows

$$\Theta = \frac{C - C_a}{C_w - C_a} \tag{2.22}$$

$$X = \frac{x}{r} \tag{2.23}$$

$$Y = \frac{y D}{V r^2} \tag{2.24}$$

When this is done, the chemical's dimensionless bulk concentration is given by

$$\Theta_B = \frac{C_B - C_a}{C_w - C_a} = \frac{\int_0^1 \Theta(X, N_{Gz})(1 - X^2)\,dX}{\int_0^1 1 - X^2\,dX} \qquad (2.25)$$

where $N_{Gz} = (l\ D)/(V\ r^2)$ is the gills' dimensionless lamellar length or Graetz number. Two important features of this expression can now be observed. First, one can easily verify that

$$1 - \Theta_B = \frac{C_w - C_B}{C_w - C_a} \qquad (2.26)$$

Consequently, Equation (2.11) can be rewritten as

$$S_g k_g = Q(1 - \Theta_B) \qquad (2.27)$$

Secondly, analytical expressions for Θ_B are readily available (Brown 1960, Grimsrud and Babb 1966, Colton et al. 1971, Walker and Davies 1974). In particular, a chemical's dimensionless bulk concentration can be evaluated by

$$\Theta_B = \sum_{m=0}^{\infty} B_m \exp(-\tfrac{2}{3}\lambda_m^2 N_{Gz}) \qquad (2.28)$$

where the coefficients B_m and exponents λ_m are known functions of the gills' dimensionless conductance or Sherwood number

$$N_{Sh} = \frac{k_m r}{D} \qquad (2.29)$$

and the fish's ventilation / perfusion volume ratio. See Appendix B. Although this infinite series solution does not have a convenient convergence formula, for Sherwood numbers and ventilation / perfusion ratios that are typical of fish gills, only the first two terms of the series are needed to estimate Θ_B with less than 1% error (see Barber et al. 1991). See **Figure 2.1** and **Figure 2.2** for displays of λ_1 and B_1 and of λ_2 and B_2, respectively.

2.3. Modeling Exchange from Food

Chemical exchange (J_i) across the intestines of fish often has been modeled as unidirectional chemical uptake assuming that fish assimilate a constant fraction of the chemical that they ingest, i.e.,

$$J_i = \alpha_c C_p F_w \qquad (2.30)$$

where α_c is the assimilation efficiency (dimensionless) for the chemical; C_p is the chemical's concentration (µg/g wet wt) in the ingested prey; and F_w is the fish's daily wet weight prey consumption (g wet wt/d) (Norstrom et al. 1976, Jensen et al. 1982, Thomann and Connolly 1984, Niimi and Oliver 1987). Because the chemical exchange across the intestine is driven by diffusive gradients (Vetter et al. 1985, Clark et al. 1990, Gobas et al. 1993), however, such formulations are thermodynamically realistic only if α_c is a decreasing function of the fish's total body concentration C_f.

A thermodynamically based description for the dietary exchange of chemicals can be formulated using the simple mass balance relationship

$$J_i = C_p F_w - C_e E_w \qquad (2.31)$$

where E_w is the fish's daily wet weight egestion (g wet wt/d) and C_e is the pollutant's chemical concentration (µg/g wet wt) in the fish's feces. When this equation is reformulated in terms of dry weight feeding and egestion (i.e., $F_d = P_{dp} F_w$ and $E_d = P_{de} E_w$ where P_{dp} and P_{de} denote the prey's and feces' dry weight fractions , respectively) the fish's net dietary exchange becomes

$$\begin{aligned} J_i &= \frac{C_p F_d}{P_{dp}} - (C_{ae} E_a + C_{de} E_d) \\ &= \frac{C_p F_d}{P_{dp}} - \left(\frac{E_a}{E_d} + \frac{C_{de}}{C_{ae}}\right) C_{ae} E_d \\ &= \frac{C_p F_d}{P_{dp}} - \left(\frac{P_{ae}}{P_{de}} + \frac{C_{de}}{C_{ae}}\right) C_{ae} E_d \\ &= \frac{C_p F_d}{P_{dp}} - \left(P_{ae} + P_{de}\frac{C_{de}}{C_{ae}}\right) \frac{C_{ae} E_d}{P_{de}} \end{aligned} \qquad (2.32)$$

where C_{ae} and C_{de} are the pollutant's chemical concentrations in the aqueous and dry phases of the fish's feces, respectively; E_a is the mass / volume of the feces' aqueous phase; and P_{ae} and P_{ap} are the aqueous fractions of the fish's feces and prey, respectively. To parameterize Equation (2.32), two assumptions are made.

The first assumption is that the concentrations of chemicals in the fish's aqueous blood, intestinal fluids, and dry fecal matter equilibrate with one another because the transit time through the gastrointestinal tract is relatively slow; consequently, $C_{ae} = C_a$. Moreover, for organic chemicals, the concentration ratio C_{de}/C_{ae} can be replaced with an organic carbon / water partition coefficient, K_{oc} (e.g., Briggs 1981, Karickhoff 1981, Chiou et al. 1986), and for metals, this ratio can be substituted with a distribution coefficient similar to that used in Equation (2.6).

Although reported values for the percent moisture of the intestinal contents of fish vary typically between 50% and 80% (Brett 1971, Marais and Erasmus 1977, Grabner and Hofer

1985), the second assumption made to parameterize Equation (2.32) assumes that the fish's intestinal contents and whole body are osmotically equilibrated; consequently, $P_{ae} = P_a$. If this assumption is reasonable, then meals with the same dry weights but different wet weights should be processed by the fish at equal rates and efficiencies since both will attain the same proximate composition relatively soon after ingestion. Having the same proximate composition implies that the concentrations of digestive enzymes acting on the meals will be comparable and that the physical forces exerted by the gut contents that control gastric mobility will also be comparable. Because Bromley (1980), Garber (1983), and Ruohonen et al. (1997) demonstrated that initial dietary moisture content had no significant effect on the assimilation efficiencies of turbot (*Scophthalmus maximus*) or on gastric evacuation rates of yellow perch (*Perca flavescens*) and rainbow trout (*Oncorhynchus mykiss*), respectively, the assumption that $P_{ae} = P_a$ seems reasonable.

Using the stated assumptions above and Equations (2.5), (2.6), and (2.7), Equation (2.32) can now be rewritten as

$$\begin{aligned} J_i &= \frac{C_p F_d}{P_{dp}} - \left[P_a + \left(1 - P_a\right) K_{oc}\right] \frac{C_f E_d}{K_f \left(1 - P_a\right)} \\ &= \frac{C_p F_d}{P_{dp}} - \frac{K_e C_f E_d}{K_f \left(1 - P_a\right)} \end{aligned} \tag{2.33}$$

where K_e is the distribution coefficient describing the chemical partitioning between the aqueous and dry organic matter phases of the fish's intestinal contents. Although BASS uses this equation to calculate a fish's net chemical dietary exchange, this equation can also be further manipulated as follows

$$\begin{aligned} J_i &= \left[1 - \frac{P_{dp} C_f K_e E_d}{\left(1 - P_a\right) C_p K_f F_d}\right] \frac{C_p F_d}{P_{dp}} \\ &= \left[1 - \left(1 - \alpha_f\right) \frac{P_{dp} C_f K_e}{P_d C_p K_f}\right] C_p F_f \end{aligned} \tag{2.34}$$

where $\alpha_f = (F_d - E_d)/F_d$ is the fish's food assimilation efficiency (g dry wt assimilated/g dry wt ingested), and $P_d = (1 - P_a)$ is the fish's dry fraction. In other words, a thermodynamically based assimilation efficiency for Equation (2.30) corresponds to

$$\alpha_c = 1 - \left(1 - \alpha_f\right) \frac{P_{dp} C_f K_e}{P_d C_p K_f} \tag{2.35}$$

Thus, Equation (2.33) is equivalent to Equation (2.30) with a chemical assimilation efficiency that decreases as the fish's whole-body chemical burdens or concentrations increase. Studies by Lieb et al. (1974), Gruger et al. (1975), and Opperhuizen and Schrap (1988) corroborate this prediction (see Barber et al. 1991). Additionally, using *in situ* preparations of channel catfish intestines Doi et al. (2000) have established clearly that pre-exposures to 3,4,3',4'-tetrachlorobiphenyl decrease intestinal uptake rates.

Although the preceding model development demonstrates the potential logical inconsistency between an assumed constant chemical assimilation efficiency model for dietary chemical uptake and a thermodynamically based model, many researchers continue to use the former assumption and model. Parameters for these constant chemical assimilation efficiency models generally have been estimated using the following equations proposed by Bruggeman et al. (1981)

$$\frac{dC_f}{dt} = \alpha_c \varphi_{ww} C_p - k_2 C_f \tag{2.36}$$

$$C_f = \left(\frac{\alpha_c \varphi_{ww} C_p}{k_2}\right) \left[1 - \exp(-k_2 t)\right] \tag{2.37}$$

where φ_{ww} is the fish's weight-specific feeding rate (g wet wt/g wet wt/d); and k_2 is the fish apparent elimination rate coefficient (g wet wt/g wet wt/d or 1/d) that is the sum of its rate coefficients of growth (γ), biotransformation (k_{bt}), and actual excretion (k_{ex}). See for example Muir et al. (1992), Dabrowska et al. (1996), and Fisk et al. (1998). Unfortunately, many researchers have failed to acknowledge that Equation (2.37) is the solution to Equation (2.36) only when initial time is $t_0 = 0$ and the fish's initial whole-body concentration is zero (i.e., $C_f(t_0) = 0$). This fact, combined with the ability of Equation (2.37) to fit experimental results statistically, has been at least partially responsible for the perpetuation of the idea of constant chemical assimilation efficiencies.

The general solution to Equation (2.36) is actually

$$C_f = \frac{\alpha_c \varphi_{ww} C_p}{k_2} + \left[C_f(t_0) - \frac{\alpha_c \varphi_{ww} C_p}{k_2}\right] \exp\left[-k_2 \left(t - t_0\right)\right] \tag{2.38}$$

When this solution is re-differentiated, one observes that

$$\frac{dC_f}{dt} = \left[\alpha_c \varphi_{ww} C_p - k_2 C_f(t_0)\right] \exp\left[-k_2 \left(t - t_0\right)\right] \tag{2.39}$$

Using this exponential form of Equation (2.36), one can analyze the parameter behavior of a dietary exposure during consecutive time segments for which φ_{ww} and C_p are constant. Therefore, let $T = (t_2 - t_0)$ denote the length of such a dietary exposure, and let t_1 denote the time when the exposure is half over. During the first half of the exposure (i.e., $t_0 < t < t_1$) the fish's bioaccumulation dynamics will be described by Equation (2.39). During the second half of the exposure, however, these dynamics will be

described by

$$\frac{dC_f}{dt} = \left[\hat{\alpha}_c \varphi_{ww} C_p - \hat{k}_2 C_f(t_1)\right] \exp\left[-\hat{k}_2 (t - t_1)\right] \qquad (2.40)$$

where $\hat{\alpha}_c$ and $\hat{k}_2$ are the fish's assimilation efficiency and apparent elimination rate coefficient that may require updating for $t_1 < t < t_2$. If an equation of the form of Equation (2.37) is assumed to describe the fish's bioaccumulation dynamics over the entire interval $[t_0, t_2]$, then the derivatives specified by Equations (2.39) and (2.40) must be equal when evaluated for $t = t_1$. This consistency condition, which is analogous to the preservation of derivatives that occurs when approximating a function with Bernstein polynomials, requires that

$$\hat{\alpha}_c \varphi_{ww} C_p - \hat{k}_2 C_f(t_1) = \left[\alpha_c \varphi_{ww} C_p - k_2 C_f(t_0)\right] \exp\left[-k_2 (t_1 - t_0)\right] \qquad (2.41)$$

which implies that

$$\hat{\alpha}_c = \frac{\hat{k}_2 C_f(t_1)}{\varphi_{ww} C_p} + \left[\alpha_c - \frac{k_2 C_f(t_0)}{\varphi_{ww} C_p}\right] \exp\left[-k_2 (t_1 - t_0)\right] \qquad (2.42)$$

When the fish's initial whole-body concentration is zero, this equation can be shown to reduce to

$$\hat{\alpha}_c = \alpha_c \left\{\frac{\hat{k}_2}{k_2} + \left(1 - \frac{\hat{k}_2}{k_2}\right) \exp\left[-k_2 (t_1 - t_0)\right]\right\} \qquad (2.43)$$

This equation shows that unless $\hat{k}_2 = k_2$, chemical assimilation efficiencies estimated for different times and initial whole-body concentration will be different. Phrased another way, this equation implies that the fish's ability to excrete, biodilute, and biotransform chemicals, as measured by $\hat{k}_2$ and k_2, contributes to the determination of the fish's realized chemical assimilation efficiencies. Because weight-specific growth rates ($\gamma = W_w^{-1} dW_w/dt$) and chemical excretion rate coefficients (k_{ex}) for fish are generally related to the fish's body size as allometric power functions, i.e.,

$$\gamma = \alpha_1 W_w^{\alpha_2} \qquad (2.44)$$

$$k_{ex} = \beta_1 W_w^{\beta_2} \qquad (2.45)$$

where $\alpha_2 < 0$ and $\beta_2 < 0$ (Barber et al. 1988, Sijm et al. 1993, Sijm and van der Linde 1995, Sijm et al. 1995), one would expect that $\hat{k}_2 < k_2$ when significant growth occurs during the experiment. Consequently, one would also expect that $\hat{\alpha}_c < \alpha_c$. Importantly, this simple analysis is corroborated by Ram and Gillet (1993) who showed that assimilation efficiencies for a variety of organochlorines by oligochaetes decreased as chemical exposures progressed.

BASS's fecal partitioning model [i.e., Equation (2.33)] is best suited to circumstances where its equilibrium assumptions are reasonably satisfied, as where the object is to predict the dietary exchange of the average individual of a population. A more kinetically based approach may be needed, however, when describing the toxicokinetics of individual fish. See for example Nichols et al. (1998). Readers are referred to Barber (2008) for a more thorough discussion and analysis of dietary uptake algorithms used to model chemical bioaccumulation in fish.

2.4. Modeling Chemical Biotransformation

BASS assumes that the metabolism of xenobiotic chemicals in fish is a simple, first-order reaction of the chemical's aqueous phase concentration, i.e.,

$$J_{bt} = (\varepsilon_a C_a)(P_a W_w) \qquad (2.46)$$

where ε_a is the fish's aqueous phase biotransformation rate coefficient (1/d); and $(P_a W_w)$ is the volume of the fish's aqueous phase. If Equations (2.9) and (2.46) are used to describe chemical bioconcentration during a water-only exposure without growth, a fish's whole-body concentration would be modeled as

$$\frac{dC_f}{dt} = \frac{1}{W_w}\frac{dB_f}{dt} = \frac{S_g k_g}{W_w}\left(C_w - \frac{C_f}{K_f}\right) - \frac{\beta P_a C_f}{K_f} = k_u C_w - (k_{ex} + k_{bt}) C_f \qquad (2.47)$$

where k_u, k_{ex}, and k_{bt} are the fish's rate coefficients of gill uptake, excretion, and biotransformation, respectively. This equation predicts that a fish's whole-body biotransformation rate k_{bt} should be inversely proportional to its thermodynamic bioconcentration factor K_f that in turn is proportional to the chemical's K_{ow}. This relationship, however, will also be influenced by any quantitative structure activity relationships (QSARs) that the fish's aqueous phase biotransformation rate ε_a might exhibit. See de Wolf et al. (1992) and de Bruijn et al. (1993).

2.5. Modeling Temperature Effects on Physiological Rates

Because temperature affects a fish's feeding, assimilation, respiration, and egestion, a discussion of how temperature modulates these processes is in order before describing how BASS actually models fish growth. Although the temperature dependence of physiological processes is often described using an exponential response equation, e.g.,

$$p_1 = p_0 \exp\left[\varepsilon (T_1 - T_0)\right] \qquad (2.48)$$

where p_0 and p_1 are the reaction rates of the process at temperatures T_0 and T_1, respectively, such descriptions are generally valid only within a range of the organism's thermal tolerance. In many cases, however, a process's reaction rate increases monotonically with temperature only up to a temperature T_1 after which it decreases. Moreover, the temperature at which a process's rate is maximum is often very close to the organism's upper thermal tolerance limit. To model this behavior, Thornton and Lessem (1978) developed a logistic multiplier to describe the temperature dependence of a wide variety of physiological processes. Although this algorithm has been used successfully in many fish bioenergetic models, BASS uses an exponential-type formulation that responds hyperbolically to increasing temperature. Importantly, such algorithms can be easily parameterized.

Let P denote the rate of a physiological process, and let T_1 denote the temperature at which the rate is at its maximum value. If this process generally exhibits an exponential response to temperature changes well below T_1, then Equation (2.48) can be used to describe this process for T and $T_0 << T_1$, i.e.,

$$P = P_0 \exp\left[\varepsilon\left(T - T_0\right)\right] \tag{2.49}$$

$$\frac{dP}{dT} = \varepsilon P \tag{2.50}$$

where P_0 is the process's rate at the low-end reference temperature T_0. To incorporate the adverse effects of high temperatures on this process, the right-hand side of Equation (2.50) can be multiplied by a hyperbolic temperature term that approaches unity as temperature decreases well below T_1; equals zero at T_1; and becomes increasingly negative as temperature approaches the fish's upper thermal tolerance limit $T_L = T_2$. Modifying Equation (2.50) in this fashion yields

$$\frac{dP}{dT} = \varepsilon P\left(\frac{T - T_1}{T - T_2}\right) \tag{2.51}$$

whose solution is

$$P = P_0 \exp\left[\varepsilon\left(T - T_0\right)\right]\left(\frac{T_2 - T}{T_2 - T_0}\right)^{\varepsilon\left(T_2 - T_1\right)} \tag{2.52}$$

If one assumes, without loss of generality, that $T_0 = 0$, the preceding equation can be simplified to

$$P = P_0 \exp\left(\varepsilon T\right)\left(1 - \frac{T}{T_2}\right)^{\varepsilon\left(T_2 - T_1\right)} \tag{2.53}$$

Figure 2.3 displays the behavior of this equation for $P_0 = 1$ and $T_2 = 36$ Celsius as a function of ε and T_1. Although these equations apparently have not been used to describe physiological responses of fish, their utility for doing so is discussed in Section 3.3. For other applications of Equations (2.52) and (2.53) see Lassiter and Kearns (1974), Lassiter (1975), and Swartzman and Bentley (1979). Note that when $T_1 = T_2$, Equation (2.53) reduces to Equation (2.49).

2.6. Modeling Growth of Fish

Although the preceding algorithms for modeling chemical bioaccumulation in fish depend on a fish's wet weight, BASS does not directly simulate the wet weight of fish. Instead, it simulates the dry weight of fish as the mass balance of feeding, egestion, respiration, and excretion and then calculates the fish's associated wet weight using the following relationships

$$W_w = W_a + W_d = W_a + W_l + W_o \tag{2.54}$$

$$P_l = l_1 W_w^{l_2} \tag{2.55}$$

$$P_a = a_0 - a_1 P_l \tag{2.56}$$

$$P_o = 1 - P_a - P_l \tag{2.57}$$

where W_a, W_d, W_l, and W_o are the fish's aqueous, dry, lipid, and non-lipid organic weights, respectively; and a_0, a_1, l_1, and l_2 are empirical constants. Whereas Equations (2.54) and (2.57) are simply assertions of mass conservation, Equations (2.55) and (2.56) are purely empirical functions. Although Equation (2.55) is assumed because simple power functions of this form adequately describe many morphometric relationships for most organisms, Equation (2.56) is based on the results of numerous field and laboratory studies (Eschmeyer and Phillips 1965, Brett et al. 1969, Groves 1970, Elliott 1976a, Staples and Nomura 1976, Craig 1977, Shubina and Rychagova 1981, Beamish and Legrow 1983, Weatherley and Gill 1983, Flath and Diana 1985, Lowe et al. 1985, Kunisaki et al. 1986, Morishita et al. 1987). These equations yield an expression for a fish's wet weight that is a monotonically increasing, but nonlinear, function of the fish's dry weight.

BASS calculates a fish's realized feeding by first estimating its expected consumption (F_d^* g dry wt/d) and then adjusting this potential by the availability of appropriate prey as described in the next section. Because a variety of models are commonly used to describe the expected feeding of fish, BASS is coded to allow users the option of using any one of four different feeding models for any particular age / size class of fish.

The first feeding model is a temperature-dependent power function

$$F_d^* = f_1 W_w^{f_2} \exp\left(f_3 T\right)\left(1 - \frac{T}{T_2}\right)^{f_3\left(T_2 - T_1\right)} \tag{2.58}$$

where f_1, f_2, f_3, T_1, and T_2 are empirical constants specific to the fish's feeding.

The second feeding model is the Rashevsky-Holling model that is defined by the equations

$$F_d^* = \varphi_{dd}\left(G_{\max} - G\right)$$
$$\frac{dG}{dt} = F_d^* - A_d - E_d \qquad (2.59)$$

where φ_{dd} is the fish's *ad libitum* feeding rate (g dry wt/g dry wt/d); G_{max} is the maximum amount of food (g dry wt/fish) that the fish's stomach / gut can hold; G is the actual amount of food (g dry wt/fish) present in the gut; and A_d and E_d are the fish's assimilation and egestion, respectively, in units of g dry wt/d (Rashevsky 1959, Holling 1966). Given a fish's gut capacity G_{max}, feeding time t_{sat} to satiation, and satiating meal size M_{sat} , φ_{dd} can be estimated using the equations

$$F_d^*(t) = \int_0^t \varphi_{dd}\left[G_{\max} - F_d^*(\tau)\right] d\tau \qquad (2.60)$$

$$\frac{dF_d^*}{dt} = \varphi_{dd}\left(G_{\max} - F_d^*\right) \qquad (2.61)$$

$$-\varphi_{dd}\, t_{sat} = \ln\left(1 - \frac{M_{sat}}{G_{\max}}\right) \qquad (2.62)$$

where $F_d^*(t)$ is the total food consumed during the interval $(0, t)$ and $M_{sat} = F_d^*(t_{sat})$ (also see Dunbrack 1988). Alternatively, φ_{dd} can be estimated by simply assuming that $M_{sat} = 0.95 \times G_{max}$ in which case

$$\varphi_{dd} = -\frac{\ln 0.05}{t_{sat}} \qquad (2.63)$$

The third feeding model, which is intended for planktivorous species and larval/juvenile fish cohorts in general, is the clearance volume model

$$F_d^* = \Psi\, Q_{cl} \qquad (2.64)$$

where Ψ is the plankton standing stock (g dry wt/L); and Q_{cl} is the planktivore's clearance volume (L/d) that is assumed to be given by

$$Q_{cl} = q_1\, W_w^{\,q_2} \exp\left(q_3\, T\right)\left(1 - \frac{T}{T_2}\right)^{q_3 (T_2 - T_1)} \qquad (2.65)$$

where q_1, q_2, q_3, T_1, and T_2 are empirical constants specific to the fish's filtering rate.

The fourth feeding model back-calculates a fish's expected feeding based on knowing the fish's expected growth and routine respiratory demands. In particular, because assimilation, egestion, specific dynamic action, and excretion are assumed to be linear functions of feeding and routine respiration as discussed subsequently, it is a straightforward matter to calculate a fish's expected ingestion given its expected growth and respiration. When users elect this feeding option, BASS assumes that the fish's weight-specific growth rate $\gamma = W_w^{-1}\, dW_w/dt$ (1/d) is given by

$$\gamma = g_1\, W_w^{\,g_2} \exp\left(g_3\, T\right)\left(1 - \frac{T}{T_2}\right)^{g_3 (T_2 - T_1)} \qquad (2.66)$$

where g_1, g_2, g_3, T_1, and T_2 are empirical constants specific to the fish's growth rate. See Thomann and Connolly (1984) for additional discussion of this feeding model.

When BASS estimates a fish's feeding rate using Equations (2.58), (2.64), or (2.66), the fish's assimilation and egestion are estimated as simple fractions of its realized ingestion F_d, i.e.,

$$A_d = \alpha_f F_d \qquad (2.67)$$

$$E_d = \left(1 - \alpha_f\right) F_d \qquad (2.68)$$

where α_f is the fish's net food assimilation efficiency that is a weighted average of its assimilation efficiencies for invertebrate, piscine, and vegetative prey. When the Rashevsky-Holling feeding model is used, however, BASS calculates these fluxes by substituting F_d with a function that describes the fish's pattern of intestinal evacuation. The general form of this function is assumed to be

$$EV = e_1\, G^{e_2} \exp\left(e_3\, T\right)\left(1 - \frac{T}{T_2}\right)^{e_3 (T_2 - T_1)} \qquad (2.69)$$

where e_1, e_2, e_3, T_1, and T_2 are empirical constants specific to the fish's gastric evacuation.

The numerical value of this function's exponent, e_2, depends on characteristics of the food being consumed and on the mechanisms that presumably control gastrointestinal motility and digestion (Jobling 1981, 1986, 1987). For example, when gut clearance is controlled by intestinal peristalsis, e_2 should approximately equal ½ since peristalsis is stimulated by circumferential pressure exerted by the intestinal contents that, in turn, is proportional to the square root of the contents mass. On the other hand, when surface area controls the rate of digestion, e_2 should be approximately either ⅔ or unity. If the fish consumes a small number of large-sized prey (e.g., a piscivore), $e_2 = ⅔$ may be the appropriate surface area model. On the other hand, if the fish consumes a large number of smaller, relatively uniform-sized prey (e.g., a planktivore or drift feeder),

$e_2 = 1$ is more appropriate since total surface area and total volume of prey become almost directly proportional to one another. When $e_2 = 1$, the Rashevsky-Holling model [i.e., Equation (2.59)] is analogous to the Elliott-Persson model for estimating daily rations of fish (Elliott and Persson 1978). Finally, Olson and Mullen (1986) outlined a process-based model that even suggests $e_2 = 0$.

A fish's specific dynamic action, i.e., the respiratory expenditure associated with the digestion and assimilation of food, is modeled as a constant fraction of the fish's assimilation. In particular,

$$SDA = \sigma A_d \tag{2.70}$$

where σ generally varies between 0.15 and 0.20 (Ware 1975, Tandler and Beamish 1981, Beamish and MacMahon 1988).

BASS assumes that body weight losses via metabolism are due entirely to the respiration of carbon dioxide and the excretion of ammonia. A fish's respiratory loss R is therefore calculated from its routine oxygen consumption, R_{O2} (g O_2/d), using a respiratory quotient, RQ (L CO_2 respired)/L O_2 consumed), as follows

$$R = \frac{12\,g\ C}{mole\ CO_2} \bullet \frac{mole\ CO_2}{22.4\,L\ CO_2} \bullet RQ \bullet \frac{22.4\,L\ O_2}{mole\ O_2} \bullet \frac{mole\ O_2}{32\,g\ O_2} \bullet R_{O2} = \frac{12}{32} \bullet RQ \bullet R_{O2} \tag{2.71}$$

BASS calculates a fish's routine oxygen consumption as a constant multiple RB of its standard basal oxygen consumption (Ware 1975) that is assumed to be a temperature-dependent power function. In particular,

$$R_{O2} = RB\ b_1 W_w^{b_2} \exp\left(b_3 T\right)\left(1 - \frac{T}{T_2}\right)^{b_3 (T_2 - T_1)} \tag{2.72}$$

where b_1, b_2, b_3, T_1, and T_2 are empirical constants specific to the fish's standard basal oxygen consumption. Although ammonia excretion could be modeled using an analogous function (Paulson 1980, du Preez and Cockroft 1988a, b), BASS calculates this flux as a constant fraction of the fish's total respiration since excretion and oxygen consumption generally track one another. For example, ammonia excretion increases after feeding, as does oxygen consumption (Savitz 1969, Brett and Zala 1975, Gallagher et al. 1984). Likewise, conditions that inhibit the passive excretion of ammonia also depress carbon dioxide excretion (Wright et al. 1989). Assuming that fish maintain a constant nitrogen/carbon ratio NC (g N/g C), BASS estimates a fish's excretory loss in body weight as

$$EX = \varepsilon NC\left(R + SDA\right) \tag{2.73}$$

where ε = 17/14 is the ratio of the molecular weight of ammonia to that of nitrogen.

2.7. Modeling Predator-Prey Interactions

BASS simulates aquatic food webs in which each age class of a species can feed upon other fish species, benthos, incidental terrestrial insects, periphyton / attached algae, phytoplankton, and zooplankton. The realized feeding of any given age class of fish is determined by the expected feeding rate of individuals within the cohort, the cohort's population size, and the biomass of prey available to the cohort; the latter quantity is the sum of the current biomass of potential prey minus the biomass of potential prey expected to be consumed by other fish cohorts that are more efficient foragers / competitors. BASS ranks the competitive abilities of different cohorts using the following assumptions:

ASSUMPTION 1. The competitive abilities and efficiencies of benthivores and piscivores are positively correlated with their body sizes (Garman and Nielsen 1982, East and Magnan 1991). Two general empirical trends support this assumption. The first of these is the trend for the reactive distances, swimming speeds, and territory sizes of fish to be positively correlated with their body size (Minor and Crossman 1978, Breck and Gitter 1983, Wanzenböck and Schiemer 1989, Grant and Kramer 1990, Miller et al. 1992, Keeley and Grant 1995, Minns 1995). Given two differently sized predators of the same potential prey, these trends suggest that the larger predator is more likely to encounter that prey than is the smaller. Having encountered the prey, the other general trend for prey handling times to be inversely correlated with body size (Werner 1974, Miller et al. 1992) suggests that the larger predator could dispatch intercepted prey and resume foraging more quickly than the smaller predator. Also see Post et al. (1999) and Railsback et al. (2002).

ASSUMPTION 2. Unlike benthivores and piscivores, the competitive abilities and efficiencies of planktivores are inversely related to their body size due to their relative morphologies (Lammens et al. 1985, Johnson and Vinyard 1987, Wu and Culver 1992, Persson and Hansson 1999). Consequently, "large" planktivores only have access to the leftovers of "small" planktivores.

BASS calculates the relative frequencies $\{..., d_i, ...\}$ of the prey consumed by a cohort using dietary electivities, i.e.,

$$e_i = \frac{d_i - f_i}{d_i + f_i} \tag{2.74}$$

where f_i is the relative availability of the i-th prey with respect to all other prey consumed by the cohort. One can easily verify that the range of dietary electivities is $-1 < e_i < 1$. One can also

verify that if the fish does not eat a potential food item *i*, $e_i = -1$. Similarly, if the fish consumes a potential prey item *i* in direct proportion to the prey's relative abundance, then $e_i = 0$. BASS actually allows users to specify a fish's diet as either a set of fixed dietary frequencies $\{\ldots,\bar{d}_i,\ldots\}$, a set of electivities $\{\ldots,\bar{e}_i,\ldots\}$, or a combination of fixed frequencies and electivities $\{\ldots,\bar{d}_i,\ldots,\bar{e}_j,\ldots\}$. To calculate a cohort's realized dietary composition, however, BASS converts all user-specified fixed dietary frequencies into their equivalent electivities using the simulated relative abundances $\{\ldots,f_i,\ldots\}$ of the cohort's potential prey. These electivities are then combined with user-specified electivities to form a set of unadjusted electivities $\{\ldots,\hat{e}_i,\ldots\}$ that is subsequently converted into a consistent set of realized electivities $\{\ldots,e_i,\ldots\}$. Finally, BASS then calculates the cohort's realized dietary frequencies using

$$d_i = \left(\frac{1 + e_i}{1 - e_i} \right) f_i \qquad (2.75)$$

The important step in this computational process is the conversion of the unadjusted electivities into a set of realized electivities. Although this conversion is sometimes unnecessary, it is generally needed to insure that the sum of the dietary frequencies calculated by Equation (2.75) equals 1. One can verify that the condition that guarantees $\Sigma\, d_i = 1$ is

$$\sum_{i=1}^{n} \frac{f_i}{1 - e_i} = 1 \qquad (2.76)$$

See Appendix C. When Equation (2.76) is not satisfied for a given set of electivities $\{\ldots,\hat{e}_i,\ldots\}$ and relative prey availabilities $\{\ldots,f_i,\ldots\}$, BASS transforms the given electivities using a linear transformation that maps $\hat{e}_i = -1$ into $e_i = -1$ and $\max(\ldots,\hat{e}_i,\ldots)$ into $e_i < 1$. The general form of this transformation is

$$e_i = m\left(\hat{e}_i + 1\right) - 1 \qquad (2.77)$$

where $0 < m < 2\max(\ldots,\hat{e}_i,\ldots)^{-1} + 1$. Besides insuring that $\Sigma\, d_i = 1$, this transformation also preserves the relative preferences represented in the original base set $\{\ldots,\hat{e}_i,\ldots\}$.

Because many studies have shown a strong positive correlation between the body sizes of piscivorous fish and the forage fish that they consume (Parsons 1971, Lewis et al. 1974, Timmons et al. 1980, Gillen et al. 1981, Knight et al. 1984, Moore et al. 1985, Stiefvater and Malvestuto 1985, Storck 1986, Jude et al. 1987, Johnson et al. 1988, Yang and Livingston 1988, Brodeur 1991, Elrod and O'Gorman 1991, Hambright 1991, Juanes et al. 1993, Mattingly and Butler 1994, Hale 1996, Madenjian et al. 1998, Margenau et al. 1998, Mittelbach and Persson 1998, Bozek et al. 1999), only a specific size range of forage fish is assumed to be available to a piscivorous cohort. BASS characterizes this size spectrum by using either linear or complementary exponential functions to describe the maximum, minimum, and mean prey body lengths ingested by a predator of a given body length. In particular, these key features of a fish's prey spectrum are described by

$$L_{\max} = \begin{cases} \alpha_1 + \alpha_2 L_{predator} \\ \alpha_1 + \alpha_2 \exp\left(\alpha_3 L_{predator}\right) \end{cases} \qquad (2.78)$$

$$L_{\min} = \begin{cases} \beta_1 + \beta_2 L_{predator} \\ \beta_1 + \beta_2 \exp\left(\beta_3 L_{predator}\right) \end{cases} \qquad (2.79)$$

$$L_{mean} = \begin{cases} \gamma_1 + \gamma_2 L_{predator} \\ \gamma_1 + \gamma_2 \exp\left(\gamma_3 L_{predator}\right) \end{cases} \qquad (2.80)$$

where α_1, α_2, and α_3 are empirical constants describing the fish's maximum length of prey; β_1, β_2, and β_3 are empirical constants describing the fish's minimum length of prey; and γ_1, γ_2, and γ_3 are empirical constants describing the fish's average length of prey. The relative frequencies f_i of forage fish available to a piscivorous cohort are then calculated relative to the sum of forage fish biomasses whose body lengths are both greater than $L_{\min}$ and less than $L_{\max}$ minus the biomass of those prey sizes predicted to be consumed by more efficient piscivorous cohorts (see Assumption 1).

When two or more cohorts of a forage species *i* can be consumed by a piscivore, the relative frequencies of those cohorts s_{ij} in the piscivore's diet are calculated assuming that prey sizes follow a simple triangular distribution defined by Equations (2.78) through (2.80). For example, let L_{i1} and L_{i2} denote the body lengths of two age classes of species *i* that are prey for the cohort. If P_{ij} is the triangular distribution function

$$\text{›}_{ij} = \begin{cases} \dfrac{2\,(L_{ij} - L_{\min})}{(L_{\max} - L_{\min})\,(L_{mean} - L_{\min})} & \text{for } L_{\min} < L_{ij} < L_{mean} \\ \dfrac{2}{(L_{\max} - L_{\min})} & \text{for } L_{ij} = L_{mean} \\ \dfrac{2\,(L_{\max} - L_{ij})}{(L_{\max} - L_{\min})\,(L_{\max} - L_{mean})} & \text{for } L_{mean} < L_{ij} < L_{ma} \end{cases} \qquad (2.81)$$

the relative frequencies of these two age classes in the cohort's diet are calculated to be $s_{i1} = d_i\,[P_{i1}/(P_{i1} + P_{i2})]$

and $s_{i2} = d_i [P_{i2}/(P_{i1} + P_{i2})]$. If only one age class of a forage species is vulnerable to the cohort, then $s_{ij} = d_i$.

If, while calculating the dietary frequencies of a piscivorous cohort, BASS predicts that the cohort's available prey is insufficient to satisfy its desired level of feeding, BASS reassigns the cohort's unadjusted electivities $\{..., \hat{e}_i, ...\}$ to simulate prey switching. These reassignments are based on the following assumption:

ASSUMPTION 3. When forage fish become limiting, piscivores switch to benthic macroinvertebrates or incidental terrestrial insects as alternative prey. However, piscivores that must switch to benthos or that routinely consume benthos in addition to fish are less efficient benthivores than are obligate benthivores (Hanson and Leggett 1986, Lacasse and Magnan 1992, Bergman and Greenberg 1994). Consequently, only the leftovers of non-piscivorous benthivores are available to benthos-feeding piscivores. If such resources are still insufficient to satisfy the piscivores' metabolic demands, piscivores are assumed to switch to planktivory (Werner and Gilliam 1984, Magnan 1988, Bergman and Greenberg 1994). In this case, piscivores have access only to the leftovers of non-piscivorous planktivores. Using this assumption, BASS first assigns the cohort's electivity for benthos to zero regardless of its previous value. BASS also reassigns any other electivity that does not equal -1, to zero.

If benthos becomes limiting for benthivores, or if plankton becomes limiting for planktivores, BASS assumes that benthivores can shift their diets to include plankton and terrestrial insects and that planktivores can shift their diets to include benthos and terrestrial insects. See, for example, Ingram and Ziebell (1983).

After BASS has calculated a cohort's dietary composition, it then assigns the cohort's individual realized feeding rate adjusted for prey availability as

$$F_d = \min\left(F_d^*,\ N^{-1} \sum_{e_j^* = -1} AB_j \right) \tag{2.82}$$

where F_d^* is the cohort's expected individual ingestion (g dry wt/fish); N is the cohort's population size (fish/ha), and AB_j is the biomass (g dry wt/ha) of prey j that is available to that cohort. Using its predicted dietary compositions and realized feeding rates, BASS then calculates the predatory mortalities for each fish cohort and non-fish compartments.

2.8. Modeling Stable Isotopes and Trophic Position

To provide a summary output variable that integrates the temporal and body size dynamics of a fish's dietary composition, BASS simulates time dynamics of each cohort's carbon and nitrogen stable isotopic signatures (i.e., $\delta^{13}C$ and $\delta^{15}N$). Although other models have been proposed for this purpose (see Hesslein et al. 1993, Harvey et al. 2002, Olive et al. 2003), BASS assumes that the change in a fish's mean stable isotope ratio during an arbitrarily "small" fraction or multiple of a day while feeding on a single prey item can be described by

$$\delta_f(t+h) = \frac{\delta_f(t)\, W(t) + \delta_p(t)\, \lambda_p\, \alpha_p (hF) - \delta_f(t)\, \mu (hR)}{W(t) + \alpha_p (hF) - (hR)} \tag{2.83}$$

where $\delta_f(t)$ and $\delta_p(t)$ denote the stable isotope ratios of the fish and its prey, respectively, at time t; λ_p denotes the fish's fractionation constant associated with prey assimilation; α_p denotes the fish's assimilation efficiency for that prey; F is the fish's dry weight ingestion rate (g dry wt·d^{-1}); h is the length (d) of the chosen time interval; μ is the fish's fractionation constant associated with its routine metabolism (i.e., respiration and excretion); and R is the fish's daily metabolic loss rate (g dry wt·d^{-1}). One can verify that Equation (2.83) is also equivalent to

$$\frac{\delta_f(t+h) - \delta_f(t)}{h} = \alpha_p \lambda_p \delta_p(t)\, \varphi - \mu \rho\, \delta_f(t) - \left[\alpha_p \varphi - \rho\right] \delta_f(t+h) \tag{2.84}$$

where $\varphi = F/W(t)$ and $\rho = R/W(t)$ are the fish's weight-specific rates (g dry wt·g dry wt^{-1}·d^{-1}) of feeding and metabolism, respectively. Passing to the limit (i.e., letting h approach zero) then yields the differential equations

$$\frac{d\delta_f}{dt} = \alpha_p \lambda_p \delta_p \varphi - \left(\alpha_p \varphi - \rho + \mu \rho\right) \delta_f \tag{2.85}$$

$$\frac{d\delta_f}{dt} = \alpha_p \lambda_p \delta_p \varphi - \left(\gamma + \mu \rho\right) \delta_f \tag{2.86}$$

where $\gamma = \alpha_p \varphi - \rho$ is the fish's weight-specific growth rate (g dry wt·g dry wt^{-1}·d^{-1}). Equation (2.86) can be reparameterized by noting that most stable isotope studies assume that the difference between the stable isotope signatures of any two successive trophic levels is a constant. For Equation (2.86), this assumption implies that

$$K = \delta_{f,eq} - \delta_p = \frac{\alpha_p \lambda_p \delta_p \varphi}{(\gamma + \mu \rho)} - \delta_p \tag{2.87}$$

where $\delta_{f,eq}$ denotes the fish's steady-state stable isotope ratio. Consequently,

$$\lambda_p = \left(\frac{K}{\delta_p} + 1 \right) \left(\frac{\gamma + \mu \rho}{\alpha_p \varphi} \right) \tag{2.88}$$

and Equation (2.86) can be rewritten as

$$\frac{d\delta_f}{dt} = (K + \delta_p)(\gamma + \mu\rho) - (\gamma + \mu\rho)\,\delta_f \qquad (2.89)$$

One can generalize Equations (2.86) and (2.89) to describe the isotope dynamics of fish feeding on multiple prey or mixed trophic levels as follows

$$\frac{d\delta_f}{dt} = \varphi \sum_{p=1}^{n} \alpha_p \beta_p \lambda_p \delta_p - (\gamma + \mu\rho)\,\delta_f \qquad (2.90)$$

$$\frac{d\delta_f}{dt} = (\gamma + \mu\rho) \sum_{p=1}^{n} \beta_p (K + \delta_p) - (\gamma + \mu\rho)\,\delta_f \qquad (2.91)$$

where β_p is the frequency of the p-th prey in the fish's diet. BASS calculates the trophic position of each fish cohort using the cohort's predicted $\delta^{15}N$ and the standard equation

$$TP = (\delta_f - \delta_{invert})/3.4 + 2 \qquad (2.92)$$

(Vander Zanden and Rasmussen 2001).

2.9. Modeling Dispersal, Non-Predatory Mortalities, and Recruitment

The algorithm that BASS employs to simulate a species' dispersal and non-predatory mortality is based on the general empirical observation that population densities of most vertebrates can be adequately characterized by the self-thinning power function relationship

$$N = a\,W_w^{-b} \qquad (2.93)$$

where N is the species' or cohort's density (fish/ha) and W_w is the species' or cohort's mean wet body weight (Damuth 1981, Peters and Raelson 1984, Juanes 1986, Robinson and Redford 1986, Dickie et al. 1987, Boudreau and Dickie 1989, Gordoa and Duarte 1992, Randall et al. 1995, Dunham and Vinyard 1997, Steingrímsson and Grant 1999, Dunham et al. 2000, Guiñez 2005). For fish the body weight exponent b generally varies from 0.75 to 1.5 (Boudreau and Dickie 1989, Grant and Kramer 1990, Gordoa and Duarte 1992, Elliott 1993, Bohlin et al. 1994, Randall et al. 1995, Dunham and Vinyard 1997, Grant et al. 1998, Dunham et al. 2000, Knouft 2002, Keeley 2003). Larger exponents ranging from 1.5 to 3.0, however, have also been reported (Steingrímsson and Grant 1999). If Equation (2.93) is differentiated with respect to time, it immediately follows that a species' population dynamics can be modeled using the linear time-varying differential equation

$$\frac{dN}{dt} = \frac{-a\,b\,W_w^{-b}}{W_w}\,\frac{dW_w}{dt} = -\,b\,\gamma\,N \qquad (2.94)$$

where $\gamma = W_w^{-1}\,dW_w/dt$ is the species' weight-specific growth rate. Consequently, $b\gamma$ corresponds to the cohort's total mortality rate. Readers interested in detailed discussions concerning the underlying process-based interpretation and general applicability of this result should consult Peterson and Wroblewski (1984), McGurk (1993, 1999), and Lorenzen (1996).

Because Equations (2.93) and (2.94) encompass the cohort's predatory and non-predatory mortality and dispersal, and because BASS separately models the cohort's predatory mortality, BASS assumes that the cohort's combined rate of dispersal (EM) and non-predatory mortality (NM) is simply a fraction δ of $b\gamma$. In particular,

$$EM + NM = \delta\,b\,\gamma\,N \qquad (2.95)$$

If community population dynamics are strongly dominated by predation, the fraction δ will be "small" (e.g., $\delta < 0.5$) for forage fishes and "large" (e.g., $\delta > 0.5$) for predatory species. However, if community population dynamics are dominated by dispersal mechanisms related to competition for food, space, or other limiting community resource, the fraction δ will be large for forage and predatory species alike.

Although BASS's basic self-thinning algorithm for predicting a cohort's combined dispersal and non-predatory mortality ($EM + NM$) may be sufficient to simulate realistically bounded populations for most species, some species may tend to exhibit unbounded or unrealistic population dynamics under certain conditions. To correct such behaviors, a simulation option that imposes an additional mortality and dispersal on all of a species' cohorts as its total biomass approaches a user-defined biomass carrying capacity has been implemented. This algorithm assumes that a cohort's realized biomass derivative, adjusted for an assumed carrying capacity, is given by

$$\frac{d\hat{X}}{dt} = \frac{dX}{dt}\left(\frac{S - K}{X - K}\right) \qquad (2.96)$$

$$N\frac{dW}{dt} - W(EM + NM + PM + KM) = \left(N\frac{dW}{dt} - W(EM + NM + PM)\right)\left(\frac{S - K}{X - K}\right) \qquad (2.97)$$

$$KM = W^{-1}\left(1 - \frac{S - K}{X - K}\right)\frac{dX}{dt} \qquad (2.98)$$

where $X = N\,W$ denotes the cohort's biomass; KM is the cohort's additional dispersal and mortality due to the species' biomass carrying capacity constraint; S is the species total biomass; and K is the species biomass carrying capacity. It is interesting to note that Equation (2.96) can also be written as

$$\frac{d\hat{X}}{dt} = \frac{dX}{dt}\left(\frac{X-(K-S+X)}{X-K}\right) = \frac{dX}{dt}\left(\frac{X-K_c}{X-K}\right) \qquad (2.99)$$

where $K_c = K - (S - X)$ corresponds to the cohort's instantaneous carrying capacity given the species' existing age class structure. That is, the cohort's biomass attains a local maximum when $X = K_c$. Consequently, the hyperbolic multipliers used in these equations are mathematically analogous to those used to model temperature effects on the cohort's physiological functions (see Section 2.5).

BASS estimates a species' recruitment by assuming that each species turns over a fixed percentage of its potential spawning biomass into new young-of-year (YOY). This percentage is referred to as the species' reproductive biomass investment (*rbi*). The species' spawning biomass is defined as the total biomass of all cohorts whose body lengths are greater than or equal to a specified minimum value (tl_{r0}) marking the species' sexual maturation. When reproduction is simulated, the body weight of each sexually mature cohort is decreased by its *rbi*, and the total number of YOY recruited into the population as a new cohort is calculated by dividing the species' total spawned biomass by its characteristic YOY body weight. Although this formulation does not address the myriad of factors known to influence population recruitment, it is logically consistent with the spawners' abundance model for fish recruitment. See Myers and Barrowman (1996) and Myers (1997).

2.10. Modeling Habitat Effects

Although BASS does not explicitly model physical habitat features of the fish community of concern, it does allow users to specify habitat suitability multipliers on the feeding, reproduction / recruitment, and dispersal / non-predatory mortality for any or all species. Because these multipliers are assumed to be analogous to subcomponents of habitat suitability indices, they are assumed to take values from 0 to 1. If these multipliers are not specified, BASS assigns them the default value of 1.

When feeding habitat multipliers ($HSI_{feeding}$) are specified, BASS uses the specified parameters as simple linear multipliers on the fish's maximum rate of ingestion, i.e.,

$$F_d(habitat) = HSI_{feeding}\, F_d^* \qquad (2.100)$$

The resulting adjusted maximum feeding rate then replaces F_d^* in Equation (2.82). These multipliers are assumed to modify the fish's ability to perceive or to intercept prey by affecting the fish's reactive distance, foraging patterns, etc. or by providing modified refuges for its potential prey. Habitat interactions that actually change the abundance of potential prey should not be specified as feeding habitat multipliers since these interactions are automatically addressed by the algorithms outlined in Section 2.7.

Like the aforementioned feeding habitat multipliers, BASS uses any specified recruitment habitat multipliers ($HSI_{recruitment}$) as simple linear multipliers on the number of young-of-year recruited into the species population, i.e.,

$$N_0(habitat) = HSI_{recruitment}\, N_0 \qquad (2.101)$$

These multipliers can represent either the availability of suitable spawning sites or the ability of otherwise successful spawns to result in the expected numbers of young-of-year as discussed in Section 2.8.

Finally, when habitat multipliers ($HSI_{survival}$) are specified for dispersal / non-predatory mortality, they are assumed to control a species' self-thinning exponent *b* (see Section 2.8) so that the exponent is maximum for $HSI_{survival} = 0$ and minimum for $HSI_{survival} = 1$. Thus, as habitat suitability decreases, dispersal and non-predatory mortality increase, and vice versa [see Equation (2.95)]. Between this range, the species self-thinning exponent is assumed to respond linearly to changing $HSI_{survival}$, i.e.,

$$b(habitat) = \left(1 - HSI_{survival}\right)\left(b_{\max} - b_{\min}\right) + b_{\min} \qquad (2.102)$$

Because constructing habitat suitability multipliers in a standard way is not a trivial issue, BASS relegates their construction to the user. Nevertheless, users might consider several obvious starting points when simulating habitat effects with BASS. Turbidity, for example, is known to affect the foraging abilities of both prey and predatory fishes, and one could readily use results of published studies (e.g., Vandenbyllaardt et al. 1991, Barrett 1992, Gregory 1993, Gregory and Northcote 1993, Miner and Stein 1996, Reid et al. 1999, Vogel and Beauchamp 1999, Bonner and Wilde 2002, de Robertis et al. 2003, Sweka and Hartman 2003) to estimate feeding multipliers for Equation (2.100) as power functions or polynomials of turbidity. Field-based HSIs are often estimated by logistic regression of presence-absence data without specifying the underlying mechanisms that actually determine habitat suitability for a species. Such HSIs could be used as habitat multipliers for species' recruitment [Equation (2.101)] or persistence/survival [Equations (2.95) and (2.102)] depending on the user's interpretation of what the indices most likely represent.

2.11. Modeling Non-fish Compartments

BASS assumes that the non-fish components of a community of concern can be treated as four lumped compartments, i.e., benthos, periphyton/attached algae, phytoplankton, and

zooplankton. These compartments can be treated either as community forcing functions or as state variables. In the latter case, the required compartmental dynamics are simulated using the simple mass balance model

$$\frac{dY}{dt} = IP - R - \hat{F} - M \tag{2.103}$$

where Y is the compartment's biomass (g dry wt/m^2); and IP, R, $\hat{F}$, and M are the compartment's ingestion or photosynthesis, respiration, mortality due to fish consumption, and non-consumptive mortality and dispersal, respectively, all of which have units of g dry wt/m^2/d. Except for $\hat{F}$, each of these fluxes is modeled as a linear function of the compartment's biomass, i.e.,

$$IP = \varphi_{dd} Y \tag{2.104}$$

$$R = \rho Y \tag{2.105}$$

$$M = \mu Y \tag{2.106}$$

where the rate coefficients (g dry wt/g dry wt/d) φ_{dd}, ρ, and μ are minimally functions of temperature and time.

For benthos, phytoplankton, and zooplankton that can be conceptualized as populations of organisms possessing similar body sizes, the rate coefficients φ_{dd}, ρ, and μ are estimated using temperature-dependent allometric relationships that describe these processes for individuals comprising the compartment of interest. For example, consider the following formulation of benthos consumption. Assuming that $\bar{W}_d$ is the average dry weight of individuals comprising the benthos compartment, it follows that the expected density of individuals within the compartment is simply

$$N = \frac{Y}{\bar{W}_d} \tag{2.107}$$

If the average consumption (g dry wt/d) of individual benthos is then assumed to be

$$C = c_1 \bar{W}_d^{\,c_2} \exp\left(c_3 T\right)\left(1 - \frac{T}{T_2}\right)^{c_3 (T_2 - T_1)} \tag{2.108}$$

it follows that the ingestion of the benthos compartment at large can be modeled as

$$\begin{aligned} IP &= C\ N \\ &= \left[c_1 \bar{W}_d^{\,c_2 - 1} \exp\left(c_3 T\right)\left(1 - \frac{T}{T_2}\right)^{c_3 (T_2 - T_1)}\right] Y \\ &= \varphi_{dd} Y \end{aligned} \tag{2.109}$$

Formulating compartmental ingestion, photosynthesis, and respiration using this method not only delineates an objective procedure to parameterize BASS, but also yields production relationships that are consistent with results reported by Plante and Downing (1989), Stockwell and Johannsson (1997), and Kuns and Sprules (2000). When estimating φ_{dd}, ρ, and μ for benthos, phytoplankton, or zooplankton using this approach, BASS assumes that

$$P = p_1 \bar{W}_d^{\,p2} \exp\left(p_3 T\right)\left(1 - \frac{T}{T_2}\right)^{p_3 (T_2 - T_1)} \tag{2.110}$$

where P is the individual's ingestion, photosynthesis, or respiration in units of g dry wt/d; and p_1, p_2, p_3, T_1, and T_2 are empirical constants specific to the process of interest. Although BASS does not attempt to simulate the average individual body sizes of benthos, phytoplankton, or zooplankton, it does allow users to vary these parameters as functions of time.

Because periphyton communities typically are complex amalgamations of filamentous and unicellular algae, it is difficult to conceptualize this compartment as a population of archetypical individuals and to employ the preceding model parameterization scheme. Consequently, for periphyton BASS assumes that φ_{dd}, ρ, and μ are generally temperature-dependent allometric functions of the compartment's biomass, i.e.,

$$\varphi_{dd} = \alpha_1 Y^{\alpha_2} \exp\left(\alpha_3 T\right)\left(1 - \frac{T}{T_2}\right)^{\alpha_3 (T_2 - T_1)} \tag{2.111}$$

$$\rho = \beta_1 Y^{\beta_2} \exp\left(\beta_3 T\right)\left(1 - \frac{T}{T_2}\right)^{\beta_3 (T_2 - T_1)} \tag{2.112}$$

$$\mu = \delta_1 Y^{\delta_2} \exp\left(\delta_3 T\right)\left(1 - \frac{T}{T_2}\right)^{\delta_3 (T_2 - T_1)} \tag{2.113}$$

The rationale for these formulations is based on the assumption that the primary production, respiration, and mortality of periphyton communities are generally limited by their surface-volume relationships that are implicitly represented by these equations.

Because φ_{dd} is generally much greater than ρ, the astute reader will recognize that Equations (2.103) - (2.106) will predict unbounded autocatalytic growth for any non-fish compartment whose predatory mortality and non-predatory mortality/dispersal does not precisely balance its intrinsic growth rate. To prevent such unrealistic dynamics, BASS internally estimates a physiologically based carrying capacity for each non-fish compartment based on its projected daily oxygen consumption and the community's prevailing dissolved oxygen content. In

particular, BASS assumes that compartmental oxygen consumption cannot exceed the dissolved oxygen content corresponding to the difference between the community's prevailing dissolved oxygen concentration (DOC) and an assumed hypoxic threshold of 4 mg O_2 /L. When the compartment's daily oxygen consumption is predicted to exceed this available dissolved oxygen content, compartmental growth is suspended by equating the compartment's feeding/photosynthesis to its projected respiration.

BASS assumes that the rates of chemical bioaccumulation in non-fish compartments are rapid enough to enable chemical concentrations within these components to be calculated using simple bioaccumulation factors. In particular,

$$C_{nf} = BAF_{nf} C_w \tag{2.114}$$

where C_{nf} is the chemical concentration (µg /g dry wt) in the compartment of concern. BASS enables users to specify the bioaccumulation factor BAF_{nf} (ml/g dry wt) for Equation (2.114) as an empirically derived constant, a quantitative structure activity relationship (QSAR), or the ratio of the chemical's uptake rate to the sum of its excretion rate and the compartment's growth rate. When BAF_{nf} is specified as a QSAR, BASS assumes that

$$BAF_{nf} = b_1 K_{ow}^{b_2} \tag{2.115}$$

where b_1 and b_2 are empirical constants. When BAF_{nf} is specified by the compartment's chemical exchange rates and growth rate, BASS assumes that

$$BAF_{nf} = \frac{k_1}{k_2 + \gamma} = \frac{k_1}{k_1 / K_{nf} + \gamma} \tag{2.116}$$

where k_1, k_2, and γ are the rates of uptake, excretion, and growth, respectively, by individuals comprising the compartment; and K_{nf} is the compartment's thermodynamic bioconcentration factor that is defined analogously to Equation (2.7). For heterotrophs, Equation (2.116) assumes that direct chemical uptake and excretion with the ambient water are dominant over dietary uptake and fecal excretion of the organisms of concern. Although this assumption is not satisfied for all benthic or planktonic heterotrophs, it does bypass the need to specify feeding rates, assimilation efficiencies, and dietary compositions for compartments that are actually mixed functional groups. For further discussions of Equation (2.116) and its generalization, readers should consult Connolly and Pedersen (1988), Thomann (1989), and Arnot and Gobas (2004).

2.12. Modeling Toxicological Effects

Narcosis is defined as any reversible decrease in physiological function induced by chemical agents. Because the potency of narcotic agents was originally found to be correlated with their olive oil / water partition coefficients (Meyer 1899, Overton 1901), it was long believed that the principal mechanism of narcosis was the disruption of the transport functions of the lipid bilayers of biomembranes (Mullins 1954, Miller et al. 1973, Haydon et al. 1977, Janoff et al. 1981, Pringle et al. 1981). More recently, however, it has been acknowledged that narcotic chemicals also partition into other macromolecular components besides the lipid bilayers of membranes. It is now widely accepted that partitioning of narcotic agents into hydrophobic regions of proteins and enzymes inhibit their physiological function by changing their conformal structure or by changing the configuration or availability of their active sites (Eyring et al. 1973, Adey et al. 1976, Middleton and Smith 1976, Richards et al. 1978, Franks and Lieb 1982, 1984, Law et al. 1985, Lassiter 1990). In either case, the idea that the presence of narcotic chemicals increases the physical dimensions of various physiological targets to some "critical volume" that renders them inactive is fundamental (Abernethy et al. 1988). Narcotic chemicals can thus be treated as generalized physiological toxicants, and narcosis itself can be considered to represent baseline chemical toxicity for organisms. Although any particular chemical can act by a more specific mode of action under acute or chronic exposure conditions, all organic chemicals can be assumed to act minimally as narcotics (Ferguson 1939, McCarty and Mackay 1993).

Studies have shown that for narcotic chemicals there is a relatively constant chemical activity within exposed organisms associated with a given level of biological activity (Ferguson 1939, Brink and Posternak 1948, Veith et al. 1983). This relationship holds true not only for exposures to a single chemical but also for exposures to chemical mixtures. In the case of a mixture of chemicals, the sum of the chemical activities for each component chemical is constant for a given level of biological activity. Because narcotic chemicals can be treated as generalized physiological toxicants, it should not be surprising that the effects of mixtures of chemicals possessing diverse specific modes of action often not only resemble narcosis but also appear to be additive in their toxic effects (Barber et al. 1987, McCarty and Mackay 1993). For example, although most pesticides possess a specific mode of action during acute exposures, the joint action of pesticides is often additive and resembles narcosis (Hermanutz et al. 1985, Matthiessen et al. 1988, Bailey et al. 1997).

BASS simulates acute and chronic mortality assuming that the chemicals of concern are an additive mixture of narcotics. Because this assumption is the least conservative assumption that one could make concerning the onset of effects, mortalities predicted by BASS should signal immediate concern. When the total chemical activity of a fish's aqueous phase exceeds its

calculated lethal threshold, BASS assumes that the fish dies and eliminates that fish's age class from further consideration. The total chemical activity of a fish's aqueous phase is simply the sum of its aqueous phase chemical activity for each chemical. BASS calculates the aqueous phase chemical activity of each chemical using the following formulae

$$A_a = \gamma_a M_a$$

$$M_a = \frac{C_a}{10^3 MW} = \frac{C_f}{10^3 MW K_f} \qquad (2.117)$$

where A_a is the chemical's aqueous activity; γ_a is the chemical's aqueous activity coefficient (L/mol), the reciprocal of its sub-cooled liquid solubility; M_a is the chemical's molarity within the aqueous phase of the fish; and MW is the chemical's molecular weight (g/mol).

BASS estimates the lethal chemical activity threshold for each species as the geometric mean of the species' LA_{50}, i.e., the ambient aqueous chemical activity that causes 50% mortality in an exposed population. These lethal thresholds are calculated using the above formulae with user-specified LC_{50}'s substituted for C_a. These calculations are based on two important assumptions. The first assumption is that the exposure time associated with the specified LC_{50} is sufficient to allow almost complete chemical equilibration between the fish and the water. The second assumption is that the specified LC_{50} is the minimum LC_{50} that kills the fish during the associated exposure interval. Fortunately, most reliable LC_{50}'s satisfy these two assumptions. See Lassiter and Hallam (1990) for a comprehensive model-based analysis of these issues.

Three points should be mentioned regarding the above approach to modeling ecotoxicological effects. First, for narcotic chemicals this approach is analogous to the toxic unit approach for evaluating the toxicity of mixtures (Calamari and Alabaster 1980, Könemann 1981a, b, Hermens and Leeuwangh 1982, Hermens et al. 1984a, Hermens et al. 1984b, Broderius and Kahl 1985, Hermens et al. 1985b, Hermens et al. 1985c, Hermens et al. 1985a, Dawson 1994, Peterson 1994). Second, the approach is also analogous to the critical body residue (CBR) and total molar body residue (TBR) approaches proposed by McCarty and Mackay (1993), Verhaar et al. (1995), and van Loon et al. (1997). Third, although sublethal effects are not presently modeled by BASS, BASS's simulation results can be used to indicate when sublethal effects induced by narcotic agents would be expected to occur. Results reported by Hermens et al. (1984b) indicate that for *Daphnia* the ratio of the EC_{50} for reproductive impairment to the LC_{50} is generally on the order of 0.15 - 0.30 for chemicals whose log K_{ow} range from 4 to 8. For individual growth inhibition, however, the mean EC_{50} to LC_{50} ratio for *Daphnia* in 16 day chronic exposures was approximately 0.77 (Hermens et al. 1984a, Hermens et al. 1985b). Also see Roex et al. (2000).

Table 2.1 Summary of the notation used for model development excluding empirical parameters describing fundamental model processes, rates, or rate coefficients.

A_a chemical activity in aqueous fraction of the fish (dimensionless)
A_d assimilation rate (g dry wt/d)
B_f chemical burden in whole fish (µg/fish)
BAF_{nf} bioaccumulation factor for non-fish prey (ml/g dry wt)
C_a chemical concentration in aqueous fraction of the fish (µg/ml)
C_{ae} chemical concentration in aqueous fraction of intestinal contents (µg/ml)
C_B chemical concentration in bulk interlamellar water (µg/ml)
C_e chemical concentration in egesta/feces (µg/ml)
C_f chemical concentration in whole fish (µg/g wet wt)
C_{de} chemical concentration in dry organic fraction of intestinal contents (µg/g dry wt)
C_l chemical concentration in lipid (µg/g dry wt)
C_{nf} chemical concentration non-fish prey (µg/g dry wt)
C_o chemical concentration in non lipid organic matter (µg/g dry wt)
C_p chemical concentration in prey (µg/g wet wt)
C_w chemical concentration in environmental water (µg/ml)
$C_{w,O2}$ oxygen concentration in environmental water (µg/ml)
d interlamellar distance (cm)
d_i the relative frequency of prey *i* in a fish's diet (dimensionless)
D aqueous diffusion coefficient (cm^2/s)
e_i the electivity prey *i* in a fish's diet (dimensionless)
E_d egestion rate (g dry wt/d)
E_w egestion rate (g wet wt/d)
EM emigration/dispersal (fish/ha/d)
EX excretory rate (g dry wt/d)
f_i the relative frequency of prey *i* in the field (dimensionless)
F_d^* expected feeding rate (g dry wt/d)
F_d realized feeding rate (g dry wt/d)
F_w realized feeding rate (g wet wt/d)
G mass of gut contents (g dry wt/fish)
h height of secondary lamellae (cm)
$HSI_{feeding}$ habitat suitability index for cohort feeding (dimensionless)
$HSI_{recruitment}$ habitat suitability index for YOY recruitment (dimensionless)
$HSI_{survival}$ habitat suitability index for cohort survival (dimensionless)
J_{bt} biotransformation of chemical (µg/s)
J_g net chemical exchange across the gills (µg/s)
J_i net chemical exchange across the intestine (µg/s)
k_2 apparent elimination rate coefficient (ml/g wet wt/d, g wet wt/g wet wt/d, or 1/d), i.e., $k_2 = (\gamma + k_{bt} + k_{ex})$
k_{bt} chemical biotransformation rate coefficient (ml/g wet wt/d, g wet wt/g wet wt/d, or 1/d)
k_{ex} chemical excretion rate coefficient (ml/g wet wt/d, g wet wt/g wet wt/d, or 1/d)
k_g overall chemical conductance across the gill from the interlamellar water to the aqueous blood (cm/s)
k_m chemical conductance through the gill membrane (cm/s)
K_e partition coefficient for fecal matter (ml/g wet wt)
K_f thermodynamic bioconcentration factor (ml/g wet wt)
K_l partition coefficient between generic lipid and water (ml/g dry wt)
K_o partition coefficient between non-lipid organic matter and water (ml/g dry wt)
K_{oc} partition coefficient between organic carbon and water (ml/g dry wt)
K_{ow} partition coefficient between n-octanol and water (ml/ml)
l lamellar length (cm)
L fish's body length (cm)

M_a chemical molarity in aqueous fraction of the fish (mol/L)
N population density (fish/ha)
N_{Gz} Graetz number (dimensionless) = $(l\ D)/(V\ r^2)$
N_{Sh} Sherwood number (dimensionless) = $(k_m\ r)/D$
NM non-predatory mortality (fish/ha/d)
P_a aqueous or moisture fraction of whole fish (g water/g wet wt = ml/g wet wt)
P_{ae} aqueous or moisture fraction of feces/egesta (g water/g wet wt = ml/g wet wt)
P_{ap} aqueous of moisture fraction of prey/food (g water/g wet wt = ml/g wet wt)
P_{de} dry fraction of feces/egesta (g dry wt/g wet wt)
P_{dp} dry fraction of prey/food (g dry wt/g wet wt)
P_d dry fraction of whole fish (g dry wt/g wet wt), i.e., $P_d = (1 - P_a) = (P_l + P_o)$
P_l lipid fraction of whole fish (g dry wt/g wet wt)
P_o non-lipid organic fraction of whole fish (g dry wt/g wet wt)
PM predatory mortality (fish/ha/d)
Q ventilation volume (cm^3/s)
r hydraulic radius of interlamellar channels (cm), i.e., $r = 0.5\ d$
R routine respiratory rate (g dry wt/d)
R_{O2} oxygen consumption rate (mg O_2/s or g O_2/d)
SDA specific dynamic action (g dry wt/d)
S_g total gill surface area (cm^2)
T temperature (Celsius)
V average velocity of interlamellar flow (cm/s)
W_a weight/volume of fish's aqueous phase (g water/fish or ml/fish)
W_d weight of fish (g dry wt/fish)
W_l weight of fish's lipid phase (g dry wt/fish)
W_o weight of fish's nonlipid organic phase (g dry wt/fish)
W_w weight of fish (g wet wt/fish)
X_g cross sectional pore area of the gill (cm^2)
α_c assimilation efficiency of chemical (dimensionless)
α_f assimilation efficiency of food (g dry wt assimilated/g dry wt ingested)
α_{O2} oxygen assimilation efficiency of the gill (dimensionless)
γ specific growth rate (g wet wt/g wet wt/d), i.e., $\gamma = W_w^{-1}\ dW_w/dt$
γ_a chemical aqueous phase activity coefficient (L/mol)
ε_a aqueous phase biotransformation rate coefficient (1/d)
φ_{dd} specific feeding rate (g dry wt/g dry wt/d)
φ_{ww} specific feeding rate (g wet wt/g wet wt/d)
η solution viscosity (poise)
ν molar volume (cm^3/mol)
ρ lamellar density (lamellae/mm)

Figure 2.1 First eigenvalue and bulk mixing cup coefficient for Equation (2.28) as a function of gill Sherwood number and ventilation / perfusion ratio.

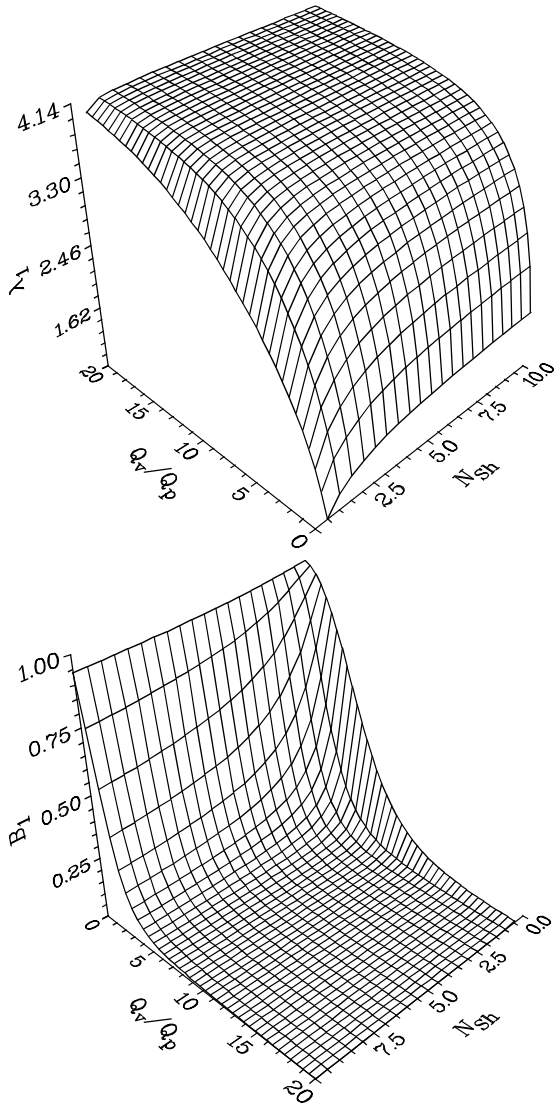


Figure 2.2 Second eigenvalue and bulk mixing cup coefficient for Equation (2.28) as a function of gill Sherwood number and ventilation / perfusion ratio.

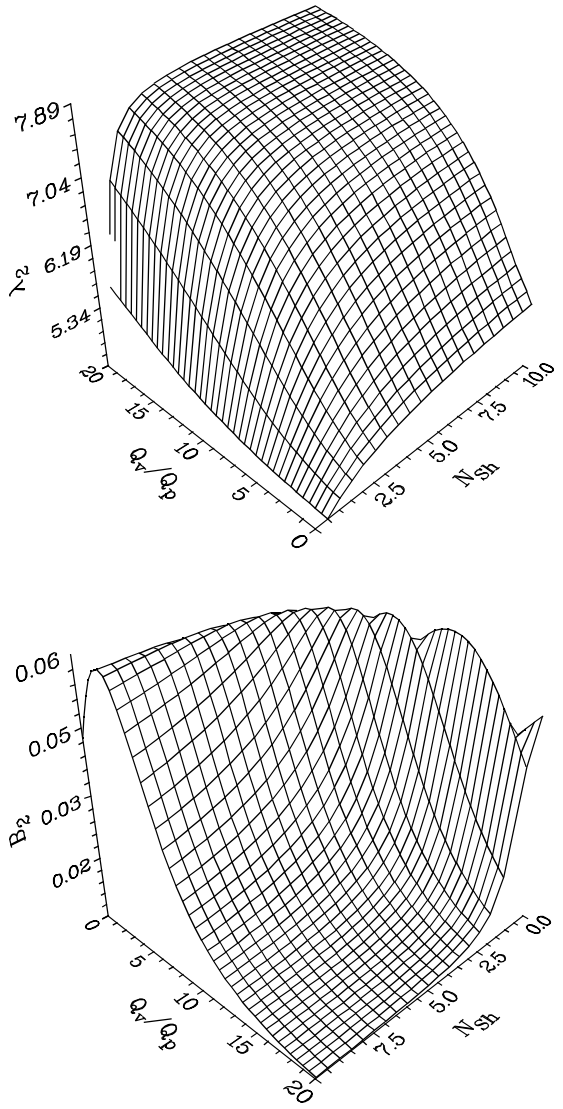
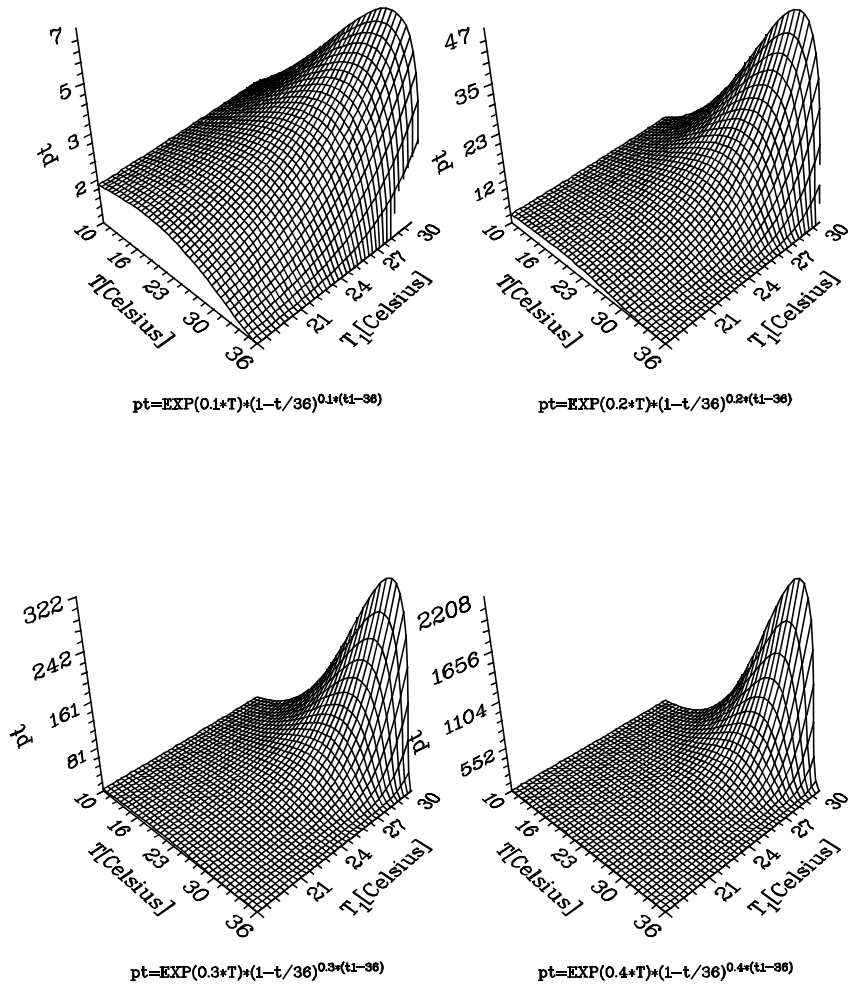


Figure 2.3 Functional behavior of Equation (2.53)



3. Model Parameterization

Because reliable application of a model depends not only on the validity of its formulation but also on its parameterization, important aspects regarding the parameterization of BASS's bioaccumulation and physiological algorithms are discussed below.

3.1. Parameterizing K_f

Superficially, estimation of a fish's thermodynamic bioconcentration factor K_f via Equation (2.7) appears to require a great deal of information. This task, however, is much simpler than it first appears. For example, given a fish's lipid fraction [see Equation (2.56)], it is a straightforward matter to calculate the fish's aqueous fraction using Equation (2.55). One can then immediately calculate the fish's non-lipid organic fraction since P_a, P_l, and P_o must sum to unity [i.e., Equation (2.57)].

For an organic chemical, the partition coefficients K_l and K_o can be estimated using the chemical's octanol / water partition coefficient K_{ow}. Although triglycerides are the principal storage lipids of fish and it would seem reasonable to estimate K_l using a triglyceride / water partition coefficient, BASS assumes that K_l equals K_{ow}. To estimate K_o, BASS assumes that a fish's non-lipid organic matter is equivalent to organic carbon and uses Karickhoff's (1981) regression between the organic carbon / water partition coefficient (K_{oc}) and K_{ow} to estimate this parameter. Specifically,

$$K_o = K_{oc} = 0.411\, K_{ow} \tag{3.1}$$

For metals or metallo-organic compounds such as methylmercury, the chemical's lipid partition coefficient K_l can again be assumed to equal its octanol / water partition coefficient K_{ow}. A metal's distribution coefficient into non-lipid organic matter, however, cannot be estimated using the K_{oc} relationship of Equation (3.1). For example, whereas the K_{ow} of methylmercury at physiological pH's is approximately 0.4 (Major et al. 1991), its distribution coefficient into environmental organic matter is on the order of 10^4 - 10^6 (Benoit et al. 1999b, Benoit et al. 1999a). O'Loughlin et al. (2000) report similar differences for organotin compounds. Whereas distribution coefficients for metals into fecal matter generally should be assigned values comparable to those used to model the environmental fate and transport of metals, distribution coefficients for metals into the non-lipid organic matter of fish should be assigned values 10 to 100 times higher to reflect the increased number and availability of sulfhydryl binding sites.

3.2. Parameters for Gill Exchange

To parameterize the gill exchange model, the fish's total gill area (S_g cm^2), mean interlamellar distance (d cm), and mean lamellar length (l cm) must be specified. Each of these morphological variables is generally assumed to be an allometric power function of the fish's body weight, i.e.,

$$S_g = s_1 W_w^{s_2} \tag{3.2}$$

$$d = d_1 W_w^{d_2} \tag{3.3}$$

$$l = l_1 W_w^{l_2} \tag{3.4}$$

Although many authors have reported allometric coefficients and exponents for total gill surface area, coefficients and exponents for the latter two parameters are seldom available. Parameters for a fish's mean interlamellar distance, however, can be estimated if the allometric function for the density of lamellae on the gill filaments, ρ (number of lamellae per mm of gill filament), i.e.,

$$\rho = \rho_1 W_w^{\rho_2} \tag{3.5}$$

is known. Fortunately, lamellar densities, like total gill areas, are generally available in the literature. See Barber (2003). BASS estimates d_1 and d_2 from ρ_1 and ρ_2 using the interspecies regression (n = 28, r = -0.92)

$$d = 0.118\, \rho^{-1.19} \tag{3.6}$$

To overcome the scarcity of published morphometrics relationships for lamellar lengths, BASS uses the default interspecific regression (n = 90, r = 0.92)

$$l = 0.0188\, W_w^{0.294} \tag{3.7}$$

Both of the preceding regressions are functional regressions rather than simple linear regressions (Rayner 1985, Jensen 1986); the data used for their development are taken from Saunders (1962), Hughes (1966), Steen and Berg (1966), Muir and Brown (1971), Umezawa and Watanabe (1973), Galis and Barel (1980), and Hughes et al. (1986).

To calculate lamellar Graetz and Sherwood numbers, BASS estimates a chemical's aqueous diffusivity (cm^2/s), using the empirical relationship,

$$D = 2.101\times10^{-7}\, \eta^{-1.4}\, \nu^{-0.589} \tag{3.8}$$

where η is the viscosity (poise) of water; and ν is the chemical's molar volume (cm^3/mol) (Hayduk and Laudie

1974). The diffusivity of a chemical through the gill membrane needed to estimate the membrane's permeability k_m is then assumed to equal half of the chemical's aqueous diffusivity (Piiper et al. 1986, Barber et al. 1988, Erickson and McKim 1990). The other quantity needed to estimate k_m is the thickness of the gill's epithelial layer. Although previous versions of BASS assumed a constant water-blood barrier thickness (β_e) equal to 0.0029 cm for all fish species, BASS now uses the interspecies allometric relationship

$$\beta_e = 9.17\times10^{-5}\, W_w^{0.261} \qquad (3.9)$$

to estimate this parameter (Barber 2003).

To calculate ventilation / perfusion ratios, BASS estimates the ventilation volumes (ml/hr) of fish from their oxygen consumption rates assuming an extraction efficiency of 60% and a saturated dissolved oxygen concentration [see Equation (2.12)]. Perfusion rates (ml/hr) are estimated using

$$Q_p = (0.23\, T - 0.78)\, 1.862\, W_w^{0.9} \qquad (3.10)$$

as the default for all species. Although this expression, in units of L/kg/hr, was developed by Erickson and McKim (1990) for rainbow trout (*Oncorhynchus mykiss*), it has been successfully applied to other fish species (Erickson and McKim 1990, Lien and McKim 1993, Lien et al. 1994).

The eigenvalues and bulk mixing cup coefficients needed to parameterize Equation (2.28) are interpolated internally by BASS from matrices of tabulated eigenvalues and mixing cup coefficients that encompass the range of Sherwood numbers ($1< N_{Sh} <10$) and ventilation / perfusion ratios ($1 < Q_v / Q_p < 20$) that are typical for fish (Hanson and Johansen 1970, Barron 1990, McKim et al. 1994, Sijm et al. 1994). See **Figure 2.1** and **Figure 2.2** of the previous chapter.

3.3. Bioenergetic and Growth Parameters

Parameterization of the physiological processes used by BASS to simulate fish growth generally poses no special problems since the literature abounds with studies that can be used for this purpose. The BASS Data Supplement summarizes literature data that have been analyzed to date for use by BASS.

3.4. Procedures Used to Generate the BASS Database

BASS's database for fish ecological, morphological, and physiological parameters is generated by its own Fortran 95 software program. This program not only decodes functional expressions for BASS model parameters that have been reported in the literature but also calculates its own regressions using data reported in the literature. Each species within the BASS database is assigned its own data file whose name corresponds to its genus and species. Thus, all literature data and regressions pertaining to largemouth bass are compiled into the BASS database file *micropterus_salmoides.dat*. Literature regressions are entered into BASS database files using the functional syntax outlined in chapter sections 4.3.3, 4.4.1, and 4.4.2 herein. Except for this syntax, all literature regressions are recorded as reported; any required unit conversions are performed by the BASS database generator.

When literature regressions are not equivalent to the functional forms used by BASS, and their associated primary data are not reported, synthetic datasets are generated to estimate the needed parameters. For example, when a fish's oxygen consumption does not exhibit a temperature optimum, BASS assumes that this parameter is given by

$$so[mg(o2)/hr] = a\, W[g]^b \exp(c * t[celsius]) \qquad (3.11)$$

or, equivalently,

$$\log so[mg(o2)/hr] = \log a + b \log W[g] + c\, t[celsius] \qquad (3.12)$$

Although many researchers use similar expressions to report a fish's oxygen consumption, some use the function

$$so[mg(o2)/hr] = a\, W[g]^b\, t[celsius]^c \qquad (3.13)$$

or, equivalently,

$$\log so[mg(o2)/hr] = \log a + b \log W[g] + c \log t[celsius] \qquad (3.14)$$

When such power functions of temperature are encountered, synthetic datasets of "observed/predicted" oxygen consumption are generated using the reported regressions for the reported range of body weights and temperatures. These synthetic data are then refitted to Equation (3.11).

A similar procedure for generating synthetic datasets is used to convert the temperature-dependent functions (Kitchell et al. 1977, Thornton and Lessem 1978) employed by the Wisconsin Bioenergetics Fish Model (Hanson et al. 1997) into the hyperbolic Arrhenius formulation assumed by BASS.

Although the BASS database generator performs most parameter estimations using univariate statistics or ordinary linear least-squares regression analysis as appropriate, nonlinear least-squares regression analysis is used to estimate weight-specific growth rates and physiological functions that are to be fitted to BASS's hyperbolic Arrhenius formulation. In these latter instances, BASS's database generator uses the NL2SOL Fortran 90 software that solves nonlinear least-squares problems using a modified Newton's method

with analytic Jacobians and a secant-updating algorithm to compute the required Hessian matrix. See Dennis et al. (1981).

Estimation of Weight-specific Growth Rates

BASS uses weight-specific growth rates ($\gamma = W^{-1}\, dW/dt$) not only to estimate a cohort's rate of dispersal and non-predatory mortality [see Equation (2.95)] but also as a parameter by which a cohort's expected ingestion rate can be back-calculated. Estimating weight-specific growth rates for BASS, however, obviously depends on the underlying model used to describe the fish's expected growth rate dynamics (i.e., dW/dt). Selecting an appropriate growth model for use by the BASS simulation software, like most model selections, was not a trivial issue since at least four different models (i.e., von Bertalanffy, Richards, Gompertz, and Parker-Larkin models) have become standard tools for characterizing the growth of fishes. See Ricker (1979) for a detailed discussion of these and other less commonly used models.

According to the von Bertalanffy model, a fish's growth rate is the simple mass balance of anabolic processes that are directly proportional to the fish's surface area and of catabolic processes that are directly proportional to the fish's body weight. Consequently, the fish's growth dynamics are governed by the following differential equation

$$\frac{dW_w}{dt} = \varphi W_w^{2/3} - \rho W_w \qquad (3.15)$$

where φ is the fish's rate of feeding and assimilation, and ρ is the fish's total metabolic rate. Assuming isometric growth (i.e., $W_w = \lambda L^3$), this model is also equivalent to

$$\frac{dL}{dt} = \frac{\rho}{3}\,(L_{max} - L) \qquad (3.16)$$

where L is the fish's body length; and $L_{max} = \varphi / (\rho\, \lambda^{1/3})$ is the fish's "maximum" body length that is obtained by setting Equation (3.15) to zero. For further discussion, see Parker and Larkin (1959) and Paloheimo and Dickie (1965).

The Richards model (Richards 1959) is a generalization of the von Bertalanffy model that relaxes the assumption of isometric growth and strict proportionality between a fish's feeding/assimilatory processes and its absorptive surface areas. In this model, the fish's feeding is simply assumed to be a power function of its body weight. The fish's growth is then described by the differential equation

$$\frac{dW_w}{dt} = \varphi_1 W_w^{\varphi_2} - \rho W_w \qquad (3.17)$$

Although the von Bertalanffy and Richards models appear to have strong physiological foundations, a critical analysis of their parameters casts doubts on such assertions. One particular point of contention is the assumption that a fish's metabolism (i.e., respiration and excretion) is directly proportional to its body weight. Although this assumption is certainly satisfied or closely approximated for some fish species, most species have metabolic demands that are best described as power functions of their body weights. Consequently, from a physiologically based perspective, a better anabolic-catabolic process model for fish growth would be

$$\frac{dW_w}{dt} = \varphi_1 W_w^{\varphi_2} - \rho_1 W_w^{\rho_2} \qquad (3.18)$$

See Paloheimo and Dickie (1965). Unlike the von Bertalanffy and Richards models, however, this model generally does not have a closed analytical solution. Furthermore, when this model is fit to observed data, there is no a priori guarantee that the fitted exponents will actually match expected physiological exponents unless the analysis is suitably constrained.

In light of these criticisms, simpler empirical growth models may be more than adequate for most applications. Two such models that have proved useful in this regard are the Gompertz and Parker-Larkin models. Both of these models are intended to describe the growth of fishes that decreases with the age or size of the individual. Whereas the Gompertz model describes fish growth by

$$\frac{dW_w}{dt} = \varepsilon_1 \exp(-\varepsilon_2 t)\, W_w \qquad (3.19)$$

the Parker-Larkin model (Parker and Larkin 1959) assumes that

$$\frac{dW_w}{dt} = \alpha W_w^{\beta} \qquad (3.20)$$

where the exponent β is less than 1.

Although each of the aforementioned models can describe very different growth trajectories, much of the discussion surrounding their use has focused on whether they predict asymptotically zero or indeterminate growth (Parker and Larkin 1959, Paloheimo and Dickie 1965, Knight 1968, Schnute 1981). Although growth rates of individual fish almost always decrease with increasing age or body size, Knight (1968) argued that the traditional notion of asymptotically zero growth is seldom, if ever, supported by studies that have focused on actual growth increments rather than on size-at-age. Because the Parker-Larkin model is the only model outlined above that assumes fish growth is fundamentally indeterminate, and because the Parker-Larkin model does not

rely on the a priori assumption that fish respiration is a linear function of their body weight as do the von Bertalanffy and Richards models, it is used exclusively by BASS when needed.

Three basic types of data have been used traditionally to calculate fish growth rates; these are: (1) length at age or capture, (2) back-calculated length at age for specific age classes sampled over multiple years, and (3) back-calculated length at age for specific year classes or cohorts. Back-calculated body lengths for the latter two data types are generally calculated by regression using measured growth increments of body scales, otoliths, pectoral spines, or other "hard" structures. Whereas for a length at age dataset each individual fish contributes only one observation (i.e., its current length), each individual fish contributes a time series of body lengths for both of the remaining types of growth data.

To estimate weight-specific growth rates for fish, body lengths at age that have been reported in the literature, whether back-calculated or not, are converted into wet body weights using weight-length regressions reported by the study of interest or other published sources. Estimated wet body weights are then fit to the analytical solution Parker-Larkin growth model,

$$\frac{dW_w}{dt} = \gamma W_w = \left(g_1 W_w^{-g_2}\right) W_w \qquad (3.21)$$

using the NL2SOLV nonlinear optimization software. The explicit solution of the Parker-Larkin growth model for any time interval $[t_0, t]$ is

$$W_w(t) = \left[g_1 g_2 (t - t_0) + W_w(t_0)^{g_2}\right]^{1/g_2} \qquad (3.22)$$

Because this expression is discontinuous at $g_2 = 0$, the growth parameters g_1 and g_2 are actually obtained by fitting calculated body weights to the equivalent expression

$$W_w(t) = \left[g_1 \exp(b)(t - t_0) + W_w(t_0)^{\exp(b)}\right]^{1/\exp(b)} \qquad (3.23)$$

where $g_2 = \exp(b)$.

Estimation of Hyperbolic Arrhenius Functions

When a fish's daily rate of maximum food ingestion, plankton filtration, gastric evacuation, respiration, or growth exhibits a temperature optimum, the BASS database generator fits the process's actual or synthetic data to the hyperbolic Arrhenius function

$$P = p_1 W_w^{p_2} \exp(p_3 T)\left(1 - \frac{T}{T_2}\right)^{p_3 (T_2 - T_1)} \qquad (3.24)$$

The BASS database generator also fits actual or synthetic data regarding satiation meal size and feeding times to satiation to the above equation when these feeding parameters exhibit temperature optima. Testing of the initial NL2SOL-based procedure developed to estimate the parameters of Equation (3.24) revealed that the convergence performance of NL2SOL could be greatly improved by reconfiguring Equation (3.24) as

$$P = p_1 W_w^{p_2} \exp(p_3 T)\left(1 - \frac{T}{T_{\max} + \delta^2}\right)^{p_3 (T_{\max} + \delta^2 - T_1)} \qquad (3.25)$$

where $T_{\max}$ is the maximum temperature of the dataset being fitted, and $T_2 = T_{\max} + \delta^2$. Because estimations of nonlinear parameters are frequently sensitive to their initial estimates, a three-step procedure was developed to estimate the parameters for Equation (3.25).

The first step estimates a mean body weight exponent $\bar{p}_2$ by fitting repeated linear least-squares regressions

$$\log P_k = p_{2,k} \log W_{w,k} + p_{0,k} \qquad (3.26)$$

to data subsets, indexed by k, whose temperature ranges are less than 3 Celsius.

The second step uses NL2SOL to estimate the parameters of the temperature response model

$$\hat{P} = \frac{P}{W_w^{\bar{p}_2}} = p_1 \exp(p_3 T)\left(1 - \frac{T}{T_{\max} + \delta^2}\right)^{p_3 (T_{\max} + \delta^2 - T_1)} \qquad (3.27)$$

Multiple sets of initial parameters are sequentially supplied to NL2SOL, and the set that produces the smallest sum of least-squares is used in the third and final step in the estimation process.

Initial parameter estimates for Equation (3.27) are generated by first fitting $\hat{P}$ to the cubic polynomial

$$\hat{P} = \xi_3 T^3 + \xi_2 T^2 + \xi_1 T + \xi_0 \qquad (3.28)$$

using ordinary linear least-squares techniques. The initial value of T_1 for each set of initial parameters is then assigned as the local maximum of this polynomial, i.e.,

$$\left.\frac{d\hat{P}}{dT}\right|_{T=T_1} = 3\xi_3 T^2 + 2\xi_2 T + \xi_1 = 0 \qquad (3.29)$$

$$\left.\frac{d^2\hat{P}}{dT^2}\right|_{T=T_1} = 6\xi_3 T + 2\xi_2 < 0 \qquad (3.30)$$

Initial estimates for δ are assigned assuming that the fish's upper tolerance temperature corresponds to equidistant temperatures within the interval

$$T_{max} < T_2 < 43 \quad (3.31)$$

Similarly, initial estimates of the process's temperature coefficient p_3 are assigned as equidistant values within the interval

$$0.05 < p_3 < 0.75 \quad (3.32)$$

Having assigned p_3, T_1, and δ, the process's rate at $T = 0$ is then assigned as the mean back-calculated rate

$$p_1 = \frac{1}{n} \sum_{i=1}^{n} \frac{\hat{P}_i}{\exp(p_3 T_i)(1 - T_i/T_2)^{p_3 (T_2 - T_1)}} \quad (3.33)$$

where $\hat{P}_i$ and T_i denote the observed data values.

In the third step, the results of steps 1 and 2 were supplied to NL2SOL as the "best" initial estimates of the parameters for Equation (3.25), and the final parameters for Equation (3.24) were determined.

Table 3.1 summarizes the results obtained using the aforementioned procedure to estimate maximum daily consumption and maximum meal size for a variety of studies reported in the open literature. **Table 3.2** summarizes the results of converting the maximum daily consumption functions used by the Wisconsin Bioenergetics Model into their "equivalent" hyperbolic Arrhenius form. **Figure 3.1** and **Figure 3.2** display selected results from **Table 3.2**.

Readers interested in obtaining the Fortran 95 subroutines used to implement this procedure can do so by simply requesting this code from the author.

3.5. Suggested Calibration Procedures

Calibrating Fish Growth Rates

Because Equations (3.21) and (3.22) do not explicitly account for either reproductive losses or temperature-dependent growth, growth rates estimated by them generally should be calibrated for the application at hand when back-calculating expected fish ingestion rates.

Having estimated a long-term average growth rate

$$\gamma = g_1 W_w^{-g_2} \quad (3.34)$$

for a species of interest, the calibration procedure developed for BASS assumes that the fish's weight-specific growth coefficient g_1 is actually an exponential function of the fish's ambient water temperature that, in turn, is assumed to be a sinusoidal function of the time of year. In particular,

$$g_1 = g_0 \exp\left[g_3 \left(T_m + \alpha \sin(\beta t + \omega)\right)\right] \quad (3.35)$$

where $g_3 = 0.1 \ln(Q_{10,G})$ defines the fish's Q_{10} relationship for growth; T_m is the mean annual water temperature experienced by the fish; and α, β, and ω are the coefficients describing the amplitude, frequency, and phase shift of the water temperatures experienced by the fish, respectively. Under this assumption a fish's growth is therefore described by

$$\frac{dW_w}{dt} = \left\{g_0 W_w^{-g_2} \exp\left[g_3 \left(T_m + \alpha \sin(\beta t + \omega)\right)\right]\right\} W_w \quad (3.36)$$

If t_0 is the day that the species' young-of-year are recruited into the population, and m is the integer age in years when the fish becomes sexually mature, it follows that a fish's pre-spawn body weight at the time of its first reproduction is given by

$$W_w(t_0 + 365\,m)^{g_2} - W_w(t_0)^{g_2} = g_0\, g_2 \int_{t_0}^{t_0 + 365\,m} \exp\left[g_3 \left(T_m + \alpha \sin(\beta \tau + \omega)\right)\right] d\tau \quad (3.37)$$

Because the integrand of this equation is a periodic function possessing an annual period, the preceding equation can be simplified to

$$W_w(t_0 + 365\,m)^{g_2} - W_w(t_0)^{g_2} = g_0\, g_2\, m\, I \quad (3.38)$$

where

$$I = \int_{t_0}^{t_0 + 365} \exp\left[g_3 \left(T_m + \alpha \sin(\beta \tau + \omega)\right)\right] d\tau \quad (3.39)$$

Once fish reach sexual maturity, their underlying growth equation [i.e., Equation (3.36)] is only piecewise differentiable since fish are assumed to lose a constant fraction (σ) of their body weight during spawning due to gamete production and increased metabolic expenditures associated with spawning behaviors. If n is the species' maximum integer age in years, Equation (3.36) can be integrated between any two consecutive spawning events $i = m, (m + 1), \ldots, (n - 1)$ as follows

$$W_w(t_0 + 365\,(i+1))^{g_2} - \left[(1 - \sigma)\, W_w(t_0 + 365\,i)\right]^{g_2} = g_0\, g_2\, I \quad (3.40)$$

$$W_w(t_0 + 365\,(i+1))^{g_2} - (1 - \rho)\, W_w(t_0 + 365\,i)^{g_2} = g_0\, g_2\, I \quad (3.41)$$

where $\rho = 1 - (1 - \sigma)^{g_2}$. Summing Equations (3.38) and (3.41) appropriately, it follows that

$$W_w(t_0 + 365\,n)^{g_2} + \rho\left(\sum_{i=m}^{n-1} W_w(t_0 + 365\,i)^{g_2}\right) - W_w(t_0)^{g_2} = g_0\,g_2\,n\,I \quad (3.42)$$

To calibrate a species growth rate using Equations (3.34), (3.39) and (3.42), one must specify the parameters (T_m, α, β, and ω) describing the application's water temperatures and the species' maximum age (n yr), mean age (m yr) of sexual maturity, annual spawning times $[t = (t_0 + 365\,m), (t_0 + 365\,(m+1)), \ldots]$, spawning loss constant (σ), initial body weight of young-of-year fish $[W_w(t_0)]$, body weight at maximum age $[W_w(t_0 + 365\,n)]$, and allometric growth exponent (g_2). The species' pre-spawn body weights for Equation (3.41) can be estimated using Equation (3.22) using the adjusted allometric growth coefficient

$$g_1 = \frac{W_w(t_0 + 365\,n)^{g_2} - W_w(t_0)^{g_2}}{g_2\,a_{\max}} \quad (3.43)$$

To demonstrate this procedure, growth rates estimated for brook trout (*Salvelinus fontinalis*) from literature data will be calibrated for a "typical" Mid-Atlantic trout stream whose annual temperature regime is assumed to be given by

$$T[Celsius] = 10.8 + 8.8\sin(0.0172 * t + 6.04) \quad (3.44)$$

This temperature function assumes that the stream's annual range of water temperatures is 2 to 19.5 Celsius, that April 1 corresponds to $t = 0$, and that January 15 is the coldest day of the year. In this stream, brook trout are assumed to be recruited into the population with an initial YOY body weight equal to 0.25 g wet wt/fish and to live a maximum of seven years. The maximum size attained by these trout is assumed to be 825 g wet wt/fish (i.e., ≈440 mm(TL) assuming $W[g] = 0.148 \times 10^{-4}\,TL[mm]^{2.93}$). Spawning and recruitment are assumed to occur on October 30. Sexual maturity is reached when trout attain a total body length of 157 mm (i.e., between the ages of 2 and 3 years), and the trout's reproductive loss constant is assumed to equal 0.2 g wet wt/g wet wt/spawn. Finally, the trout's growth Q_{10} is assumed to equal 2 (i.e., $g_3 = 0.069$). Using data compiled by Carlander (1969), the BASS database analysis program estimated the following weight-specific growth rate for brook trout

$$\gamma = 0.0196\,W_w^{-0.455} \quad (3.45)$$

Calibrating this growth rate to predict with the trout's assumed maximum and YOY body weights and maximum age using Equation (3.43) yields

$$\gamma = 0.0178\,W_w^{-0.455} \quad (3.46)$$

When this adjusted growth rate is used to project pre-spawn body weights for Equation (3.42) using Equation (3.22), the weight-specific growth rate of brook trout calibrated for reproductive losses and temperature dependencies is

$$\gamma = 0.0107\,W_w^{-0.455}\exp[0.069\,(10.8 + 8.75\sin(0.0172\,t + 6.04))] \quad (3.47)$$

When weight-specific feeding rates (φ_{dd} g dry wt/g dry wt/d) are back-calculated monthly, using this equation and standard salmonid metabolic relationships [i.e., food assimilation efficiencies, specific dynamic action (SDA) to ingestion ratios, oxygen consumption rates, respiratory quotients (RQ), and ammonia excretion to oxygen consumption quotients (AO)] as outlined by Barber (2003), the following allometric regression can be calculated

$$\varphi_{dd} = 0.0251\,W_w^{-0.205}\exp(0.064\,T) \quad (n = 84;\ r^2 = 0.98) \quad (3.48)$$

This regression agrees well with results of Sweka and Hartman (2001) who estimated the maximum consumption of brook trout at 12 Celsius to be

$$\varphi_{ww} = 0.13\,W_w^{-0.20} \quad (3.49)$$

Taken together, the preceding equations imply that the realized ingestion rate of brook trout at 12 Celsius would be approximately 42% of their maximum ingestion rate. This result agrees well with that reported by Elliott and Hurley (1998).

A Fortran 95 executable program (BASS_FILES.EXE) is provided with the BASS simulation software to perform the aforementioned growth rate calibration and back-calculated feeding rate estimation. See Section 5.6.

Estimating Initial Conditions

Although most fish surveys typically report only total species densities (fish/ha) or total species biomass (kg wet wt/ha), such data can be easily converted into BASS initial conditions if one assumes that the recruitment strength for each cohort of observed population density has been relatively constant or has been fluctuating around a long-term average. To perform this conversion, BASS's assumed self-thinning model Equation (2.94), is first rewritten as

$$\frac{dN}{N} = -b\,\frac{dW_w}{W_w} \tag{3.50}$$

This equation can then be reintegrated to obtain

$$\ln\frac{N(t)}{N(t_0)} = -b\,\ln\left(\frac{W_w(t)}{W_w(t_0)}\right)$$
$$N(t) = N(t_0)\,\exp\left[-b\,\ln\left(\frac{W_w(t)}{W_w(t_0)}\right)\right] \tag{3.51}$$

A species total population density can be estimated by applying Equation (3.51) to each of its cohorts, i.e.,

$$N(t) = \sum_i N_i(t)$$
$$N(t) = \sum_i N_i(t-a_i)\,\exp\left\{-b\ln\left[\frac{W_{w,i}(t)}{W_{w,i}(t-a_i)}\right]\right\} \tag{3.52}$$

where N_i, $W_{f,i}$, and a_i denote the density, average wet body weight, and age, respectively, of the i-th cohort. Assuming that each cohort is recruited into the species' total population with the same initial body weight [$W_{w,i}(t-a_i) = W_0$] and population density [$N_i(t-a_i) = N_0$], the preceding equation can be simplified to

$$N(t) = N_0\sum_i \exp\left\{-b\,\ln\left[\frac{W_{w,i}(t)}{W_0}\right]\right\} \tag{3.53}$$

If the growth rate trajectories of each cohort have also remained relatively constant, it follows that an expected decomposition of a species total population density into its component cohort densities would be

$$N(t) = N_0\sum_i \exp\left\{-b\,\ln\left[\frac{W_{w,i}(a_i)}{W_0}\right]\right\} \tag{3.54}$$

It also follows that an expected decomposition of a species total biomass into its component cohort biomasses would be

$$B(t) = \sum_i W_{w,i}(a_i)\,N_i(t)$$
$$= N_0\sum_i W_{w,i}(a_i)\,\exp\left\{-b\,\ln\left[\frac{W_{w,i}(a_i)}{W_0}\right]\right\} \tag{3.55}$$

From Equations (3.54) and (3.55) it should be reasonably clear that given a species total population density (N) or total biomass (B) and given a model for the species body growth [i.e., Equations (3.21) and (3.22)], one can straightforwardly calculate the species' apparent long-term year-class strength N_0. Having done so, one can estimate the species' cohort densities and also convert the species' total population density into its expected total biomass and vice versa.

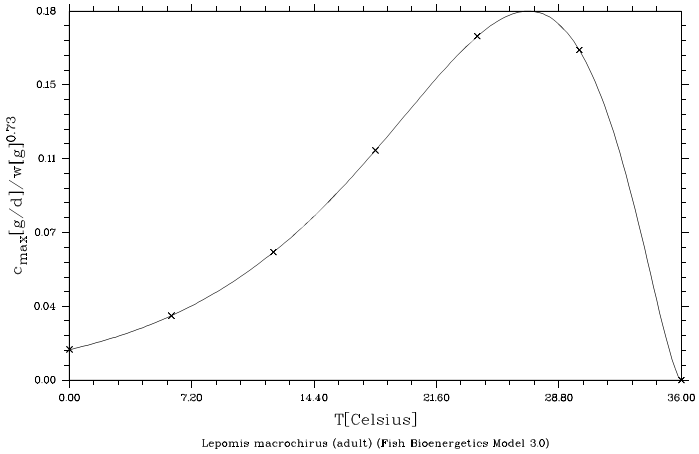
To corroborate the density-to-biomass conversion procedure outlined above, a database of studies that have reported measured fish densities and associated fish biomasses was compiled from the literature (Miles 1978, Quinn 1988, Reed and Rabeni 1989, Ensign et al. 1990, Buynak et al. 1991, Flick and Webster 1992, Bettoli et al. 1993, Waters et al. 1993, Maceina et al. 1995, Mueller 1996, Allen et al. 1998, Radwell 2000, Dettmers et al. 2001, Pierce et al. 2001, Habera et al. 2004). Reported fish densities were converted into estimated biomasses assuming evenly spaced self-thinning exponents b ranging from -0.5 to -1.0 at 0.025 increments. Reduced major axis (RMA) regressions were then calculated for each assumed self-thinning exponent. The self-thinning exponent that minimized the intercurve area between the calculated RMA regression line and the identity relationship $B_{obs} = B_{est}$ was b = -0.825. This regression was

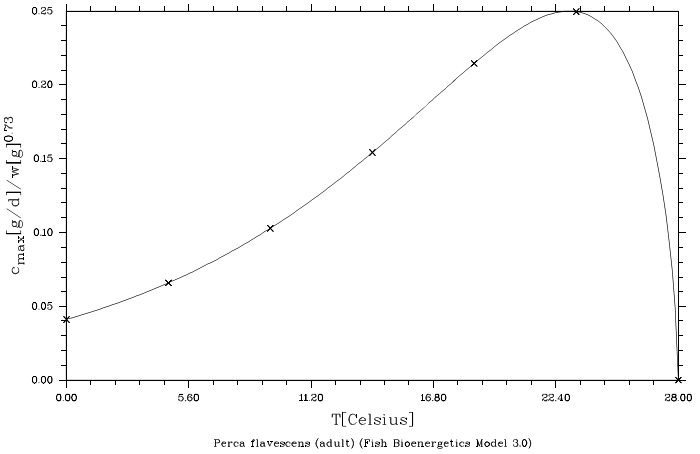
$$\ln B_{obs} = 0.827\,\ln B_{est} - 0.0528\ \ (n = 512;\ r^2 = 0.64)$$
$$B_{obs} = 0.949\ B_{est}^{0.827} \tag{3.56}$$

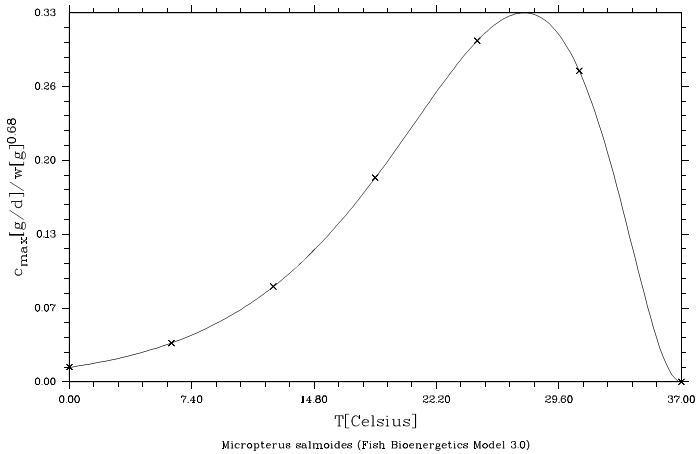
Figure 3.3 displays the data for the regression (3.56) and the identity relationship $B_{obs} = B_{est}$.

In addition to calibrating fish growth rates and back-calculating feeding rates, the auxiliary BASS program BASS_FILES.EXE described in the preceding section estimates initial body weights and cohort densities for users given a target initial total species density or a target initial total species biomass. See Section 5.6.

Figure 3.1 Selected results for fitting Equation (2.58) to maximum consumption rates calculated by the algorithms and parameters used by the Wisconsin Bioenergetics Model. Observed data corresponds to the maximum daily consumption of fish weighing 1, 25, 50, 75, and 100 g wet wt/fish at seven equally spaced temperatures between 0 Celsius and the fish's upper tolerance limit.







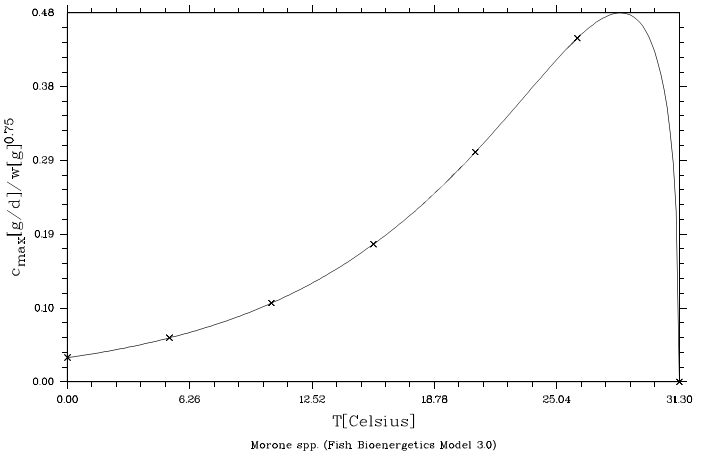
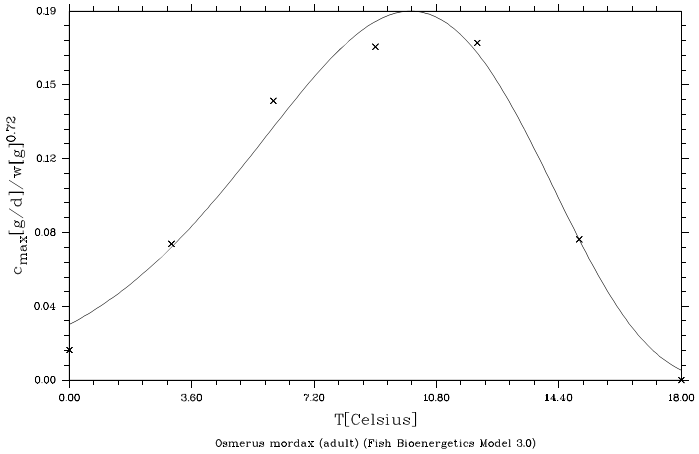
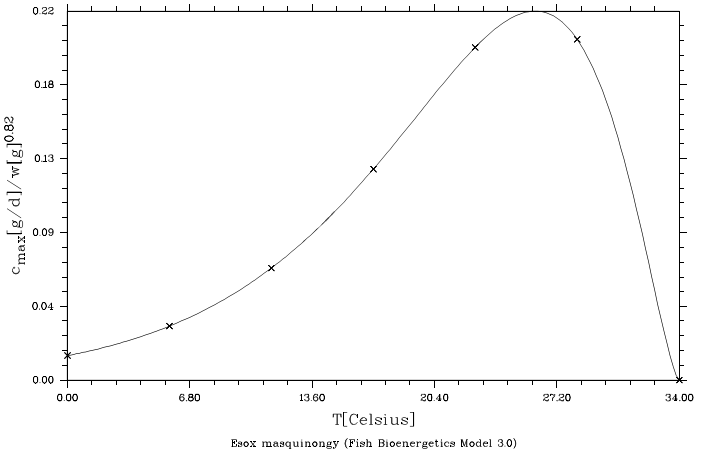
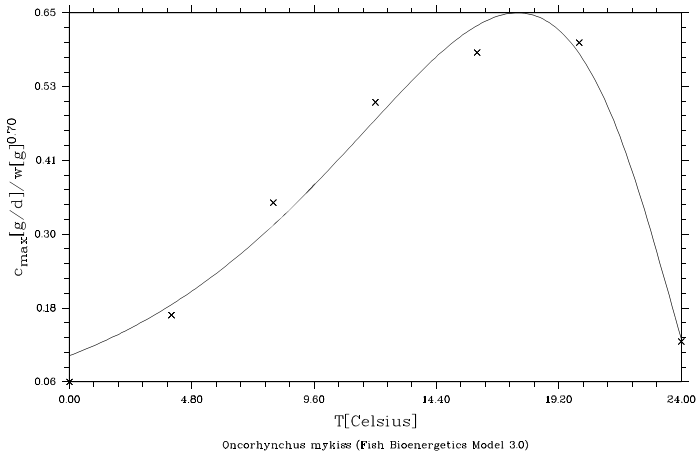


Figure 3.2 Selected results for fitting Equation (2.58) to maximum consumption rates calculated by the algorithms and parameters used by the Wisconsin Bioenergetics Model. Observed data corresponds to the maximum daily consumption of fish weighing 1, 25, 50, 75, and 100 g wet wt/fish at seven equally spaced temperatures between 0 Celsius and the fish's upper tolerance limit.







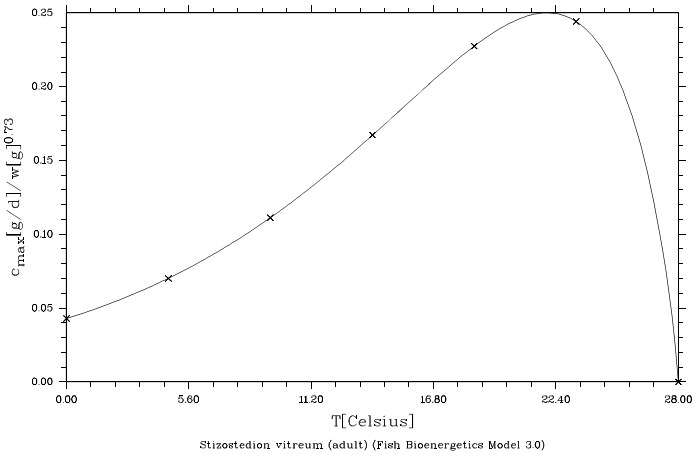


Figure 3.3 Observed fish biomass versus fish biomass predicted by cohort self-thinning BASS's algorithm.

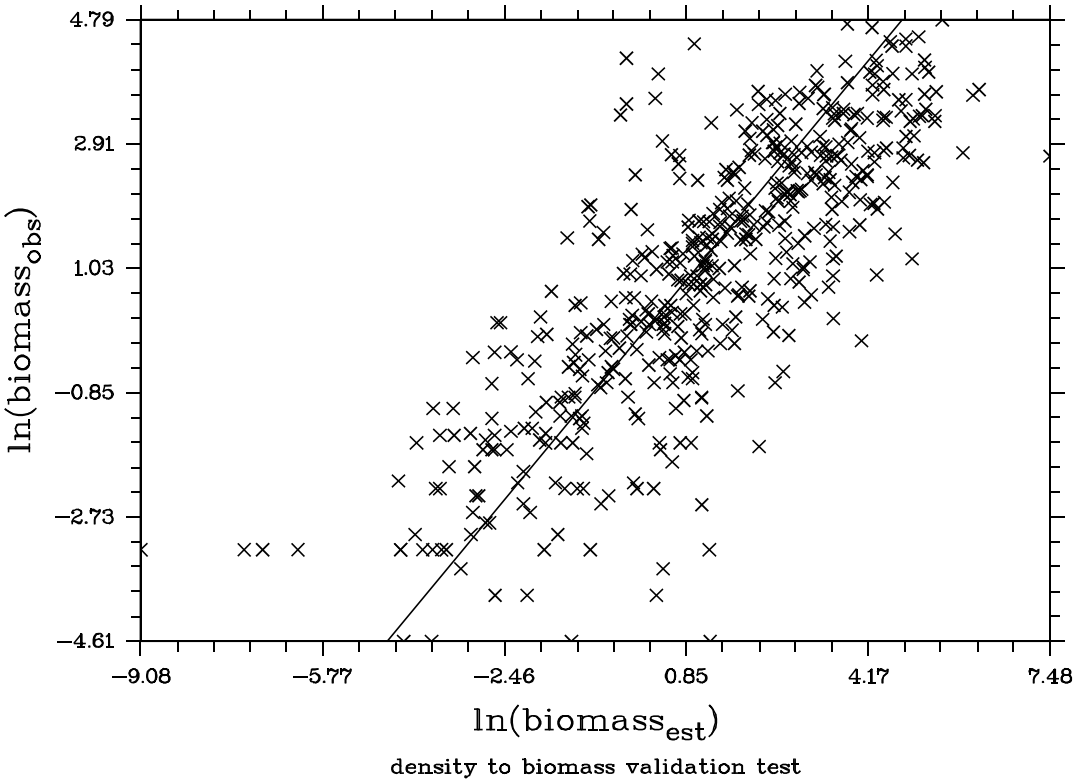


Table 3.1 Summary of NL2SOL regressions for Equation (3.24) fitted to maximum daily consumption rates and satiation meal size reported in the literature.

Species	Process	p_1	p_2	p_3	T_1	T_2	r^2
[1] *Channa argus*	c_{max}[g/d]	0.00741	0.52	0.425	29.2	51.3	0.99
[2] *Coregonus hoyi*	c_{max}[g/g/d]	0.159	-0.54	0.320	16.8	26.0	0.96
[3] *Morone saxatilis*	c_{max}[g/g/d]	0.000945	0.00	0.708	25.9	58.7	0.97
[4] *Morone saxatilis*	c_{max}[g/g/d]	0.00542	0.00	0.455	21.6	42.1	0.85
[5] *Pomoxis annularis*	c_{max}[g/d]	0.00213	0.03	1.051	23.1	43.0	0.50
[6] *Salmo trutta*	c_{max}[Kcal/d]	0.0100	0.76	0.262	18.5	21.8	1.00
[7] *Salmo trutta*	sm[mg(dw)]	1.54	0.69	0.596	15.0	29.3	1.00
[8] *Salmo trutta*	sm[mg(dw)]	0.731	0.78	2.000	13.8	67.8	1.00
[9] *Salmo trutta*	sm[mg(dw)]	0.843	0.76	2.000	13.6	69.5	0.99
[10] *Salmo trutta*	sm[mg(dw)]	1.72	0.79	0.463	14.9	24.1	1.00
[11] *Salmo trutta*	sm[mg(dw)]	0.906	0.80	0.437	15.1	24.2	0.99
[12] *Salvelinus alpinus*	c_{max}[g(dw)/g/d]	0.00123	0.00	0.489	16.5	29.0	0.79
[13] *Salvelinus confluentus*	c_{max}[g/g/d]	0.00840	0.00	0.288	14.0	29.0	0.98
[14] *Siniperca chuatsi*	c_{max}[g/d]	0.0267	0.60	0.212	30.3	44.5	0.99
[15] *Tilapia zillii*	c_{max}[g/g/d]	7.300E-07	0.00	2.000	30.6	75.1	0.94

Data sources and notes

[1] Liu et al. (1998). Rates estimated by regression assuming no feeding or lethality at 43 Celsius.
[2] Binkowski and Rudstam (1994). Rates as reported in Table 1 assuming no feeding or lethality at 26 Celsius.
[3] Cox and Coutant (1981). Rates as reported in Table 2 assuming no feeding or lethality at 43 Celsius.
[4] Hartman and Brandt (1993). Rates estimated from Figure 1 assuming no feeding or lethality at 43 Celsius.
[5] Hayward and Arnold (1996). Rates as reported in Table 1 assuming no feeding or lethality at 43 Celsius.
[6] Elliott (1976b). Rates generated by regressions reported in Table 2.
[7] Elliott (1975). Data as reported in Table 4 for *Baetis*.
[8] Elliott (1975). Data as reported in Table 4 for *Hydropsyche*.
[9] Elliott (1975). Data as reported in Table 4 for chironomids.
[10] Elliott (1975). Data as reported in Table 4 for mealworms (*Tenebrio molitor*).
[11] Elliott (1975). Data as reported in Table 4 for oligochaetes.
[12] Larsson and Berglund (1998). Rates as reported in Table 1 assuming no feeding or lethality at 26 Celsius.
[13] Selong et al. (2001). Rates calculated from data reported in Table 2 assuming no assuming or lethality at 26 Celsius.
[14] Liu et al. (1998). Rates estimated by regression assuming no feeding or lethality at 43 Celsius.
[15] Platt and Hauser (1978). Rates estimated from Figure 1 assuming no feeding or lethality at 43 Celsius.

Table 3.2 Summary of NL2SOL regressions for Equation (2.58) fitted to maximum consumption rates (g wet wt/day) estimated by the Wisconsin Bioenergetics Model 3.0 and its distributed database. Observed data corresponds to the maximum daily consumption of fish weighing 1, 25, 50, 75, and 100 g wet wt/fish at seven equally spaced temperatures between 0 Celsius and the fish's upper tolerance limit.

Species	f_1	f_2	f_3	T_1	T_2	r^2
Alosa psuedoharengus (adult)	0.102	0.70	0.426	15.5	29.3	0.99
Alosa psuedoharengus (juvenile)	0.112	0.70	0.214	19.6	27.3	0.98
Alosa psuedoharengus (yoy)	0.0919	0.70	0.196	21.8	29.2	0.99
Chrosomus spp.	0.0590	0.69	0.094	26.0	29.0	1.00
Clupea harengus (adult)	0.08	0.74	0.644	12.9	29.5	0.99
Clupea harengus (juvenile)	0.0808	0.74	0.535	14.4	31.5	0.99
Coregonus hoyi	0.159	0.46	0.320	16.8	26.0	1.00
Coregonus spp.	0.159	0.68	0.320	16.8	26.0	1.00
Esox masquinongy	0.0147	0.82	0.188	26.0	34.0	1.00
Lates niloticus	0.0112	0.73	0.235	27.5	38.0	1.00
Lepomis macrochirus (adult)	0.0150	0.73	0.172	27.0	36.0	1.00
Lepomis macrochirus (juvenile)	0.0113	0.73	0.138	31.0	37.0	1.00
Micropterus dolomieui	0.00139	0.69	0.296	29.0	36.0	1.00
Micropterus salmoides	0.0129	0.68	0.222	27.5	37.0	1.00
Morone saxatilis (adult)	0.0336	0.75	2.000	21.8	213.9	0.95
Morone saxatilis (age 0)	0.014	0.75	2.000	21.3	153.6	0.99
Morone saxatilis (age 1)	0.0310	0.75	2.000	22.4	221.1	0.98
Morone saxatilis (age 2)	0.0376	0.75	2.000	23.8	268.5	0.96
Morone spp.	0.0314	0.75	0.128	28.3	31.3	1.00
Oncorhynchus gorbuscha	0.142	0.73	0.102	17.0	25.9	0.99
Oncorhynchus kisutch	0.0460	0.73	0.320	15.6	25.8	0.98
Oncorhynchus mykiss	0.102	0.70	0.220	17.6	25.3	0.99
Oncorhynchus nerka	0.142	0.73	0.102	17.0	25.9	0.99
Oncorhynchus tshawytscha	0.0330	0.72	0.230	15.0	18.0	1.00
Osmerus mordax (adult)	0.0304	0.73	0.680	10.0	22.3	0.99
Osmerus mordax (juvenile)	0.0472	0.72	0.207	13.1	18.0	0.98
Osmerus mordax (yoy)	0.0587	0.73	0.143	17.9	26.1	0.98
Perca flavescens (adult)	0.0411	0.73	0.125	23.0	28.0	1.00
Perca flavescens (juvenile)	0.0317	0.73	0.094	29.0	32.0	1.00
Perca flavescens (larvae)	0.0647	0.58	0.094	29.0	32.0	1.00
Petromyzon marinus	0.0766	0.65	0.150	18.0	25.0	1.00
Sarotheradon spp.	0.00643	0.64	0.172	30.0	37.0	1.00
Stizostedion vitreum (adult)	0.0428	0.73	0.138	22.0	28.0	1.00
Stizostedion vitreum (juvenile)	0.0802	0.73	0.094	25.0	28.0	1.00
Theraga chalcogramma (adult)	0.146	0.41	0.270	8	15.0	1.00
Theraga chalcogramma (juvenile)	0.0994	0.41	0.461	8	15.0	1.00

4. BASS User Guide

Although BASS versions 1.0 and 1.1 were written in Fortran 77, BASS version 2.0 and higher are coded in Fortran 95. The model enables users to simulate the population and bioaccumulation dynamics of age-structured fish communities using the temporal and spatial resolution of a day and a hectare, respectively. Although BASS implicitly models the dispersal of fish out of the simulated hectare, it does not explicitly simulate the immigration of fish into the simulated hectare. Monthly or yearly age classes can be used for any species. This flexibility enables users to simulate small, short-lived species such as daces, live bearers, and minnows together with larger, long-lived species such as bass, perch, sunfishes, and trout. The community's food web is specified by defining one or more foraging classes for each fish species based on body weight, body length, or age. The user then specifies the dietary composition of these foraging classes as a combination of benthos, incidental terrestrial insects, periphyton, phytoplankton, zooplankton, and/or other fish species, including its own. Standing stocks of non-fish compartments can be simulated as external forcing functions or as state variables.

Although BASS was developed to simulate the bioaccumulation of chemical pollutants within a community or ecosystem, it can also simulate population and community dynamics of fish assemblages that are not exposed to chemical pollutants. For example, in its present form BASS could be used to simulate the population and community dynamics of fish assemblages that are subjected to altered thermal regimes that might be associated with a variety of hydrological alterations or industrial activities. BASS could also be used to investigate the impacts of exotic species or sport fishery management programs on population or community dynamics of native fish assemblages.

The model's output includes:

- Summaries of all model input parameters and simulation controls.
- Tabulated annual summaries for the bioenergetics of individual fish by species and age class.
- Tabulated annual summaries of chemical bioaccumulation within individual fish by species and age class.
- Tabulated annual summaries for the community level consumption, production, and mortality of each fish species by age class.
- Comma-separated values (CSV) files that users can import into Excel or other graphical software create customized plots.

Please report any comments, criticisms, problems, or suggestions regarding the model software or user manual to

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4.1. General Model Structure and Features

The following features are available in BASS v2.3:

- There are no restrictions on the number of fish species that can be simulated.
- There are no restrictions on the number of cohorts that a fish species can have.
- There are no restrictions on the number of foraging classes that a fish species can have, and seasonal diets can be specified for any or all foraging classes. See the fish command /ECOLOGICAL_PARAMETERS option **diet(.,.)={...}**.
- Refuge levels at which cohorts of potential prey species become unavailable to piscivores can be specified. See the fish command /ECOLOGICAL_PARAMETERS option **refugia[]=*fnc***.
- Size-dependent harvest and stocking functions can be specified for any or all species to simulate fisheries management practices. See the fish command /FISHERY_PARAMETERS.
- Habitat suitability indices (HSI) can be specified to adjust a fish's realized feeding/growth, recruitment/spawning, and combined dispersal and non-predatory mortality. See the fish command /HABITAT_PARAMETERS.
- Benthos, periphyton, phytoplankton, and zooplankton can be simulated either as forcing functions or as state variables. Incidental insects, however, can only be simulated as a forcing function.
- There are no restrictions on the number of chemicals that can be simulated.

- Biotransformation of chemicals can be simulated with or without daughter products.

- Integration of BASS's differential equations is performed using a fifth-order Runge-Kutta method with adaptive step sizing that monitors the accuracy of its integration. BASS's Runge-Kutta integrator is patterned on the fifth-order Cash-Karp Runge-Kutta algorithm outlined by Press et al. (1992).

4.2. New Features

The following features were not available in BASS v2.2 and earlier

- Stable isotope dynamics of carbon and nitrogen are simulated to estimate an operational trophic position of each fish cohort within the community of interest; for details see Section 2.8. Users can modify the parameters of this algorithm using the new simulation control command /ISOTOPE_PARAMETERS and the new arguments **del_c13[-]=α** and **del_n15[-]=β** for the non-fish commands /BENTHOS, /TERRESTRIAL_INSECTS, /PERIPHYTON, /PHYTOPLANKTON, and /ZOOPLANKTON.

- BASS can simulate an additional mortality and dispersal (*KM*), over and above a cohort's self-thinning mortality and dispersal (*NM* and *EM*, respectively) and its predatory mortality (*PM*), that are associated with a species-specific biomass carrying capacity. Species-specific biomass carrying capacities are calculated internally by BASS based on each species initial relative biomasses and a user-specified total fish biomass carrying capacity for the community of interest. See the new simulation control command /FISH_CARRYING_CAPACITY.

- To facilitate its linkage to numerous fate and transport models [e.g., see Johnson et al. (2011)], BASS simulations are now conducted to acknowledge when leap years occur. See the new simulation control command /FIRST_LEAP_YEAR.

- The BASS v2.1 plotting commands /ANNUAL_PLOTS and /SUMMARY_PLOTS and their associated code have been deprecated. Users can now generate three different types of CSV files which can be used to create even more customized plots using Excel or other graphical software programs. See **Section 4.7. Command Line Options**.

4.3. Input File Structure

The general structure of a BASS's input or project file is:

/$command_1$ argument(s)
/$command_2$ argument(s)
⋮ ⋮
/$command_n$ argument(s)
/end

The leading slash (/) identifies the line as a command. Blanks or tabs before or after the slash are not significant. The keyword or phrase (i.e., $command_n$) that follows each slash identifies the type of data being specified by that record. Keywords must be spelled in full without embedded blanks and must be separated from the record's remaining information by at least one blank or tab. Arguments are either integers (e.g., 7), real numbers (e.g., 0, 3.7e-2, 1.3, etc.), or character strings. If the command allows multiple arguments or options, each argument must be separated by a semicolon. Commands can be continued by appending an ampersand (&) to the end of the record; therefore, the following commands are equivalent

/command arg_1; arg_2; arg_3; arg_4; arg_5; arg_6

/command arg_1; arg_2; arg_3; &
arg_4; arg_5; arg_6

Because each record is transliterated to lowercase before being decoded, the case of the input file is not significant. Likewise, because consecutive blanks or tabs are collapsed into a single blank, spacing within a command is not significant. The maximum length of a command line, including continuation lines, is 1024 characters.

An exclamation mark (!) in the first column of a line identifies that line as a comment. An exclamation mark can be also placed elsewhere within a record to start an end-of-line comment, i.e., the remainder of the line, including the exclamation mark, will be ignored.

The last command in any BASS project file must be /END. This command terminates program input and any text or commands following it are ignored. BASS checks the syntactical accuracy of each input command as it is read. If no syntax errors are encountered, BASS then checks the specified input parameters for completeness and internal inconsistency.

BASS input data and commands are broadly classified into four categories: simulation control parameters, chemical parameters, fish parameters, and non-fish biotic parameters. Simulation control parameters provide information that is applicable to the simulation as a whole, e.g., length of the simulation, the ambient water temperature, water column depth, and any desired output options. Chemical parameters specify the chemical's physico-chemical properties (e.g., the chemical's molecular weight,

molecular volume, n-octanol / water partition coefficient, etc.) and the chemical's exposure concentrations in various media. Fish parameters specify the fish's feeding and metabolic demands, dietary composition, predator-prey relationships, gill morphometrics, body composition, and initial conditions for the body weights, whole-body chemical concentrations, and population sizes of a fish's cohorts. Non-fish biotic parameters specify how benthos, terrestrial insects, periphyton, and plankton will be simulated.

A BASS project file is actually constructed and managed as a series of include files which are blocks of closely related input commands. These files are specified using the include statement

include *'filename'*

where *filename* is the name of the file containing the desired commands. Each include file specifies data for either a chemical, a fish species, or a non-fish biotic component. Consequently, a typical BASS project file is structured as follows:

```
! file: bass_input_file.prj
! notes: a BASS project file as specified by include files
!
/ command1   simulation control_data
/ command2   simulation control_data
/ command3   simulation control_data
# include   'data_for_chemical_1'
# include   'data_for_chemical_2'
# include   'data_for_fish_1'
# include   'data_for_fish_2'
# include   'data_for_fish_3'
# include   'data_for_fish_4'
# include   'data_for_benthos'
# include   'data_for_insects'
# include   'data_for_periphyton'
# include   'data_for_phytoplankton'
# include   'data_for_zooplankton'
/end
```

BASS's graphical user interface (GUI) enables users to create and edit BASS project files and include files in a modular fashion. The actual file structure used by the BASS GUI is detailed in Section 4.5., following the discussion of the BASS input commands below.

4.3.1. Simulation Control Commands

These commands establish the length of the simulation, the ambient water temperature, the community's water level, and other simulation options. These data are specified by the following block of commands

/SIMULATION_CONTROL	no argument/option required
/ANNUAL_OUTPUTS	*integer*
/BIOTA	$string_1$; ...; $string_n$
/FIRST_LEAP_YEAR	*integer*
/FISH_CARRYING_CAPACITY	*string*
/FGETS	no argument/option required
/HEADER	*string*
/ISOPTOPE_PARAMETERS	$string_1$; $string_2$
/LENGTH_OF_SIMULATION	*string*
/LESLIE_MATRIX_SIMULATION	no argument/option required
/MONTH_T0	*string*
/NONFISH_QSAR	$string_1$; ...; $string_n$
/TEMPERATURE	$string_1$; $string_2$
/WATER_LEVEL	$string_1$; $string_2$

Although the command /SIMULATION_CONTROL must be the first command in the block since it identifies the start of these data, the order of the remaining commands is not significant. The use of these commands is described below in alphabetical order.

■ **/ANNUAL_OUTPUTS *integer***

This command specifies the time interval, in years, between BASS's annual tabulated outputs. This number must be a nonnegative integer. BASS assumes a default value of zero that signifies that no annual outputs will be generated.

■**/BIOTA *string*$_1$; ...; *string*$_n$**

This BASS v2.1 command specifies non-fish standing stocks that are to be generated as forcing functions rather than as simulated state variables. Although this command has been superceded in BASS v2.2 and higher by the commands /BENTHOS, /TERRESTRIAL_INSECTS, /PERIPHYTON, /PHYTOPLANKTON, and /ZOOPLANKTON (see Section 4.3.4), it has been retained for upward compatibility. Valid options are:

- **benthos[*yunits*] = *fnc*** to generate benthic standing stocks according to the function ***fnc***. The units string ***yunits*** must be dimensionally equivalent to g dry wt/m^2.

- **insects[*yunits*] = *fnc*** to generate incidental terrestrial insect standing stocks according to the function ***fnc***. The units string ***yunits*** must be dimensionally equivalent to g dry wt/m^2.

- **periphyton[*yunits*] = *fnc*** to generate periphyton standing stocks according to the function ***fnc***. The units string ***yunits*** must be dimensionally equivalent to g dry wt/m^2.

- **phytoplankton[*yunits*] = *fnc*** to generate phytoplankton standing stocks according to the function ***fnc***. The units

string ***yunits*** must be dimensionally equivalent to g dry wt/L.

- **zooplankton[*yunits*] = *fnc*** to generate zooplankton standing stocks according to the function ***fnc***. The units string ***yunits*** must be dimensionally equivalent to g dry wt/L.

Valid specifications for the function strings ***fnc*** are :

- ***nonfish_name*[*yunits*] = α** to generate a constant compartmental standing stock of **α** (*yunits*) for the simulation.

- ***nonfish_name*[*yunits*] = α + β*sin(ω + φ*t[*xunits*])** to generate a sinusoidal compartmental standing stock for the simulation where **α** is the mean standing stock for the chosen time period, **β** is its amplitude (*yunits*), **ω** is its phase angle (radians), and $\varphi = 2\pi$ / period is its frequency (1/*xunits*).

- ***nonfish_name*[*yunits*] = file(*filename*)** to read and interpolate the specified compartmental standing stock from the file ***filename***. See Section 4.4.3.

Unless specified otherwise, BASS assumes that the first day of simulation is April 1 and that the 365-th simulation day is March 31. This assignment can be changed using the command /MONTH_T0.

These options are only required when the user is simulating fish that feed on these resources (see the "diet" option for /ECOLOGICAL_PARAMETERS). Note, however, because BASS assumes that piscivorous fish switch to benthic invertebrates and incidental terrestrial insects when appropriate forage fish are unavailable, the benthos and insect options should be specified even when simulating only piscivorous fish. Also note that if project file uses the FGETS option described below, the only /BIOTA option that might be required is the **zooplankton[*yunits*]=*fnc*** option. This option is required only if the user specifies a fish's feeding to be simulated using the clearance model formulation described in Equation (2.64).

If multiple options are selected, each option must be separated by a semicolon.

■ **/FGETS**

This command enables users to run BASS without simulating the assemblage's population dynamics, i.e., only the growth and bioaccumulation of individual fish are simulated. The command's function and name are based on the FGETS (Food and Gill Exchange of Toxic Substances) model (Barber et al. 1987, 1991) that is BASS's predecessor.

■ **/FIRST_LEAP_YEAR *integer***

This command specifies which year of the simulation corresponds to the first leap year, i.e., contains the first February 29. If not specified, BASS assumes that the fourth year of any simulation is the first leap year.

■ **/FISH_CARRYING_CAPACITY *string***

This command specifies an optional total fish biomass carrying capacity of the community of interest which is used to impose an additional mortality and dispersal (*KM*) on all cohorts of each species over and above their self-thinning mortality and dispersal (*NM* and *EM*, respectively) and their predatory mortality (*PM*). See Equations (2.96) - (2.98) in Section 2.9. The valid syntax for *string* is

- **α[*units*]**

where **α** is a nonnegative real value, and *units* is a string that must be dimensionally equivalent to kg wet wt/ha. Using this input and the initial relative biomass of each species, BASS then internally estimates corresponding species-specific biomass carrying capacities.

■ **/HEADER *string***

This is an optional command that specifies a title to be printed on each page of the output file. The maximum length of the quoted string is 80 characters.

■ **/ISOTOPE_PARAMETERS *string*$_1$; *string*$_2$**

This command specifies how BASS will estimate a fish's operational trophic position ***TP*** from its simulated stable isotope fractions $\delta^{13}C$ and $\delta^{15}N$ using the equations

$$\delta^{13}C_{fish} = \alpha\left(TP_{fish} - TP_{benthos}\right) + \delta^{13}C_{benthos} \qquad (4.1)$$

$$\delta^{15}N_{fish} = \beta\left(TP_{fish} - TP_{benthos}\right) + \delta^{15}N_{benthos} \qquad (4.2)$$

Valid options for this command are:

- **del_c13_tp[-]=α**
- **del_n15_tp[-]=β**

If not specified, BASS assumes the defaults values of $\alpha = 0.8$ and $\beta = 3.4$ (see Vander Zanden and Rasmussen 2001).

■ **/LENGTH_OF_SIMULATION *string***

This command specifies the desired length of the simulation. The valid syntax for *string* is

- **α[*units*]**

where **α** is a nonnegative real value. The time unit specified with brackets is converted into days for internal use and subsequent model output.

■ **/LESLIE_MATRIX_SIMULATION**

This command enables users to run BASS in a mode that is computationally intermediate between BASS's FGETS and full community modes. When this option is specified, BASS simulates fish population dynamics using the conceptual framework of a multispecies Leslie matrix population model. A cohort's mortality is predicted using a single, lumped, self-thinning mortality rate [i.e., Equation (2.94)] without attempting to partition its total mortality into predatory and non-predatory mortality and dispersal as outlined in Sections 2.7 and 2.8. Although predatory mortality is not simulated, the dietary composition of each cohort is nevertheless predicted using the methods described in Section 2.7. While this simulation option is designed partially to lessen the need for detailed food web information and the work required to calibrate a full community simulation, it is also designed to simulate more realistically the population dynamics of communities in which the dominant process driving cohort mortality and self-thinning is dispersal rather than predation.

■ **/NONFISH_QSAR *string*$_1$; ...; *string*$_n$**

This command specifies the quantitative structural activity relationships for the bioconcentration / bioaccumulation factors of the non-fish compartments benthos, periphyton, phytoplankton, and zooplankton that are to be applied to all chemicals. Valid string options are:

- **BCF[-](*nonfish_name*)=α*Kow[-]^β**

where Kow[-] is the chemical's n-octanol / water partition coefficient; and **α** and **β** are real or integer empirical constants. Also see the chemical command **/NONFISH_BCF**. When this command is used, the specified QSARs supercede any BCFs specified by /NONFISH_BCF or exposures specified by /EXPOSURE.

■ **/MONTH_T0 *string***

This is an optional command that specifies the month that corresponds to the start of the simulation. If not specified, BASS assumes a default start time of April 1.

■ **/SIMULATION_CONTROL**

This command specifies the beginning of input data that will apply to the simulation at large, e.g., the type of simulation to be performed, the length of the simulation, ambient water temperature and depth, output options, etc.

■ **/TEMPERATURE *string*$_1$; *string*$_2$**

This command specifies a community's ambient water temperatures. For an unstratified water body only one string option is specified. In this case valid options for this command are:

- **temp[celsius]=α** generates a constant ambient water temperature for the simulation.

- **temp[celsius]=α + β*sin(ω + φ*t[*xunits*])** generates a sinusoidal ambient water temperature for the simulation where **α** is the mean temperature for the chosen time period, **β** is its amplitude (*yunits*), **ω** is its phase angle (radians), and **φ**=2π / period is its frequency (1/*xunits*).

- **temp[celsius]=file(*filename*)** to read and interpolate the ambient water temperature from the file ***filename***. See Section 4.4.3.

For a stratified water body, users must specify the temperature of both the epilimion and hypolimnion. In this case valid options are:

- **temp_epilimnion[meter]=α**
- **temp_epilimnion[meter]=α + β*sin(ω + φ*t[*xunits*])**
- **temp_epilimnion[meter]=file(*filename*)**

- **temp_hypolimnion[meter]=α**
- **temp_hypolimnion[meter]=α + β*sin(ω + φ*t[*xunits*])**
- **temp_hypolimnion[meter]=file(*filename*)**

Note that unless specified otherwise BASS assumes that its first day of simulation is April 1 and that the 365-th simulation day is March 31. This assignment can be changed using the command /MONTH_T0.

■ **/WATER_LEVEL *string*$_1$; *string*$_2$**

This command specifies a community's actual water level. For an unstratified water body only one string option is specified. In this case, valid options for this command are:

- **depth[meter]=α** generates a constant water level for the simulation.

- **depth[meter]=α + β*sin(ω + φ*t[*xunits*])** generates a sinusoidal water level for the simulation where **α** is the mean water level for the chosen time period, **β** is its amplitude (*yunits*), **ω** is its phase angle (radians), and **φ**=2π / period is its frequency (1/*xunits*).

- **depth[meter]=file(*filename*)** to read and interpolate the water levels from the file ***filename***. See Section 4.4.3.

For a stratified water body, users must specify the depth of both the epilimion and the hypolimnion. In this case, valid options are:

- **depth_epilimnion[meter]=α**
- **depth_epilimnion[meter]=α + β*sin(ω + φ*t[*xunits*])**
- **depth_epilimnion[meter]=file(*filename*)**

- **depth_hypolimnion[meter]=α**
- **depth_hypolimnion[meter]=α + β*sin(ω + φ*t[*xunits*])**
- **depth_hypolimnion[meter]=file(*filename*)**

Note that unless specified otherwise, BASS assumes that its first day of simulation is April 1 and that the 365-th simulation day is March 31. This assignment can be changed using the command /MONTH_T0.

4.3.2. Chemical Input Commands

The physico-chemical properties and exposure concentrations of each chemical of interest are specified by a block of twelve commands, i.e.,

/CHEMICAL *string*
/EXPOSURE $string_1$; ...; $string_n$
/LETHALITY $string_1$; ...; $string_n$
/LOG_AC *real number*
/LOG_KB1 *real number*
/LOG_KB2 *real number*
/LOG_P *real number*
/MELTING_POINT *real number*
/METABOLISM $string_1$; ...; $string_n$
/MOLAR_VOLUME *real number*
/MOLAR_WEIGHT *real number*
/NONFISH_BCF $string_1$; ...; $string_n$

The command /CHEMICAL must be the first command in the block since it identifies the start of a new set of chemical parameters. The order of the remaining commands, however, is not significant. The use of these commands will now be described in alphabetical order.

■ **/CHEMICAL *string***

This command specifies the start of the input for a new chemical. Each chemical name must be a single character string without embedded blanks or hyphens. If a two-part name is desired, the user should use an underscore "_" as a separating character. This command must precede the commands /EXPOSURE, /LETHALITY, /LOG_AC, /LOG_KB1, /LOG_KB2, /LOG_P, /METABOLISM, /MOLAR_WEIGHT, /MOLAR_VOLUME, and /MELTING_POINT. The name specified by this command is used in conjunction with the command /INITIAL_CONDITIONS to input initial whole-body concentrations of chemicals in each age class of the fish of concern and with the command /METABOLISM to specify daughter products of chemical biotransformation. If the user specifies chemical exposures via the file option, the indicated name is also used to direct reading of the specified exposure files. Otherwise, this name is used only for output purposes; BASS does not use this name to link to any chemical database.

■ **/EXPOSURE $string_1$; ...; $string_n$**

This command enables the user to specify the temporal dynamics of chemical exposures to fish via water or contaminated sediments or via the ingestion of benthic invertebrates, incidental terrestrial insects, or plankton. Exposure concentrations specified by these options are assumed to be completely bioavailable to the fish. For example, water concentrations are assumed to be actual dissolved concentrations and not total water concentrations that include particle-bound chemical. If multiple options are selected, each option must be separated by a semicolon. Valid options are:

- **cbenthos[*yunits*]=*fnc*** generates potential dietary exposures to fish via benthic organisms according to the function ***fnc***. Note in BASS 2.1 the six-lettered name **cbnths** was used to specify this exposure function.

- **cinsects[*yunits*]=*fnc*** generates potential dietary exposures to fish via incidental terrestrial insects according to the function ***fnc***. Note in BASS 2.1 the six-lettered name **cinsct** was used to specify this exposure function.

- **cperiphyton[*yunits*]=*fnc*** generates potential dietary exposures to fish via periphyton according to the function ***fnc***. Note in BASS 2.1 the six-lettered name **cphytn** was used to specify this exposure function.

- **cphytoplankton[*yunits*]=*fnc*** generates potential dietary exposures to fish via phytoplankton according to the function ***fnc***. Note in BASS 2.1 the six-lettered name **cpplnk** was used to specify this exposure function.

- **csediment[*yunits*]=*fnc*** generates sediment exposure

concentrations according to the function ***fnc***. Note in BASS 2.1 the six-lettered name **csdmnt** was used to specify this exposure function.

- **cwater[*yunits*]=*fnc*** generates aqueous exposure concentrations according to the function ***fnc***.

- **czooplankton[*yunits*]=*fnc*** generates potential dietary exposures to fish via zooplankton according to the function ***fnc***. Note in BASS 2.1 the six-lettered name **czplnk** was used to specify this exposure function.

The concentration units for each exposure function are specified within the indicated brackets. As previously noted for the simulation control functions, unless specified otherwise, BASS assumes that the first day of simulation is April 1 and that the 365-th simulation day is March 31 for all time-dependent exposure functions discussed in the following. This assignment can be changed using the command /MONTH_T0.

Valid expressions for dietary exposures via benthos, periphyton, phytoplankton, or zooplankton and for benthic sediments are:

- ***nonfish_name*[*yunits*]=α** generates a constant concentration of toxicant in benthos, periphyton, phytoplankton, sediment, or zooplankton.

- ***nonfish_name*[*yunits*]=α*cwater[*xunits*]** generates chemical concentrations in benthos, periphyton, phytoplankton, sediment, or zooplankton as a chemical equilibrium with the ambient environmental water. If this equilibrium is assumed to be thermodynamic, then the coefficient **α** generally is equal to the product of the component's dry organic fraction and the chemical's K_{ow}. Also see /NONFISH_BCF.

- ***nonfish_name*[*yunits*]=file(*filename*)** to read and interpolate the concentration of toxicant in benthos, periphyton, phytoplankton, sediment, or zooplankton from the file ***filename***. See Section 4.4.3.

Valid expressions for insect dietary exposures are:

- **cinsects[*yunits*]= α** generates a constant concentration of the toxicant in incidental terrestrial insects.

- **cinsects[*yunits*]=file(*filename*)** to read and interpolate the concentration of the toxicant in incidental terrestrial insects from the file ***filename***. See Section 4.4.3.

Valid expressions for direct aqueous exposures are:

- **cwater[*yunits*]=α** generates a constant aqueous concentration for the chemical of concern.

- **cwater[*yunits*]=α*csediment[*xunits*]** generates aqueous exposure concentrations as a chemical equilibrium with the benthic sediments. If this equilibrium is assumed to be thermodynamic, then the coefficient **α** generally is assumed to equal the product of the sediment's organic fraction and the chemical's K_{oc}.

- **cwater[*yunits*]=α+β*exp(γ*t[*xunits*])** generates an exponential dissolved chemical water concentration where **α** and **β** have units of ***yunits*** and **γ** has units of 1/***xunits***. This option can be used to simulate a chemical spill or one-time application of a pesticide.

- **cwater[*yunits*]=α+β*sin(ω+φ*t[*xunits*])** generates a sinusoidal dissolved chemical water concentration where **α** is the mean dissolved chemical water concentration (***yunits***) (over one period), **β** is the amplitude (***yunits***), **ω** is its phase angle (radians), and **φ**=2π / period is its frequency (1/***xunits***). This option might be used to simulate the mobilization of sediment bound contaminants during spring or fall turnover.

- **cwater[*yunits*]=file(*filename*)** to read and interpolate the dissolved aqueous concentration of toxicant from the file ***filename***. See Section 4.4.3.

Users should be cautious and judicious when using more than one of the above options since an exposure scenario that is inconsistent with theoretical constraints on the fate and distribution of contaminants in aquatic systems can easily be constructed.

■ **/LETHALITY *string*$_1$; ...; *string*$_n$**

This optional command specifies species-specific LC_{50}'s for the chemicals of concern either as an actual concentration value or as a QSAR function. Valid string options are:

- **LC50[units](*fish_name*)=α**

- **LC50[units](*fish_name*)=α*Kow[-]^β**

where *fish_name* is the common name of the fish species to be simulated; Kow[-] is the chemical's n-octanol / water partition coefficient; and **α** and **β** are real or integer empirical constants. BASS converts user-specified LC_{50}s into their corresponding aqueous chemical activities and then uses the geometric mean of these lethal activities to trigger mortality during the simulation.

If the user desires, simulation of mortality associated with the accumulation of a lethal aqueous chemical activity can be turned-off by using the command line option "-l" as discussed in Section 4.5. When this is done, however, BASS still calculates the fish's total aqueous phase chemical activity and reports it as a fraction of the fish's estimated lethal chemical activity to provide the user with a useful monitor of the total chemical status of the fish.

■ **/LOG_AC *real number***

This command specifies the $\log_{10}$ of the chemical's aqueous activity coefficient. For organic chemicals, if this parameter is not specified, BASS will estimate the chemical's activity coefficient using its melting point and n-octanol / water partition coefficient.

■ **/LOG_KB1 *real number***

This command specifies the $\log_{10}$ of a metal's binding constant for non-lipid organic matter [see Equation (2.6)]. This parameter is input only for metals and organometals.

■ **/LOG_KB2 *real number***

This command specifies the $\log_{10}$ of a metal's binding constant for refractory organic matter. This parameter is used to calculate metal binding to the fish's dry fecal matter and input only for metals and organometalics.

■ **/LOG_P *real number***

This command specifies the chemical's $\log_{10} K_{ow}$, where K_{ow} is the n-octanol / water partition coefficient. /LOG_P must be specified for all organic chemicals.

■ **/MELTING_POINT *real number***

This command specifies the chemical's melting point (Celsius). This datum, together with the chemical's logP, is used to calculate the aqueous activity coefficient for organic chemicals when that parameter is not specified by the user. See Yalkowsky et al. (1983)

■ **/METABOLISM *string*$_1$; ...; *string*$_n$**

This optional command specifies species-specific rates of biotransformation for the chemical of concern either as a constant rate or as a QSAR function. Valid string options are:

- **BT[units](*fish_name, chemical_name*)=α**
- **BT[units](*fish_name, chemical_name*)=α*Kow[-]^β**
- **BT[units](*fish_name*, none)=α**
- **BT[units](*fish_name*, none)=α*Kow[-]^β**

where BT specifies the whole-body-referenced biotransformation rate k_{bt} in Equation (2.47); *fish_name* is the common name of the fish species that can metabolize the chemical of concern; *chemical_name* is the name of the daughter product generated by the metabolism of the chemical of concern; Kow[-] is the chemical's n-octanol / water partition coefficient: and **α** and **β** are real or integer empirical constants. If the user does not wish to simulate daughter products because they are insignificant or assumed to be harmless, *chemical_name* can be assigned the value *none*. When daughter products are specified, the user must specify all physico-chemical properties of the identified by-product in the same way that the physico-chemical properties of the parent compound are specified.

■ **/MOLAR_VOLUME *real number***

This command specifies the chemical's molecular volume (cm^3/mol) that is used to calculate the chemical's aqueous diffusivity, i.e.,

$$D = 2.101\times10^{-7}\,\eta^{1.4}\,\nu^{-0.589} \qquad (4.3)$$

where D is the toxicant's aqueous diffusivity (cm^2/sec); η is the viscosity of water (poise); and ν is the chemical's molecular volume (cm^3/mol) (Hayduk and Laudie 1974). The viscosity of water over its entire liquid range is represented with less than 1% error by

$$\log_{10}\frac{\eta_{20}}{\eta_T} = \frac{1.37\,(T-20) + 8.36\times10^{-4}\,(T-20)^2}{109 + T} \qquad (4.4)$$

where η_T is the viscosity (centipoise) at temperature T (Celsius), and η_{20} is the viscosity of water at 20 Celsius (1.002 centipoise) (Atkins 1978).

■ **/MOLAR_WEIGHT *real number***

This command specifies the chemical's molecular weight (g/mol).

■ **/NONFISH_BCF *string*$_1$; ...; *string*$_n$**

This command specifies the bioconcentration / bioaccumulation factors for the non-fish compartments benthos, periphyton, phytoplankton, and zooplankton either as a numerical constant or as a QSAR function. Valid string options are:

- **BCF[-](*nonfish_name*)=α**

- **BCF[-](*nonfish_name*)=α*Kow[-]^β**

where Kow[-] is the chemical's n-octanol / water partition coefficient; and **α** and **β** are real or integer empirical constants. Note that this command or **/NONFISH_QSAR** must be specified for any non-fish compartment that is simulated as a community state variable.

4.3.3. Fish Input Commands

Model parameters for each fish species of interest are specified by a block of thirteen commands, i.e.,

/COMMON_NAME *string*
/SPECIES *string*
/AGE_CLASS_DURATION *string*
/SPAWNING_PERIOD *string*
/FEEDING_OPTIONS $string_1$; ...; $string_n$
/PREY_SWITCHING _OFF
/INITIAL_CONDITIONS $string_1$; ...; $string_n$
/COMPOSITIONAL_PARAMETERS $string_1$; ...; $string_n$
/ECOLOGICAL_PARAMETERS $string_1$; ...; $string_n$
/MORPHOMETRIC_PARAMETERS $string_1$; ...; $string_n$
/PHYSIOLOGICAL_PARAMETERS $string_1$; ...; $string_n$
/FISHERY_PARAMETERS $string_1$; ...; $string_n$
/HABITAT_PARAMETERS $string_1$; ...; $string_n$

The command /COMMON_NAME must be the first command in the block since it is the identifier for the start of a new set of fish parameters. The order of the remaining commands is not significant. The use of these commands will now be described in alphabetical order.

■ **/AGE_CLASS_DURATION *string***

This command specifies the duration of each age class. Two character strings, "month" and "year", are recognized as valid options.

■ **/COMMON_NAME *string***

This command specifies the start of input data for a fish species. The command's specified common name *string* is used for model output and as a label for specifying the dietary composition of other fish species. Each common name must be a single character string without embedded blanks. If a two-part name is desired, the user should use an underscore "_" as a separating blank. See the **diet** option for the command /ECOLOGICAL_PARAMETERS.

■ **/COMPOSITIONAL_PARAMETERS $string_1$; ...; $string_n$**

This command specifies aqueous and lipid fractions of the fish. Valid options that must be separated by semicolons are:

- **pa[-]=α + β*pl[-]** specifies the fish's aqueous fraction as a linear function of the fish's lipid fraction.

- **pl[-]=α*W[*xunits*]^β** specifies the fish's lipid fraction as an allometric function of its body weight. If a fish's average lipid content is independent of its body weight (i.e., **β** equals zero), however, this parameter can be specified simply as **pl[*yunits*]=α**.

where **α** and **β** are real or integer empirical constants.

■ **/ECOLOGICAL_PARAMETERS $string_1$; ...; $string_n$**

This command specifies the ecological parameters describing the fish's trophic interactions, non-predatory mortality, and recruitment. Valid options that must be separated by semicolons are:

- **ast_yoy[-]=f(b[-]=α, *yoy*[*xunits*]=β, *pop*[*yunits*]=γ)** specifies parameters for implementing accelerated self-thinning of young-of-year fish (YOY), or more accurately recently recruited cohorts, that often occurs due to intraspecies competition for territories, refugia, or other habitat resources. The functional argument **b[-]=α** specifies the desired accelerated self-thinning exponent. The functional argument ***yoy*[*xunits*]=β** defines the age, length, or wet weight threshold below which cohorts will be subject to accelerated self-thinning. Valid expressions for ***yoy*** are either "**age**", "**tl**", or "**wt**". The final functional argument specifies the population threshold that triggers accelerated self-thinning. Depending on the assumed nature of the competition, this threshold can be specified either as the total density of cohorts satisfying the condition ***yoy*[*xunits*]≤β**, or as the total density of cohorts satisfying the condition ***yoy*[*xunits*]>β**. For the former case, ***pop*** equals "**pop_yoy**" whereas for the latter case, ***pop*** equals "**pop_adults**".

- **diet(*class*, *time*) = {$prey_1$ = ε $_1$, ..., $prey_n$ = ε $_n$}** specifies the dietary composition for fish of the age or size class ***class*** during the months specified by ***time***. The right-hand side of the option specifies the prey items ($prey_n$) and their contribution (ε_n) to the fish's diet. Each $prey_n$ is either the common name of a simulated fish species, "benthos", "insects", "periphyton", "phytoplankton", or "zooplankton" (see commands /BIOTA and /COMMON_NAME). Depending on its value, ε_n is interpreted either as a constant percent contribution or as a prey electivity. In particular, if $1<\varepsilon_n<100$, then ε_n designates the relative frequency of that prey in the fish's

diet independent of its relative abundance in the field. On the other hand, if $-1<\varepsilon_n<1$, then ε_n is considered a prey electivity [see Equation (2.74)]. For any foraging class, users can specify both constant dietary percentages and prey electivities.

Valid expressions for ***class*** are:

α< a[*xunits*]<β for age-based dietary classes

α< l[*xunits*]<β for length-based dietary classes

α<w[*xunits*]<β for weight-based dietary classes

where **α** and **β** are real or integer empirical constants. Although for a given species all ***class*** types must be the same (i.e., age, length, or weight), the ***class*** types between species can be different.

Valid expressions for ***time*** are either the name of a month or the names of two months separated by a hyphen. For example,

month1, e.g., **July**, or

month1-month2, e.g., **July-December**.

If the diet of a specified age / size class is independent of time of year, "**,** ***time***" can be omitted. In this case, ***time*** = "January-December" is assumed.

The **diet(.,.)={...}** option can be repeated as many times as needed to define a complete lifetime sequence of diets for the fish.

- **lp[*yunits*]= *fnc*** specifies the average length of prey consumed by a fish whose body length is L[***xunits***]. Unlike most fish command options, two valid function strings are recognized, i.e.,

  lp[*yunits*]=α + β*L[*xunits*] or

  lp[*yunits*]=α + β*exp(γ*L[*xunits*])

  where **α**, **β**, and **γ** are real or integer empirical constants. If a fish's average prey size is independent of its body length (i.e., **β** equals zero), this parameter can be specified simply as **lp[*yunits*]=α**. If not specified, BASS assigns the default value **lp[cm]=0.2*L[cm]**.

- **lp_max[*yunits*]= *fnc*** specifies the maximum length of prey consumed by a fish whose body length is L[***xunits***]. Like the option for a fish's average prey length, two valid function strings are recognized, i.e.,

  lp_max[*yunits*]=α + β*L[*xunits*] or

  lp_max[*yunits*]=α + β*exp(γ*L[*xunits*])

  where **α**, **β**, and **γ** are real or integer empirical constants. If a fish's maximum prey size is independent of its body length (i.e., **β** equals zero), this parameter can be specified simply as **lp_max[*yunits*]=α**. If not specified, BASS assigns the default value **lp_max[cm]=0.5*L[cm]**.

- **lp_min[*yunits*]=*fnc*** specifies the minimum length of prey consumed by a fish whose body length is L[***xunits***]. Like the option for a fish's average prey length, two valid function strings are recognized, i.e.,

  lp_min[*yunits*]=α + β*L[*xunits*] or

  lp_min[*yunits*]=α + β*exp(γ*L[*xunits*])

  where **α**, **β**, and **γ** are real or integer empirical constants. If a fish's minimum prey size is independent of its body length (i.e., **β** equals zero), this parameter can be specified simply as **lp_min[*yunits*]=α**. If not specified, BASS assigns the default value **lp_min[cm]=0.1*L[cm]**.

- **mls[*yunits*]=α** specifies the species' maximum longevity or life span.

- **nm[-]=α*b(β:γ)*sg_mu[-]** specifies a cohort's rate of dispersal and non-predatory mortality as a function of its habitat suitability and long-term weight-specific growth rate **sg_mu[-]**. Whereas **α** specifies the fraction of the species' total "mortality" that is attributable to dispersal and non-predatory mortality, **β** and **γ** specify the species' minimum and maximum self-thinning exponents, respectively. See Equations (2.95) and (2.102). If the user elects not to simulate habitat effects on dispersal and non-predatory mortality, this parameter can be specified simply as

  nm[-] = α*b(β)*sg_mu[-]

  where **β** is the species' average self-thinning exponent. Also see the /ECOLOGICAL_PARAMETERS option **sg_mu[]**.

- **rbi[-]=α** specifies the species' reproductive biomass investment (i.e., grams gametes per gram spawning fish) where **α** is real empirical constant. If not specified, BASS assigns the default value **rbi[-]=0.2**.

- **refugia[*yunits*]=α** specifies a refuge population size for each cohort that can be prey for community piscivores where **α** is real or integer constant. ***Yunits*** must be dimensionally equivalent to fish/ha. If not specified, BASS assumes no refuge level (i.e., **refugia[*yunits*]=0**)

- **sg_mu[*yunits*]=α*W[*xunits*]^β** specifies the species' mean long-term weight-specific growth rate where **α** and β are real or integer empirical constants. ***yunits*** must be dimensionally equivalent to day^{-1}, and ***xunits*** must be dimensionally equivalent to g wet wt/fish. If not specified, BASS can estimate this parameter provided that the user specifies the species' expected body weight at its maximum age. See /ECOLOGICAL_PARAMETERS option **wt_max[]** for details.

- **tl_r0[*yunits*]=α** specifies the species' minimum total length when sexual maturity is reached where **α** is a real or integer empirical constant.

- **wl[*yunits*]=α*L[*xunits*]^β** specifies the species' wet weight as an allometric function of its total length where **α** and **β** are real or integer empirical constants.

- **wt_max[*yunits*]=α** specifies the species' expected wet body weight at its maximum age where **α** is a real or integer empirical constant. This parameter is required only when the user has not specified the species' mean long-term weight-specific growth rate using the /ECOLOGICAL_PARAMETERS option **sg_mu[]**. When **sg_mu[]** is not specified, BASS will estimate the species' long-term weight-specific growth rate based on its maximum life span **mls[]**, young-of-year body weight **yoy[]**, and **wt_max[]**. If the user has specified the species' temperature-dependent weight-specific growth rate

  sg[*yunits*]=α*W[*xunits*]^β*H(γ,T_1,T_2)

  (see /PHYSIOLOGICAL_ PARAMETERS option **sg[]**), BASS estimates the species' long-term weight-specific growth rate by

  sg_mu[1/d] = $\bar{\alpha}$*W[g]^β

  where $\bar{\alpha}$ is back-calculated as outlined by Equation (3.43). If **sg[]** has not been specified, BASS estimates the species' long-term weight-specific growth rate by

  sg_mu[1/d] = $\bar{\alpha}$*W[g]^(-0.584)

  where $\bar{\alpha}$ is back-calculated as outlined by Equation (3.43) using the mean interspecies weight-specific growth exponent (i.e., -0.584) estimated from the BASS model database. Also see Barber (2003).

- **yoy[*yunits*]=α** specifies the wet weight of fish recruited into the population as age class 1 where **α** is a real or integer empirical constant.

■ **/FEEDING_OPTIONS *string*$_1$; ...; *string*$_n$**

This command instructs BASS how to calculate ingestion for a particular age or size range of fish. Valid options for this command are :

- **allometric(*class*)** to model expected feeding using Equation (2.58).

- **clearance(*class*)** to model expected feeding using Equation (2.64).

- **holling(*class*)** to model expected feeding using Equation (2.59).

- **linear(*class*)** to model expected feeding using Equation (2.66).

Valid expressions for ***class*** are:

α < a[*xunits*] < β if the fish's age determines its feeding algorithm;

α< l[*xunits*] < β if the fish's length determines its feeding algorithm;

α < w[*xunits*] < β if the fish's weight determines its feeding algorithm.

where **α** and **β** are real or integer empirical constants. Although for a given species all class types must be the same type (i.e., age, length, or weight), class types between species can be different. The parameters for these models are specified using the /PHYSIOLOGICAL_PARAMETERS command.

■ **/FISHERY_PARAMETERS *string*$_1$; ...; *string*$_n$**

This command specifies stocking and harvest rates for sport fishes. Valid options for this command are:

- **stocking[*sunits*](age[*aunits*]=α, size[*bunits*]=β, season=*time*, frequency = *schedule*) = γ** specifies the stocking rate of fish of age **α** and body size **β** (i.e., total length or wet weight) during the time interval specified by ***time*** and the stocking frequency specified by ***schedule***.

The units of the specified stocking rate ***sunits*** must be dimensionally equivalent to fish/ha. Valid expressions for ***time*** are given below. Valid options for ***schedule*** are: "weekly", biweekly", "monthly", or "one_time". If ***schedule = weekly***, then a new cohort of **γ** individuals is added to the species' population once a week throughout the specified period. If ***schedule = monthly***, then a new cohort of **γ** individuals is added to the species' population once a month throughout the specified period.

- **harvest[*hunits*](α<L[units]<β, *time*) = γ** specifies the fractional harvest rate of fish of the specified length class during the indicated time period. The units of the specified harvest rate ***hunits*** must be dimensionally equivalent to 1/d.

Valid expressions for ***time*** are two month-day combinations separated by a hyphen. For example,

March 15 - September 1.

Both of these fishery options can be repeated as many times as needed to define the species stocking and harvest. Additionally, only nonzero stocking and harvesting rates need to be specified.

Fishing mortality and harvest can be turned off without deleting the user's harvest parameters using the command line option "-f". Similarly, stocking can be turned off without deleting the user's stocking parameters using the command line option "-s". See Section 4.5 for details.

■ **/HABITAT_PARAMETERS *string*$_1$; ...; *string*$_n$**

This command specifies habitat preferences, tolerances, and suitability indices for the species.

Valid options for habitat preferences are:

- **tpref[celsius](*class*) = γ** specifies the preferred or optimum temperature of the age or size class specified within the parentheses.

Valid expressions for ***class*** are:

α < a[*xunits*] < β
α< l[*xunits*] < β
α < w[*xunits*] < β

where **α** and **β** are real or integer empirical constants. This option can be specified repeatedly as needed. Although for a given species all class types must be the same type (i.e., age, length, or weight), class types between species can be different.

Valid options for habitat suitability multipliers are:

- **hsi_feeding[-] = *fnc*** specifies the species' HSI for feeding by the time function ***fnc***. This HSI is used as a simple linear multiplier on a cohort's maximum ingestion rate when feeding is modeled with either an allometric, Holling, or clearance volume formulation. When a cohort's ingestion is back-calculated from its expected growth rate, the specified HSI is used as a simple linear multiplier on the cohort's weight-specific growth rate. See Section 2.9.

- **hsi_recruitment[-] = *fnc*** specifies the species's HSI for recruitment by the time function ***fnc***. This HSI is used as a simple linear multiplier on the species' YOY recruitment. See Section 2.9.

- **hsi_survival[-] = *fnc*** specifies the species' HSI for dispersal and non-predatory mortality by the time function ***fnc***. This HSI is used to control the species' self-thinning exponent that determines, in combination with the fish's growth rate, a cohort's estimated dispersal and non-predatory mortality rate. See Section 2.9.

Valid expressions for these HSI functions are:

- ***hsi_name*[-]= α** generates a constant HSI for the entire simulation.

- ***hsi_name*[-]=file(*filename*)** generates time-varying HSIs either by reading and interpolating HSIs specified by the file ***filename*** or by reading and interpolating habitat variables and then calculating HSIs using user-specified logistic regressions. See Sections 4.4.3.

When HSI multipliers are calculated using user-specified logistic regressions, the desired regressions are specified using the following options:

- **hsi_feeding_equation[-] = *regression***

- **hsi_recruitment_equation[-] = *regression***

- **hsi_survival_equation[-] = *regression***

where ***regression*** specifies a linear combination of habitat variables X_i that are transformed or raised to an integer or real power. Transformations recognized by BASS include:

LN(X_i**)** => $\ln X_i = \log_e X_i$
LN_1(X_i**)** => $\ln (X_i + 1) = \log_e (X_i + 1)$
LOG(X_i**)** => $\log (X_i) = \log_{10} (X_i)$

LOG_1(X_i) => $\log\ (X_i + 1) = \log_{10}\ (X_i + 1)$

SQRT(X_i) => $\sqrt{X_i}$

ASIN_SQRT(X_i) => $\arcsin\left(\sqrt{X_i}\right)$

ASIN_SQRT_PCT(X_i) => $\arcsin\left(\sqrt{0.01\ X_i}\right)$

Habitat variables must be specified with units enclosed by brackets, and must match in name and units to column variables specified by the data file ***filename***. After evaluating the specified logistic regression, BASS calculates the fish's HSI multiplier using the standard equation

hsi_name **= 1 / (1 + EXP (- *hsi_name*_equation))**

If HSI functions are not specified, BASS assigns the default value of 1 to each unspecified HSI function.

■ **/INITIAL_CONDITIONS** ***string*$_1$; ...; *string*$_n$**

This command specifies the species' initial ages, whole-body chemical concentrations, wet body weights, and population sizes. Valid options for this command are:

- **age[*units*]={x_1, ..., x_n}** to initialize the age of each cohort with the specified vector. The units enclosed by brackets must be dimensionally equivalent to days.

- ***chemical_name*[*units*]={x_1, ..., x_n}** to initialize the whole-body concentration of each cohort for the named chemical by the specified vector. Each name must correspond exactly to a name specified by one of the /CHEMICAL commands. The units enclosed by brackets must be dimensionally equivalent to µg/g wet wt.

- **wt[*units*]={x_1, ..., x_n}** to initialize the body size of each age class with the specified vector. The units enclosed by brackets must be dimensionally equivalent to g wet wt/fish.

- **pop[*units*]={x_1, ..., x_n}** to initialize the population density of each age class with the specified vector. The units enclosed by brackets must be dimensionally equivalent to fish/ha.

■ **/MORPHOMETRIC_PARAMETERS** ***string*$_1$; ...; *string*$_n$**

This command specifies the species' morphometric parameters that are needed to describe the exchange of chemicals across its gills. Each ***string*** specifies a required morphometric parameter as a simple allometric power function of the fish's body weight. Valid options, which must be separated by semicolons, are:

- **ga[*yunits*]=α*W[*xunits*]^β** specifies the fish's total gill surface area where **α** and **β** are real or integer empirical constants. ***yunits*** must be dimensionally equivalent to cm^2 or cm^2/g wet wt.

- **id[*yunits*]=α*W[*xunits*]^β** specifies the interlamellar distance between adjacent lamellae where **α** and **β** are real or integer empirical constants. ***yunits*** must be dimensionally equivalent to cm or cm/g wet wt.

- **ld[*yunits*]=α*W[*xunits*]^β** specifies the density of secondary lamellae on the primary gill filaments (i.e., number of lamellae per mm gill filament) where **α** and **β** are real or integer empirical constants.

- **ll[*yunits*]=α*W[*xunits*]^β** specifies the fish's lamellar length where **α** and **β** are real or integer empirical constants. ***yunits*** must be dimensionally equivalent to cm or cm/g wet wt.

Note that if the exponent **β** equals zero for any of these parameters, the resulting term **W[*xunits*]^0** does not have to be specified.

■ **/PHYSIOLOGICAL_PARAMETERS** ***string*$_1$; ...; *string*$_n$**

This command specifies the species' physiological parameters for simulating growth. Each ***string*** specifies a physiological parameter of the fish as a constant or temperature-dependent power function of its body weight. In particular,

- **ae_plant[-]=α** specifies the fish's assimilation efficiency for periphyton and phytoplankton where **α** is a real empirical constant less than or equal to one.

- **ae_invert[-]=α** specifies the fish's assimilation efficiency for benthos, insects, and zooplankton where **α** is a real empirical constant less than or equal to one.

- **ae_fish[-]=α** specifies the fish's assimilation efficiency for fish where **α** is real a empirical constant less than or equal to one.

- **ge[*yunits*]=α*G[*xunits*]^β*H(γ,T_1,T_2)** specifies the fish's gastric evacuation where **G** is the mass of food resident in the intestine, and where **α**, **β**, **γ**, $\mathbf{T_1}$, and $\mathbf{T_2}$ are real or integer empirical constants. ***yunits*** must be dimensionally equivalent to g dry wt/d. In general, γ=½, ⅔, or 1 (Jobling 1981). This parameter is required only if the feeding option **holling(·)** is used.

- **kf_min[-]=α** specifies the minimum condition factor for

a fish's continuing existence. In BASS, a fish's condition factor is defined by the ratio

$$kf = \frac{W_w}{\alpha L^{\beta}} \qquad (4.5)$$

where W and L are the fish's current wet body weight and total length, respectively; and **α** and **β** are the coefficient and exponent for the fish's weight-length relationship (see **/PHYSIOLOGICAL_PARAMETERS** option **wl[·]**).

- **mf[*yunits*]=α*W[*xunits*]^β*H(γ,T$_1$,T$_2$)** specifies the fish's maximum filtering rate where **α**, **β**, **γ**, **T$_1$**, and **T$_2$** are real or integer empirical constants. ***yunits*** must be dimensionally equivalent to L/d. This parameter is required only if the feeding option **clearance(·)** is used.

- **mi[*yunits*]=α*W[*xunits*]^β*H(γ,T$_1$,T$_2$)** specifies the fish's mean ingestion rate where **α**, **β**, **γ**, **T$_1$**, and **T$_2$** are real or integer empirical constants. ***yunits*** must be dimensionally equivalent to g dry wt/d. This parameter is required only if the feeding option **allometric(·)** is used.

- **rq[-]=α** specifies the fish's respiratory quotient; (i.e., $L(CO_2)$ respired/$L(O_2)$ consumed) where **α** is a real empirical constant.

- **rt:std[-]=α** specifies the ratio of a fish's routine respiration to its standard respiration where **α** is a real empirical constant.

- **sda:in[-]=α** specifies the ratio of a fish's SDA to its ingestion where **α** is a real empirical constant.

- **sg[*yunits*]=α*W[*xunits*]^β*H(γ,T$_1$,T$_2$)** specifies the fish's weight-specific growth rate where **α**, **β**, **γ**, **T$_1$**, and **T$_2$** are real or integer empirical constants. ***yunits*** must be dimensionally equivalent to day^{-1}. This parameter is required only if the feeding option **linear(·)** is used.

- **sm[*yunits*]=α*W[*xunits*]^β*H(γ,T$_1$,T$_2$)** specifies the size of the satiation meal consumed during the interval (0, st) where **α**, **β**, **γ**, **T$_1$**, and **T$_2$** are real or integer empirical constants. ***yunits*** must be dimensionally equivalent to g dry wt/d. See option **st[*yunits*]** below. This parameter is required only if the feeding option **holling(·)** is used.

- **so[*yunits*]=α*W[*xunits*]^β*H(γ,T$_1$,T$_2$)** specifies the fish's standard oxygen consumption where **α**, **β**, **γ**, **T$_1$**, and **T$_2$** are real or integer empirical constants. ***yunits*** must be dimensionally equivalent to mg O_2/hr or mg O_2/g wet wt/hr.

- **st[*yunits*]=α*W[*xunits*]^β*H(γ,T$_1$,T$_2$)** specifies the time to satiation when feeding with an initially empty stomach where **α**, **β**, **γ**, **T$_1$**, and **T$_2$** are real or integer empirical constants. See option **sm[*yunits*]** above. This parameter is required only if the feeding option **holling(·)** is used.

For the options **ge[*yunits*]**, **mf[*yunits*]**, **mi[*yunits*]**, **sg[*yunits*]**, **sm[*yunits*]**, **so[*yunits*]**, and **st[*yunits*],**

$$H(\gamma, T_1, T_2) = \exp(\gamma T)\left(1 - \frac{T}{T_2}\right)^{\gamma(T_2 - T_1)} \qquad (4.6)$$

where T_1 is the temperature at which each particular process's rate is maximum and T_2 is the upper temperature at which the process is no longer operative. If the process does not exhibit a temperature optimum, then the hyperbolic function **H(γ,T$_1$,T$_2$)** should be substituted with the exponential function **exp(γ*T[celsius])**. Consequently, each of these temperature-dependent power functions can also be specified as

α*W[*xunits*]^β*exp(γ*T[celsius])

As noted for the fish's morphometric parameters, if the exponent **β** equals zero for any of these temperature-dependent power functions, the term **W[*xunits*]^0** does not have to be specified.

If a required parameter is not specified, the program will terminate with an appropriate error message.

■ **/PREY_SWITCHING_OFF**

This command disables BASS's prey-switching algorithms when a cohort's expected feeding level cannot be satisfied using the dietary compositions specified by the user. By default, BASS's prey-switching algorithms are enabled.

■ **/SPAWNING_PERIOD *string***

This command specifies the months during which spawning occurs. Valid character strings for this command are either the name of a month or the names of two months separated by a hyphen. For example,

/SPAWNING_PERIOD may

OR

/SPAWNING_PERIOD April-June

The names of the months must be spelled-out in full.

■ **/SPECIES *string***

This optional command specifies the scientific name (genus and species) of the fish to be simulated. Users should note, however, that the BASS parameterization software (BASS_FILES.EXE) inserts this command into all of its generated FSH files to inform users what species data have been used to create the files of interest.

4.3.4. Non-fish Input Commands

These commands specify simulation parameters for benthos, periphyton, incidental terrestrial insects, phytoplankton and zooplankton. The syntax for these commands is as follows

/BENTHOS	$string_1$; ...; $string_n$
/TERRESTRIAL_INSECTS	$string_1$; ...; $string_n$
/PERIPHYTON	$string_1$; ...; $string_n$
/PHYTOPLANKTON	$string_1$; ...; $string_n$
/ZOOPLANKTON	$string_1$; ...; $string_n$

Depending on the options selected, BASS generates the standing stocks of these non-fish compartments either as community forcing functions or as community state variables. Although these compartments can be simulated for any desired community, only those identified as fish prey must be specified (see the **diet(.,.)={...}** option for /ECOLOGICAL_PARAMETERS). Note, however, that because piscivorous fish are assumed to switch to benthic invertebrates and incidental terrestrial insects when appropriate forage fish are unavailable, the benthos and insect options should be specified even when simulating only piscivorous fish.

When benthos, periphyton, incidental terrestrial insects, phytoplankton or zooplankton are treated as community forcing functions, a single option of the form

- **biomass[*yunits*]=*string***

is specified. Valid expressions for this option are:

biomass[*yunits*]=α for a constant non-fish standing stock

biomass[*yunits*]=α + β*sin(ω + φ*t[*xunits*]) for a sinusoidal non-fish standing stock where **α** is the mean standing stock for the chosen time period, **β** is its amplitude (*yunits*), **ω** is its phase angle (radians), and **φ**=2π / period is its frequency (1/*xunits*).

biomass[*yunits*]=file(*filename*) to read and interpolate a non-fish standing stock from the file ***filename***. See Section 4.4.3.

Whereas ***yunits*** must be dimensionally equivalent to g dry wt/m^2 for benthos, incidental terrestrial insects, and periphyton, ***yunits*** must be dimensionally equivalent to g dry wt/L for phytoplankton and zooplankton. As previously noted, BASS assumes that the first day of simulation is April 1 and that the 365-th simulation day is March 31. This assignment can be changed using the command /MONTH_T0. This command-option combination is equivalent to the BASS v2.1 simulation control command /BIOTA

When benthos, periphyton, phytoplankton or zooplankton are treated as community state variables, the following five options must be specified:

- **initial_biomass[*yunits*]=*number***. This option specifies the initial compartmental standing stock of the designated component and is required to simulate the designated non-fish compartment as a BASS state variable. ***yunits*** must be dimensionally equivalent to g dry wt/m^2.

- **mean_weight[*yunits*]=*fnc***. This option specifies the average body weight of individuals within the designated non-fish compartment. This parameter is required to simulate the designated non-fish compartment as a BASS state variable. ***yunits*** must be dimensionally equivalent to g dry wt/ind. Valid expressions for ***fnc*** are:

  mean_weight[*yunits*]=α generates a constant average individual body weight for the designated prey.

  mean_weight[*yunits*]=α + β*sin(ω + φ*t[*xunits*]) generates the average individual body weight of the designated prey as a sinusoidal function of time where **α** is the mean body weight for the chosen time period, **β** is its amplitude (*yunits*), **ω** is its phase angle (radians), and **φ**=2π / period is its frequency (1/*xunits*).

  mean_weight[*yunits*]=file(*filename*) reads and interpolates the average individual body weight of the designated prey from the file ***filename***. See Section 4.4.3.

  Unless specified otherwise, BASS assumes that the first day of simulation is April 1 and that the 365-th simulation day is March 31. This assignment can be changed using the command /MONTH_T0.

- **ingestion[*yunits*]=α*W[*xunits*]^β*H(γ,T_1,T_2)** specifies the ingestion rate of individuals within the designated compartment as a function of their average body weight and temperature where **α**, **β**, **γ**, $\mathbf{T_1}$, and $\mathbf{T_2}$ are real or integer empirical constants. This parameter is required to

simulate either benthos or zooplankton as a BASS state variable. ***yunits*** must be dimensionally equivalent to g dry wt/d, and ***xunits*** must be dimensionally equivalent to g dry wt/ind.

- **photosynthesis[*yunits*]=α*W[*xunits*]^β*H(γ,T_1,T_2)** specifies the photosynthetic rate of individuals within the designated compartment as a function of their average body weight and temperature where **α**, **β**, **γ**, $\mathbf{T_1}$, and $\mathbf{T_2}$ are real or integer empirical constants. This parameter is required to simulate either periphyton or phytoplankton as a BASS state variable. ***yunits*** must be dimensionally equivalent to g dry wt/d, and ***xunits*** must be dimensionally equivalent to g dry wt/ind. Currently, photosynthesis is not treated as a function of nutrients and light availability.

- **respiration[*yunits*]=α*W[*xunits*]^β*H(γ,T_1,T_2)** specifies the rate of dry organic mater respiration for the designated compartment as a function of average individual body weight and temperature where **α**, **β**, **γ**, $\mathbf{T_1}$, and $\mathbf{T_2}$ are real or integer empirical constants. This parameter is required to simulate the designated non-fish compartment as a BASS state variable. ***yunits*** must be dimensionally equivalent to g dry wt/d, and ***xunits*** must be dimensionally equivalent to g dry wt/ind.

Although BASS enables users to simulate benthos, periphyton, phytoplankton or zooplankton as community state variables, incidental terrestrial insects are always treated as a community forcing function.

Regardless of how the biomass of benthos, incidental terrestrial insects, periphyton, phytoplankton, or zooplankton is specified as BASS inputs, or not as in the case of the FGETS simulation mode, users can specify the stable isotope fractions $\delta^{13}C$ and $\delta^{15}N$ of these compartments using the optional arguments

- **del_c13[-]=α**
- **del_n15[-]=β**

If not specified, BASS will assign default values to these parameters and output those values in the project's message file.

4.4. Input Data Syntax

4.4.1. Units Recognized by BASS

Most BASS commands require the specification of units (or combination of units) as part of an option. This section describes the syntax for units that are recognized by BASS's input algorithms. The conversion of user-specified units to those actually used by BASS is accomplished by referencing all units to the MKS system (i.e., meter, kilogram, second). **Table 4.1** and **Table 4.2** summarize prefixes and fundamental units, respectively, that are recognized by BASS's unit conversion subroutines. **Table 4.2** also summarizes the dimensionality and the conversion factor to the MKS system standard unit. **Table 4.3** summarizes units that are recognized by BASS's unit conversion subroutines for specifying ecological, morphometric, and physiological units.

Units and their prefixes can be specified in either upper or lower case. When prefixes are used, there must be no embedded blanks between the prefix and the unit name, e.g., "milligram" is correct, "milli gram" is incorrect. Unit names for wet and dry masses are appended, without blanks, with the parenthetic identifiers "(ww)" and "(dw)", respectively. Similarly, an analogous convention is used to specify mass units of specific chemical compounds. For example, "grams oxygen" is specified as "g(o2)". The circumflex (^) denotes exponentiation (e.g., cm^{-2} is presented as cm^-2). The slash (/) denotes division. If multiple slashes are used to specify a unit, they are interpreted according to strict algebraic logic. For example, both "mg/liter", and "mg liter^-1" are equivalent specifications. Similarly, the weight specific units "mg/g/day" and "mg g^-1 day^-1" are equivalent.

4.4.2. User-specified Functions

The following syntax rules apply to specifying these options

- Brackets are used only to delineate units. Dimensionless parameters like assimilation efficiency, lipid fraction, and K_{ow} must be specified with null units "[-]".

- The order of addition and multiplication is not significant. Thus, the following specifications are valid and equivalent.

  temp[celsius]=α+β*sin(ω + φ*t[*xunits*]) <=>
  temp[celsius]=β sin(φ*t[*xunits*]+ω) + α

  czplnk[*yunits*]=α*cwater[*xunits*] <=>
  czplnk[*yunits*]=cwater[*xunits*]*α

- Options that are temperature-dependent or temperature-independent power functions can be specified by $\log_{10}$ or ln transforms. For example, the following options are valid

  ln(so[*yunits*])=α + β*ln(W[*xunits*]) + γ*T[celsius]

  log(so[*yunits*])=α + β*log(W[*xunits*]) + γ*T[celsius]

- User-specified functions do not have to be in reduced form. For example, temperature-dependent power functions can be specified with a reference temperature other than 0°Celsius. Thus, BASS will correctly decode the following functions

  so[*yunits*]=α*W[*xunits*]^β*exp(γ*(T[celsius]-20))

  ln(so[*yunits*])=α+ β*ln(W[*xunits*]) + γ*(T[celsius]-20)

  log(so[*yunits*])= α+ β*log(W[*xunits*]) + γ*(T[celsius]-20)

- If the temperature dependency is unknown, temperature-dependent power functions can be input for a specific temperature, γ Celsius, in which case BASS assumes a default Q_{10}=2. If this feature is used, the reference temperature must be enclosed by parentheses and follow the units specification of the independent variable. For example, the following specifications are valid

  so[*yunits*](γ)=α*W[*xunits*]^β

  ln(so[*yunits*](γ))=α + β*ln(W[*xunits*])

  log(so[*yunits*](γ))=α + β*log(W[*xunits*])

- If either the slope of a linear function or the exponent of a power function is zero, the function can be input as a constant without specifying the expected independent variable. For example, the following specifications are equivalent

  lp[cm]=4.5 <=> lp[cm]=4.5 + 0.0*L[cm]

  pl[-]=0.05 <=> pl[-]=0.05*W[g(ww)]^0.0

- Operators (^* / +-) may not be concatenated. For example, the following options have invalid syntax

  so[mg(o2)/g/hr]=
  0.1*exp(0.0693*T[celsius])*W[g(ww)]**^-**0.2

  ln(so[mg(o2)/g/hr])=
  - 2.30+0.0693*T[celsius]+-0.2*ln(W[g(ww)])

  The correct syntax for these options would be

  so[mg(o2)/g/hr]=
  0.1*exp(0.0693*T[celsius])*W[g(ww)]^(-0.2)

  ln(so[mg(o2)/g/hr])=
  -2.30+0.0693*T[celsius]- 0.2*ln(W[g(ww)])

4.4.3. User-specified Parameter Files

If the user specifies a file option for the /EXPOSURE, /TEMPERATURE, /WATER_LEVEL, /BIOTA, /BENTHOS, /TERRESTRIAL_INSECTS, /PERIPHYTON, /PHYTOPLANKTON, /ZOOPLANKTON, or /HABITAT_PARAMETERS commands, the designated files must exist and be supplied by the user. The general format of a BASS exposure file allows a user to specify multiple exposure conditions within a single file. Each file record specifies exposure conditions for a specific time. The general format of a BASS exposure file is as follows

```
!
! file: exposure.dat
!
/001   time[units]    ! see ensuing discussion
/C1  string
⋮    ⋮
/CM   string
/START_DATA
v1,1    v1,2    ...   v1,MV   ! comment
v2,1    v2,2    ...   v2,MV   ! comment
⋮       ⋮       ...   ⋮
vNR,1   vNR,2   ...   vNR,MV  ! comment
```

Records beginning with a slash (/) followed by an integer CJ identify the type of data (time, exposure concentration, temperature, etc.) contained in CJ-th column of each data record. In this example, NR is the total number of data records in the file, MV is the number of variables per record, and C1...CM are the column positions of M exposure variables that are to be read. Note, however, that MV can be greater than CM and that C1...CM need not be consecutively numbered. To simplify the reading of multiple exposure files, BASS requires that "time" be the first column of any user-specified exposure file. Valid character strings for specifying the remaining data columns include:

- **bbenthos[*units*]** to read the standing stock of benthic invertebrates;
- **binsects[*units*]** to read the standing stock of incidental terrestrial insects;
- **bperiphyton[*units*]** to read the standing stock of periphyton or benthic algae;
- **bphytoplankton[*units*]** to read the standing stock of phytoplankton;
- **bzooplankton[*units*]** to read the standing stock of zooplankton;

- **cbenthos[*units*](*ChemicalName*)** to read the concentration of ***ChemicalName*** in benthic invertebrates;
- **cinsects[*units*](*ChemicalName*)** to read the concentration of ***ChemicalName*** in incidental terrestrial insects;
- **cperiphyton[*units*](*ChemicalName*)** to read the concentration of ***ChemicalName*** in periphyton;
- **cphytoplankton[*units*](*ChemicalName*)** to read the concentration of ***ChemicalName*** in phytoplankton;
- **csediment[*units*](*ChemicalName*)** to read the sediment concentration of ***ChemicalName***;
- **cwater[*units*](*ChemicalName*)** to read the unbound, aqueous concentration of ***ChemicalName***;
- **czooplankton[*units*](*ChemicalName*)** to read the whole-body concentration of ***ChemicalName*** in zooplankton;
- **depth[*units*]** to read water depth;
- **hsi_feeding[-](*FishName*)** to read the feeding/growth HSI for the fish species ***FishName***;
- **hsi_recruitment[-](*FishName*)** to read the recruitment/ spawning HSI for the fish species ***FishName***;
- **hsi_survival[-](*FishName*)** to read the dispersal/non-predatory mortality HSI for the fish species ***FishName***;
- **temperature[*units*]** to read ambient water temperature;
- **wbenthos[*units*]** to read the mean body weight of benthic invertebrates;
- **winsects[*units*]** to read the mean body weight of incidental terrestrial insects;
- **wperiphyton[*units*]** to read the mean body weight of periphyton or benthic algae;
- **wphytoplankton[*units*]** to read the mean body weight of phytoplankton;
- **wzooplankton[*units*]** to read the mean body weight of zooplankton.

If column names other than those listed above are specified, BASS simply ignores them. Data records can be continued by appending an ampersand (&) to the end of the record; for example, the following data records are equivalent.

$$v_{i,1}\ v_{i,2}\ \ldots\ v_{i,j}\ v_{i,j+1}\ \ldots\ v_{i,MV}$$

$$v_{i,1}\ v_{i,2}\ \ldots\ v_{i,j}\ \&$$
$$v_{i,j+1}\ v_{i,j+2}\ \ldots\ v_{i,MV}$$

File records must be sequenced so that time is non-decreasing (i.e., $t_i \le t_{i+1}$, i =1, 2, ..., N-1). The time increment between consecutive records can be constant or variable. BASS calculates the exposure conditions between specified time points by simple linear interpolation.

4.5. BASS Include File Structure

As mentioned in Section 4.1, BASS's input processing routines allow a BASS project file to be specified using include files of related parameters. This capability is the cornerstone upon which the BASS GUI has been developed.

To select an appropriate project / include file hierarchy for implementation in the BASS GUI, careful consideration was given to the perceived needs of researchers and environmental regulators who would routinely analyze and evaluate similar scenarios that might differ either in the chemical exposures of interest or in the communities of concern. For example, the USEPA Office of Chemical Safety and Pollution Prevention (OCSPP) evaluates different pesticides for registration based on their expected fate and effects in series of canonical aquatic habitats / ecosystems. Similarly, OCSPP evaluates the pre-manufacturing registration of industrial chemicals in much the same way. Such examples suggested that a practical working BASS project / include file hierarchy should be structured as follows:

- All data specifying the bioenergetic, compositional, and morphological parameters for a specific fish species that can be considered to be independent of the particular community in which the fish resides, should be contained within a single include file that is assigned the reserved extension FSH.
- All data specifying the structure and function of a particular fish community should be contained within a single include file that is assigned the reserved extension CMM. These files should use FSH files (as include files) interleaved with the necessary fish commands to define each species' (1) dietary composition, (2) initial ages, body weights, population densities, and chemical residues, (3) habitat multipliers, (4) fishery parameters, and (5) any fish commands contained within a FSH file that the user wants to have superceded.

- All data specifying the physico-chemical properties for a specific chemical of concern should be contained within a single include file that is assigned the reserved extension PRP.

- All data specifying a chemical exposure scenario should be contained within a single include file that is assigned the reserved extension CHM. These files should use PRP files (as include files) interleaved with the necessary chemical commands needed to specify each chemical's (1) aqueous concentration, (2) dietary exposures via benthos, insects, periphyton, phytoplankton, and zooplankton, (3) effects concentrations for specific fish, and (4) relevant rates of biotransformation by specific fish.

- Lastly, all BASS project files should use CMM and CHM files (as include files) to specify the fish community and the chemical exposures of concern, respectively. All such project files will be assigned the reserved extension PRJ.

Based on these considerations, the general structure of a BASS project file is as follows:

```
! file: name.prj
! notes: general structure of a BASS project file
!
/ SIMULATION_CONTROL
/ HEADER <string>
/ MONTH_T0 <string>
/ LENGTH_OF_SIMULATION  α[year]
/ TEMPERATURE temp[celsius] = fnc
/ WATER_LEVEL depth[meter] = fnc
! specify chemical exposures (if any)
#include 'exposures.chm'
! specify fish community
#include 'community.cmm'
/ END
```

The chemical exposure scenario file EXPOSURES.CHM specified in this project file has the following general form

```
! file: exposures.chm
! notes: general structure of a chemical
!        exposure scenario file
!
! specify physico-chemical parameters
#include 'chemical_1.prp'
/ EXPOSURE cwater[ppm] = fnc; &
    cbenthos[ppm] = fnc; &
    cinsects[ppm] = fnc; &
    cperiphyton[ppm] = fnc; &
    cphytoplankton[ppm] = fnc; &
    czooplankton[ppm] = fnc
/ NONFISH_BCF &
    bcf[-](benthos) = fnc; &
    bcf[-](periphyton) = fnc; &
    bcf[-](phytoplankton) = fnc; &
    bcf[-](zooplankton) = fnc
/ LETHALITY &
    lc50[units](fish_1) = fnc; &
    lc50[units](fish_2) = fnc
/ METABOLISM &
    bt[units](fish_1,chem_n) = fnc; &
    bt[units](fish_2,chem_n) = fnc
! repeat above chemical data block as needed
⋮
! end exposures.chm
```

The general structure of the chemical property file CHEMICAL_1.PRP specified in the above exposure scenario file is

```
! file: chemical_1.prp
! notes: general structure of a chemical
!        property file
!
/ CHEMICAL <string>
/ LOG_AC   <real number>
/ LOG_P    <real number>
/ LOG_KB1  <real number>
/ LOG_KB2  <real number>
/ MOLAR_WEIGHT   <real number>
/ MOLAR_VOLUME   <real number>
/ MELTING_POINT  <real number>
! end chemical_1.prp
```

The community file COMMUNITY.CMM specified for the above project file has the following general form

```
! file: community.cmm
! notes: general structure of a community file
!
#include 'fish_1.fsh'
/ ECOLOGICAL_PARAMETERS &
  diet(α<x[units]<β)={benthos=α,…,fish_n=β,…}; &
  diet(α<x[units]<β)={benthos=α,…,fish_n=β,…}; &
  diet(α<x[units]<β)={benthos=α,…,fish_n=β,…}; &
  diet(α<x[units]<β)={benthos=α,…,fish_n=β,…}; &
  nm[-]=α*b(β:γ)*sg_mu[-]; &
  ast_yoy[-]=f(bb[-]=α, size=β, pop=γ)
/ INITIAL_CONDITIONS &
  age[yr]={α,…,β}; &
  wt[g(ww)]={α,…,β}; &
  pop[fish/ha]={α,…,β}
/ FISHERY_PARAMETERS &
  stocking[fish/ha](age[yr]=α,size[g(ww)]=β,&
    season=s1,frequency=s2)=γ; &
  harvest[1/yr](α<l[cm]<β,season_string)=γ
/ HABITAT_PARAMETERS &
  hsi_feeding[-]=fnc; &
  hsi_recruitment[-]=fnc; &
  hsi_survival[-]=fnc
! repeat above fish data block as needed
⋮
! specify non-fish compartments/forcing functions
/ BENTHOS  &
  initial_biomass[units]=α; &
  mean_weight[g(dw)]=fnc; &
  ingestion[g(dw)/day]= α*w[g(dw)]^β*h(γ,t1,t2); &
  respiration[g(dw)/day]=α*w[g(dw)]^β*h(γ,t1,t2)
/ TERRESTRIAL_INSECTS biomass[units]=fnc
⋮
! end community.cmm
```

The general structure of the fish parameter file FISH_1.FSH specified in the above community file is

```
! file: fish_1.fsh
! notes: general structure of a fish file
```

```
!
/ COMMON_NAME <string>
/ SPECIES <string>
/ AGE_CLASS_DURATION <string>
/ SPAWNING_PERIOD <string>
/ FEEDING_OPTIONS &
  allometric(α<x[units]<β); &
  clearance(α<x[units]<β); &
  holling(α<x[units]<β); &
  linear(α<x[units]<β)
/ COMPOSITIONAL_PARAMETERS &
  pa[-]=α*pl[-]+β; &
  pl[-]=α*w[g(ww)]^β
/ ECOLOGICAL_PARAMETERS &
  yoy[g(ww)]=α; wt_max[g(ww)]=α; mls[yr]=α; &
  tl_r0[cm]=α; rbi[-]=α; &
  lp[cm]=α*l[cm]+β; &
  lp_max[cm]=α*l[cm]+β; &
  lp_min[cm]=α*l[cm]+β; &
  sg_mu[1/d]=α*w[g(ww)]^β; &
  wl[g(ww)]=α*l[cm]^β
/ MORPHOMETRIC_PARAMETERS &
  ga[cm^2]=α*w[g(ww)]^β; &
  id[cm]=α*w[g(ww)]^β; &
  ld[cm]=α*w[g(ww)]^β; &
  ll[cm]=α*w[g(ww)]^β
/ PHYSIOLOGICAL_PARAMETERS &
  ae_fish[-]=α; ae_invert[-]=α; ae_plant[-]=α; &
  rq[-]=α; rt:std[-]=α; sda:in[-]=α; &
  ge[g(dw)/d]=α*g[g(ww)]^β*h(γ,t1,t2); &
  mf[l/d]=α*w[g(ww)]^β*h(γ,t1,t2); &
  mi[g(dw)/d]=α*w[g(ww)]^β*h(γ,t1,t2); &
  sg[1/d]=α*w[g(ww)]^β*h(γ,t1,t2); &
  sm[g(dw)]=α*w[g(ww)]^β*h(γ,t1,t2); &
  so[mg(o2)/h]=α*w[g(ww)]^β*h(γ,t1,t2); &
  st[minute]=α*w[g(ww)]^β*h(γ,t1,t2)
! end fish_1.fsh
```

In addition to the file hierarchy outlined above, it was also concluded that the BASS software and GUI should operate within a fixed directory structure that accommodates both project-specific include files and canonical include files that could be copied and edited as needed for new applications. Consequently, the BASS installation software creates the directory structure shown below

```
C:\BASS
    |-- BASS_V23.EXE
    |
    |-- BASS GUI executables and DLLs
    |
    |-- \FISH -- *.FSH
    |
    |-- \COMMUNITY -- *.CMM
    |
    |-- \PROPERTY -- *.PRP
    |
    |-- \PROJECTS -- \project1 -- *.PRJ
                     |            *.CHM
                     |            *.DAT
                     |
                     \project2
                     |
                     ⋮
```

The \FISH subdirectory contains canonical versions of the *.FSH files that specify the bioenergetic, compositional, ecological, and morphological parameters of individual fish species and that are used as include files for constructing fish community files.

The \COMMUNITY subdirectory contains canonical versions of the *.CMM files that specify the composition, trophic structure, and initial conditions for the community's fishes as well as any desired fishery and habitat suitability parameters.

The \PROPERTY subdirectory contains canonical versions of the *.PRP files that specify the physico-chemical properties of individual chemicals and that are used as include files for chemical exposure files.

The \PROJECTS directory contains subdirectories that are created by the user for a particular model application. In general, each application should be assigned its own subdirectory. Three types of BASS data files will generally reside in each PROJECTS folder. These file types are: (1) *.PRJ files that define the desired application and any desired variants of the application, (2) *.CHM files that specify chemical exposures and properties, and (3) *.DAT files that specify chemical exposures, habitat suitability multipliers, non-fish standing stocks, water temperature, and water depth when these parameters are supplied by the "file" option. A project subdirectory can also contain local copies of either *.FSH, *.CMM, or *.PRP files that have been created or modified for a particular project. Such files may have been created from scratch or may have been constructed from canonical files residing in the \FISH, \COMMUNITY, or \PROPERTY subdirectories.

BASS's input subroutines process project files assuming that the paths of **all** specified include files are relative to the project file that is currently being read. Therefore, in the case of *.FSH, *.CMM, or *.PRP files, BASS initially attempts to find these include files in the current project file's subdirectory. If these files cannot be found in the current subdirectory, BASS uses the extension of the specified include files to search the \FISH, \COMMUNITY, or \PROPERTY subdirectories. This prioritized input processing means that a user can specify a canonical *.CMM file that uses both canonical and local *.FSH files.

4.6. Output Files Generated by BASS

BASS generates the following types of output files

- an output file that summarizes the user's input parameters, any input errors detected by BASS, and any warnings / errors encountered during an actual simulation. This file has the same name of the executed project file with extension "MSG". For example, when BASS executes the project file INPUT.PRJ, the message file INPUT.MSG is generated. If this message file already exists, it is silently overwritten.

- an output file that tabulates selected results of the simulation. Tabulated summaries include: (1) annual bioenergetic fluxes and growth statistics (e.g., mean body weight, mean growth rate, etc.) of individual fish by species and age class; (2) annual bioaccumulation fluxes and statistics (e.g., mean whole-body concentrations, mean BAF and BMF, etc.) of individual fish by species and age class; and (3) annual community fluxes and statistics (e.g., mean population densities and biomasses, mean production, etc.) of each fish species by age class. This file has the same name of the executed project file with extension "BSS". For example, when BASS executes the project file INPUT.PRJ, the output file INPUT.BSS is generated. If this file already exists, it is silently overwritten.

- one or more CSV files that enable users to create a variety of custom figures or plots using Excel or other graphical software. See the "-csv" command line options described in the following section. If these files already exist, they are silently overwritten.

4.7. Command Line Options

To run a BASS simulation that is specified by the project file INPUT.PRJ, BASS can be invoked either from the BASS GUI or using the UNIX like command line

```
C:\BASS23> bass_V23 -i input.prj
```

Although the "-i filename" option is the only required command line option, the following additional options are available

```
-a =>  enable default accelerated YOY self-thinning;
-c =>  report distribution of cpu time in major subroutines;
-cc number => total fish carrying capacity as a multiple of
              total initial biomass;
-cmm =>  generate updated cmm file using the ending valued
         for age, weight, density, and cfish;
-csv1 number => generate Excel CSV file of fish variables;
              number=print interval in days;
-csv2 number => generate Excel CSV file of non-fish
              variables; number=print interval in days;
-csv3 number =>  generate Excel CSV file of cfish X weight
              for year=number;
-e =>  tabulate realized monthly diets for elective feeding;
-ef =>   tabulate realized monthly diets for elective feeding
         and report FGETS style diets
-echo =>  echo input commands;
-f =>  turn off fishing;
-h =>  print this help list and stop (also see -?);
-hsi =>  turn off HSI functions (i.e. assume HSI=1);
-l =>  turn off lethal effects;
-m =>   enable monthly spawning for species with annual age
         classes;
-mba =>  output mass balance analysis with annual
         summaries;
-n =>  internally calculate rate-based BCF for non-fish;
-p =>  turn on messages associated with feeding and predation;
-s =>  turn off fish stocking;
-t =>  run test of BASS integrators and stop;
-tp =>   report trophic positions;
-tte =>  report net trophic transfer efficiencies;
-w => write input data no execution attempted;
-? =>  print this help list and stop (also see -h)
```

For example, the command line

```
C:\BASS22> bass_V23 -i input.prj -l -c
```

will execute the project file INPUT.PRJ without simulating acute or chronic chemical lethality and report the distribution of cpu time spent within various key BASS subroutines.

Table 4.1 Valid Unit Prefixes.

Prefix Name	Conversion Factor
atto	10^{-18}
centi	10^{-02}
deca	10^{+01}
deci	10^{-01}
exa	10^{+18}
femto	10^{-15}
giga	10^{+09}
hecto	10^{+02}
kilo	10^{+03}
mega	10^{+06}
micro	10^{-06}
milli	10^{-03}
myria	10^{+04}
nano	10^{-09}
peta	10^{+15}
pico	10^{-12}
tera	10^{+12}

Table 4.2 Valid Unit Names for Length, Area, Volume, Mass, Time, and Energy. This list is not exhaustive and summarizes only commonly used unit names that BASS's units conversion program recognizes.

Unit Name	Conversion Factor to SI	Metre	Kg	Second	Description
acre	2.471×10^{-04}	2	0	0	4840 yards^2
are	1.000×10^{-02}	2	0	0	100 meter^2
btu	9.479×10^{-04}	2	1	-2	
calorie	2.388×10^{-01}	2	1	-2	
cc	$1.000\times10^{+06}$	3	0	0	cm^3
cm	$1.000\times10^{+02}$	1	0	0	
day	1.157×10^{-05}	0	0	1	
decade	3.169×10^{-09}	0	0	1	10 years
erg	$1.000\times10^{+07}$	2	1	-2	
fathom	5.468×10^{-01}	1	0	0	6 feet
feet	$3.281\times10^{+00}$	1	0	0	
foot	$3.281\times10^{+00}$	1	0	0	
ft	$3.281\times10^{+00}$	1	0	0	feet, foot
g	$1.000\times10^{+03}$	0	1	0	grams
gallon	$2.642\times10^{+02}$	3	0	0	3.785 liter
gm	$1.000\times10^{+03}$	0	1	0	grams
gram	$1.000\times10^{+03}$	0	1	0	
gramme	$1.000\times10^{+03}$	0	1	0	
hectare	1.000×10^{-04}	2	0	0	100 are
hour	2.778×10^{-04}	0	0	1	
hr	2.778×10^{-04}	0	0	1	hour
imperialgallon	$2.200\times10^{+02}$	3	0	0	4.54 liter
inch	$3.937\times10^{+01}$	1	0	0	
joule	$1.000\times10^{+00}$	2	1	-2	
kg	$1.000\times10^{+00}$	0	1	0	kilograms
km	1.000×10^{-03}	1	0	0	kilometer
l	$1.000\times10^{+03}$	3	0	0	liter
lb	$2.205\times10^{+00}$	0	1	0	pound
liter	$1.000\times10^{+03}$	3	0	0	
litre	$1.000\times10^{+03}$	3	0	0	
m	$1.000\times10^{+00}$	1	0	0	meter
meter	$1.000\times10^{+00}$	1	0	0	
metre	$1.000\times10^{+00}$	1	0	0	
mg	$1.000\times10^{+06}$	0	1	0	milligrams
micron	$1.000\times10^{+06}$	1	0	0	10^{-6} meter
mile	6.214×10^{-04}	1	0	0	5280 feet
min	1.667×10^{-02}	0	0	1	minute
minute	1.667×10^{-02}	0	0	1	
ml	$1.000\times10^{+06}$	3	0	0	
mm	$1.000\times10^{+03}$	1	0	0	

Table 4.3 Valid ecological, morphometric, and physiological units. BASS uses these units to convert user-specified units for lamellar density, initial populations densities, fish body weights, and oxygen consumption to standard model units.

Unit Name	Conversion Factor to SI	Metre	Kg	Second	Description
fish	n.a.	0	0	0	treated as an amount as is mole
individuals	n.a.	0	0	0	treated as an amount as is mole
inds	n.a.	0	0	0	treated as an amount as is mole
ha	1.000×10^{-4}	2	0	0	hectare
lamellae	n.a.	0	0	0	treated as an amount as is mole
g(dw)	242.5	0	1	0	used for wet-to-dry conversions
kg(dw)	0.2425	0	1	0	used for wet-to-dry conversions
mg(dw)	2.425×10^{5}	0	1	0	used for wet-to-dry conversions
ug(dw)	2.425×10^{8}	0	1	0	used for wet-to-dry conversions
g(ww)	1.0×10^{3}	0	1	0	used for wet-to-dry conversions
kg(ww)	1.0	0	1	0	used for wet-to-dry conversions
mg(ww)	1.0×10^{6}	0	1	0	used for wet-to-dry conversions
ug(ww)	1.0×10^{9}	0	1	0	used for wet-to-dry conversions
g(O2)	7.3718×10^{-5}	2	1	-2	gram of oxygen
mg(O2)	7.3718×10^{-2}	2	1	-2	milligram of oxygen
ug(O2)	7.3718×10	2	1	-2	microgram of oxygen
kcal	2.388×10^{-4}	2	1	-2	kilocalorie
ul(O2)	5.1603×10	2	1	-2	microliter oxygen STP = micromole
ml(O2)	5.1603×10^{-2}	2	1	-2	milliliter oxygen STP = millimole
l(O2)	5.1603×10^{-5}	2	1	-2	22.4 liters STP = mole
umol(O2)	2.3037	2	1	-2	micromole of oxygen
mmol(O2)	2.3037×10^{-3}	2	1	-2	millimole of oxygen
mol(O2)	2.3037×10^{-6}	2	1	-2	mole of oxygen

Notes:

1. For unit conversions, a fish's kilogram wet weight is treated as its SI weight. Therefore, kg(ww)≡kg, g(ww)≡g, and mg(ww)≡mg

2. For unit conversions, all units associated with oxygen consumption are treated dimensionally as joules.

5. BASS Model Software and Graphical User Interface

5.1. Software Overview

The BASS v2.3 model and Graphical User's Interface (GUI) software are provided via two downloads from the USEPA Center for Exposure Assessment Modeling (CEAM) website (http://www.epa.gov/ceampubl/). These downloads are:

1. **BASS_V23.zip**: A compressed WinZip file that installs only the BASS modeling and parameterization software, user's manual, and distribution examples for DOS/Windows systems.

2. **BASS_V23_GUI.zip**: A compressed WinZip file that installs the BASS modeling and parameterization software, user's manual, GUI, and distribution examples for DOS/Windows systems.

BASS_V23.zip creates a BASS modeling directory as shown below

```
PATH\BASS_V23
     BASS_FILES.EXE
     BASS_FILES_ABSOFT_15.EXE
     BASS_FILES_LAHEY_77_AM.EXE
     BASS_FILES_LAHEY_77_VS.EXE
     BASS_V23.EXE
     BASS_V23_ABSOFT_15.EXE
     BASS_V23_LAHEY_77_AM.EXE
     BASS_V23_LAHEY_77_VS.EXE
     BASS_FISH_DATA.DB
     PISCES_DATA.DB
     LIBGOMP.DLL
     LIBGOMPX64.DLL
     PTHREADVC2.DLL
     PTHREADVC2_64.DLL
     CLEAN_EXAMPLES.BAT
     RUN_EXAMPLES.BAT
     COMPARE_BASS_EXEs.BAT
     BASS_CMD_OPTIONS.TXT
     \BASS_DATABASES
       \BASS_BD
       \EIGEN
       \OXYREF
     \COMMUNITY
     \DOCUMENTS
       \BASS_FGETS_APPLICATIONS_REVIEWS
       \FACT_SHEETS
       \MANUAL
       \PPT_PRESENTATIONS
       \QA
     \FISH
     \PROPERTY
     \PROJECTS
       \0EX_EVERGLADES_CANAL_HG_ABSOFT_15
       \0EX_EVERGLADES_CANAL_HG_LAHEY_77_AM
       \0EX_EVERGLADES_CANAL_HG_LAHEY_77_VS
       \EX_EVERGLADES_CANAL
       \EX_EVERGLADES_CANAL_FISHING
       \EX_EVERGLADES_CANAL_HG
       \EX_EVERGLADES_CANAL_HG_FGETS
       \EX_EVERGLADES_CANAL_HG_LESLIE
       \EX_EVERGLADES_HG_HOLES
       \EX_EVERGLADES_HG_MARSH
       \EX_L_HARTWELL
       \EX_L_HARTWELL_PCB
       \EX_L_HARTWELL_PCB_TRANS
       \EX_L_ONTARIO_PCB
       \EX_SE_FARM_POND
       \EX_SE_FARM_POND_XMS
     \SOURCE_CODE
       \BASS_FILES_ABSOFT_15
       \BASS_FILES_LAHEY_77_AM
       \BASS_FILES_LAHEY_77_AM
       \BASS_v23_ABSOFT_15
       \BASS_v23_LAHEY_77_AM
       \BASS_v23_LAHEY_77_VS
```

where *PATH* = C:\USERS\USER_NAME unless changed by the user. The contents of this directory include:

1. **BASS_V23.EXE** is the active BASS model executable. Although it is assigned to be BASS_V23_LAHEY_77_AM.EXE by default, users can reassign it to be BASS_V23_ABSOFT_15.EXE or BASS_V23_LAHEY_77_VS.EXE to obtain faster simulations depending on their CPU specifications.

2. **BASS_V23_ABSOFT_15.EXE** is the most current BASS model executable that has been created with the Absoft version 2015 Fortran 95 compiler using a 64-byte Windows 10 operating system. Depending on a user's CPU, this executable may run faster or slower than the Lahey-Fujitsu executables below. Also see Section 7.2.7.

3. **BASS_V23_LAHEY_77_AM.EXE** is the most current BASS model executable that has been created with the Lahey-Fujitsu Fortran 95 version 7.7 compiler using its AutoMake software. This executable is used as the default BASS software executable **BASS_V23.EXE**. Also see Section 7.2.7.

4. **BASS_V23_LAHEY_77_VS.EXE** is the most current BASS model executable that has been created with the Lahey-Fujitsu Fortran 95 version 7.7 compiler using its Visual Studio shell. Also see Section 7.2.7.

5. **BASS_FILES.EXE** is the active executable for the BASS parameterization software that uses the data files BASS_FISH_DATA.DB and PISCES_DATA.DB to enable users to generate fish and community files. Although this executable was created with the Lahey-Fujitsu 7.7 compiler using AutoMake, executables compiled with Absoft 2015 and Lahey-Fujitsu 7.7 using Visual Studio, are also available. See Section 5.6.

6. **\BASS_DATABASES** contain three data subdirectories with associated Fortran 95 executables that generate input data for BASS_FISH_DATA.DB and Fortran 95 code for BASS_FILES.EXE and BASS_V23.EXE. The directory \BASS_DB contains the software and data subdirectory \BASS_DB\FISH_DATA that generates the BASS database supplement and an internal database of fish growth rates for BASS_FILES.EXE. The directory \EIGEN contains the software that generates an internal database of eigenvalues and mixing coefficients for BASS's gill exchange model described in Section 2.2. Lastly, the directory \OXYREF contains the software and the OXYREF database (Thurston and Gehrke 1993) that generates family-specific oxygen consumption rates for BASS_FILES.EXE.

7. **\COMMUNITY** is the folder designed to be a repository of community files (*.CMM) that the user wishes to save as a canonical library for constructing future BASS projects. Although this folder is empty, it must be present for the BASS software to function correctly. See Section 4.5 (page 56).

8. **\DOCUMENTS** contains five document subdirectories related to the application and use BASS.

9. **\FISH** is the folder designed to be a repository of fish files (*.FSH) that the user wishes to save as a canonical library for constructing future BASS projects. This folder must be present for the BASS software to function correctly, and it is initially populated with default FSH files generated by BASS_FILES.EXE for 661 species of North American and European fishes. These files can be regenerated by double clicking on the DOS batch file **REGENERATE_FSH_FILES.BAT** See Section 5.6.

10. **\PROJECTS** contains the BASS v2.3 distribution example projects that are described in Section 6.1 (page 75). All of these examples can be executed by double clicking on the DOS batch file **RUN_EXAMPLES.BAT**. The three projects, whose names begin with "0EX_", are also included to allow users to compare the relative execution speeds of the Absoft and Lahey-Fujitsu BASS executables. These performance projects can be executed by double clicking on the DOS batch file **COMPARE_BASS_EXES.BAT**.

11. **\PROPERTY** is the folder designed to be a repository of chemical property files (*.PRP) that the user wishes to save as a canonical library for constructing future BASS projects. This folder must be present for the BASS software to function correctly, and it is initially populated with chemical property files used by the BASS distribution examples. This folder also contains the folder **\BARBER_2003** which contains chemical property files for the chemicals analyzed in Barber's review paper of gill exchange models (Barber, M.C. 2003. Environ. Toxicol. Chem. 22: 1963-1992). See Section 4.5 (page 56).

12. **\SOURCE_CODE** contains the current Fortran 95 source code for BASS_V23.EXE and BASS_FILES.EXE. This folder is included for those users who would like to review the BASS code or to adapt it for other purposes.

In addition to the aforementioned BASS modeling directory, the WinZip file **BASS_V23_GUI.zip** creates a \BASS GUI subdirectory and installs the BASS GUI executable and its associated dynamic link libraries (DLLs).

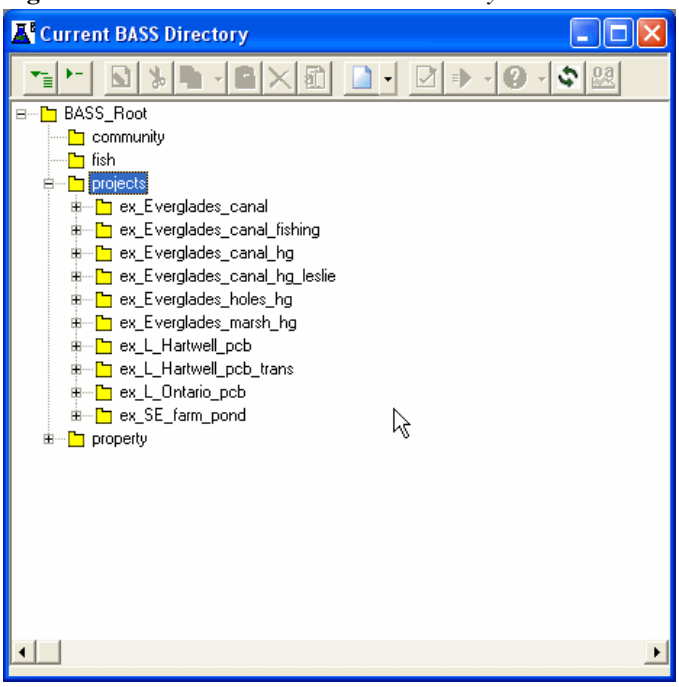
5.2. Installation Procedures

For complete installation procedures users are referred to the BASS installation readme file at the USEPA Center for Exposure Assessment Modeling (CEAM) website (http://www.epa.gov/ceampubl/).

5.3. BASS GUI Operation

The BASS GUI has been designed to emulate Microsoft's Windows Explorer in much of its form and function. After the BASS GUI is opened, the first window that users see is the GUI's *Current BASS Directory* (see **Figure 5.1**). If this window is inadvertently closed, it can be reopened using the *View* button found on the toolbar of the GUI's host window.

Figure 5.1 BASS GUI *Current BASS Directory* window.



Double-clicking on a folder's name, icon, or directory node expands or collapses the folder's contents into or out of the

user's view, respectively. Double-clicking on a file name opens the file with one of six GUI file editors based on the selected file's extension. The GUI's file editors can also be invoked by:

1. Left-clicking on the file and pressing the *Enter* key.
2. Right-clicking on the file and then left-clicking on *Edit*.
3. Left-clicking on the file and left-clicking on the *Edit* icon  found on the *Current BASS Directory* toolbar.

When users are editing a BASS project file that contains include files, users can also open file editors for those include files by

4. Left-clicking on the desired include command and then left-clicking on the resulting activated *Open Include File* link (see Section 5.4.1).

BASS output files (i.e., *.BSS, *.MSG, and *.XML), are not displayed in the *Current BASS Directory* window. These files, if they exist, are accessed via the project files (*.PRJ) that generated them.

BASS message files (*.MSG) and simulation summary files (*.BSS) can be reviewed by right-clicking on the relevant project file and then left-clicking on *View Project Message File* or *View BSS File*, respectively. These files can also be reviewed by left-clicking on the desired project file and then left-clicking on the arrow of the *File Viewing* icon  found on the *Current BASS Directory* toolbar. The *File Viewing* icon has an associated drop-down selection that enables users to specify which output file type is to be viewed. If the *File Viewing* icon is left-clicked directly, the project's message file is opened by default.

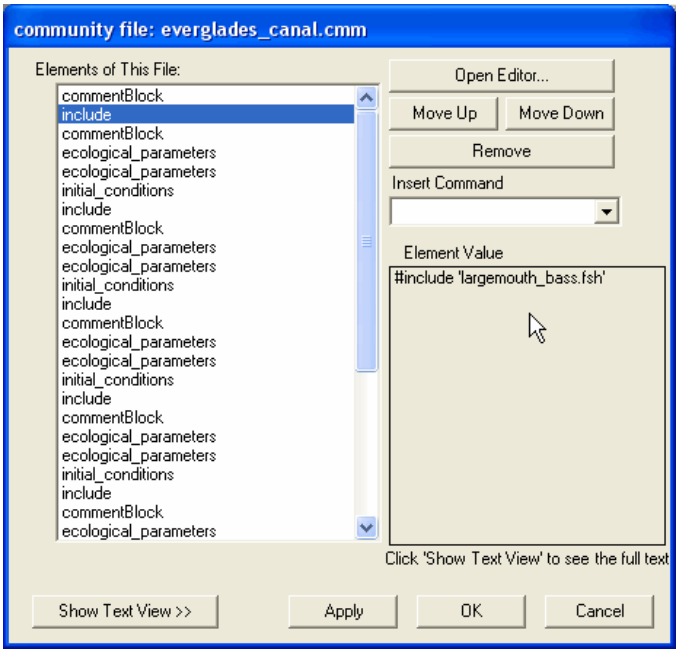
BASS project files are executed either by right-clicking on the desired project file and then left-clicking on *Run Project* or by left-clicking on the desired project file and then left-clicking on the arrow of the *Execution* icon  on the *Current BASS Directory* toolbar. Like the *File Viewing* icon, the *Execution* icon has an associated drop-down selection that enables users to specify command line options as described in Section 4.7 (page 57). When a project file is being executed, all other GUI functions are unavailable until the simulation is completed.

BASS project files can be checked for their syntax and data completeness before attempting execution either by right-clicking on the desired project file and then left-clicking on *Validate Project* or by left-clicking on the desired project file and then left-clicking on the *Validate Project* icon  on the *Current BASS Directory* toolbar. If the project file has syntax errors or missing input data, the GUI's *Event Viewer* will automatically open and display validation status of the project as well as associated errors and warnings. Most users, however, will find it easier to review these errors by opening the project's MSG file, as outlined previously, and search for the phrase "ERROR:" to determine the needed corrective actions.

5.3.1. BASS File Editors

All six GUI file editors have the same essential format and function as displayed in **Figure 5.2**. Commands, include files, and comment blocks contained within the file being edited are displayed in abbreviated form and in order of their appearance within the *Elements of This File* box. The full details of these elements can be viewed individually within the *Element Value* box or as they appear within the file by left-clicking on the *Show Text View* toggle button. Elements can be edited by either double-clicking on the element name or by left-clicking on the element and then left-clicking on the *Open Editor...* button.

Figure 5.2 General structure of BASS GUI file editors.



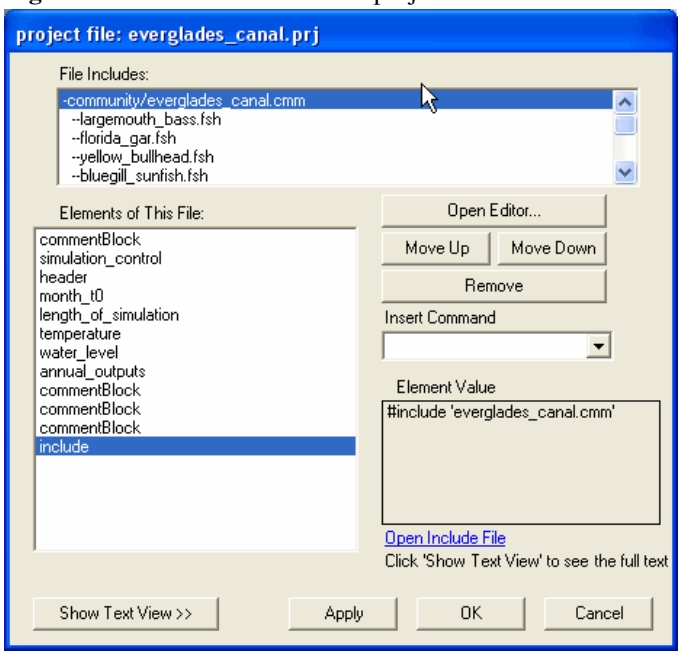
The position of elements can be changed by using the *Move Up* and *Move Down* buttons. Existing elements can be removed and new elements added by using the *Remove* button and *Insert Command* box, respectively. When elements are either added, removed, or reordered, however, users must first left-click on the *Apply* button before opening any GUI command editor. The *Apply* button is also used to save editorial changes at any time during an editing session.

Because the typical *Close* "X" button has been disabled on all

GUI file editors, users can exit GUI file editors only by using the *OK* and *Cancel* buttons. These buttons either save or cancel any editorial changes since the last invocation of the *Apply* button. This GUI behavior is designed to preserve the integrity of the GUI's Document Object Model (DOM).

Figure 5.3 displays the structure of the BASS GUI project file editor. This editor differs from the GUI's other five file editors in two ways. First, this editor explicitly identifies all include files that will be used by the project. Secondly, any include file that is directly referenced by the project file can be opened and edited by left-clicking on the *Open Include File* hyperlink that appears below the *Element Value* box whenever an include statement is highlighted in the *Elements of This File* box.

Figure 5.3 Structure of BASS GUI project file editor.



5.3.2. BASS Command Editors

GUI command editors are opened from GUI file editors as outlined in Section 5.4.1. In terms of their appearance and functionality, there are 17 basic command editor types that are described in the following:

- Simple String Editors that edit the commands /CHEMICAL, /COMMON_NAME, /HEADER, /SPECIES, and include file specifications (i.e., #INCLUDES . . .). See **Figure 5.4**.
- Simple String Editor with pull-down selection that edits the commands /AGE_CLASS_DURATION and /MONTH_T0. See **Figure 5.5**.
- Numeric Editor with units that edits the command /LENGTH_OF_SIMULATION. See **Figure 5.6**.
- Numeric Editor without units that edits the commands /ANNUAL_OUTPUTS, /LOG_AC, /LOG_KB1, /LOG_KB2, /LOG_P, /MELTING_POINT, /MOLAR_VOLUME, and /MOLAR_WEIGHT. See **Figure 5.7**.
- Forcing Function Editor that edits the commands /BIOTA, /EXPOSURE, /HABITAT_PARAMETERS, /TEMPERATURE, and /WATER_LEVEL. See **Figure 5.8**.
- Feeding Model Editor that edits the command /FEEDING_OPTIONS. See **Figure 5.9**.
- Compositional and Morphometric Editor that edits the commands /COMPOSITIONAL_PARAMETERS and /MORPHOMETRIC_PARAMETERS. See **Figure 5.10**.
- Ecological Editor that edits the command /ECOLOGICAL_PARAMETERS. See **Figure 5.11** and **Figure 5.12**.
- Physiological and Growth Editor that edits the command /PHYSIOLOGICAL_PARAMETERS. See **Figure 5.13**.
- Cohort Initial Conditions Editor that edits the command /INITIAL_CONDITIONS. See **Figure 5.14**.
- Spawning Period Editor that edits the command /SPAWNING_PERIOD See **Figure 5.15**.
- Fishery Editor that edits the command /FISHERY_PARAMETERS. See **Figure 5.16**.
- Non-fish Biotic Editor that edits the commands /BENTHOS, /PERIPHYTON, /PHYTOPLANKTON, /TERRESTRIAL_INSECTS, and /ZOOPLANKTON. See **Figure 5.17** and **Figure 5.18**.
- Non-fish BCF Editor that edits the command /NONFISH_BCF. See **Figure 5.19**.
- Chemical Metabolism Editor that edits the command /METABOLISM. See **Figure 5.20**.
- Chemical Toxicity Editor that edits the command /LETHALITY. See **Figure 5.21**.
- Plot Selection Editor that edits the commands /ANNUAL_PLOTS and /SUMMARY_PLOTS. See **Figure 5.22**.

As noted with the GUI file editors, the typical *Close* "X" button has been disabled on all GUI command editors. Users can only exit or close a command editor by using the *OK* and *Cancel* buttons. These buttons either save or cancel any editorial changes since the editor was opened. This GUI behavior is designed to preserve the integrity of the GUI's Document Object Model (DOM).

5.3.3. Special Function Editors

In addition to the file and command editors described in the previous section, the BASS GUI has two special function editors, i.e.,

- Comment Block Editor that is used to insert comment blocks before or after BASS commands, as opposed to end-of-line comments associated with the individual options of BASS commands. See **Figure 5.23**.

- Time Series Data Editor for editing external data files that are specified as file functions (e.g., /BIOTA, /EXPOSURE, /HABITAT_PARAMETERS, /TEMPERATURE, and /WATER_LEVEL). See **Figure 5.24**.

5.3.4. File and Folder Operations

Using the GUI's *Current BASS Directory* window, users can create new files and project folders either from scratch or from existing files and project folders.

To create a BASS project or include file from scratch, users must first left-click on the subdirectory (i.e., \COMMUNIY, \FISH, or \PROPERTY) or project folder where the file is to be created. The user then must left-click on the drop-down arrow head of the *Add New File* icon  . When the *Add New File* drop-down menu appears, the user must left-click on the desired file type to be created. Finally, after the new file appears in the *Current BASS Directory* window, the user must complete the naming of the new file. New project folders can be created following these same steps.

Users can create a file from an existing file by

1. Left-clicking on the desired file and then left-clicking on the *Copy* icon  .
2. Left-clicking on the desired destination folder or subdirectory and left-clicking on the *Paste* icon  .

Users can also create a new file from an existing file by

1. Right-clicking on the file to be copied and then left-clicking on *Copy*.
2. Right-clicking on the destination folder or subdirectory and then left-clicking on *Paste*.

Lastly users can create a new file from an existing file by

1. Left-clicking on the file to be copied and then pressing CTRL-c.
2. Left-clicking on the destination folder or subdirectory and then pressing CTRL-v

New project folders can be created from existing projects using the same procedures.

5.4. The BASS Output Analyzer

The BASS Output Analyzer (OA) was a dual purpose post-processor that enabled users to construct customized graphs and tables. This software could be invoked either from within the BASS GUI or as a standalone application. Using this software, users could create two and three-dimensional graphs of any state variable that is a valid option for the BASS v2.1 plotting commands /ANNUAL_PLOTS or /SUMMARY_PLOTS. The BASS OA also enabled users to create customized versions of the summary tables generated for BSS output files. This software, however, which was based on the Olectra Chart software (now ComponentOne Chart), is no longer functional or supported by the BASS GUI.

To replace the lost plotting features of the BASS OA, users can now generate three different types of CSV files which can be used to create even more customized plots using Excel or other graphical software programs. See **Section 4.7. Command Line Options**.

5.5. The BASS Parameterization Software

The BASS parameterization software BASS_FILES.EXE was created and is distributed with the BASS modeling software to assist users in constructing BASS FSH files and CMM files. Using a combination of an internal database of fish growth rates and two external database files (BASS_FISH_CODES.DB and PISCES_DATA.DB), this software currently can generate FSH files for 661 species of North American and European freshwater fish. The most current versions of these files are distributed with BASS and reside in the data directory \FISH. All FSH files generated by this software use BASS's allometric feeding model. Users can also use this software to construct a default CMM file and associate FSH files for an arbitrary selection of the aforementioned 661 fish species. This software, however, does not have an associated GUI and must be executed by the user from a DOS command prompt.

To generate a FSH file for a single species of interest, the user should open a DOS command prompt window and navigate to the project folder in which they want the file to be generated. Assuming that the user's BASS root directory is C:\BASS_V23, the DOS command

```
>c:\bass_V23\bass_files.exe -g "lepomis macrochirus"
-m "January 15" -l 10 -u 33
```

will generate a FSH file for bluegill sunfish whose growth rate has been calibrated to an annual sinusoidal water temperature cycle that varies from 10 to 33 Celsius and whose minimum annual temperature occurs on January 15.

To generate a CMM file and associated FSH files for a selection of fish, the user should again open a DOS command prompt window and navigate to the project folder in which the user wants the files to be generated. Assuming that the user's BASS root directory is C:\BASS_V23, the DOS command

```
...>c:\bass_v23\bass_files.exe -i fishes.dat
```

will generate a CMM file and associated FSH files for the fish species identified in the file *fishes.dat*. The file *fishes.dat* must reside in the desired project folder and be structured as illustrated below

```
! File:bass_bluegill_catfish.dat

CMM_FILE_NAME bass_bluegill_catfish.cmm
MONTH_TO August
COLDEST_DAY January 15
TEMPERATURE_MAXIMUM 30
TEMPERATURE_MINIMUM 10

FISH_START micropterus salmoides
COMMON_NAME largemouth bass
SPAWNING_PERIOD april-may
parameter_option_1; comment/reference
parameter_option_2; comment/reference
⋮
parameter_option_n; comment/reference
biomass[kg/ha]= number
or density[fish/ha]= number
FISH_END

FISH_START Lepomis macrochirus
COMMON_NAME bluegill sunfish
SPAWNING_PERIOD april-october
parameter_option_1; comment/reference
parameter_option_2; comment/reference
⋮
parameter_option_n; comment/reference
biomass[kg/ha]= number
or density[fish/ha]= number
FISH_END

FISH_START ictalurus puntatus
COMMON_NAME channel catfish
SPAWNING_PERIOD may-june
parameter_option_1; comment/reference
parameter_option_2; comment/reference
⋮
parameter_option_n; comment/reference
biomass[kg/ha]= number
or density[fish/ha]= number
FISH_END
```

where *parameter_option_i* is any valid option for the BASS fish commands \COMPOSITIONAL_PARAMETERS, \ECOLOGICAL_PARAMETERS, \MORPHOLOGICAL_PARAMETERS, or \PHYSIOLOGICAL_PARAMETERS that the user wants to supercede the default assignment made by BASS_FILES.EXE. All CMM files and associated FSH files used by the example BASS distribution projects have been generated using this software.

Figure 5.4 GUI command editor for simple strings.

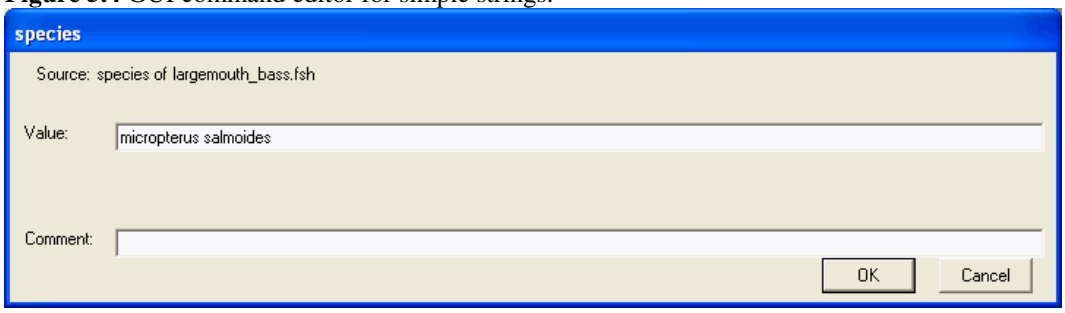


Figure 5.5 GUI command editor for simple strings with drop-down selection.

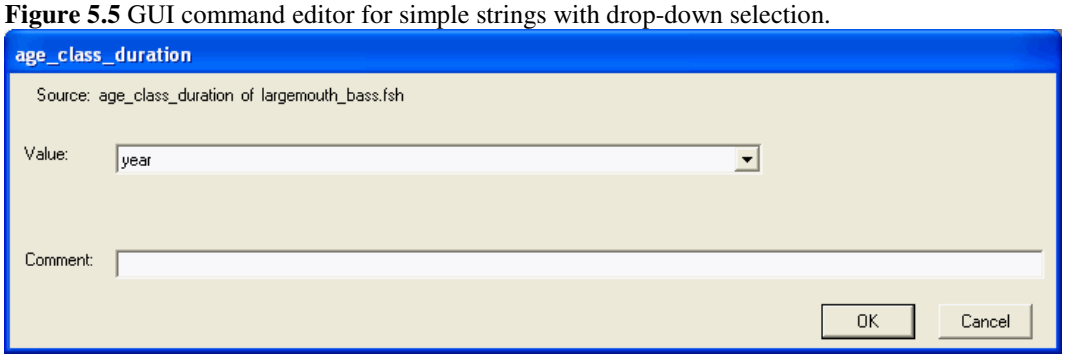


Figure 5.6 GUI command editor for numeric data with user-specified units.

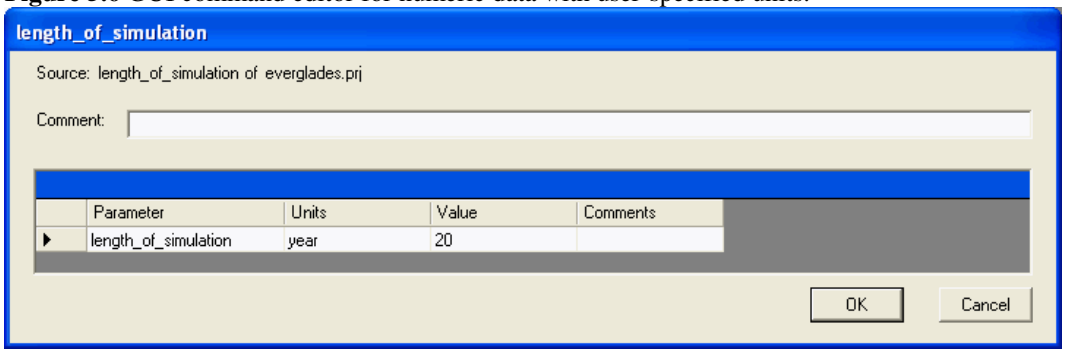


Figure 5.7 GUI command editor for numeric data fixed units.

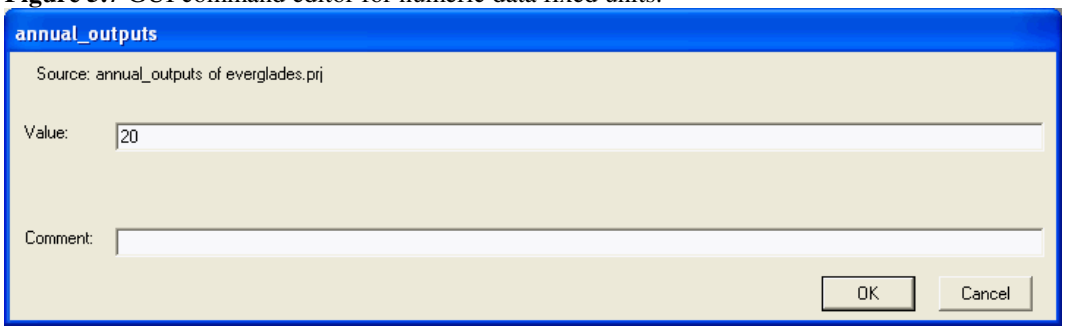


Figure 5.8 GUI command editor for forcing functions.

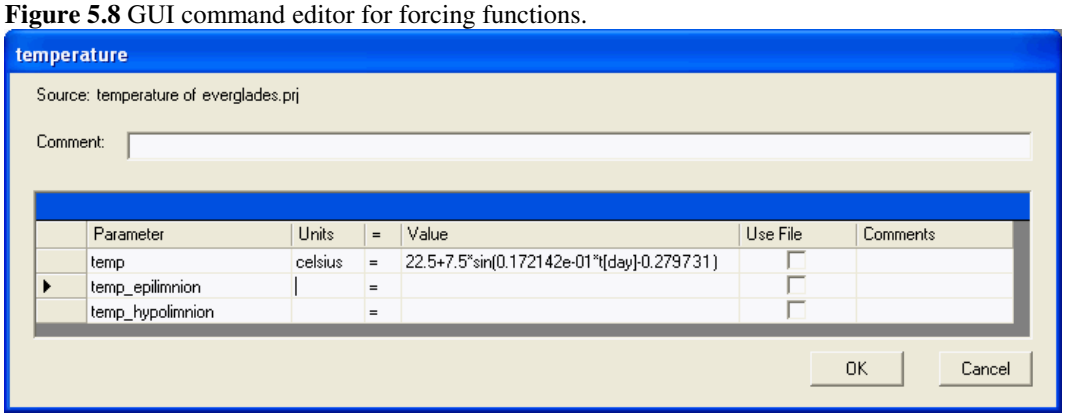


Figure 5.9 GUI command editor for feeding model options.

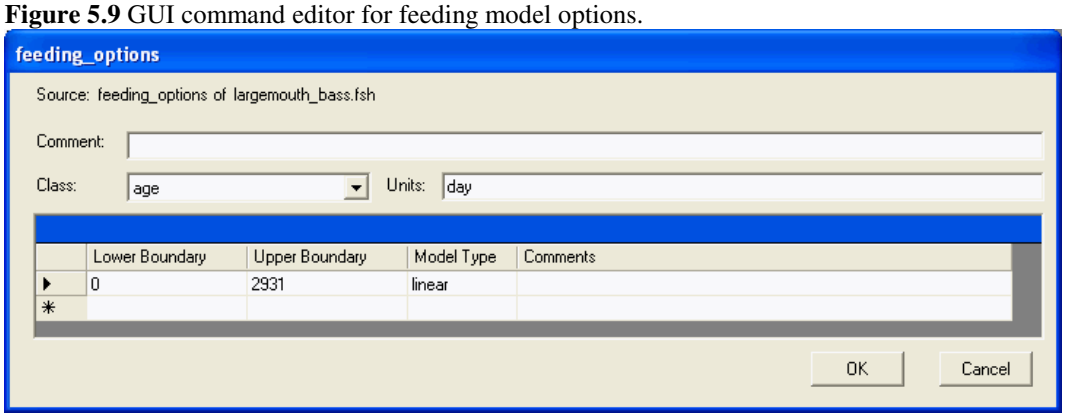


Figure 5.10 GUI command editor for compositional and morphometric parameters.

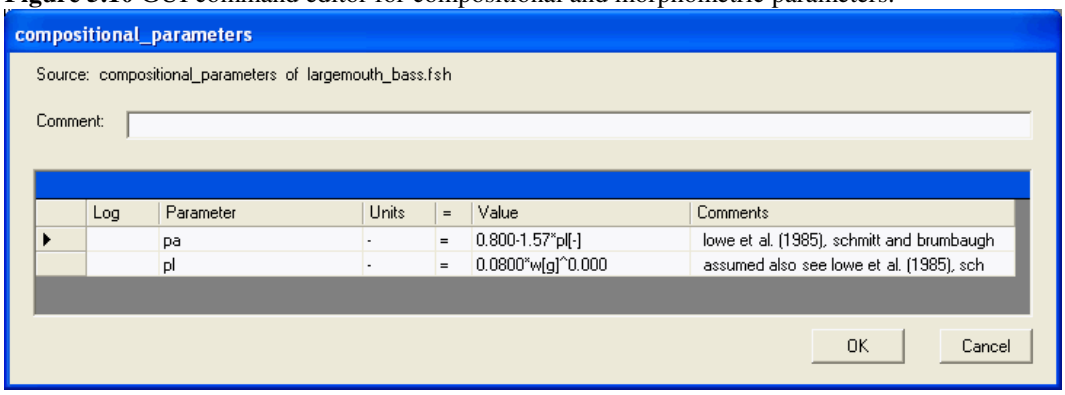


Figure 5.11 GUI command editor for nondiet ecological parameters.

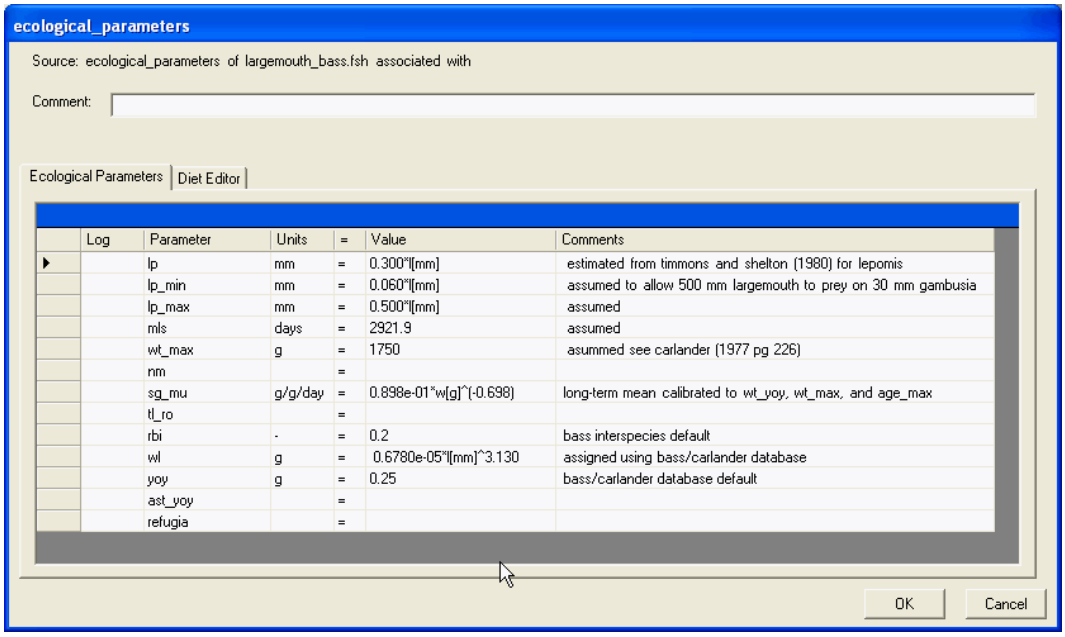


Figure 5.12 GUI command editor for fish diets.

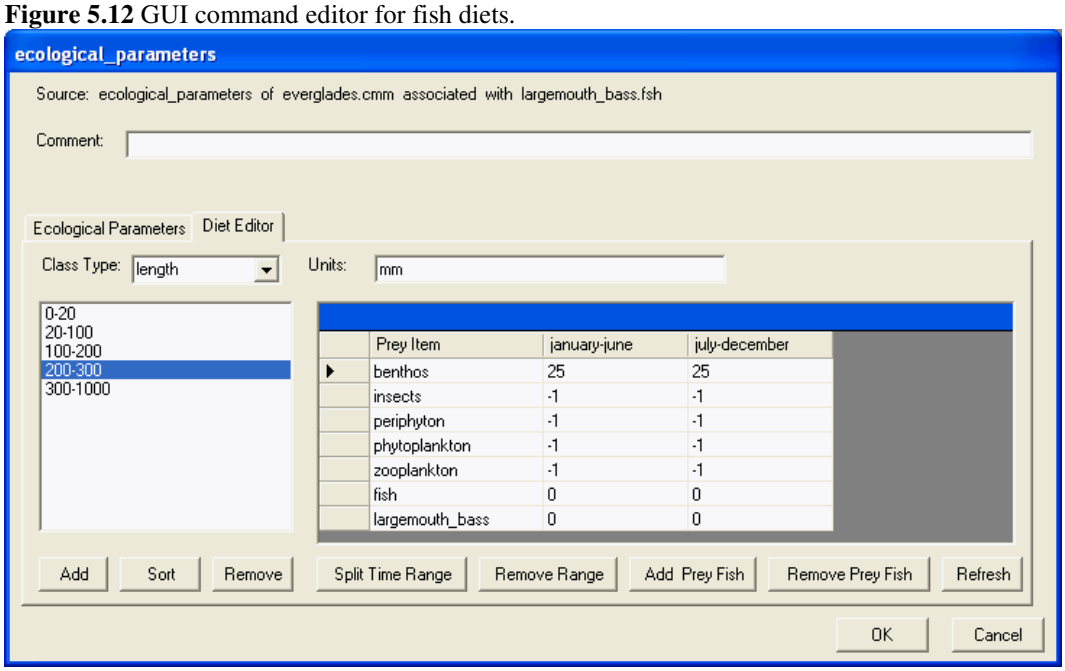


Figure 5.13 GUI command editor for physiological parameters.

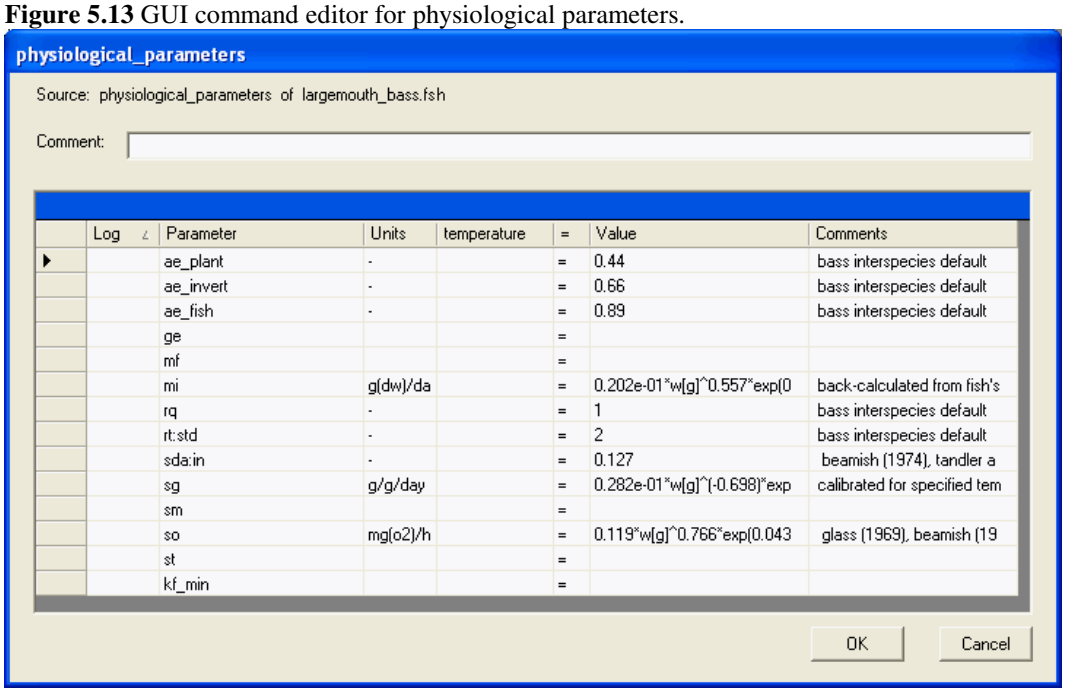


Figure 5.14 GUI command editor for cohort initial conditions.

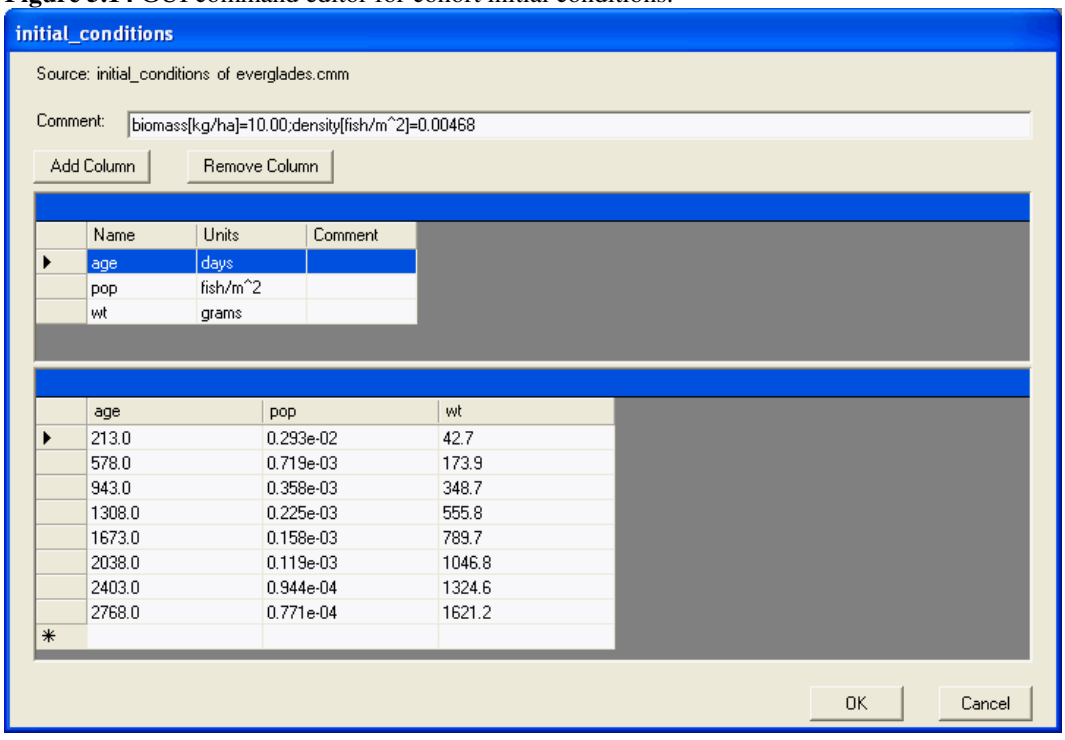


Figure 5.15 GUI command editor for spawning parameters.

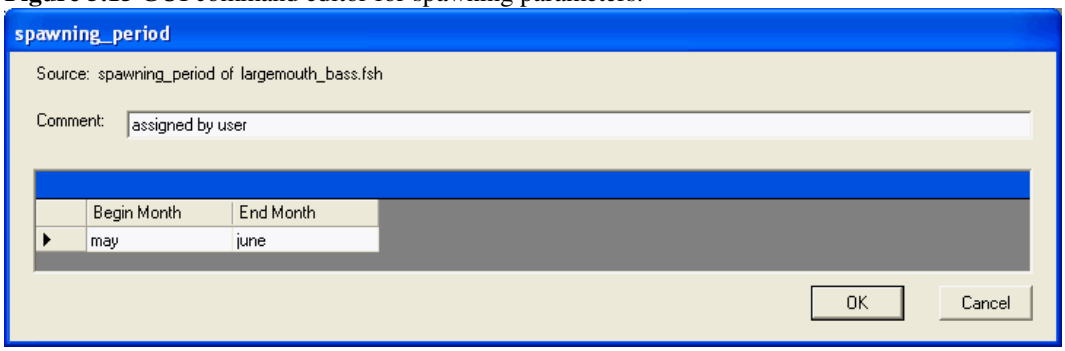


Figure 5.16 GUI command editor for fishery parameters.

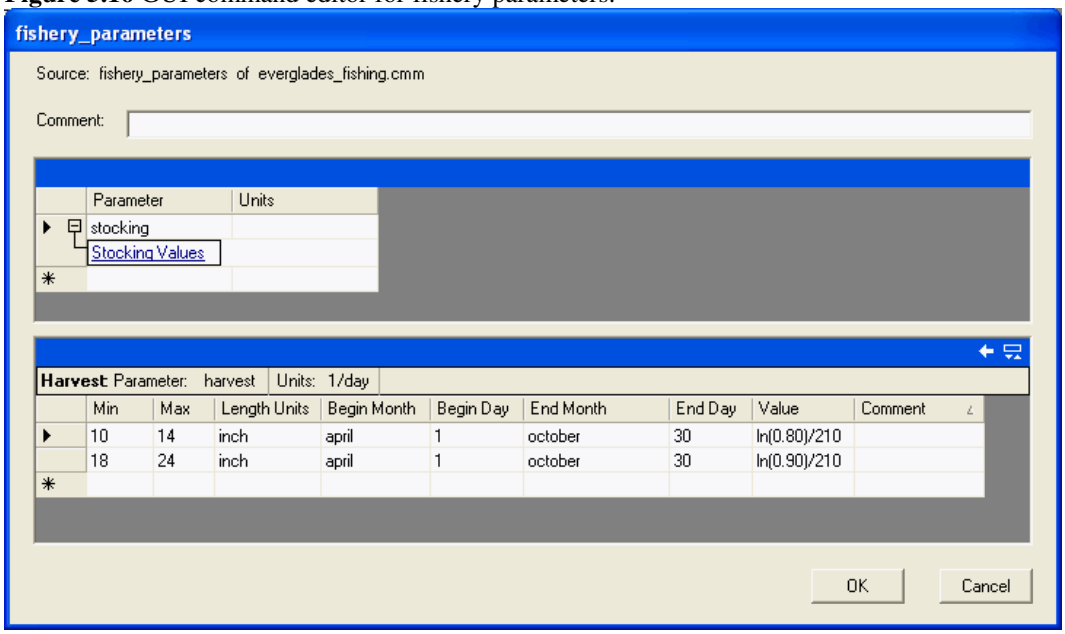


Figure 5.17 GUI command editor for non-fish biota as forcing functions.

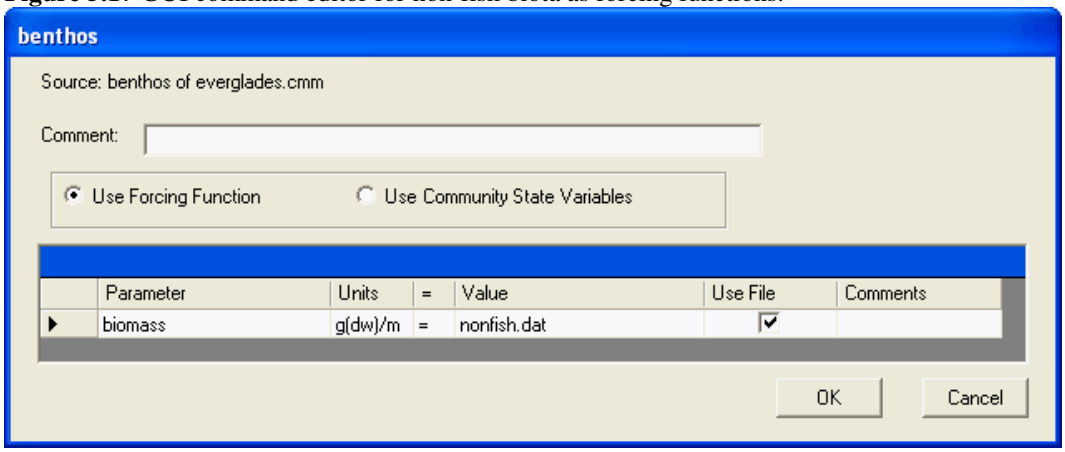


Figure 5.18 GUI command editor for non-fish biota as state variables.

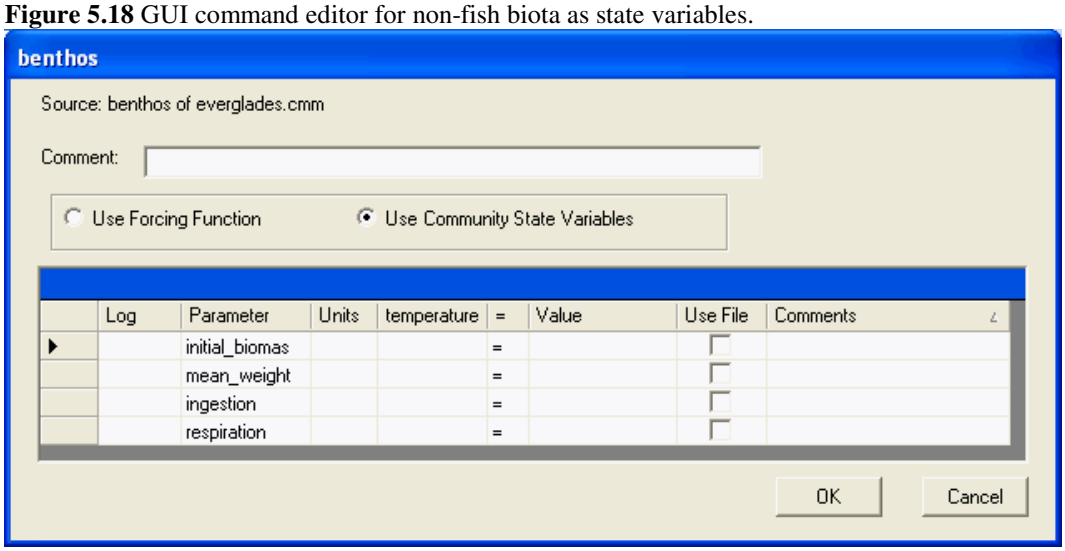


Figure 5.19 GUI command editor for non-fish bioaccumulation factors.

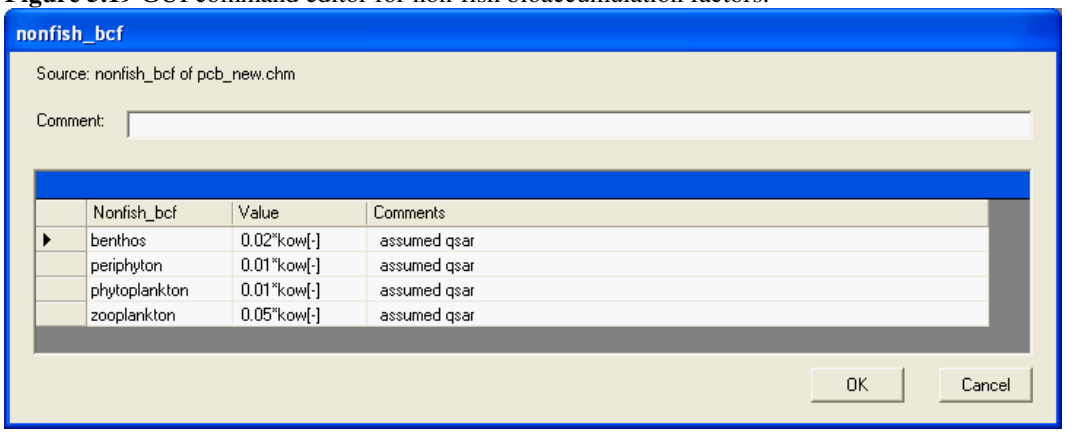


Figure 5.20 GUI command editor for chemical biotransformation parameters.

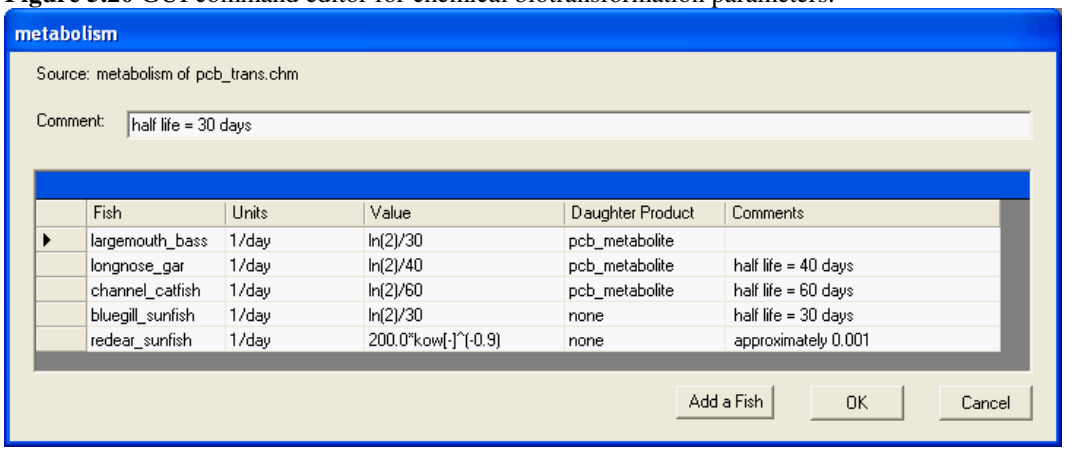


Figure 5.21 GUI command editor for chemical toxicity parameters.

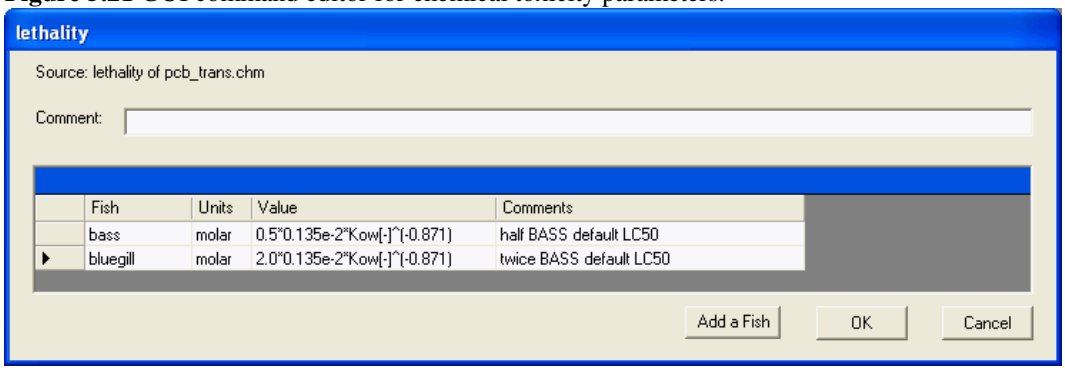


Figure 5.22 GUI command editor for automatic graphing selections.

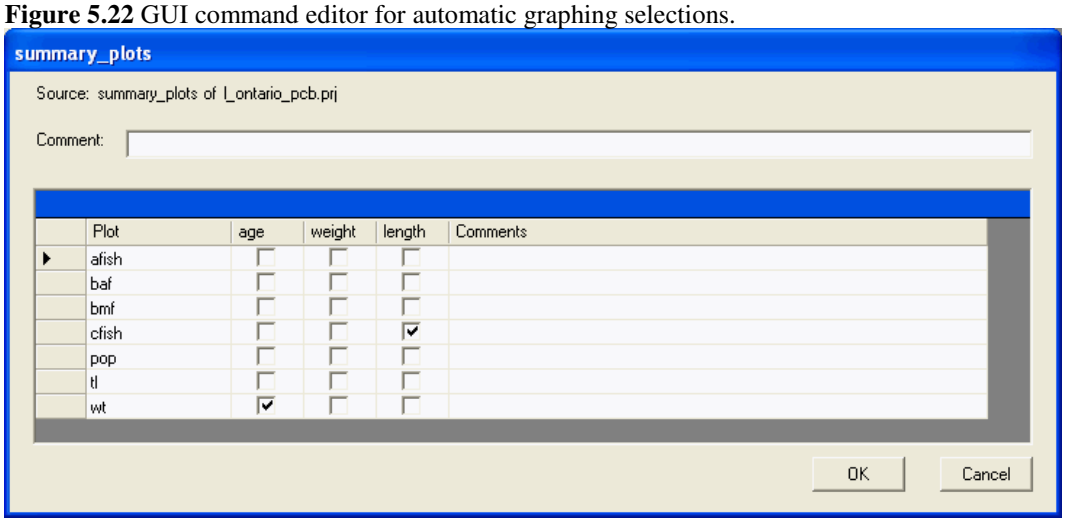


Figure 5.23 GUI Block comment editor.

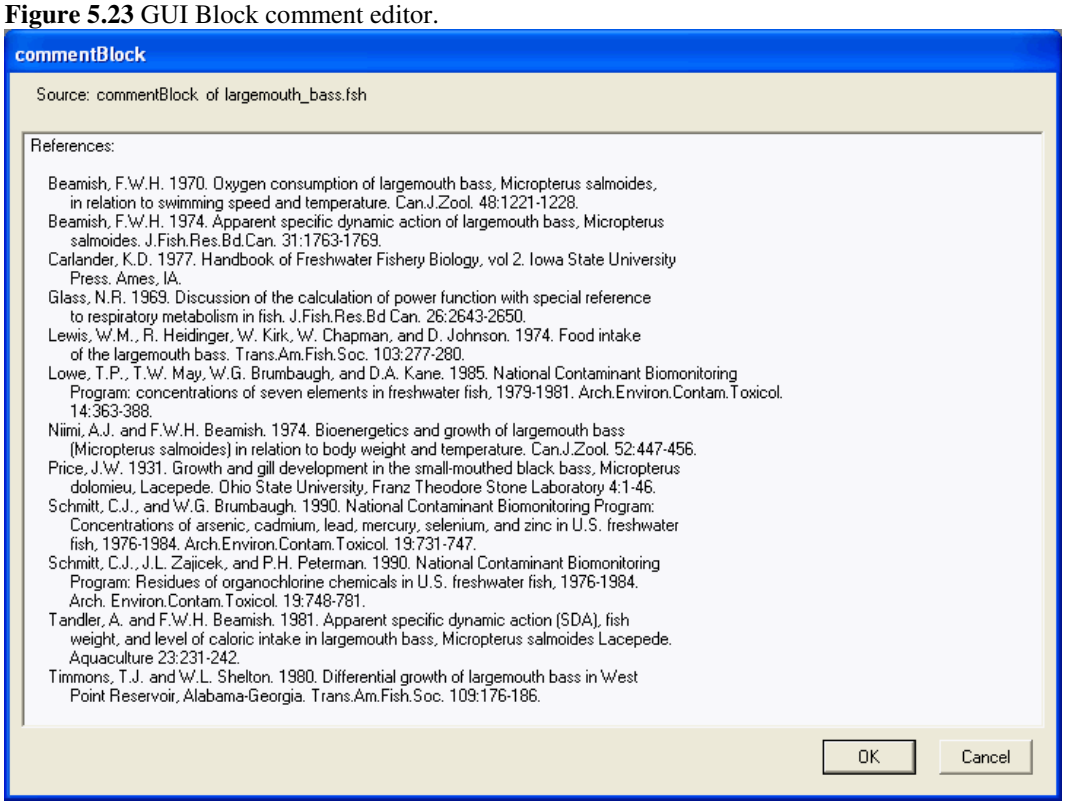
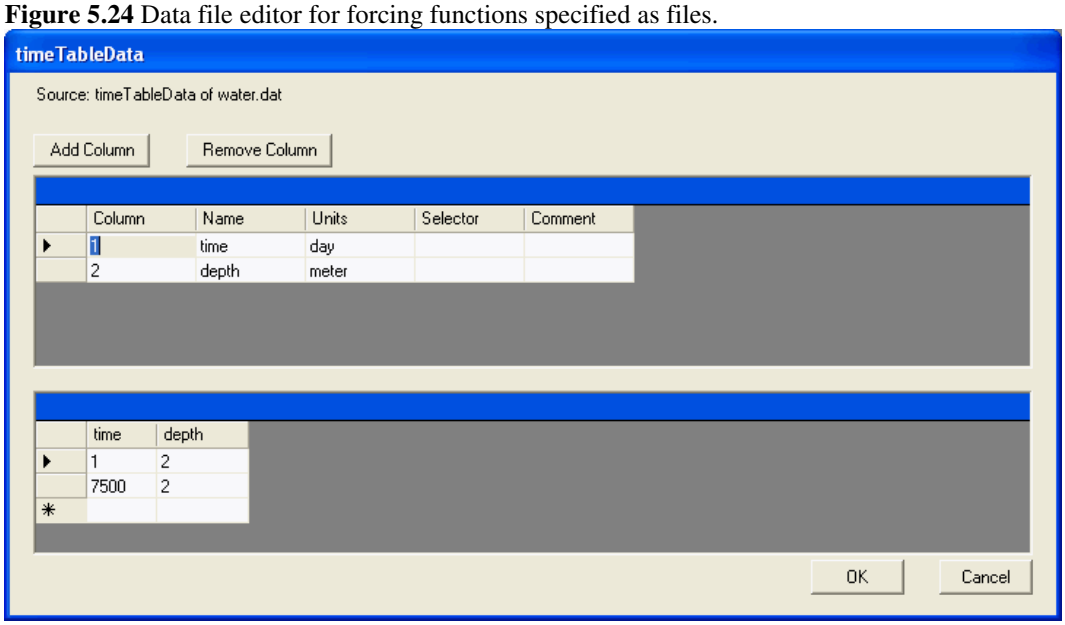


Figure 5.24 Data file editor for forcing functions specified as files.



6. Example Applications

6.1. BASS Software Distribution Examples

Thirteen example projects are provided with the BASS model software and GUI. Each project resides in its own folder within the \PROJECTS subdirectory. These projects have been updated extensively for the October 2018 release of BASS V2.3 and now use only FSH files generated by the BASS parameterization software BASS_FILES.EXE.

The project EX_EVERGLADES_CANAL simulates the growth and population dynamics of fish in an Everglades canal community in Florida, USA using the project file EVERGLADES_CANAL.PRJ. The fish species in this community are bluegill (*Lepomis macrochirus*), eastern mosquitofish (*Gambusia holbrooki*), Florida gar (*Lepisosteus platyrhincus*), largemouth bass (*Micropterus salmoides*), redear sunfish (*Lepomis microlophus*), and yellow bullhead (*Ameiurus natalis*). The project's CMM file and associated FSH files are generated by BASS_FILES.EXE using the input file EVERGLADES_CANAL_SPECIES.DAT. The canal's water depth and non-fish biomasses are supplied by the data files EVERGLADES_CANAL_WATER.DAT and EVERGLADES_NONFISH.DAT, respectively.

The project EX_EVERGLADES_CANAL_FISHING simulates the growth and population dynamics of fish in the aforementioned canal community assuming that bluegill, largemouth bass, and redear sunfish are harvested by fishing. Its project file EVERGLADES_CANAL_FISHING.PRJ uses the community file EVERGLADES_CANAL_FISHING.CMM, which was created by inserting assumed fishing mortality rates into a CMM file that is identical to the one used by the project EX_EVERGLADES_CANAL. The canal's water depth and non-fish biomasses are again specified using the data files EVERGLADES_CANAL_WATER.DAT and EVERGLADES_NONFISH.DAT, respectively.

The project EX_EVERGLADES_CANAL_HG simulates the growth, population, and methylmercury (MeHg) bioaccumulation dynamics of fish in an Everglades canal using the project file EVERGLADES_CANAL_HG.PRJ. This project uses the same CMM and FSH files as does the project EX_EVERGLADES_CANAL. The community's MeHg exposures are supplied by the include file EVERGLADES_MERCURY.CHM, which, in turn, uses the chemical property file \PROPERTY\METYL_HG.PRP. The canal's water depth and the non-fish biomasses are again supplied by the data files EVERGLADES_CANAL_WATER.DAT and EVERGLADES_NONFISH.DAT, respectively.

The project EX_EVERGLADES_CANAL_HG_FGETS simulates the growth and MeHg bioaccumulation dynamics of fish in an Everglades canal using the FGETS simulation option. With the exception of its PRJ and CMM files, this project uses the same parameter files as the project EX_EVERGLADES_CANAL_HG. To create the project's CMM file, a project file identical to EVERGLADES_CANAL_HG.PRJ was executed using the command line option "-ef" which instructs BASS to output FGETS-style diets for all fishes using the project's simulated trophic dynamics. These diets were then inserted into the project's CMM file which was renamed to EVERGLADES_CANAL_FGETS.CMM.

The project EX_EVERGLADES_CANAL_HG_LESLIE simulates the growth, population, and MeHg bioaccumulation dynamics of fish in an Everglades canal using the Leslie matrix simulation option. This project uses the same CMM and FSH files as does the project EX_EVERGLADES_CANAL_HG, and its MeHg exposures and properties are again provided by EVERGLADES_MERCURY.CHM. Similarly, the canal's water depth and non-fish biomasses are again provided by the data files EVERGLADES_CANAL_WATER.DAT and EVERGLADES_NONFISH.DAT, respectively.

The project EX_EVERGLADES_HG_HOLES simulates the growth, population, and MeHg dynamics of fish in an Everglades alligator hole community using the project file EVERGLADES_HG_HOLES.PRJ. The fish species in these communities are assumed to be bluegill, eastern mosquitofish, Florida gar, largemouth bass, least killifish (*Heterandria formosa*), redear sunfish, spotted sunfish (*Lepomis puntatus*), warmouth (*Lepomis gulosus*), and yellow bullheads. The project's CMM file and associated FSH files are generated by BASS_FILES.EXE using the input file EVERGLADES_HOLES_SPECIES.DAT. The alligator hole's water depth and non-fish biomasses are assigned in the project and community files EVERGLADES_HG_HOLES.PRJ and EVERGLADES_HG_HOLES.CMM, respectively. Lastly, MeHg exposures and properties are assigned by the include file EVERGLADES_MERCURY.CHM.

The project EX_EVERGLADES_HG_MARSH simulates the growth, population, and MeHg dynamics of fish in an Everglades marsh community using the project file EVERGLADES_HG_MARSH.PRJ. The fish species in these communities are assumed to be bluefin killifish (*Lucania goodei*), eastern mosquitofish, Florida gar, golden topminnow (*Fundulus chrysotus*), largemouth bass, least killifish, spotted sunfish, warmouth, and yellow bullheads. The project's CMM file and FSH files are generated by BASS_FILES.EXE using the input file EVERGLADES_MARSH_SPECIES.DAT. The marsh's

water depth and non-fish biomasses are assigned by the project and community files EVERGLADES_HG_MARSH.PRJ and EVERGLADES_HG_MARSH.CMM, respectively. The community's MeHg exposures are provided by the include file EVERGLADES_MERCURY.CHM.

The project EX_L_HARTWELL simulates the growth and population dynamics of fish in the Twelve-Mile Creek arm of Lake Hartwell, SC, USA which was contaminated by the Sangamo Weston Superfund site in Pickens, SC (USEPA 1994). The fish species simulated by this project are bluegill, channel catfish (*Ictalurus punctatus*), common carp (*Cyprinus carpio*), gizzard shad (*Dorosoma cepedianum*), largemouth bass, redbreast sunfish (*Lepomis auritus*), threadfin shad (*Dorosoma petenense*), and yellow perch (*Perca flavescens*). The project's CMM file and associated FSH files are generated by BASS_FILES.EXE using the input file TWELVEMILE_CREEK_SPECIES.DAT.

The project EX_L_HARTWELL_PCB simulates the growth, population, and polychlorinated biphenyl (PCB) dynamics of fish in the Twelve-Mile Creek arm of Lake Hartwell, SC, USA which was contaminated by the Sangamo Weston Superfund site in Pickens, SC (USEPA 1994). This project uses the same CMM file and associated FSH files as does the project EX_L_HARTWELL. Total PCBs are modeled as the sum of tetra-, penta-, hexa-, and hepta-PCB homologs. Exposure concentrations and chemical properties of these PCB homologs are provided by the include files TWELVEMILE_CREEK.CHM \PROPERTY\PCB_TETRA.PRP, \PROPERTY\PCB_PENTA.PRP, \PROPERTY\PCB_HEXA.PRP, and \PROPERTY\PCB_HEPTA.PRP, respectively. This project demonstrates BASS's ability to simulate the bioaccumulation of chemical mixtures.

The project EX_L_HARTWELL_PCB_TRANS simulates the bioaccumulation of tetra-PCB by fish in the Twelve-Mile Creek arm of Lake Hartwell assuming that tetra-PCB can be metabolized by bluegill, channel catfish, common carp, and largemouth bass. This project, however, is a contrived example that is intended only to demonstrate how BASS simulates the biotransformation of organic chemicals.

The project EX_L_ONTARIO_PCB simulates the bioaccumulation of tetra-, penta-, hexa-, and hepta-PCBs in Lake Ontario salmonids and alewife using the FGETS option and the project file BARBER_ET_AL_1991.PRJ. This project is a BASS implementation of the FGETS application published by Barber et al. (1991). Whereas salmonid feeding is simulated using BASS's Holling feeding option, the feeding by alewife is simulated using BASS's clearance feeding option.

The project EX_SE_FARM_POND simulates the growth and population dynamics of a typical southeastern US farm pond community using the project file SE_FARM_POND.PRJ. The principal fish species in these communities are assumed to be bluegill, channel catfish, largemouth bass, and redear sunfish. The project's CMM file and FSH files are generated by BASS_FILES.EXE using the input file SE_FARM_POND_SPECIES.DAT. The resulting community file SE_FARM_POND.CMM assigns not only the ecological and physiological parameters and the initial conditions for these fishes but also the biomasses of benthos, periphyton, and zooplankton.

The project EX_SE_FARM_POND_XMS simulates the growth, population, and pesticide bioaccumulation dynamics of a typical southeastern US farm pond community using the project file SE_FARM_POND_XMS.PRJ. The project's CMM file and FSH files are identical to those used by the project EX_SE_FARM_POND. The project's pesticide exposure file was generated by the USEPA's Office of Pesticide Programs using the EXAMS fate and transport model (Burns 2004). The identify of this pesticide is not specified since this project was designed only to illustrate the functionality of an EXAMS-BASS file transfer linkage.

6.2. Simulating Methylmercury Bioaccumulation in an Everglades Fish Community

The BASS example project EX_EVERGLADES_CANAL_HG simulates methylmercury contamination in a canal fish community of the Florida Everglades and is constructed as outlined in Section 4.5. For this application bluegill, eastern mosquitofish, Florida gar, largemouth bass, redear sunfish, and yellow bullhead are assumed to be the dominant species in the habitats of interest. The ecological, morphological, and physiological parameters used by this example are documented in the project's associated FSH files. Turner et al. (1999) reported the mean biomass of large and small fishes across various Everglades habitats to be approximately 60 kg wet wt/ha. Initial biomasses of bluegill, eastern mosquitofish, Florida gar, largemouth bass, redear sunfish, and yellow bullhead were assigned to be 50, 5, 10, 5, 25, and 10 kg wet wt/ha, respectively, for a total community biomass of 105 kg wet wt/ha. The dissolved water concentration of MeHg for the simulation was assigned to be a constant 0.2 ng/L (Stober et al. 1998) and the BAF's for benthos and zooplankton were assigned to be $10^{6.09}$ and $10^{5.90}$, respectively (Loftus et al. 1998). The simulation's length was set to be 24 years which allowed transient dynamics associated with assumed initial conditions to dissipate and a dynamic steady state to be approximated (see Barber et al. 2016).

Figure 6.1 displays the simulated time dynamics of each fish species in this Everglades canal community. During the final year of the simulation, the mean annual biomasses of bluegill, eastern mosquitofish, Florida gar, largemouth bass, redear sunfish, and yellow bullhead were 37.7, 3.94, 19.3, 9.22, 25.0, and 9.18 kg wet wt/ha, respectively, for a total community biomass of 104 kg wet wt/ha.

Figure 6.2 displays the time dynamics of each species' average daily MeHg concentration which is weighted by the species' cohort densities. During the final year of the simulation, the mean annual MeHg concentrations for bluegill, eastern mosquitofish, Florida gar, largemouth bass, redear sunfish, and yellow bullhead were 0.195, 0.160, 0.456, 0.314, 0.224, and 0.196 mg/kg wet wt, respectively. These simulated concentrations are intermediate to observed concentrations reported for the Everglades National Park (ENP) and the Everglades Water Conservation Areas (WCAs). Data reported by Loftus et al. (1998) for the ENP yield average concentrations of total mercury (T-Hg) in bluegill, eastern mosquitofish, Florida gar, largemouth bass, redear sunfish, and yellow bullhead equal to 0.550, 0.313, 1.20, 0.967, 0.247, and 0.547 mg/kg wet wt, respectively. Julian et al. (2015) report that T-Hg concentration of sunfish, sampled across the ENP and WCAs from 1999 to 2014, averaged 0.18 mg/kg wet wt (SD=0.16; n=3440). Julian et al. (2015) also report that the median T-Hg concentration of eastern mosquitofish, sampled across the ENP and WCAs for the same period of record, was 0.06 mg/kg wet wt (n=685). Lastly, Julian et al. (2015) report that the median T-Hg concentration of largemouth bass, sampled across the ENP and WCAs from 1989 to 2014, was 0.54 mg/kg wet wt (n=4991). Regarding the results reported by Julian et al. (2015), readers should note that whereas the median and mean concentrations for eastern mosquitofish and sunfish, respectively, are based on whole-body data, the median concentration for largemouth bass is based on filet data. Using the filet to whole-body conversion regression of Peterson et al. (2007), the median whole-body T-Hg concentration of largemouth bass would be estimated to be 0.322 mg/kg wet.

6.3. Simulating PCB Bioaccumulation in a Fish Community Impacted by a Superfund Site

The project EX_L_HARTWELL_PCB simulates the growth, population, and polychlorinated biphenyl (PCB) dynamics of fish in the Twelve-Mile Creek arm of Lake Hartwell, SC which was contaminated by the Sangamo Weston Superfund site in Pickens, SC (USEPA 1994). The fish species simulated by this project are bluegill, channel catfish, common carp, gizzard shad, largemouth bass, redbreast sunfish, redear sunfish, threadfin shad, and yellow perch. Total PCBs are modeled as the sum of tetra-, penta-, hexa-, and hepta-PCB homologs. The ecological, morphological, and physiological parameters used by this example are documented in the project's associated FSH files. Using data from Lake Hartwell fish surveys conducted by the Georgia Department of Natural Resources in 1987, 1990, and 1995, initial biomasses of bluegill, channel catfish, common carp, gizzard shad, largemouth bass, redbreast sunfish, threadfin shad, and yellow perch were assumed to be 23.9, 4.26, 17.2, 16.3, 8.77, 2.98, 20.8, and 2.70 kg wet wt/ha, respectively, for a total community biomass of 96.8 kg wet wt/ha. The community's carrying capacity was assumed to be three times its estimated initial biomass. The dissolved water concentrations of tetra-, penta-, hexa-, and hepta-PCB were back-calculated using their average concentrations in Twelve-Mile Creek crayfish (*Procambarus* spp.) reported by Brockway et al. (1996) and BAFs predicted by the KABAM steady-state bioaccumulation model (Garber 2009). BAFs for benthos, periphyton, phytoplankton, and zooplankton were assigned to be their KABAM-predicted counterparts. The length of this simulation was set to be 24 years which allowed for transient dynamics associated with assumed initial conditions to dissipate and for a dynamic steady state to be approximated (see Barber et al. 2016).

Figure 6.3 displays the simulated biomass dynamics of each fish species in this Twelve-Mile creek community. During the final year of the simulation, the mean annual biomasses of bluegill, channel catfish, common carp, gizzard shad, largemouth bass, redbreast sunfish, threadfin shad, and yellow perch were 64.7, 9.14, 43.1, 38.0, 24.1, 6.87, 21.6, and 7.73 kg wet wt/ha, respectively, for a total community biomass of 215 kg wet wt/ha.

Figure 6.4 displays the time dynamics of each species' average daily total PCB concentration which is weighted by the species' cohort densities. During the simulation's final year, the mean annual total PCB concentrations for bluegill, channel catfish, common carp, gizzard shad, largemouth bass, redbreast sunfish, threadfin shad, and yellow perch were 22.9, 16.9, 20.2, 33.7, 32.5, 5.16, 20.5, and 30.6 mg/kg wet wt, respectively. Although data reported by Brockway et al. (1996) yield average observed concentrations of total PCBs in bluegill, channel catfish, and largemouth bass equal to 9.96 (SD=8.52; n=42), 8.05 (SD=5.85; n=14), and 21.4 (SD=15.9; n=21) mg/kg wet wt, respectively, direct comparisons between these observed and simulated concentrations are difficult due to the range and distribution of body weights within each dataset and due to that fact that the observed concentrations include three lake sites and two creek sites which could not be sampled equally well.

Figures 6.5, 6.6, and 6.7 display the time dynamics of total

PCB concentrations of bluegill, channel catfish, and largemouth bass, respectively, plotted by year classes. Considering only sampled and simulated fish having comparable body weights, the ranges of observed and simulated concentrations (mg/kg wet wt) for bluegill are 0.965-45.9 and 1.15-24.8, respectively. Similarly, ranges of observed and simulated concentrations (mg/kg wet wt) for channel catfish are 1.15-23.1 and 0.562-18.8, respectively, and the ranges of observed and simulated concentrations (mg/kg wet wt) for largemouth bass are 1.72-64.7 and 0.651-33.5, respectively.

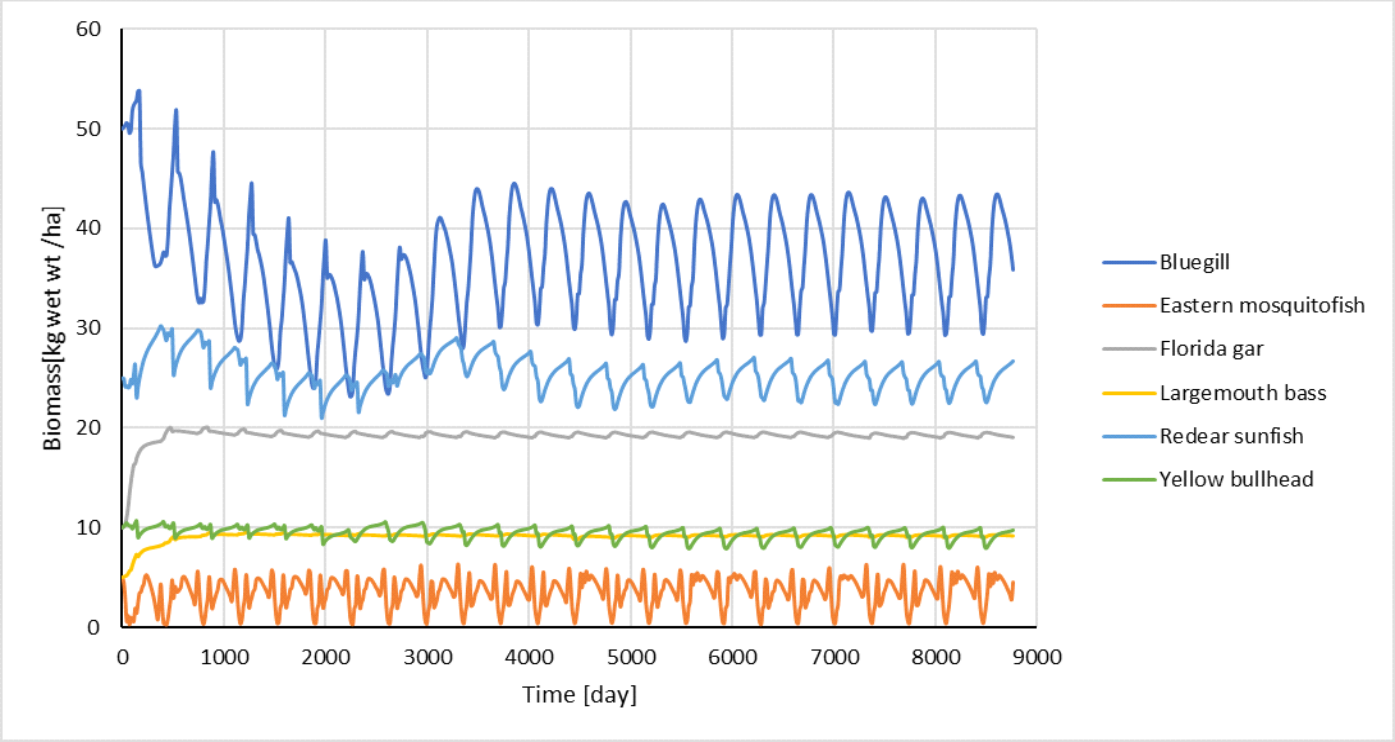


Figure 6.1 Simulated biomasses (kg wet wt/ha) of fishes in an Everglades canal.

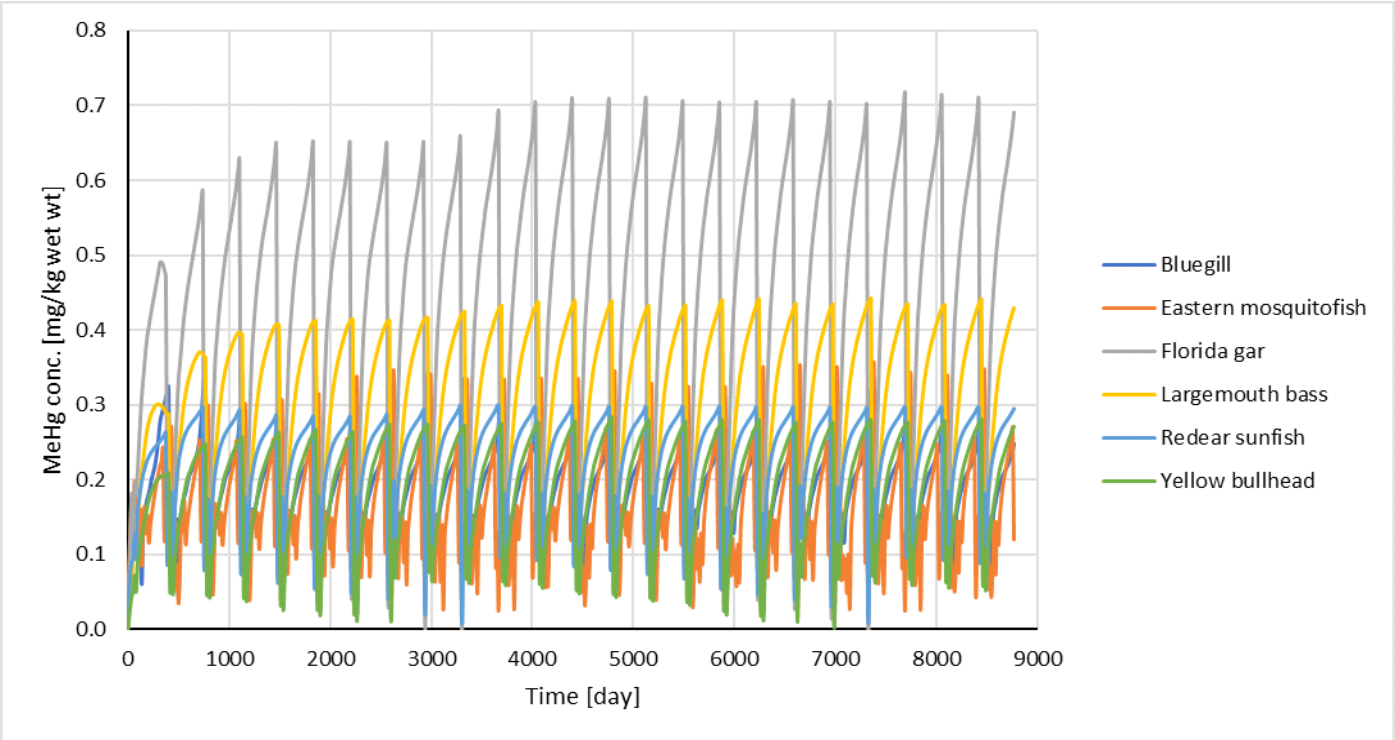
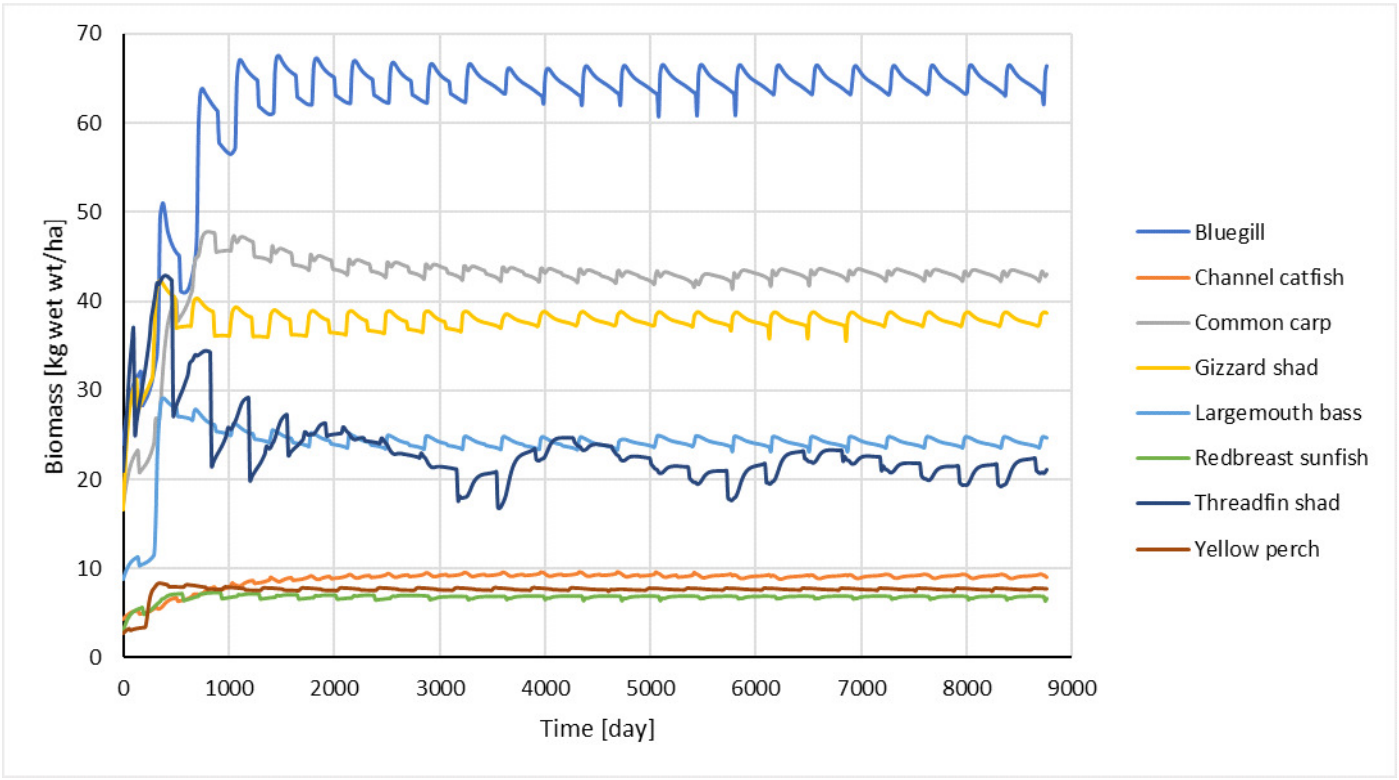


Figure 6.2 Simulated MeHg concentrations (mg/kg wet wt) of fishes in an Everglades canal.

Figure 6.3 Simulated biomasses (kg wet wt/ha) of fishes in Twelve-Mile Creek, SC.



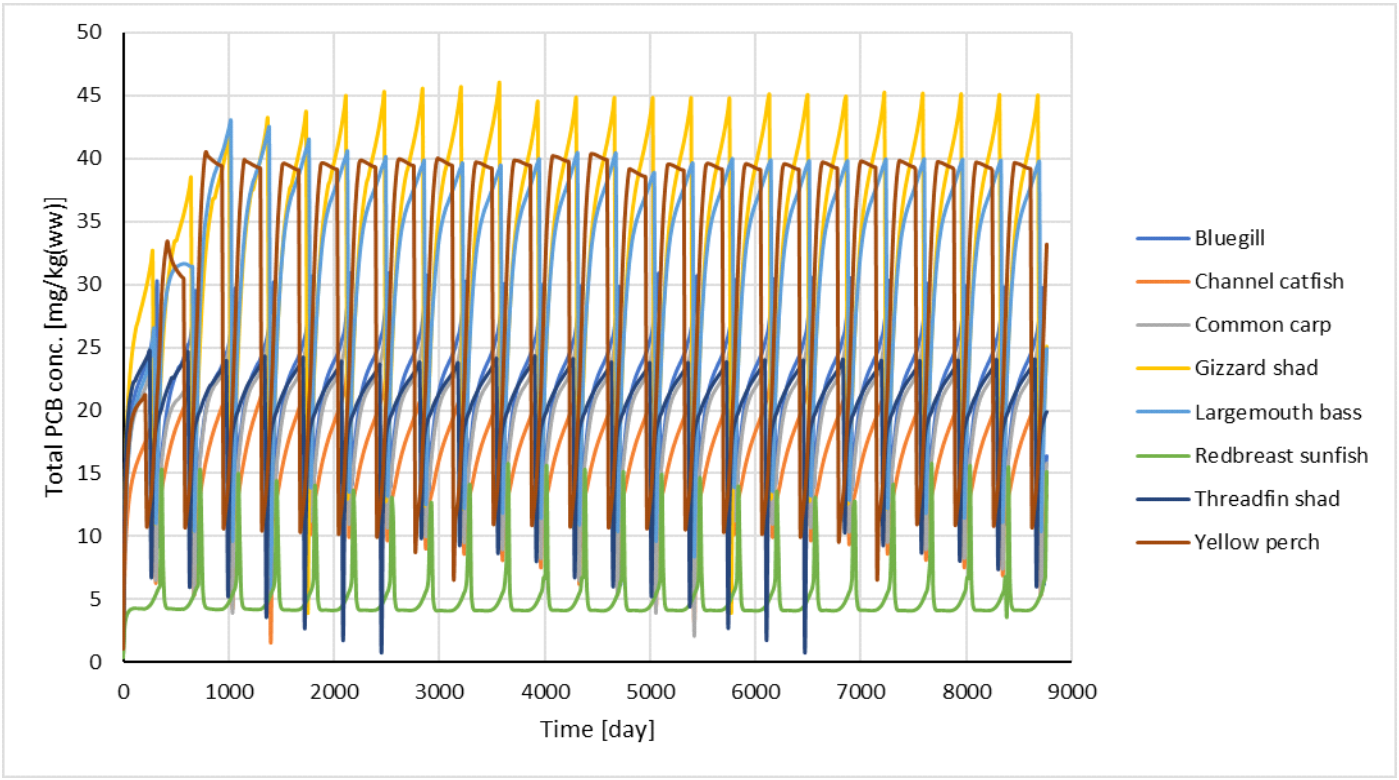


Figure 6.4 Simulated total PCB concentrations (mg/kg wet wt) of fishes in Twelve-Mile Creek, SC.

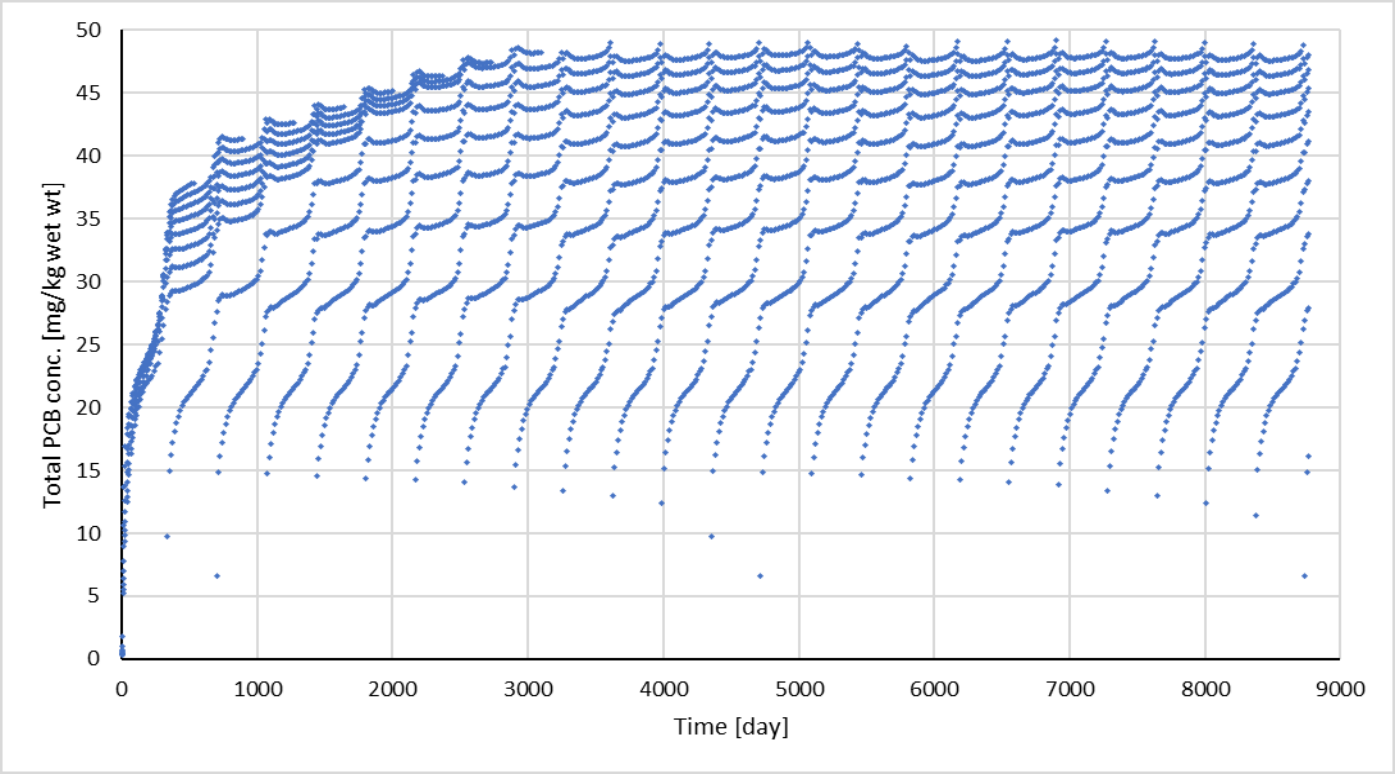


Figure 6.5 Simulated total PCB concentrations (mg/kg wet wt) of Bluegill by year class in Twelve-Mile Creek, SC.

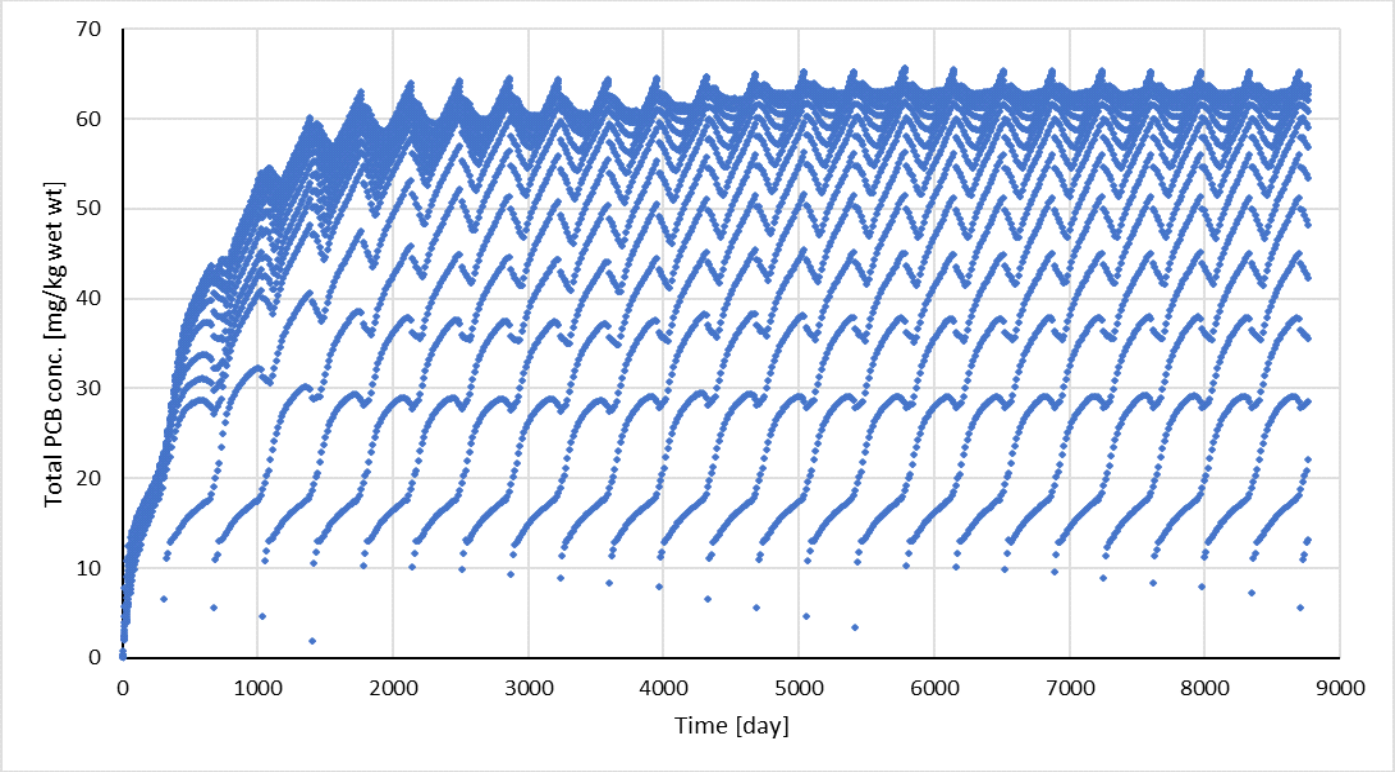


Figure 6.6 Simulated total PCB concentrations (mg/kg wet wt) of Channel catfish by year class in Twelve-Mile Creek, SC.

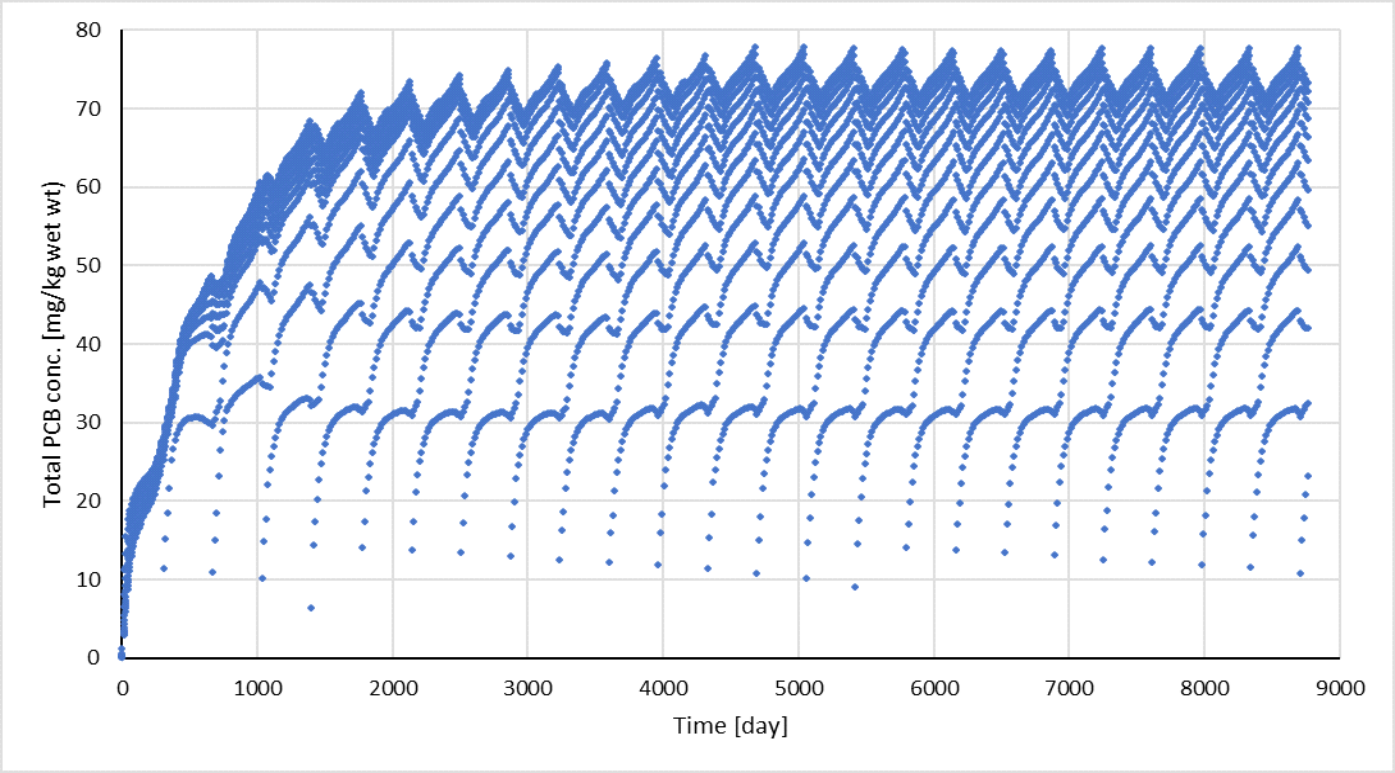


Figure 6.7 Simulated total PCB concentrations (mg/kg wet wt) of Largemouth bass by year class in Twelve-Mile Creek, SC.

7. Model Quality Assurance

Quality Assurance (QA) and Quality Control (QC) for the BASS simulation model have been addressed with respect to:

1. The model's theoretical foundations, i.e., does the model's conceptual and mathematical framework standup to scientific / engineering peer view?
2. The model's implementation, i.e., does the code actually do what it is intended to do?
3. The model's documentation and application, i.e., can the model be used by the outside research and regulatory community in a meaningful way?

7.1. Questions Regarding QA of a Model's Scientific Foundations

7.1.1. Is the model's theoretical foundation published in the peer reviewed literature?

With the exception of its population and trophodynamic algorithms, BASS is based on the FGETS bioaccumulation and bioenergetics model that has been published in the peer reviewed literature (Barber et al. 1988, 1991). These algorithms have been reviewed and compared to other bioaccumulation models to document their scientific foundation and to verify their predictive performance (see Barber 2003, 2008). The bioenergetic modeling paradigm that BASS uses to simulate fish growth has been employed by many researchers in the peer-reviewed literature (Norstrom et al. 1976, Kitchell et al. 1977, Minton and McLean 1982, Stewart et al. 1983, Thomann and Connolly 1984, Cuenco et al. 1985, Stewart and Binkowski 1986, Beauchamp et al. 1989, Barber et al. 1991, Stewart and Ibarra 1991, Lantry and Stewart 1993, Rand et al. 1993, Roell and Orth 1993, Hartman and Brandt 1995a, Petersen and Ward 1999, Rose et al. 1999, Schaeffer et al. 1999). Since their construction, BASS and FGETS have been included in numerous reviews and discussions of aquatic bioaccumulation models (Chapra and Boyer 1992, Olem et al. 1992, Dixon and Florian 1993, Cowan et al. 1995, Campfens and Mackay 1997, Feijtel et al. 1997, Exponent 1998, Howgate 1998, Vorhees et al. 1998, Wania and Mackay 1999, Mackay and Fraser 2000, Koelmans et al. 2001, Limno-Tech 2002, Nichols 2002, Barber 2003, Exponent 2003, Imhoff et al. 2004, Imhoff et al. 2005, Brooke and Crookes 2007, Barber 2008, Mackay and Milford 2008, Arnot 2009, Nichols et al. 2009, Brooke et al. 2012, EPRI 2013, Radomyski et al. 2018).

Two criticisms have been lodged against FGETS in the literature. The first of these is that FGETS attempts to prove that the gill exchange of chemicals is more important than other routes of exchange (Madenjian et al. 1993). Madenjian et al. (1993) took exception to FGETS predictions that "excretion of PCB through the gills is an important flux in the PCB budget of lake trout". Madenjian et al. claimed that this result was not supported by any laboratory study on trout and cited Weininger (1978) as proof that gill excretion was, in fact, negligible. Nevertheless, Madenjian et al. used a single, unidentified excretion constant in their model that simply lumps all excretion pathways (i.e., gill, intestinal, urinary, and dermal) into one. Thus, what Madenjian et al. are really questioning is not FGETS per se but rather the need to use thermodynamically based diffusion models for bioaccumulation in general.

The second criticism is that FGETS is overly complex and requires too much additional data to parameterize (McKim et al. 1994, Stow and Carpenter 1994, Jackson 1996). Since FGETS's bioenergetic model for fish growth is not significantly different from those used by several other authors (Norstrom et al. 1976, Weininger 1978, Thomann and Connolly 1984, Madenjian et al. 1993, Luk and Brockway 1997), this criticism is also generally aimed at BASS's gill exchange model. A recent review and comparison of gill exchange models, however, clearly demonstrated that there is more than ample literature data to parameterize the gill exchange formulations used by FGETS and BASS (Barber 2003).

7.1.2. How has the model or its algorithms been corroborated or used?

BASS's dietary and gill exchange algorithms have been corroborated by comparing its predicted dietary assimilation efficiencies and gill uptake and excretion rates to those published in the peer-reviewed literature (Barber et al. 1988, Barber 2003, 2008). BASS's dietary exchange algorithms have also been cited by other researchers to explain results of actual exposure studies (e.g., Dabrowska et al. 1996, Doi et al. 2000). For validation of BASS's bioenergetic growth algorithms, the reader is referred to Barber et al. (2016) and the examples herein.

BASS and FGETS have been used to predict the bioaccumulation of persistent bioaccumulative toxicants (PBTs) in both lakes and rivers (Barber et al. 1991, Hunt et al. 1992, USEPA 1994, PNL 1995, Panzieri and Hallam 1999, Simon 1999, Marchettini et al. 2001, Panzieri et al. 2001, Murphy 2004, Rashleigh et al. 2004, USEPA 2005, Knightes et al. 2009, Johnston et al. 2011, Knightes et al. 2012, RTI International 2013, Reese et al. 2015a, Reese et al. 2015b, Sokol 2015, Barber et al. 2016, Barber et al. 2017, Johnston et al. 2017). Additionally, both models have been cited in numerous guidance documents issued by USEPA, ECHA (The European Chemical Agency), OECD (The Organisation for Economic Co-operation and Development) and other federal agencies (USEPA 1991a, b, 1993, LaPoint et al. 1995, USEPA

1995, 1998, ECOFRAM 1999, USEPA 2000, 2003, 2006, ECHA 2008, USEPA 2008a, b, 2010, OECD 2011b, a, ECHA 2012b, a, OECD 2012b, c, a, 2013b, a, ECHA 2014a, d, c, b, 2016, OECD 2016b, a, ECHA 2017c, b, a).

Several researchers (Lassiter and Hallam 1990, ECOFRAM Aquatic Effects Subcommittee et al. 1998, ECOFRAM 1999, Boxall et al. 2001, Boxall et al. 2002, Reinert et al. 2002) have used BASS's predecessor, FGETS, to predict acute and chronic lethality, and the EPA's Office of Water's AQUATOX modeling system uses the FGETS/BASS lethal effects algorithm as its principal effects module (Park and Clough 2004). Additionally, the Office of Water recognized BASS as one of the leading models available for simulating time dynamic bioaccumulation for applications when steady-state methods (e.g., BAFs or BSAFs) are considered insufficient (USEPA 2003). The Commonwealth of Virginia identified BASS as an accepted tool for its PCB bioaccumulation assessments (VDEQ 2005). BASS has also been recommended to the states of Michigan and Washington as an assessment tool (Exponent 1998, 2003).

Hallam and Deng (2006) implemented the FGETS/BASS bioaccumulation framework within sophisticated McKendrick-von Foerster partial differential equation models for age-structured populations, and Cohen and Cooter (2002a, 2002b) incorporated simpler forms of this framework into their fate and transport exposure software. Lastly, Apeti et al. (2005) modified FGETS to simulate metal bioaccumulation in shellfish.

7.1.3. What is the mathematical sensitivity of the model with respect to parameters, state variables (initial value problems), and forcing functions / boundary conditions? What is the model's sensitivity to structural changes?

There are four major classes of mathematical sensitivity regarding a model's behavior. These are the model's sensitivity to parameter changes, forcing functions, initial state variables, and structural configuration. The first three of these classes generally are formally defined in terms of the following partial derivatives

$$\frac{\partial X_i}{\partial p_j}; \qquad \frac{\partial X_i}{\partial Z_j}; \qquad \frac{\partial X_i}{\partial X_j(0)} \tag{7.1}$$

where X_i is a state variable of interest; p_j is some state parameter of concern; Z_j is some external forcing function; and $X_j(0)$ is the initial value of some state variable of interest that may be X_i itself. Structural sensitivity, which generally cannot be formulated as a simple partial derivative, typically concerns the number and connectivity between the system's state variables. An excellent question regarding structural sensitivity for a model like BASS might be how does a predator's population numbers or growth rate change with the introduction or removal of new or existing prey items?

Because sensitivity is simply a mathematical characteristic of a model, model sensitivity in and of itself is neither good nor bad. Sensitivity is desirable if the real system being modeled is itself sensitive to the same parameters, forcing functions, initial state perturbations, and structural changes to which the model is sensitive. Even though model sensitivity can contribute to undesirable model uncertainty or prediction error, it is important to acknowledge that model sensitivity and uncertainty are not one and the same (Summers et al. 1993, Wallach and Genard 1998). Model uncertainty, or at least one of its most common manifestations, is the product of both the model's sensitivity to particular components and the statistical variability associated with those components.

A generalized sensitivity analysis of BASS without explicit specification of a fish community of concern is infeasible. Furthermore, the results of a sensitivity analysis for one community generally cannot be extrapolated to other communities. Issues related to BASS's sensitivity must be evaluated on a case-by-case basis.

7.2. Questions Regarding QA of a Model's Implementation

7.2.1. Did the input algorithms properly process all user input?

As part of its routine output, BASS generates a *.MSG file that summarizes all input data used for a particular simulation. This summary includes not only a line by line summary of the user's input commands but also a complete summary of all control, chemical and fish parameters that BASS assigned based on the user's specified input file(s). The onus is on the user to verify that their input data has been properly processed. If not, the user should report their problem to the technical contact identified in the BASS user's guide.

BASS has a series of subroutines that check for the completeness and consistency of the user's input data. When missing or inconsistent data are detected, error messages are written to the *.MSG file, and an error code is set to true. If this error code is true after all input has been processed, BASS terminates without attempting further execution.

To insure that all program subroutines, functions, and procedures are transmitting and receiving the correct variables, all BASS subroutines and functions are called using implicit interfaces generated by the Absoft and Lahey-Fujitsu Fortran 95 compilers. Subroutines and functions are packaged together within Fortran 95 modules according to their function and degree of interaction. The BASS v2.3 software is coded with one main program PROGRAM BASS_MAIN (see BASS_PROGRAM.F90) and 30

procedure modules. These modules are:

- MODULE ADAMS_GEAR - subroutines for performing EXAMS Adams-Gear integrations (see EXAMS_ADAM_GEAR.F90).
- MODULE BASS_ALLOC - subroutines for allocating and reallocating derive type pointers (see BASS_ALLOC.F90).
- MODULE BASS_CHECK - subroutines for checking the completeness and consistency of user input (see BASS_CHECK.F90).
- MODULE BASS_DEBUG - subroutines for program debugging. Used only for program development (see BASS_DEBUG.F90).
- MODULE BASS_DEFINED - functions for determining whether program parameters and variables have been initialized or assigned (see BASS_DEFINED.F90).
- MODULE BASS_EXP - subroutines for calculating chemical exposures, community forcing functions, and habitat suitability multipliers (see BASS_EXP.F90).
- MODULE BASS_INI - subroutines for initialization of program variables (see BASS_INI.F90).
- MODULE BASS_INPUT - subroutines for decoding user input (see BASS_INPUT.F90).
- MODULE BASS_INT - subroutines for Adams-Gear, Euler, and Runge-Kutta integrations (see BASS_INT.F90).
- MODULE BASS_INT_LOADER - subroutines for loading BASS derived type variables into standard integration vectors (see BASS_INT_LOADER.F90).
- MODULE BASS_IO - subroutines for processing user input and output (see BASS_IO_*.F90 for the Absoft and Lahey-Fujitsu compilers).
- MODULE BASS_ODE - subroutines for the computational kernel of the BASS software (see BASS_ODE.F90).
- MODULE BASS_TABLES - subroutines for generating output tables for BASS v2.1 and earlier as well as for code development and maintenance (see BASS_TABLES.F90).
- MODULE BASS_WRITE_CSV - subroutines for generating CSV output files for import into Excel workshets (see BASS_CSV.F90).
- MODULE BASS_WRITE_XML - subroutines for generating XML output files for post processing by the BASS GUI (see BASS_XML.F90).
- MODULE DECODE_FUNCTIONS - subroutines for decoding constant, linear, and power functions from character strings (see UTL_DCOD_FNC.F90).
- MODULE ERROR_MODULE - subroutines for printing error codes encountered with general utility modules (see UTL_ERRORS_V2.F90).
- MODULE F2KCLI - subroutines for extracting arguments from a command line (see F2KCLI.F90).
- MODULE FILESTUFF - subroutines for parsing file names and obtaining version numbers or time stamps (see UTL_FILESTUFF_V2_*.F90 for the Absoft and Lahey-Fujitsu compilers).
- MODULE FLOATING_POINT_COMPARISONS - operators for testing equality or inequality of variables with explicit consideration of their computer representation and spacing characteristics (see UTL_FLOATCMP.F90).
- MODULE GETNUMBERS - subroutines for extracting numbers from character strings (see UTL_GETNUMS.F90).
- MODULE IOSUBS - subroutines for assigning, opening, and closing logical units (see UTL_IOSUBS_V2.F90).
- MODULE MODULO_XFREAD - subroutines for reading files that contain comments, continuation lines, and include files (see UTL_XFREAD_V2_*.F90 for the Absoft and Lahey-Fujitsu compilers).
- MODULE MSORT - subroutines for sorting and generating permutation vectors for lists and vectors (see UTL_MSORT.F90).
- MODULE REALLOCATER - subroutines for allocating and reallocating integer, logical, and real pointers (see UTL_ALLOC.F90).
- MODULE SEARCH - subroutines for finding the location of a key phrase within a sorted list (see UTL_SEARCH_V2.F90).
- MODULE SEARCH_LISTS - subroutines for finding the location of a value within a sorted list (see UTL_SEARCH_LISTS.F90).
- MODULE STRINGS - subroutines for character string manipulations and printing multiline character text (see UTL_STRINGS_*.F90 for the Absoft and Lahey-Fujitsu compilers).
- MODULE TABLE_UTILS - subroutines for generating self-formating tables (see UTL_PTABLE.F90).
- MODULE UNITSLIBRARY - subroutines for defining and performing units conversions (see UTL_UNITSLIB_*.F90 for the Absoft and Lahey-Fujitsu compilers).

In general, these procedure modules are coded with minimal scoping units. Consequently, their component subroutines and functions explicitly initialize all required internal variables. This safeguard prevents inadvertent use of uninitialized variables. Whenever possible, subroutine and function arguments are declared with INTENT(IN) and INTENT(OUT) declarations to preclude unintentional reassignments.

Although global constants and Fortran parameters are supplied to program procedures via modules (see question 7.2.3), data exchanges between program procedures are performed via formal subroutine / function parameters whenever possible. The only notable exceptions to this coding policy are modules that must be used to supply auxiliary parameters to "external" subroutines that are used as arguments to certain mathematical subroutines (e.g., root finding subroutines). Working areas used by BASS are not

used for data transfers between internal and external procedures.

To simplify the construction and maintenance of the formal parameter lists of many BASS subroutines and functions and to prevent the inadvertent transposition of formal parameters, BASS makes extensive use of derived type data structures. Each derived type definition is specified within its own module, and all derive type definition modules are maintained in a single file (BASS_TYPES.F90.) Derived types used by BASS v2.3 are:

- MODULE BASS_TYPE_CHEM_PAR - type definition for chemical parameters
- MODULE BASS_TYPE_DIET_MEAN - type definition used to summarize average realized diets.
- MODULE BASS_TYPE_DIET_PAR - type definition used by derived type BASS_TYPE_FOODWEB_PAR
- MODULE BASS_TYPE_DIETS - type definition used for input processing of user-specified fish diets
- MODULE BASS_TYPE_FISH_INT - type definition for integrated fish variables and fluxes
- MODULE BASS_TYPE_FISH_PAR - type definition for fish parameters
- MODULE BASS_TYPE_FISH_VAR - type definition for current fish variables and fluxes
- MODULE BASS_TYPE_FOODWEB_PAR - type definition for the decoded user-specified fish diets and community trophic structure.
- MODULE BASS_TYPE_HSI_PAR - type definition for fish habitat multipliers
- MODULE BASS_TYPE_NONFISH_INT - type definition for integrated non-fish variables and fluxes
- MODULE BASS_TYPE_NONFISH_PAR - type definition for non-fish parameters
- MODULE BASS_TYPE_NONFISH_VAR - type definition for current non-fish variables and fluxes
- MODULE BASS_TYPE_PREY_ITEMS - type definition used by derived type BASS_TYPE_FISH_VAR to store a fish's currently realized dietary composition
- MODULE BASS_TYPE_QSAR_DATA - type definition for linked list used during data input
- MODULE BASS_TYPE_QSAR_LINKED_LIST - type definition for linked list used during data input
- MODULE BASS_TYPE_QSAR_NODE - type definition for linked list used during data input
- MODULE BASS_TYPE_TROPHIC - definition used for the calculation of realized diet composition and consumption
- MODULE BASS_TYPE_VMATRIX_LOGICAL - type definition for logical matrices having rows with varying number of columns.
- MODULE BASS_TYPE_VMATRIX_REAL - type definition for for real matrices having rows with varying number of columns.
- MODULE BASS_TYPE_ZFUNCTION_PAR - type definition for user-specified exposure and forcing functions

A good example of BASS's use of derived type data structures is the derived type variable used to store and transfer the ecological, physiological, and morphometric data for a particular fish species. This derived type is defined by the following module

```
MODULE bass_type_fish_par
USE bass_type_hsi_par
TYPE:: fish_par
   CHARACTER (LEN=80) :: ageclass, ast_type, ast_var, common_name, &
      fmodel_var, genus_species, spawning_interval, temp_var
   INTEGER :: fmodel_cls=0, harvests=0, spawnings=0, &
      stockings=0, temperatures=0
   INTEGER,DIMENSION(:),POINTER:: fmodel=>NULL()
   INTEGER,DIMENSION(:),POINTER:: spawn_dates=>NULL()
   INTEGER,DIMENSION(:),POINTER:: harvest_date1=>NULL()
   INTEGER,DIMENSION(:),POINTER:: harvest_date2=>NULL()
   INTEGER,DIMENSION(:),POINTER:: stock_dates=>NULL()
   LOGICAL :: bb_constant=.TRUE., prey_switching_on=.TRUE.
   REAL :: ae_fish, ae_invert, ae_plant, ast_bb, ast_bnds, ast_pop, &
      biomass_cc, dry2live_ab, dry2live_aa, dry2live_bb, dry2live_cc, &
      gco2_d, kf_min, la, longevity, mgo2_s, rbi, refugia, rq, rt2std, &
      sda2in, tl_r0, wt_max, yoy
   REAL, DIMENSION(2) :: ga, id, ld, ll, lw, pa, pl, sg_mu, wl
   REAL, DIMENSION(3) :: nm
   REAL, DIMENSION(4) :: lp, lp_max, lp_min
   REAL, DIMENSION(5) :: ge, mf, mi, sg, sm, so, st
   REAL, DIMENSION(:), POINTER :: fmodel_bnds=>NULL()
   REAL, DIMENSION(:), POINTER :: harvest_len1=>NULL()
   REAL, DIMENSION(:), POINTER :: harvest_len2=>NULL()
   REAL, DIMENSION(:), POINTER :: harvest_rate=>NULL()
   REAL, DIMENSION(:), POINTER :: stock_age=>NULL()
   REAL, DIMENSION(:), POINTER :: stock_rate=>NULL()
   REAL, DIMENSION(:), POINTER :: stock_tl=>NULL()
   REAL, DIMENSION(:), POINTER :: stock_wt=>NULL()
   REAL, DIMENSION(:), POINTER :: temp_bnds=>NULL()
   REAL, DIMENSION(:), POINTER :: temp_pref=>NULL()
   TYPE(hsi_par) :: hsi_feed, hsi_persist, hsi_recruit
END TYPE fish_par
END MODULE bass_type_fish_par
```

Many components of this derived type are user input parameters that have already been discussed. For example, the array ga(2) stores the coefficient and exponent of a species' gill area function (see /MORPHOMETRIC_PARAMETERS page 49). Other components are secondary parameters that are calculated from the user's input data. For example, dry2live_ab, dry2live_aa, dry2live_bb, and dry2live_cc are constants that are used to calculate a fish's wet weight from its dry weight (see introduction to Section 2.6. Modeling Growth of Fish). Using a declaration of the form

```
TYPE(fish_par), DIMENSION(nspecies) :: par
```

all data defined by the above derived type can be passed to a BASS subroutine by the simple calling statement

CALL sub1(...., par, ...)

without fear of data misalignment.

To insure that all program subroutines, functions, and procedures use the same global constants or parameters, such constants are declared and defined within a set of 15 data modules. These modules include:

- MODULE ADAM_DATA - stores control parameters for the EXAMS Adams-Gear integrators (see EXAMS_ADAM_GEAR_MODULES.F90).
- MODULE BASS_CONSTANTS - specifies various biological and physical constants used by BASS's computational subroutines (see BASS_GLOBALS.F90).
- MODULE BASS_GRAETZ - specifies parameters used to calculate chemical exchange across the fish gills (see BASS_GLOBALS.F90).
- MODULE BASS_IOFILES - specifies logical unit numbers for input and output devices (see BASS_GLOBALS.F90).
- MODULE BASS_NAMES - stores user-specified fish and chemical names (see BASS_GLOBALS.F90).
- MODULE BASS_NOVALUE - specifies values for integer, real, and character variables that have not been initialized (see BASS_GLOBALS.F90).
- MODULE BASS_PRECISION - specifies the precision of floating point variables as either single, double, or quad precision variables. (see BASS_GLOBALS.F90).
- MODULE BASS_UNITS - specifies unit conversion factors that are specific to BASS for use by MODULE UNITSLIBRARY (see BASS_UNITS.F90).
- MODULE BASS_WORKING_DIMENSIONS - specifies "standard" sizes for character variables, input records, etc. (see BASS_GLOBALS.F90).
- MODULE CONSTANTS - constants used by utility subroutines (see UTL_CONSTANTS.F90).
- MODULE GEAR_DATA - stores control parameters for the EXAMS Adams-Gear integrators (see EXAMS_ADAM_GEAR_MODULES.F90).
- MODULE LOCAL_GEAR_DATA - stores control parameters for the EXAMS Adams-Gear integrators (see EXAMS_ADAM_GEAR_MODULES.F90).
- MODULE STEP_DATA - stores control parameters for the EXAMS Adams-Gear integrators (see EXAMS_ADAM_GEAR_MODULES.F90).
- MODULE STIFF_DATA - stores control parameters for the EXAMS Adams-Gear integrators (see EXAMS_ADAM_GEAR_MODULES.F90).
- MODULE UNITS_PARAMETERS - specifies parameters used by the units conversion subroutines (see UTL_UPARAMS.F90)

BASS v2.3 uses the following modules (see BASS_WORK_AREAS.F90) to define work areas that are common to two or more functions or subroutines:

- MODULE BASS_CPU_PERFORMANCE
- MODULE BASS_FOODWEB_WORK_AREA
- MODULE BASS_HSI_MEANS
- MODULE BASS_MULTISORT_WORK_AREA
- MODULE BASS_ODE_WORK_AREA
- MODULE BASS_OUTPUT_WORK_AREA

7.2.3. Is the developer reasonably confident that all program subroutines, functions, and procedures are using the same global constants or parameters?

All global constants are defined within their own individual modules. These modules include:

- MODULE BASS_CONSTANTS - constants used by BASS's computational subroutines (see BASS_GLOBALS.F90).
- MODULE BASS_NOVALUE - specifies values for integer, real, and character variables that have not been initialized (see BASS_GLOBALS.F90).
- MODULE BASS_PRECISION - specifies the precision of floating point variables as either single, double, or quad precision variables. This module also assigns certain associated floating point constants (see BASS_GLOBALS.F90).
- MODULE BASS_WORKING_DIMENSIONS - specifies "standard" sizes for character variables, input records, etc. (see BASS_GLOBALS.F90).
- MODULE CONSTANTS - constants used by utility subroutines (see UTL_CONSTANTS.F90).

7.2.4. Do all strictly mathematical algorithms do what they are supposed to? For example, are root finding algorithms functioning properly?

During execution, BASS must employ root finding algorithms for two important types of calculations. The first of these is the calculation of a fish's wet weight from its dry weight given an allometric relationship between its wet body weight and its fraction lipid, and linear relationships between its moisture, lipid, and non-lipid organic matter fractions. The second type of calculation involves the linear transformation of unconditioned dietary electivities into self-consistent sets of dietary electivities. These calculations are performed using the combined bisection / Newton-Raphson algorithm outlined by Press et al. (1992).

BASS integrates its governing differential equations using a fifth-order Runge-Kutta method with adaptive step sizing. This integrator is patterned on the fifth-order Cash-Karp Runge-Kutta

algorithm outlined by Press et. al. (1992) and was tested using the following system of equations:

$$
\begin{aligned}
dy_1/dx &= 1.0 \\
dy_2/dx &= x \\
dy_3/dx &= \cos(x) \\
dy_4/dx &= \cosh(x) \\
dy_5/dx &= \exp(x) \\
dy_6/dx &= 1.0/(1.0 + x) \\
dy_7/dx &= 1.0/(1.0 + x^2) \\
dy_8/dx &= 1.0/\sqrt{1.0 + x^2} \\
dy_9/dx &= -100\,(y_9 - \sin(x)) \qquad y_9(0) = 1 \\
du/dx &= 998\,u + 1998\,v \qquad u(0) = 1 \\
dv/dx &= -999\,u - 1999\,v \qquad v(0) = 0
\end{aligned}
\tag{7.2}
$$

The analytical solution to this system of equations is

$$
\begin{aligned}
y_1 &= x - x_0 \\
y_2 &= 0.5\,(x^2 - x_0^2) \\
y_3 &= \sin(x) - \sin(x_0) \\
y_4 &= \sinh(x) - \sinh(x_0) \\
y_5 &= \exp(x) - \exp(x_0) \\
y_6 &= \ln(1 + x) - \ln(1 + x_0) \\
y_7 &= \arctan(x) - \arctan(x_0) \\
y_8 &= asinh(x) - asinh(x_0) \\
y_9 &= \frac{10101}{10001}\exp(-100\,x) \\
&\quad - \frac{100}{10001}\cos(x) + \frac{10000}{10001}\sin(x) \\
u &= 2\exp(-x) - \exp(-1000\,x) \\
v &= -\exp(-x) + \exp(-1000\,x)
\end{aligned}
\tag{7.3}
$$

On the interval [0<x<10], the above solutions range in value from v=0.453999E-04 to y_5=0.220255E+05. Besides their large numerical range, the last three equations in this system are numerically stiff (Press et al. 1992, Ascher and Petzold 1998). When integrated on the interval [0<x<10], the ratio of the numerical solutions and the corresponding analytical solutions equaled unity with an absolute error of $<10^{-6}$.

BASS's Runge-Kutta algorithm has also been compared to the adaptive Adams-Gear algorithm employed by the widely used EXAMS fate and transport model. These comparisons demonstrated that BASS's Runge-Kutta algorithm was not only as accurate as the EXAMS Adams-Gear algorithm but was also computationally faster.

7.2.5. Are mathematical algorithms implemented correctly, i.e., are the assumptions of the procedure satisfied by the problem of interest?

Because BASS is a differential equation model, a question of paramount concern is how its integration between points of discontinuity / nondifferentiability is controlled. Like many ecological models, BASS utilizes threshold responses, absolute value functions, maximum and minimum functions, and linear interpolations between time series in its formulation and implementation. Although most BASS parameters are updated continuously, some parameters that change very slowly and that are computationally intensive to evaluate (e.g., dietary compositions) are updated only daily. All of these features create points of discontinuity or nondifferentiability. Although there is nothing intrinsically wrong with using such formulations in differential equation models, numerical integrations of such models must proceed from one point of discontinuity / nondifferentiability to another.

With these considerations in mind, BASS's computational kernels (subroutines BASS_ODESOLVR and FGETS_ODESOLVR) are designed to integrate BASS's differential equations for a single day of the desired simulation period. Immediately following the call of these computational kernels, BASS calculates the dietary composition of each fish that will be held constant for that day. The progress of the subsequent numerical integration within the day is then controlled by any condition that results in a point of nondifferentiability. The two most important conditions in this regard occur when BASS must read an exposure file to update the parameters for the linear interpolation of one or more exposure variables, or when one or more cohorts are eliminated from the community. In the latter case, BASS recalculates the dietary compositions of the remaining fish that will remain constant for the remainder of the day. Note that recruitment of new cohorts into the simulated community does not create a point of nondifferentiability for BASS since such amendments to the community's structure are performed before calling the computational kernels BASS_ODESOLVR or FGETS_ODESOLVR and, therefore, constitutes only a simple reinitialization problem.

7.2.6. Are simulated results consistent with known mathematical constraint of the model? For example, if state variables are supposed to be non-negative, are they? Similarly, if the model is supposed to mass balance, does it?

BASS's state variables, like those of most physical or biological models, must be non-negative by definition. However, insuring that the numerical integration of a differential equation model remains constrained to its appropriate state space is not a trivial issue. Consider, for example, the case when one wants to take a simple Eulerian step for a non-negative state variable that has a

negative derivative. If the state variable is to remain non-negative, then the largest allowable size for the integration step can be calculated as follows

$$y(t+h) = y(t) + h\,y'(t)$$

$$0 < y(t) + h\,y'(t) \qquad (7.4)$$

$$\frac{-y(t)}{y'(t)} > h \qquad \text{where} \quad y'(t) < 0$$

If h is greater than the numerical spacing of t (i.e., $t + h \neq t$), then an integration step is possible. If the converse is true, however, the function $y(t)$ is approximating a step function in which case the desired integration can simply be restarted with $y(t) = 0$. There are at least two situations that can occur during a BASS simulation that might necessitate this corrective action. The first can occur when a cohort experiences intense predation or other mortality that drives its population to extinction; the second can occur when there is the rapid excretion of a hydrophilic contaminant following the disappearance of an aqueous exposure. When the derivative for a fish's body weight, population density, or body burden is negative, BASS verifies whether the current integration step will, in fact, yield non-negative state values. If so, BASS executes a simple Euler step of the appropriate size and restarts the integration with the appropriate state variables initialized to zero.

Using the "-mba" command line option, BASS performs a comprehensive mass balance analysis of its fundamental differential equations [i.e., Equations (2.1), (2.2), and (2.3)]. BASS also calculates and reports mass balances for each cohort's total biomass and the community's total predicted predatory mortality and total predicted piscivorous consumption. For the example projects EX_EVERGLADES_CANAL_HG and EX_L_HARTWELL_PCB presented herein, these mass balances were -5.239E-10 and -5.821E-11 g dry wt/ha/yr, respectively. Since the total piscivory of these communities were 2.832E+04 and 3.124E+04 g dry wt/ha/yr, respectively, these mass balance checks would have relative errors of less than 10^{-13}.

7.2.7. Are simulation results consistent across machines or compilers?

BASS was originally developed on a DEC 3000 workstation using the DEC Fortran 90 compiler. In November 1999, it was ported to the Windows operating system on the DELL OptiPlex using the Lahey LF90 v4.5 compiler. Although the results of these two implementations agree with one another up to single precision accuracy, due to differences in compiler optimization, model computations must be performed in double precision to obtain this level of consistency. Since November 1999, BASS has also been compiled and tested using the Lahey-Fujitsu Fortran LF95 versions 5.0, 5.5, 5.6, 5.7, 7.0, 7.1, and 7.6. Currently, BASS is compiled on standard USEPA DELL laptops and desktops, running 64-byte Windows 10, using the Lahey-Fujitsu 7.7 compiler.

In September 2004, BASS was ported to an IBM Intellistation A Pro workstation equipped with dual 64-byte Opteron processors and a Windows XP operating system. The BASS source code was then recompiled using the Absoft multiprocessor Fortran 90/95 compilers 8.2 MP and 9.0 MP. Although initial compilations using these compilers failed due to compiler bugs that were acknowledged by Absoft Technical Support, workarounds for these bugs were successfully implemented. Simulation results using these executables were in excellent agreement with those obtained using Lahey-Fujitsu single processor executables. BASS has also been compiled on standard USEPA single processor DELL laptops and desktops, running 32-byte Windows XP, using the Absoft Pro Fortran 2012 compiler with similar results. Currently, BASS is compiled on standard USEPA DELL laptops and desktops, running 64-byte Windows 10, using the Absoft 15.0 compiler.

Finally, in June 2010, BASS ported to a DELL Latitude 8400 laptop equipped with Windows XP and a single dual core Intel processor and recompiled using the Intel Fortran 95 compilers 11.0 and XE 2011.

7.2.8. Have test and reference / benchmark data sets been documented and archived?

The 13 BASS projects discussed in Section 6.1 serve not only as BASS distribution examples but also as test projects that track changes in the operation of BASS associated with code maintenance and updates. These project files are used as benchmarks to verify that code modifications that should not change BASS's computational results also do not change BASS's simulation output.

7.3. Questions Regarding QA of Model Documentation and Applications

7.3.1. Is the model intended for absolute or comparative prediction?

Although BASS can be used to analyze results from actual field studies or predict the expected future condition of specific real communities, its principal intended use is to predict and compare outcomes of alterative management options associated with pollution control, fisheries management, and / or ecosystem restoration activities.

7.3.2. Does the User Guide provide the information needed to

appropriately apply and use the model?

The BASS User's Guide summarizes the model's theoretical foundations and assumptions, the model's input command structure, issues related to user file and project management, and software installation. The User's Guide also presents and discusses the results of two of the 13 example projects that are distributed with the BASS software.

7.3.3. What internal checking can be made to help insure that the model is being used appropriately?

Currently, the only internal checking performed by BASS is to verify that all parameters needed by the model for a particular simulation have, in fact, been specified by the user. Although BASS does assign default values for a limited number of parameters, most unassigned parameters are fatal errors. Future versions of BASS will perform bounds checking on many of its physiological and morphological parameters.

7.3.4. Has the developer anticipated computational problem areas that will cause the model to "bomb"?

Several key mathematical calculations have been identified as potential problem areas for a BASS simulation. In general, these problem areas involve either the unsuccessful resolution of a root of a nonlinear equation or the unsuccessful integration of BASS's basic state variables. Examples of the former include situations when BASS's calculated dietary compositions do not sum to unity or when a fish's wet weight is calculated to be less or equal to its dry weight. Examples of the latter include situations when the current integration step is less than the numerical spacing of the current time point, or when BASS's integration error exceeds 10^{-5}. When such situations are encountered, BASS terminates execution and issues an appropriate error message to the current *.MSG file.

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APPENDICES

Appendix A. Equilibrium complexation model for metals

As reviewed by Mason and Jenkins (1995), metals can be classified into three different categories based on their complexation behavior and preference for different ligands. These groups are generally designated as class A, class B, and borderline metals. Of these, however, class B and borderline metals are the most important from an ecotoxicological point of view. Class B metals (e.g., Au, Ag, Cu, Hg, and Pb) preferentially bind to marcromolecules such as proteins and nucleotides that are rich in sulfhydryl groups and heterocyclic nitrogen. Borderline metals (e.g., As, Cd, Co, Cr, Ni, Sn, and Zn) bind not only to the same sites as do class B metals but also to those sites preferred by class A metals (i.e., carboxylates, carbonyls, alcohols, phosphates, and phosphodiesters). Although factors determining the preference of borderline metals for a particular binding site are complex, the fact that the transport and storage of these metals in fish and other biota are regulated by metallothioneins via sulfhydryl complexation reactions suggests that the total availability of sulfhydryl groups within organisms plays a key role in their internal distribution and accumulation.

To formulate complexation reactions for class B and borderline metals, one can assume that protein sulfhydryl groups are the only significant ligand for these metals, i.e.,

$$RSH + M^+ \leftrightharpoons RSM + H^+ \tag{A.1}$$

The stability constant for this reaction is

$$Kb = \frac{[RSM]\,[H^+]}{[RSH]\,[M^+]} = \frac{RSM\,[H^+]}{RSH\,[M^+]} \tag{A.2}$$

where $[H^+]$ is the hydrogen ion concentration (molar); $[M^+]$ is the concentration of free metal (molar); $[RSH]$ is the concentration of reactive sulfhydryls (molar); $[RSM]$ is the concentration of sulfur bound metal (molar); RSM is the moles of metal bound to sulfhydryls; and RSH is the moles of free, non-disassociated sulfhydryl. If a fish's metal concentrations (i.e., C_a , C_l , C_o , and C_f) are expressed on a molar basis, then the following identities hold

$$[M^+] = C_a \tag{A.3}$$

$$RSM = C_o P_o W_w \tag{A.4}$$

$$C_f = \left(P_a + P_l K_{ow} + P_o \frac{C_o}{C_a} \right) C_a \tag{A.5}$$

where W_w is the fish's kilogram wet weight. Substituting Equations (A.3) and (A.4) into Equation (A.2), one can verify that

$$\frac{P_o C_o}{C_a} = \frac{Kb\,RSH}{W_w\,[H^+]} \tag{A.6}$$

and consequently

$$C_f = \left(P_a + P_l K_{ow} + \frac{Kb\,RSH}{W_w\,[H^+]} \right) C_a \tag{A.7}$$

To parameterize Equation (A.7) for RSH, the following mass balance for the fish's sulfhydryl content is then assumed

$$\begin{aligned} TS &= RSH + RS^- + \sum_i RSM_i \\ &= RSH + \frac{RSH\,K_a}{[H^+]} + \sum_i \frac{Kb_i C_{a_i} RSH}{[H^+]} \\ &= RSH \left(1 + \frac{K_a}{[H^+]} + \sum_i \frac{Kb_i C_{a_i}}{[H^+]} \right) \end{aligned} \tag{A.8}$$

where TS is the total moles of sulfhydryl ligands; RS^- is the moles of disassociated sulfhydryls; and K_a is the sulfhydryl's disassociation constant. Therefore,

$$RSH = \frac{TS\,[H^+]}{[H^+] + K_a + \sum_i Kb_i C_{a_i}} \tag{A.9}$$

Using Equation (A.7), however, this expression can be rewritten as

$$RSH = \frac{TS}{1 + \frac{K_a}{[H^+]} + \sum_i \frac{Kb_i B_{f_i}}{\left(P_a + P_l K_{ow_i}\right) W_w [H^+] + Kb_i RSH}} \tag{A.10}$$

where $B_{f_i} = C_{f_i} W_w$ is the fish's total burden (mol/fish) of metal i. For most class B metals, however,

$$\left(P_a + P_l K_{ow_i}\right) W_w [H^+] \ll Kb_i RSH \tag{A.11}$$

Consequently, Equation (A.10) can be simplified to

$$RSH = \frac{TS}{1 + \frac{K_a}{[H^+]} + \sum_i \frac{B_{f_i}}{RSH}} = \frac{TS - \sum_i B_{f_i}}{1 + \frac{K_a}{[H^+]}} \tag{A.12}$$

This expression can then be substituted into Equation (A.7) to

calculate the fish aqueous phase metal concentrations.

To use the aforementioned complexation model [i.e., Equation (A.12) substituted into Equation (A.7)], one must specify both the metal's stability constant [see Equation (A.2)] and the total concentration of sulfhydryl binding sites *TS* (mol SH/g dry wt) within the fish. Although numerous studies have investigated the sulfhydryl content of selected fish tissues, it appears that no study has attempted to quantify the total sulfhydryl content of fish. A reasonable approximation of this parameter, however, can still be made since data do exist for the major tissues (i.e., muscle, liver, kidney, gill, and intestine) typically associated with metal bioaccumulation.

Itano and Sasaki (1983) reported the sulfhydryl content of Japanese sea bass (*Lateolabrax japonicus*) muscle to be 11.5 µmol SH/g(sacroplasmic protein) and 70.5 µmol SH/g(myofibrillar protein). Using these authors' reported values of 0.0578 g(sarcoplasmic protein)/g(muscle) and 0.120 g(myofibrillar protein)/g(muscle), the total sulfhydryl content of Japanese sea bass muscle is estimated to be 9.12 µmol(SH)/g(muscle) or 45.6 µmol(SH)/g(dw muscle). Opstevedt et al. (1984) reported the sulfhydryl content of Pacific mackerel (*Pneumataphorus japanicus*) and Alaska pollock (*Theragra chalcogramma*) muscle to be 6.6 and 6.2 mmol(SH)/16 g(muscle N), respectively. Using conversion factors reported by these authors, these values are equivalent to 48.7 and 56.7 µmol/g(dw muscle). Chung et al. (2000) determined the sulfhydryl content of mackerel (*Scomber australasicus*) muscle to be 88.2 µmol(SH)/g(protein). Using the conversion factor 0.83 g(protein)/g(dw muscle) (Opstevdt et al. 1984), this value is equivalent to 73.2 µmol(SH)/g(dw muscle). Several studies have determined sulfhydryl contents of the actomyosin and myosin components of fish myofibrillar proteins (Connell and Howgate 1959, Buttkus 1967, 1971, Takashi 1973, Itoh et al. 1979, Sompongse et al. 1996, Benjakul et al. 1997, Lin and Park 1998). Because the results of these studies agree well with the actomyosin analysis reported by Itano and Sasaki (1983), the results of Itano and Sasaki (1983), Opstevedt et al. (1984), and Chung et al. (2000) can be assumed to be representative of fish in general. Consequently, the sulfhydryl content of fish muscle can be assumed to be on the order of 45-70 µmol(SH)/g(dw muscle).

Although the sulfhydryl contents of liver, kidney, gills, and intestine have not been measured directly, the sulfhydryl content of these tissues can be estimated from their metallothionein concentrations. Metallothioneins (MT) are sulfur-rich proteins that are responsible for the transport and storage of heavy and trace metals and that are also usually considered to be the principal source of sulfhydryl binding sites in these tissues (Hamilton and Mehrle 1986, Roesijadi 1992). Numerous researchers have investigated the occurrence of MTs in the liver, kidney, and gills of fish, and most have shown that tissue concentrations of MTs generally vary with metal exposures. Under moderate exposures, typical hepatic MT concentrations in fish are on the order of 0.03 - 0.30 µmol(MT)/g(liver) (Brown and Parsons 1978, Roch et al. 1982, Klaverkamp and Duncan 1987, Dutton et al. 1993). Using data from Takeda and Shimizu (1982) who report the sulfhydryl content of skipjack tuna (*Katsuwonus pelamis*) MTs to be approximately 25 mol(SH)/mol(MT) and assuming a dry to wet weight ratio equal 0.2, these MT concentrations would be equivalent to 3.75 - 37.5 µmol(SH)/g(dw liver). This range of values suggests that the hepatic sulfhydryl content of fish, that includes both baseline MT and cytoplasmic components that can be converted into MT, might be on the order of 40 µmol(SH)/g(dw liver). This latter value, however, is probably too conservative. Consider, for example, the observation that the ratios of mercury concentrations in liver to those in muscle often vary from 1.5 to 6 or more (Lockhart et al. 1972, Shultz et al. 1976, Sprenger et al. 1988). If liver and muscle are equilibrating with the same internal aqueous phase, then either the MT sulfhydryls are more available than are the sacroplasmic and myofibrillar sulfhydryls or the inducible concentrations of hepatic MT are much higher than 40 µmol(SH)/g(dw liver). Of these two possibilities, the latter appears more likely.

Although gill, kidney, and intestine MTs have not been studied in the same detail as hepatic MTs, it appears that MT, and hence sulfhydryl, concentrations in gills and kidney are lower and not as inducible as hepatic concentrations (Hamilton et al. 1987a, b, Klaverkamp and Duncan 1987). Klaverkamp and Ducan (1987) estimated the concentrations of gill MT in white suckers (*Catostomus commersoni*) to be 33 µg(MT)/g(gill) which is equilvalent to 3.3 nmol(MT)/g(gill) or 0.0825 µmol(SH)/g(gill). This latter value agrees well with the estimated concentrations of unidentified binding sites [0.03 - 0.06 µmol/g(gill)] for copper on the gills of rainbow trout (*Oncorhynchus mykiss*) and brook trout (*Salvelinus fontinalis*) (MacRae et al. 1999), but is somewhat higher than the concentration of unidentified binding sites [0.013 - 0.03 µmol/g(gill)] for copper, cadmium, and silver on the gills of rainbow trout and fathead minnows (*Pimephales promelas*) (Playle et al. 1993, Janes and Playle 1995).

Based on these considerations and the acknowledgment that many other important organic compounds contain sulfhydryl groups, e.g., enzymes involved in fatty acid synthesis, glutathione, etc., it seems reasonable to assume that the sulfhydryl content of fish is approximately 70 µmol(SH)/g dry wt. Because Davis and Boyd (1978) reported the mean sulfur content of 17 fish species to be 206 µmol(S)/g dry wt, this assumption implies that almost 1/3 of a fish's sulfur pool exists as sulfhydryl groups.

The aforementioned complexation model was implemented within BASS using 70 μmol(SH)/g dry wt to calculate the fish's total sulfhydryl content. The mean dissociation constant for organic sulfhydryls was then assigned as $pK_a = 9.25$ (i.e., the SPARC estimated pK_a for cysteine). Using literature values for the stability constants of methylmercury, however, BASS over predicted the bioaccumulation of methylmercury in fish by at least an order of magnitude. Consequently, a much simpler distribution coefficient algorithm was adopted.

Appendix B. Modeling diffusive chemical exchange across fish gills with ventilation and perfusion effects. See Section 2.2 for background information and notation.

If chemical exchange across fish gills is treated as steady-state, convective mass transport between parallel plates, then the following PDE and boundary conditions can be used to model chemical uptake from and excretion to the interlamellar water:

$$\frac{3}{2}\left(1-\frac{x^2}{r^2}\right)V\frac{\partial C}{\partial y}=D\frac{\partial^2 C}{\partial x^2} \tag{B.1}$$

$$\left.\frac{\partial C}{\partial x}\right|_{x=0}=0 \tag{B.2}$$

$$D\left.\frac{\partial C}{\partial x}\right|_{x=r}=-k_m\left[C(r,y)-C_a-\frac{2hD}{q_p}\int_y^l\left.\frac{\partial C}{\partial x}\right|_{x=r}dv\right] \tag{B.3}$$

To obtain a canonical solution for this gill model, these equations can be nondimensionalized using the following transformations:

$$\Theta=\frac{C-C_a}{C_w-C_a} \tag{B.4}$$

$$X=\frac{x}{r} \tag{B.5}$$

$$Y=\frac{yD}{Vr^2} \tag{B.6}$$

Applying these transformations, chemical exchange across a fish's gills is described by the following dimensionless PDE and boundary conditions:

$$\frac{3}{2}\left(1-X^2\right)V\frac{\partial\Theta}{\partial Y}=\frac{\partial^2\Theta}{\partial X^2} \tag{B.7}$$

$$\left.\frac{\partial\Theta}{\partial X}\right|_{X=0}=0 \tag{B.8}$$

$$\left.\frac{\partial\Theta}{\partial X}\right|_{X=1}=-N_{Sh}\left[\Theta(1,Y)-\frac{2rhV}{q_p}\int_Y^{N_{Gz}}\left.\frac{\partial\Theta}{\partial X}\right|_{X=1}dv\right] \tag{B.9}$$

where $N_{Sh}=k_m r D^{-1}$ is the gills' dimensionless lamellar permeability (i.e., Sherwood number); and $N_{Gz}=l D V^{-1} r^{-2}$ is the gills' dimensionless lamellar length (i.e., Graetz number).

The boundary condition (B.9) describing exchange across the secondary lamellae, however, can be simplified by noting that the solution of Equation (B.7) is separable, i.e., $\Theta(X, Y)=\Phi(X)\Psi(Y)$ and that $q_v = 2\ rhV$ is the ventilation volume of an individual interlamellar channel. Using these observations, one can then write

$$\Psi(Y)\left.\frac{d\Phi}{dX}\right|_{X=1}=-N_{Sh}\left[\Phi(1)\Psi(Y)-\frac{q_v}{q_p}\left.\frac{d\Phi}{dX}\right|_{X=1}\int_Y^{N_{Gz}}\Psi(v)\,dv\right] \tag{B.10}$$

that can then be differentiated with respect to Y to obtain

$$\left.\frac{d\Psi}{dY}\frac{d\Phi}{dX}\right|_{X=1}=-N_{Sh}\left[\Phi(1)\frac{d\Psi}{dY}+\Psi(Y)\frac{q_v}{q_p}\left.\frac{d\Phi}{dX}\right|_{X=1}\right] \tag{B.11}$$

Because $\Psi(Y)=\exp(-\frac{2}{3}\lambda^2 Y)$ where λ is the constant of separation for Equation (B.7), the preceding equation is equivalent to

$$-\tfrac{2}{3}\lambda^2\left.\frac{d\Phi}{dX}\right|_{X=1}=-N_{Sh}\left[-\tfrac{2}{3}\lambda^2\Phi(1)+\frac{q_v}{q_p}\left.\frac{d\Phi}{dX}\right|_{X=1}\right] \tag{B.12}$$

which can be rearranged to yield

$$\left.\frac{d\Phi}{dX}\right|_{X=1}=-\left(\frac{\tfrac{2}{3}\lambda^2 N_{Sh}}{\tfrac{2}{3}\lambda^2-\left(q_v/q_p\right)N_{Sh}}\right)\Phi(1) \tag{B.13}$$

Although this boundary condition is dependent on the eigenvalue λ, the eigenvalue expansion for the solution of Equation (B.7) is still straightforward (Walter 1973, Fulton 1977). Note that as the fish's perfusion rate increases, this boundary condition converges to

$$\left.\frac{d\Phi}{dX}\right|_{X=1}=-N_{Sh}\Phi(1) \tag{B.14}$$

which is the boundary condition originally used by Barber et al. (1991).

See Barber et al. (1991) for the method used to construct the series solution for the dimensionless bulk concentration of the aforementioned PDE gill exchange model [i.e., Equation (2.28)].

Appendix C. Derivation of the consistency condition for feeding electivities.

To derive a self consistency condition for a fish's electivities and relative prey availabilities such that its calculated dietary frequencies will sum to unity, consider the following

$$e_i = \frac{d_i - f_i}{d_i + f_i} \tag{C.1}$$

$$e_i \left(d_i + f_i\right) = d_i - f_i \tag{C.2}$$

$$d_i = \left(\frac{1 + e_i}{1 - e_i}\right) f_i \tag{C.3}$$

Summing Equation (C.2) over all *i* then yields

$$\sum_{i=1}^{n} e_i \left(d_i + f_i\right) = \sum_{i=1}^{n} d_i - \sum_{i=1}^{n} f_i \tag{C.4}$$

$$\sum_{i=1}^{n} e_i \left(d_i + f_i\right) = 0 \tag{C.5}$$

When Equation (C.3) is substituted into Equation (C.5), one then obtains

$$\sum_{i=1}^{n} e_i \left(\frac{1 + e_i}{1 - e_i} f_i + f_i\right) = \sum_{i=1}^{n} \frac{2 e_i f_i}{1 - e_i} = 0 \tag{C.6}$$

or equivalently

$$\sum_{i=1}^{n} \frac{e_i f_i}{1 - e_i} = 0 \tag{C.7}$$

Finally, adding $\Sigma f_i = 1$ to each side of Equation (C.7), the following consistency condition is obtained

$$\begin{gathered} \sum_{i=1}^{n} \left(\frac{e_i f_i}{1 - e_i} + f_i\right) = 1 \\ \sum_{i=1}^{n} \frac{f_i}{1 - e_i} = 1 \end{gathered} \tag{C.8}$$

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