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Bioaccumulation and Aquatic System Simulator (BASS) User's Manual Beta Test Version 2.1

by

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Notice

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Foreword

This report describes the theoretical development, parameterization, and application software of a generalized, community-based, bioaccumulation model called BASS (**B**ioaccumulation and **A**quatic **S**ystem **S**imulator). This model is designed to predict the population and bioaccumulation dynamics of age-structured fish communities that are 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 rather a reference and user's guide. The intended audience of this report and associated software is research fisheries ecologists, bioaccumulation researchers, and EPA environmental scientists and ecologists who must routinely analyze and estimate bioaccumulation of chemicals in fish for ecological or human health exposure assessments.

BASS version 2.1 is a beta test version that is being released on a targeted basis to EPA Program and Regional Offices and to the academic research community for comment and testing. Although the model has not been extensively field-tested, its process-based algorithms for predicting chemical bioaccumulation, growth of individual fish, predator-prey interactions, and population dynamics either have been corroborated or have been formulated using widely accepted ecological and ecotoxicological principles. Even when a process-based model has undergone only limited field testing, it can be an extremely useful tool. Process-based models 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. If the conceptualization and construction of process-based models are both comprehensive (i.e., holistic) and reasonable, then their output, validated or not, can still be used for comparative analyses. A model's ability to simulate trends and comparative dynamics are, in fact, often more important measures of a model's utility than is its ability to replicate a specific field or laboratory study. Although BASS can be used to analyze results from actual field studies, its principal intended use is to predict and compare the outcomes of alternative management options that are associated with pollution control or ecosystem management or restoration activities.

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Abstract

BASS (**B**ioaccumulation and **A**quatic **S**ystem **S**imulator) is a Fortran 95 simulation program that predicts the population and bioaccumulation dynamics of age-structured fish assemblages that are exposed to hydrophobic organic pollutants and class B and 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. The model's exchange algorithms consider both biological attributes of fishes and physico-chemical properties of the chemicals of concern that 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 are 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 specified by defining one or more foraging classes for each fish species based on either its body weight, body length, or age. The dietary composition of each of these feeding 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 community's food web and standing stocks, size dependent physiological mortality rates, the maximum longevity of species, and toxicological responses to chemical exposures. The model's temporal and spatial scales of resolution are a day and a hectare, respectively. Currently, BASS ignores the migration of fish into and out of the simulated hectare.

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1. Introduction

Fish health can be defined from both an ecological and a human health/value perspective in a wide variety of ways. Questions relating to fish health from an ecological perspective often include:

1) Is 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 for the fish to attain it's 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 chemical considerations?
4) Are regional fish assemblages maintaining their expected level of productivity based on biogeographical and physical chemical 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?

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

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

Some of the important metrics or indicators that have been typically used 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, sediment loading, etc., 2) community species and functional diversity, 3) total community biomass (kg/ha or kg/km), 4) the population density (fish/ha or fish/km) or biomass (kg/ha or kg/km) of the community's dominant species, 5) the age or size class structure of the community's dominant species, 6) annual productivity of the community and its dominant species, 7) individual growth rates or condition factors (i.e., the fish's current body weight normalized to an expected body weight based on its current length), and 8) levels of chemical contaminants in muscle or whole fish for human or ecological exposure assessments, respectively.

From the perspective of evaluating alternative management options or of assessing expected future consequences of existing conditions, simulation models that can predict the individual and population growth of fish and their patterns of chemical bioaccumulation are important tools for analyzing several of the dimensions of fish health identified above.

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), are becoming the models of choice for predicting the growth of fish. Because these models predict fish growth as 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 the population dynamics and productivity of fish, 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 in assessing the ecological and human health risks of chemical pollutants. Not only are accurate estimates needed to predict realistic dietary exposures to humans and piscivorous wildlife but such estimates are also needed to assess more accurately potential ecological risks to fish assemblages themselves. Although exposure-referenced toxicological benchmarks such as the LC_{50} and the EC_{50} have been widely used to make hazard assessments, most deleterious effects of chemical pollutants are caused by the internal accumulation of those compounds, rather than their environmental concentrations per se. Numerous 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 need to consider chemical bioaccumulation explicitly 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 the concentrations of moderately hydrophobic chemicals in fish often can 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 in either direction, with calculated contamination levels being both considerably above and 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 linear, first order kinetic 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 species of concern is relatively short lived, the time needed for equilibrium can exceed their expected life span. Even when there is sufficient time for equilibration, whole body concentrations of fish can be much lower than that expected from thermodynamic partitioning due to physical dilution of the chemical that accompanies body growth or to the biotransformation and metabolism of the parent compound.

One of two possible assumptions are implicitly made whenever equilibrium-based estimators are used. The first of these assumptions is that only the selected reference route of exposure is significant in determining the total chemical accumulation in fish. The alternative to this assumption is that there are actually multiple routes of exposure which are all covariant with the chosen reference pathway in a fixed and constant manner. In the case of bioconcentration factors (BCFs), the implicit assumption is that virtually all of the fish's accumulated body 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 burdens for extremely hydrophobic chemicals. This shift in the relative significance of the direct aqueous versus the dietary pathway 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/day, is the product of its ventilation volume, Q mL/day, and the chemical's aqueous concentration, C_w μg/mL. Similarly, the fish's dietary exposure, DE μg/day, is the product of its feeding rate, F g/day, and the chemical's concentration in the fish's prey, C_p μg/g. Assuming that 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

$$\begin{aligned} AE &= DE \\ Q\ C_w &= F\ C_p \\ Q\ /\ F &= BCF \end{aligned} \qquad (1\text{-}1)$$

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 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 $10^{5.6}$. For extremely hydrophobic chemicals, not only will fish be more exposed via food but they probably will assimilate chemicals from food more effectively than from the water. 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 the chemical concentrations of the fish's gut contents to increase (Connolly and Pedersen 1988; Gobas et al. 1988). Predicting residue levels for 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 generally 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 the kinetic exchange of chemicals from food and water and the growth of fish provide objective and scientifically defensible tools that can overcome

many of the limitations of equilibrium-based predictors of bioaccumulation identified above. Although numerous models have been developed to describe the dynamics of chemical bioaccumulation in fish, (Norstrom et al. 1976; Thomann 1981, 1989; Jensen et al. 1982; Thomann and Connolly 1984; Gobas et al. 1988; Barber et al. 1991; Thomann et al. 1992; Gobas 1993; Madenjian et al. 1993), these models differ significantly with regard to how food web structure and dietary exposures are represented.

This report describes the theoretical framework, parameterization, and use of a generalized, community-based, bioaccumulation model called BASS (**B**ioaccumulation and **A**quatic **S**ystem **S**imulator). This 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 such 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 SPARC (Carreira et al. 1994; http://ibmlc2.chem.uga.edu/sparc/style/welcome.cfm), 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 the growth of individuals and populations within an age-structured fish community, BASS solves the following system of differential equations for each age class of fish

$$\frac{dB}{dt} = J_g + J_i - M \qquad (2\text{-}1)$$

$$\frac{dW_d}{dt} = F - E - R - EX - SDA \qquad (2\text{-}2)$$

$$\frac{dN}{dt} = - NM - PM \qquad (2\text{-}3)$$

where B and W_d denote the chemical body burden (μg/fish) and dry body weight (g(DW)/fish) of the average individual within the age class and N denotes the age class's population density (fish/ha). In Eq.(2-1) J_g and J_i denote the net chemical exchange across a fish's gills from the water and across its intestine from food, respectively, and M denotes the chemical's biotransformation or metabolism. In Eq.(2-2) F, E, R, EX, and SDA denote the fish's feeding, egestion, routine respiration, excretion, and specific dynamic action (i.e., the additional respiratory expenditure in excess of R required to assimilate food), respectively. Although many physiologically based models for fish growth are formulated in terms of energy content and fluxes (e.g., kcal/fish and kcal/d), formulating a physiologically based growth model in terms of dry weight is fundamentally identical to the former since the energy densities of fish depend on their dry weight (Kushlan et al. 1986; Hartman and Brandt 1995b). Finally, in Eq.(2-3) NM and PM denote the age class's non-predatory and predatory mortality, respectively. Although migration can be a significant process in determining population sizes, this process is presently ignored in BASS. Though it may not be immediately apparent from the above notation, these equations are tightly coupled to one another. 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 the 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 1 summarizes the definitions of all 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 units conversion is necessary to make the coupled system of equations dimensionally consistent. The reader should also note that whereas the growth of fish is described in terms of dry weight, modeling the bioaccumulation of chemicals in fish requires knowledge of their live weights since the following formulations of the bioaccumulation process will be developed in terms of diffusive exchange 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 it be the surrounding ambient water or the aqueous phases of the fish's intestinal contents. Consequently, to model these exchanges one must first consider how chemicals distribute with the bodies of fish. If individual fish are conceptualized as a three-phase solvent consisting of water, lipid, and non-lipid organic matter, then their whole body chemical concentration can be expressed as

$$\begin{aligned} C_f = \frac{B}{W_f} &= P_a C_a + P_l C_l + P_o C_o \\ &= \left(P_a + P_l \frac{C_l}{C_a} + P_o \frac{C_o}{C_a} \right) C_a \end{aligned} \qquad (2\text{-}4)$$

where W_f is the fish's live weight (g(FW)); 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 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, 1986b), internal equilibration between these three phases can be assumed to be rapid in comparison to external exchanges. For organic chemicals this assumption means that Eq.(2-4) simplifies to

$$C_f = \left(P_a + P_l K_l + P_o K_o \right) C_a \qquad (2\text{-}5)$$

where K_l and K_o are partition coefficients between lipid and water and between organic carbon and water, respectively.

For metals, however, Eq.(2-4) is in theory 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 it would seem that the term $P_o C_o / C_a$ in Eq.(2-4) should 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, this algorithm greatly overestimated metal (in particular 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 to be inappropriate to the time scales of most of the 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, the same approach was adopted for BASS. Thus, for a metal

$$C_f = \left(P_a + P_l K_l + P_o K_d\right) C_a \qquad (2\text{-}6)$$

where K_l is again an appropriate partition coefficients between lipid and water and K_d is an appropriate metal specific distribution coefficient. Although this equation appears identical to Eq.(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_w equals C_a at equilibrium, it follows from Eq.(2-4) that the thermodynamic bioconcentration factor ($K_f = C_f/C_w$ at equilibrium) for a chemical in fish would be

$$K_f = \begin{cases} P_a + P_l K_l + P_o K_o & \textit{for organics} \\ P_a + P_l K_l + P_o K_d & \textit{for metalics} \end{cases} \qquad (2\text{-}7)$$

2.2. Modeling Exchange from Water

Because chemical exchange across the gills of fish occurs by simple diffusion, such exchanges can be modeled by Fick's first law of diffusion as follows

$$J_g = S_g \, k_g \left(C_w - C_a\right) \qquad (2\text{-}8)$$

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 concentrations (μg/mL) in the environmental water. See Yalkowsky et al. (1973), Mackay (1982), Mackay and Hughes (1984), Gobas et al. (1986), Gobas and Mackay (1987), and Erickson and McKim (1990). When Eqs.(2-4) and (2-7) are substituted into this equation, one then obtains

$$J_g = S_g k_g \left(C_w - \frac{C_f}{K_f}\right) \qquad (2\text{-}9)$$

Although according to Fick's first law the conductance k_g of a chemical across a fish's gill 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 because the thickness of the boundary layer varies along the length of the gill's secondary lamellae and is a function of the gill's ventilation velocity. To circumvent this problem, a fish's net chemical exchange rate, $S_g k_g$, can be objectively estimated by reformulating the gill's net chemical exchange as

$$J_g = Q\left(C_w - C_B\right) \qquad (2\text{-}10)$$

where Q is the fish's ventilation volume (cm^3/s) and C_B is the bulk concentration of the chemical in the water expired from the gills. When Eqs. (2-8) and (2-10) are equated, it follows that

$$S_g k_g = Q\left(\frac{C_w - C_B}{C_w - C_a}\right) \qquad (2\text{-}11)$$

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

$$Q = \frac{O_2}{\alpha_{O_2} C_{w,O_2}} \qquad (2\text{-}12)$$

where O_2 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 water's dissolved oxygen concentration (μg/mL). And if one now makes certain assumptions concerning the geometry of the interlamellar spaces and the nature of mass transport between the secondary lamellae, the normalized bulk concentration of the exhalant gill water $(C_w\text{-}C_B)/(C_w\text{-}C_a)$ can also be formulated.

Because the gill's secondary lamellae form flat channels having very high aspect ratios (i.e., mean lamellar height / interlamellar distance), the lamellae can be considered 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 exhalant 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.,

$$\frac{3}{2}\left(1 - x^2\right) V \frac{\partial C}{\partial y} = D \frac{\partial^2 C}{\partial x^2} \qquad (2\text{-}13)$$

where V (cm/s) is the gill's mean interlamellar flow velocity, D (cm^2/s) is the chemical's aqueous diffusivity, and x and y are the lateral and longitudinal coordinates of the channel along which diffusion and convection occurs, respectively. In this equation $C = C(x, y)$ denotes 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 $x = \pm h$ where h is the hydraulic radius of the lamellar channel which equals one half of the interlamellar distance d (cm). The midline between adjacent lamellae is therefore denoted by x=0. The mean interlamellar flow velocity, V (cm/s), can be formulated as the ratio of the fish's ventilation volume to the cross sectional pore area, X_g (cm^2), of its gills. Because this pore area is related to the gill's lamellar surface area by

$$X_g = \frac{S_g\, d}{l} \tag{2-14}$$

where d (cm) is the mean interlamellar distance and l (cm) is the mean lamellar length (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 the above PDE 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

$$D \left.\frac{\partial C}{\partial x}\right|_{x=h} = -k_m \left(C(h,y) - C_a\right) \tag{2-17}$$

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

$$\begin{aligned} D \left.\frac{\partial C}{\partial x}\right|_{x=h} &= -k_m \left(C(h,y) - C_a(y)\right) \\ &= -k_m \left(C(h,y) - \left(C_a(l) + \frac{U(y,l)}{q_p} \right) \right) \end{aligned} \tag{2-18}$$

where $C_a(y)$ denotes the aqueous phase concentration of the chemical at point y along the length of a secondary lamella, $C_a(l) = C_a$ denotes the chemical' s concentration in the afferent lamellar blood, $U(y, l)$ is the chemical's accumulated rate of 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 uptakes chemical, then $U(y, l)$ can be formulated as

$$\begin{aligned} U(y,l) &= 2 \int_y^l \int_0^z D \left.\frac{\partial C}{\partial x}\right|_{x=h} dz\, dy \\ &= 2\, z\, D \int_y^l \left.\frac{\partial C}{\partial x}\right|_{x=h} dy \end{aligned} \tag{2-19}$$

where z denotes the height (cm) of the secondary lamella. Using this expression, the boundary condition (2-18) can now be written as

$$D \left.\frac{\partial C}{\partial x}\right|_{x=h} = -k_m \left(C(h,y) - C_a - \frac{2\, z\, D}{q_p} \int_y^l \left.\frac{\partial C}{\partial x}\right|_{x=h} dy \right) \tag{2-20}$$

Once the solution of Eq.(2-13) for these boundary conditions has been obtained, the chemical's bulk concentration in the exhalant gill water can be evaluated using the weighted average

$$C_B = \frac{\int_0^h C(x,l) \left(1 - x^2\right) dx}{\int_0^h \left(1 - x^2\right) dx} \tag{2-21}$$

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

A canonical solution to Eq.(2-13) can be obtained by nondimensioning $C(x, y)$, x, and y as follows

$$\Theta = \frac{C - C_a}{C_w - C_a} \tag{2-22}$$

$$X = \frac{x}{h} \tag{2-23}$$

$$Y = \frac{y\, D}{V\, h^2} \tag{2-24}$$

where h is the hydraulic radius of the lamellar channel (i.e., one-half the interlamellar distance). When this is done, the chemical's dimensionless bulk concentration is given by

$$\Theta_B = \frac{C_B - C_a}{C_w - C_a} = \frac{\int_0^1 \Theta(X, N_{Gz}) \left(1 - X^2\right) dx}{\int_0^1 \left(1 - X^2\right) dX} \tag{2-25}$$

where $N_{Gz} = (l\, D) / (V\, h^2)$ is the lamellae's dimensionless length or Graetz number. Two important points concerning this expression can now be made. Firstly, one can easily verify that

$$1 - \Theta_B = \frac{C_w - C_B}{C_w - C_a} \tag{2-26}$$

and therefore Eq. (2-11) can be rewritten as

$$S_g k_g = Q\, (1 - \Theta_B) \tag{2-27}$$

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

$$\Theta_B = \sum_{m=0}^{\infty} B_m \exp\left(-\tfrac{2}{3}\,\lambda_m^2\, N_{Gz}\right) \qquad (2\text{-}28)$$

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

$$N_{Sh} = \frac{k_m h}{D} \qquad (2\text{-}29)$$

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 evaluate Θ_B with less than 1% error (also see Barber et al. 1991).

2.3. Modeling Exchange from Food

Chemical uptake from food has usually been modeled by assuming that a fish can assimilate a constant fraction of the chemical it ingests, i.e.,

$$J_i = \alpha_c\, C_p\, F_f \qquad (2\text{-}30)$$

where α_c is an assimilation efficiency (dimensionless) for the chemical, C_p is the chemical's concentration (μg/g(FW)) in the ingested prey, and F_f is the fish's wet weight consumption (Norstrom et al. 1976; Jensen et al. 1982; Thomann and Connolly 1984; Niimi and Oliver 1987). However, because the chemical exchange across the intestine is driven by diffusive gradients (Vetter et al. 1985; Clark et al. 1990; Gobas et al. 1993), such formulations would be thermodynamically realistic only if α_c is a decreasing function of the fish's total body concentration C_f. A thermodynamically sound description for the dietary uptake of chemicals can be formulated using the simple mass balance relationship

$$J_i = C_p F_f - C_e E_f \qquad (2\text{-}31)$$

where E_f is the fish's daily wet weight egestion and C_e is the chemical's concentration (μg/g(FW)) in the fish's feces.

Because the transit time through the gastrointestinal tract is relatively slow, it is reasonable to assume that the concentrations of chemicals in the fish's aqueous blood, intestinal fluids, and dry fecal matter equilibrate with one another. Connell (1989) made similar assumptions to analyze the ratio of a predator's chemical concentration to that of its prey. Using this assumption, a fish's total fecal elimination of a chemical can be calculated as

$$\begin{aligned} C_e E_f &= C_a E_a + C_d E \\ &= \left(E_a + E\,\frac{C_d}{C_a}\right) C_a \\ &= \left(\frac{P_{ia}}{1-P_{ia}} + \frac{C_d}{C_a}\right) \frac{C_f}{K_f}\, E \\ &= \frac{K_e}{K_f}\, C_f E \end{aligned} \qquad (2\text{-}32)$$

where E_a is the aqueous phase volume of the fish's feces $P_{ia} = E_a/(E_a+E)$ is the aqueous fraction of the fish's feces, and C_d is the chemical's concentrations in the feces's dry organic phase. For organic chemicals, the concentration ratio C_d/C_a can be replaced with an organic carbon/water partition coefficient K_{oc} (e.g., Karickhoff 1981; Briggs 1981; Chiou et al. 1986) whereas for metals, this ratio can be substituted with the distribution coefficient similar to the one used in Eq.(2-6). Although reported values for the percent moisture of the intestinal contents of fish vary between 50 and 80% (Brett 1971; Marais and Erasmus 1977; Grabner and Hofer 1985), in general one can assume that $P_{ia} = P_a$ due to rapid osmotic equilibration between the fish's intestinal contents and its whole body. If this assumption is indeed reasonable, then meals with the same dry weight but different moisture contents should be processed by the fish at the same rate and efficiency since they will attain the same proximate composition relatively soon after ingestion. Having the same proximate composition implies not only that the concentrations of digestive enzymes acting on such meals should be comparable but also that physical forces exerted by the volume of the gut contents which controls peristalsis and gastric mobility should likewise be comparable. Because Bromley (1980) and Garber (1983) demonstrated that initial dietary moisture content had no significant effect on the assimilation efficiencies of turbot (*Scophthalmus maximus*) or gastric evacuation rates of yellow perch (*Perca flavescens*), respectively, the assumption that $P_{ia} = P_a$ does seem to be reasonable.

When Eq.(2-32) is substituted into Eq.(2-31) and the resulting expression is equated to Eq.(2-30), one can verify that.

$$\alpha_c = 1 - (1 - \alpha_f)\,\frac{K_e C_f}{K_f C_p} \qquad (2\text{-}33)$$

where α_f is the fish's food assimilation efficiency. This expression predicts that a fish's chemical assimilation efficiency decreases as its whole body chemical burden or concentration increases and increases as the whole body concentration of its prey increases. Observing these predictions experimentally,

however, is not without problems since the fish's food assimilation efficiency can vary significantly with feeding rate, food quality, temperature and other factors. Nevertheless, the results of studies by Lieb et al. (1974), Gruger et al. (1975) , and Opperhuizen and Schrap (1988) which are analyzed and discussed in Barber et al. (1991) corroborate these predicted tends. Recent studies by Dori et al. (2000) who used in situ preparations of channel catfish intestines, have clearly established that preexposures to 3,4,3',4'-tetrachlorobiphenyl does indeed decrease intestinal uptake rates.

Muir et al. (1992), Dabrowska et al. (1996), and Fisk et al.(1998) have investigated chemical assimilation efficiencies of rainbow trout and channel catfish using a model proposed by Bruggeman et al. (1981), i.e.,

$$\frac{d\,C_f}{dt} = \alpha\ f\ C_p - k_2\,C_f \qquad (2\text{-}34)$$

$$C_f = \alpha\ f\ C_p\ \frac{1-\exp(-k_2\ t)}{k_2} \qquad (2\text{-}35)$$

where α is a constant assimilation efficiency, f is the fish's specific rate of feeding (g/g/d), and k_2 is the chemical's apparent elimination rate which necessarily must include actual excretion, biotransformation, and growth dilution. Eq.(2-35), however, is only the solution to Eq.(2-34) when $C_f(0) = 0$. The general solution to Eq.(2-34) is actually

$$\begin{aligned} C_f &= \alpha\ f\ C_p\ \frac{1-\exp(-k_2\ t)}{k_2} + C_f(0)\ \exp(-k_2\ t) \\ &= \frac{\alpha\ f\ C_p}{k_2} + \left(C_f(0) - \frac{\alpha\ f\ C_p}{k_2} \right)\ \exp(-k_2\ t) \end{aligned} \qquad (2\text{-}36)$$

Acknowledging this fact is of paramount importance to interpret the results reported by Muir et al. (1992), Dabrowska et al. (1996), or Fisk et al. (1998) correctly in light of the fecal partitioning model proposed herein. When this solution is redifferentiated, one observes that

$$\frac{d\,C_f}{d\,t} = -\left(C_f(0) - \frac{\alpha\,f\,C_p}{k_2} \right)\ k_2\ \exp(-k_2\ t) \qquad (2\text{-}37)$$

Now let T denote the length of a bioaccumulation experiment in which $C_f(0)$=0 and f and C_p are constant, i.e., such as those studies cited above. Also let α and k_2 denote the assimilation efficiency and apparent depuration rate that were estimated for this experiment. When the experiment is half over, the rate of change in the fish's whole body concentration would be calculated by Eq.(2-37) to be

$$\left.\frac{d\,C_f}{d\,t}\right|_{t=T/2} = \alpha\ f\ C_p\ \exp(-k_2\ T/2) \qquad (2\text{-}38)$$

If one now elects to arbitrary restart time, the bioaccumulation dynamics for the second half of the experiment would be described by

$$C_f = \frac{\hat{\alpha}\,f\,C_p}{\hat{k}_2} + \left(C_f(T/2) - \frac{\hat{\alpha}\,f\,C_p}{\hat{k}_2} \right)\ \exp(-\hat{k}_2\,\tau) \qquad (2\text{-}39)$$

where $\hat{\alpha}$ and $\hat{k}_2$ denote updated estimates for the fish's assimilation efficiency and apparent depuration rate for $0 \le \tau \le T/2$. This equation can also be differentiated to yield

$$\frac{d\,C_f}{d\,\tau} = -\left(C_f(T/2) - \frac{\hat{\alpha}\,f\,C_p}{\hat{k}_2} \right)\ \hat{k}_2\ \exp(-\hat{k}_2\,\tau) \qquad (2\text{-}40)$$

which can be evaluated at $\tau = 0$ to yield

$$\left.\frac{d\,C_f}{d\,\tau}\right|_{\tau=0} = \hat{\alpha}\ f\ C_p - \hat{k}_2\ C_f(T/2) \qquad (2\text{-}41)$$

For logical as well as mathematically consistency this derivative should equal the derivative given by Eq.(2-38), i.e.,

$$\hat{\alpha}\ f\ C_p - \hat{k}_2\ C_f(T/2) = \alpha\ f\ C_p\ \exp(-k_2\ T/2) \qquad (2\text{-}42)$$

Solving for $\hat{\alpha}$ then yields

$$\begin{aligned} ; &= \frac{\alpha\ f\ C_p\ \exp(-k_2\ T/2) + \hat{k}_2\ C_f(T/2)}{f\ C_p} \\ &= \alpha\ \exp(-k_2\ T/2) + \frac{\hat{k}_2}{f\ C_p}\ C_f(T/2) \\ &= \alpha\ \exp(-k_2\ T/2) + \frac{\hat{k}_2}{f\ C_p}\left(\alpha\,f\,C_p\,\frac{1-\exp(-k_2\ T/2)}{k_2} \right) \\ &= \alpha\left(\exp(-k_2\ T/2) + \frac{\hat{k}_2}{k_2}\left(1-\exp(-k_2\ T/2)\right) \right) \end{aligned} \qquad (2\text{-}43)$$

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. Specific growth rates and chemical excretion rates for fish, however, are generally related to the fish's body size as allometric power functions, i.e.,

$$r = \rho_1\,W^{\rho_2}$$

where in general $\rho_2 < 0$ (Barber et al. 1988; Sijm et al. 1993, 1995; Sijm and van der Linde 1995). Therefore, if any

significant growth occurs during the experiment, which is often the case, one would not expect that $k_2 = \hat{k}_2$ and consequently one would not expect $\alpha = \hat{\alpha}$. In point of fact one would generally expect $\alpha > \hat{\alpha}$. Importantly, this simple analysis is corroborated by findings of Ram and Gillet (1993) who showed that assimilation efficiencies for a variety of organochlorines by oligochaetes decreased as chemical exposures progressed.

In terms of application the above fecal partitioning model is best suited to circumstances where its equilibrium assumptions are best met such as the case herein where the object is to predict the dietary exchange of average individual of an explicit or implicit population. A more kinetically based approach may be needed, however, when trying to describe the toxicokinetic of individual fish. See for example Nichols et al. (1998).

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.,

$$M = -\beta\, C_a\, (P_a\, W) \qquad (2\text{-}45)$$

where M is the total amount of chemical metabolized (µg / ml), β is the fish's biotransformation rate (1/day), and (P_a W) is the volume of the volume of the fish's aqueous phase. If Eqs. (2-9) and (2-45) are used to described the bioconcentration of a chemical in fish during a water only exposure without growth, then a fish's whole body concentration would be modeled as

$$\begin{aligned} \frac{dC_f}{dt} &= \frac{1}{W}\frac{dB_f}{dt} \\ &= \frac{S_g k_g}{W}\left(C_w - \frac{C_f}{K_f}\right) - \frac{\beta\, P_a\, C_f}{K_f} \qquad (2\text{-}46) \\ &= k_u C_w - (k_e + k_m)\, C_f \end{aligned}$$

where k_u, k_e, and k_m are the fish's uptake rate, elimination rate, and biotransformation rate, respectively, which are often reported in the literature. In terms of quantitative structure activity relationships (QSARs), one should note that this model predicts that the whole body biotransformation rate k_m should be inversely proportional to the fish's thermodynamic bioconcentration factor K_f which in turn is proportional to the chemical's K_{ow}. This relationship, however, will also be influenced by any QSAR dependencies which the fish's aqueous phase biotransformation rate β might have. See de Wolf et al. (1992) and de Bruijn et al. (1993).

2.5. Modeling Temperature Effects on Physiological Rates

Because temperature effects a fish's feeding, assimilation, respiration, and egestion, a general 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 are often described using an exponential response equation, e.g.,

$$k_1 = k_0\, e^{\epsilon\,(T_1 - T_0)} \qquad (2\text{-}47)$$

where k_0 and k_1 are the process's reaction rates at temperatures T_0 and T_1, respectively, such descriptions are generally valid only within a range of the organism's thermal tolerances. In most cases, the process's reaction rate increases exponentially with increasing temperature up to a temperature T_1 after which it decreases. Moreover, in most cases the temperature at which a process's rate is maximal is very close to the organism's upper thermal limit. To address this problem, 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 a variety of fish bioenergetic models, BASS uses an exponential-type formulation that is assumed to response hyperbolically to increasing temperature. Importantly, such algorithms can be easily parameterized.

Let P denote the rate of a physiological process and T_1 denote the temperature at which this rate is maximal. If this process generally exhibits an exponential response to temperature changes well below T_1, then

$$P = P_0\, e^{\beta\,(T - T_0)} \qquad (2\text{-}48)$$

$$\frac{d\,P}{d\,T} = \gamma\, P \qquad (2\text{-}49)$$

where P_0 is the process's rate at an appropriate lower-end reference temperature T_0. To incorporate the adverse effects of high temperatures on this process, the right hand side of Eq.(2-49) can be multiplied by a hyperbolic temperature term that approaches unity as temperature decreases below T_1, equals zero at T_1, and becomes increasingly negative as temperatures approach the fish's upper thermal tolerance limit $T_L = T_2$. Modifying Eq.(2-49) in this fashion subsequently yields

$$\frac{d\,P}{d\,T} = \gamma\, P\left(\frac{T - T_1}{T - T_2}\right) \qquad (2\text{-}50)$$

whose solution is

$$P = P_0\, e^{\gamma\,(T - T_0)}\left(\frac{T_2 - T}{T_2 - T_0}\right)^{\gamma\,(T_2 - T_1)} \qquad (2\text{-}51)$$

Figure 1 displays the predicted temperature response of the maximum feeding of a 50 g brown trout (*Salmo trutta*) based on data reported by Elliott (1976b, Tables 2 and 9). For this figure

it is assumed that $T_0 = (3.8 + 6.6)/2$, $T_1 = 17.8$, and $T_2=25$. The parameters $P_0 = 340$ and $\gamma = 0.50$ were then calibrated using the results of a non-linear least squares analysis as a starting point. For other applications of this model see Lassiter and Kearns (1974) and Swartzman and Bentley (1979). Note that when $T_1 = T_2$, the Eq.(2-51) reduces to Eq.(2-48).

2.6. Modeling Growth of Fish

Although the preceding formulations of the processes that determine the bioaccumulation of chemicals in fish depend on a fish's live weight, BASS does not directly simulate the live 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

$$\begin{aligned} W &= W_a + W_d \\ &= W_a + W_l + W_o \end{aligned} \qquad (2\text{-}52)$$

$$P_l = \lambda_0 \, W^{\lambda_2} \qquad (2\text{-}53)$$

$$P_a = \alpha_0 - \alpha_1 \, P_l \qquad (2\text{-}54)$$

$$P_o = 1 - P_a - P_l \qquad (2\text{-}55)$$

where W_a, W_d, W_l, and W_o denotes the fish's aqueous, dry, lipid, and non-lipid organic weights, respectively. Whereas Eqs.(2-52) and (2-55) are simply assertions of mass conservation, Eqs. (2-53) and (2-54) are purely statistical in nature. Although Eq. (2-53) is assumed because simple power functions of this form generally describe a wide variety of morphometric relationships for most organisms, the appropriateness of Eq. (2-54) 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. 1985; Morishita et al. 1987). These equations yield an expression for a fish's live weigh that is a monotonically increasing but non-linear function of the fish's dry weight.

BASS calculates a fish's realized feeding by first estimating its maximum *ad libitum* consumption and then adjusting this potential by the availability of appropriate prey as described in the next section. Because a wide variety of models and methods have been used to describe maximum feeding of fish, BASS is coded to allow a user the option of using any one of four different models to simulate the feeding of any particular age/size class of fish. The first formulation that can be used is a temperature-dependent power function

$$C_{\max} = c_1 \, W^{c_2} \, e^{c_3 (T - T_0)} \left(\frac{T_2 - T}{T_2 - T_0} \right)^{c_3 (T_2 - T_1)} \qquad (2\text{-}56)$$

where the temperatures T_0, T_1, and T_2 are specific to the fish's feeding. A commonly used alternative to this model is the process-based Rashevsky-Holling model that is defined by the equations

$$\begin{aligned} C_{\max} &= \phi \left(I_{\max} - I \right) \\ \frac{dI}{dt} &= C_{\max} - A - E \end{aligned} \qquad (2\text{-}57)$$

where ϕ is the fish's *ad libitum* feeding rate (day^{-1}) that is generally a temperature-dependent power function of body weight, I_{max} is the maximum amount of food (g(DW)) that the fish's stomach/intestine can hold, I is the actual amount of food (g(DW)) present in the intestine, and A and E again are the fish's assimilation (g(DW)/day) and egestion (g(DW)/day) , respectively (Rashevsky 1959; Holling 1966). The feeding rate ϕ can be estimated using the following equations

$$M(t) = \int_0^t \phi \left(I_{\max} - M(\tau) \right) d\tau \qquad (2\text{-}58)$$

$$\frac{dM(t)}{dt} = \phi \left(I_{\max} - M(t) \right) \qquad (2\text{-}59)$$

$$-\phi \, t = \ln \left(1 - \frac{M(t)}{I_{\max}} \right) \qquad (2\text{-}60)$$

where $M(t)$ denotes the total amount of food consumed during the interval $(0,t]$ (also see Dunbrack 1988). Although given a fish's gut capacity I_{max}, satiation meal size M_{sat}, and time t_{sat} required to ingest M_{sat} one can readily calculate ϕ, one can also simply assume that $M_{sat} = 0.95 \times I_{max}$ in which case

$$\phi = -\frac{\ln(0.05)}{t_{sat}} \qquad (2\text{-}61)$$

For planktivores BASS can also estimate a fish's maximum ingestion using the clearance volume model

$$\begin{aligned} C_{\max} &= \Psi \; Q_{cl} \\ Q_{cl} &= q_1 \, W^{q_2} \, e^{q_3 (T - T_0)} \left(\frac{T_2 - T}{T_2 - T_0} \right)^{q_3 (T_2 - T_1)} \end{aligned} \qquad (2\text{-}62)$$

where Ψ is the plankton standing stock (g(DW)/L), Q_{cl} is the planktivore's clearance volume (L/day), and the temperatures T_0, T_1, and T_2 are specific to the fish's filtering rate. The fourth and final option is based on knowing the fish's projected growth and routine respiratory demands. In particular, because assimilation, egestion, specific dynamic action, and excretion can be calculated as linear functions of feeding and routine respiration as discussed below, it is then a straightforward matter to calculate a fish's expected ingestion given its projected growth and respiration. When a user elects this feeding option, BASS assumes that the fish's specific growth rate γ (day^{-1}) is given by

$$\gamma = W^{-1}\frac{dW}{dt} = g_1 W^{g_2} e^{g_3(T-T_0)}\left(\frac{T_2 - T}{T_2 - T_0}\right)^{g_3(T_2 - T_1)} \quad (2\text{-}63)$$

where the temperatures T_0, T_1, and T_2 are specific to the fish's growth rate. See Thomann and Connolly (1984) for additional discussion of the use of this feeding model.

If Eqs. (2-56), (2-62), or (2-63) are used to estimate a fish's maximum consumption, then BASS calculates the fish's assimilation and egestion as a simple fraction of its realized ingestion F, i.e.,

$$A = \alpha_f F \quad (2\text{-}64)$$

$$E = \left(1 - \alpha_f\right) F \quad (2\text{-}65)$$

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

$$D = d_1 I^{d_2} e^{d_3(T-T_0)}\left(\frac{T_2 - T}{T_2 - T_0}\right)^{d_3(T_2 - T_1)} \quad (2\text{-}66)$$

The numerical value of this function's exponent, d_2, depends both on characteristics of the food item being consumed and on the mechanisms that presumably control gastro-intestinal motility and digestion (Jobling 1981, 1986, 1987). For example, when gut clearance is controlled by intestinal peristalsis, d_2 should approximately equal ½ since peristalsis is stimulated by circumferential pressure exerted by the intestinal contents which, in turn, is proportional to the square root of its mass. On the other hand, when surface area controls the rate of digestion, d_2 should be approximately either ⅔ or unity. If the fish consumes a small number of large-sized prey (e.g., a piscivore), d_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), d_2 = 1 is more appropriate since total surface area and total volume of prey become almost directly proportional to one another. When d_2 = 1, the above Rashevsky-Holling model is analogous to the Elliott-Persson model for estimating daily rations of fish (Elliott and Persson 1978). Finally, Olson and Mullen (1986) outlined a hypothetical, process-based model that even suggests d_2 = 0 as an appropriate model.

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,

$$SDA = \sigma A \quad (2\text{-}67)$$

where σ is generally on the order of 0.15 to 0.20 (Ware 1975; Tandler and Beamish 1981; Beamish and MacMahon 1988).

In BASS, it is assumed that body weight losses via metabolism are due entirely to the respiration of carbon dioxide and the excretion of ammonia. A fish's respiratory losses are therefore calculated from its routine oxygen consumption, O_r (g O_2/day) using respiratory quotients RQ (L (CO_2) respired)/ L (O_2) consumed) as follows

$$R = \frac{12\,g\,C}{mole\,CO_2}\cdot\frac{mole\,CO_2}{22.4\,L\,CO_2}\cdot RQ\cdot\frac{22.4\,L\,O_2}{mole\,O_2}\cdot\frac{mole\,O_2}{32\,g\,O_2}\cdot($$
$$= \frac{12}{32}\cdot RQ\cdot O_r \quad (2\text{-}68)$$

BASS then calculates a fish's routine oxygen consumption as a constant multiple of its basal or standard oxygen consumption (Ware 1975) which is specified using the temperature-dependent power function

$$O_b = b_1 W^{b_2} e^{b_3(T-T_0)}\left(\frac{T_2 - T}{T_2 - T_0}\right)^{b_3(T_2 - T_1)} \quad (2\text{-}69)$$

Although the ammonia excretion could be modeled using an analogous function (Paulson 1980; du Preez and Cockroft 1988a, 1988b), in BASS this flux is formulated 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

$$EX = \epsilon\, NC\,(R + SDA) \quad (2\text{-}70)$$

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

2.7. Modeling Trophic Interactions and Predatory Mortalities

BASS is designed to simulate 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 maximum or desired feeding rate of an individual of that cohort, the cohort's population size, and the biomass of prey available to the cohort which is the sum of the prey's compartmental biomasses minus the biomass of those components which are expected to be consumed by other 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 would suggest that the larger predator is more likely to encounter that prey than is the smaller. Having encountered the prey, the trend for prey handling times to be inversely correlated with body size (Werner 1974; Miller et al. 1992) would also suggest that the larger predator could dispatch the prey and resume its foraging more quickly than the smaller predator.

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 different prey consumed by a cohort using dietary electivities, i.e.,

$$e_i = \frac{d_i - f_i}{d_i + f_i} \qquad (2\text{-}71)$$

where f_i is the relative availability of the i-th prey with respect to all other prey consumed by the cohort. These electivities are calculated dynamically by BASS using dietary data specified by the user and the relative availabilities of the cohort's prey currently predicted by BASS. As described in the discussion of BASS' sdiet command (see page 38), BASS allows a user to specify a fish' s diet as either a set of fixed dietary frequencies $\{..., \hat{d}_i, ...\}$, a set of electivities $\{..., \hat{e}_i, ...\}$, or a combination of fixed frequencies and electivities $\{..., \hat{d}_i, ..., \hat{e}_j, ...\}$. In order to calculate the cohort's realized dietary composition, BASS first converts all fixed dietary frequencies specified by the user into their equivalent electivities using Eq. (2-71) and the current relative availabilities $\{..., f_i, ...\}$ of all potential prey. These electivities are then combined with any user specified electivities to form a set of unadjusted electivities $\{..., \hat{e}_i, ...\}$ which in general must then be converted into a consistent set of realized electivities $\{..., e_i, ...\}$. Using these realized electivities, BASS finally calculates the cohort's realized dietary frequencies using

$$d_i = \frac{1 + e_i}{1 - e_i} f_i \qquad (2\text{-}72)$$

The important step in this computational process is the conversion of the unadjusted electivities $\{..., \hat{e}_i, ...\}$ into a set of realized electivities $\{..., e_i, ...\}$. Although this conversion is sometimes unnecessary, it is generally needed to insure that the sum of the dietary frequencies $\{..., d_i, ...\}$ calculated by Eq.(2-72) equals 1. One can verify that the condition that guarantees $\Sigma d_i = 1$ is

$$\sum \frac{f_i}{1 - e_i} = 1 \qquad (2\text{-}73)$$

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

$$e_i = \alpha (\hat{e}_i + 1) - 1 \qquad (2\text{-}74)$$

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

Because numerous food web studies have shown that there is generally 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), when BASS uses the above procedure to calculate piscivorous interactions, only a specific size range of forage fish are assumed to be available to a piscivorous cohort. More specifically, BASS assumes that the body lengths of forage fish available to such a cohort are distributed normally with mean

$$L_{prey} = \alpha + \beta L_{predator} \qquad (2\text{-}75)$$

BASS estimates the variance of this distribution by assuming that the body length of the largest prey typically taken by a piscivore approximately equals 50% of its own body length (Juanes 1994). If less than 1% of a predator' s prey exceeds this upper limit, the variance of the predator's prey size distribution can be calculated from the corresponding standardized Z-score as

$$\sigma = \frac{0.5\ L_{predator} - L_{prey}}{2.33} \qquad (2\text{-}76)$$

When BASS calculates the relative frequency d_i of a forage fish species *i* in a cohort's diet, the relative availability of that species is calculated as the sum of all cohort biomasses whose body lengths are less than $0.5\ L_{predator}$ minus the biomass of those cohorts that are calculated to be consumed by other cohorts that

are more efficient piscivores (see assumption 1 above). If more than one age class of species *i* can be consumed by the cohort, the relative frequencies of these age classes s_{ij} in the cohort's diet are calculated using the cohort's prey size distribution . 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} denotes the probabilistic density

$$P_{ij} = \frac{1}{\sqrt{2\ \pi}\ \sigma} \exp\left(-\frac{(L_{ij} - L_{prey})^2}{2\ \sigma^2} \right) \qquad (2\text{-}77)$$

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 species is vulnerable to the cohort, then $s_{ij} = d_i$.

If during the calculation of 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 $\{..., e_i^*, ...\}$ in a manner to simulate prey switching. These reassignments as 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 benthic feeding piscivores. If such resources are still insufficient to satisfy the piscivores' metabolic demands, piscivores are assumed to then switch to planktivory (Werner and Gilliam 1984; Magnan 1988; Bergmann 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 0 regardless of its previous value. BASS also reassigns any other electivity which does not equal -1, to 0.

After BASS has calculated a cohort's dietary composition, it then assigns the realized feeding rate of cohort as

$$F = \max\left(N^{-1} \sum_{e_j \neq -1} AB_j\,,\ F_{\max} \right) \qquad (2\text{-}78)$$

where F_{max} is the cohort's maximum or desired individual ingestion, *N* is the cohort's population size, and AB_j is the biomass 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 cohort and non-fish biotic resource.

2.8. Modeling Non Predatory Mortalities and Recruitment

Numerous studies (Damuth 1981; Peters and Raelson 1984; Juanes 1986; Robinson and Redford 1986; Boudreau and Dickie 1989; Gordoa and Duarte 1992; Randall et al. 1995 Dunham and Vinyard 1997; Steingrímsson and Grant 1999) have shown that the population densities of vertebrates are generally correlated with their mean body size. In particular,

$$N = a\ W^{-b} \qquad (2\text{-}79)$$

where *N* is the population density (inds/area) of the species or cohort and *W* is the mean body weight of that species or cohort. Although an interspecific analysis of data for a variety of fish by Randall et al. (1995) suggests a mean exponent close to unity, data reported by Boudreau and Dickie (1989) and Gordoa and Duarte (1992) for individual fish species suggest an average exponent of approximately 0.75. An expression for a species' total mortality rate can be obtained by differentiating Eq. (2-79) as follows

$$\frac{dN}{dt} = -b\ a\ W^{-b} \left(W^{-1}\ \frac{dW}{dt} \right) = -b\ N\ \gamma \qquad (2\text{-}80)$$

where γ is the species specific growth rate. Based on this equation, one could therefore conclude that a species' total mortality rate is simply $\mu = b\ \gamma$. Readers interested in detailed discussions concerning the underlying process-based interpretation and general applicability of this result should consult Peterson and Wroblewski (1984) and McGurk (1993, 1999). Because BASS assumes that the specific growth rates of a species are allometric functions of its body sizes, it follows that

$$\mu = b\ \gamma_1\ W^{\gamma_2} \qquad (2\text{-}81)$$

Also see Lorenzen (1996). Because this equation actually includes both a species' predatory and non-predatory mortality, BASS assumes that a species' non-predatory mortality rate is simply some fraction δ of μ. In general, this fraction will be small for forage fish and large for predatory species. During the course of the simulation BASS calculates the daily non-predatory mortality each cohort using Eq.(2-81) parameterized with the cohort's current body weight.

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 to be the total biomass of all cohorts whose body length is 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 decremented by its rbi and the

total number of YOY which are recruited into the population as a new cohort is estimated by simply dividing the species' spawned biomass by the species' 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)).

2.9. Modeling Toxicological Effects

Narcosis is defined to be any reversible decrease in physiological function that is induced by chemical agents. Because the potency of narcotic agents was originally found to be correlated 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 either 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; Franks and Lieb 1978, 1982, 1984; Richards et al. 1978; Law et al. 1985; Lassiter 1990). In either case, however, the idea that the presence of narcotic chemicals increases the physical dimensions of various physiological targets to some "critical volume" which renders them inactive is fundamental (Abernethy et al. 1988). Consequently, narcotic chemicals can be treated as generalized physiological toxicants and narcosis itself can be considered to represent baseline chemical toxicity for organisms. Although any particular chemical may 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 any given level of biological activity (Fergusion 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 as noted above, it should not be too surprising that the effects of mixtures of chemicals possessing diverse specific modes of action not only often resemble narcosis but also appear to be additive in terms of their toxic effects (Barber et al. 1987; McCarty and Mackay 1993). For example, even though most pesticides possess a specific mode of action is 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 would 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 it's calculated lethal threshold, BASS assumes that the fish dies and then eliminates that fish's age class from further consideration. The total chemical activity of a fish's aqueous phase is simply the sum of the fish's aqueous phase chemical activity for each chemical. BASS calculates the aqueous phase chemical activity of each chemical using the following formulae

$$A_a = \gamma_a M_a$$

$$M_a = \frac{C_a}{10^3 MW} \qquad (2\text{-}82)$$

$$C_a = \frac{C_f}{K_f}$$

where A_a is the chemical's aqueous activity, γ_a is the chemical's aqueous activity coefficient (L/mol) which is 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 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.

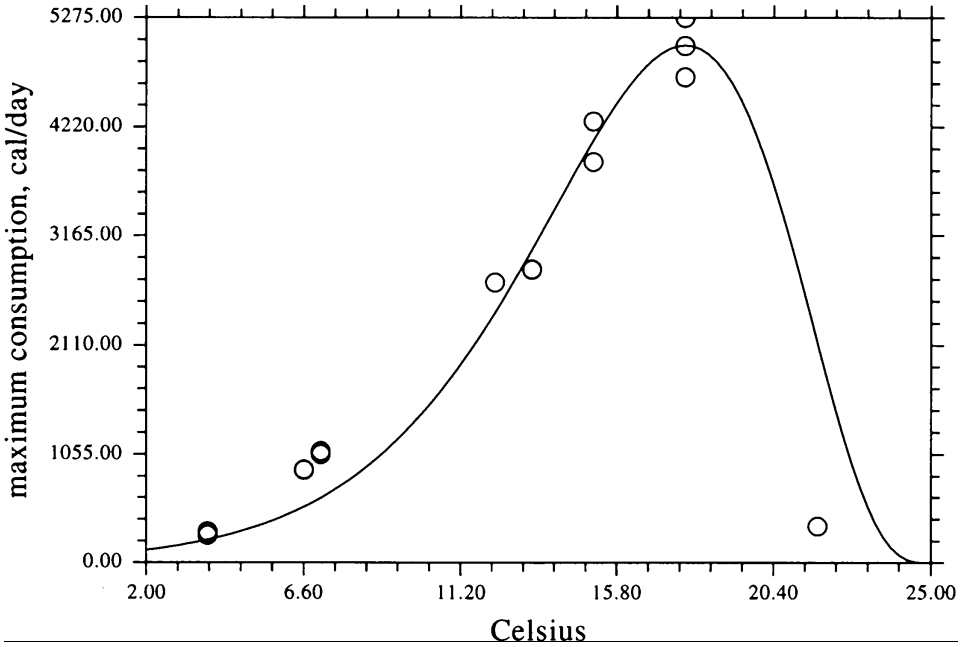
Three points should be mentioned regarding the above approach to modeling ecotoxicological effects. Firstly, it should be noted that for narcotic chemicals this approach is analogous to the

toxic unit approach for evaluating the toxicity of mixtures (Calamari and Alabaster 1980; Könemann 1981a, 1981b; Hermens and Leeuwangh 1982; Hermens et al. 1984a, 1984b, 1985a, 1985b, 1985c; Broderius and Kahl 1985; Dawson 1994; Peterson 1994). Secondly, 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). Lastly, although sublethal effects are not presently modeled by BASS, BASS's simulation results can be used to indicate when sublethal effects that are induced by narcotic agents would be expected to occur. Results reported by Hermens et al (1984a) 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 at. 1984a, 1985a). Also see Roex et al. (2000).

Table 1. Symbols used for model development

B	chemical burden in whole fish (μg)
C_a	chemical concentration in aqueous fraction of the fish (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(FW))
C_{ia}	chemical concentration in aqueous fraction of intestinal contents (μg/mL)
C_{io}	chemical concentration in organic fraction of intestinal contents (μg/mL)
C_l	chemical concentration in lipid (μg/g(FW))
C_o	chemical concentration in non lipid organic matter (μg/g(FW))
C_w	chemical concentration in environmental water (μg/mL)
d	interlamellar distance (cm)
D	aqueous diffusion coefficient (cm^2/s)
E	egestive flux (g(FW)/day)
EX	excretory flux (g(FW)/day)
F	feeding flux (g(FW)/day)
h	hydraulic radius of interlamellar channels (cm) = 0.5d
I	mass of food resident in the intestine (g(FW))
J_g	net chemical exchange across the gills (μg /s)
J_i	net chemical exchange across the intestine (μg /s)
K_l	partition coefficient between generic lipid and water (dimensionless)
K_e	partition coefficient for fecal matter (dimensionless)
K_f	thermodynamic bioconcentration factor (dimensionless)
K_{oc}	partition coefficient between organic carbon and water (dimensionless)
K_{ow}	partition coefficient between n-octanol and water (dimensionless)
K_o	partition coefficient between non-lipid organic matter and water (dimensionless)
k_g	conductance in interlamellar water (cm/s)
k_m	conductance of the gill membrane (cm/s)
l	lamellar length (cm)
L	fish's body length (cm)
M	metabolism of chemical (μg /s)
N	population density (inds/ha)
N_{Gz}	Graetz number (dimensionless) = $(l\ D)/(V\ r^2)$
N_{Sh}	Sherwood number (dimensionless) = $(k_m\ h)/D$
NM	non-predatory mortality (inds·ha^{-1}·day^{-1})
P_a	fraction of whole fish that is aqueous (dimensionless)
P_{ia}	fraction of intestinal contents that is aqueous (dimensionless)
P_{io}	fraction of intestinal contents that is organic (dimensionless)
P_l	fraction of whole fish that is lipid (dimensionless)
P_o	fraction of whole fish that is non-lipid organic matter (dimensionless)
PM	predatory mortality (inds·ha^{-1}·day^{-1})
O_2	oxygen consumption (mg/s)
Q	ventilation volume (cm^3/s)
R	routine respiratory flux (g(FW)/day)
SDA	specific dynamic action (g(FW)/day)
S_g	total gill surface area (cm^2)
T	temperature (Celsius)
V	average velocity of interlamellar flow (cm/s)
W	weight of fish (g(FW) or g(DW))
X_g	cross sectional pore area of the gill (cm^2)
α_c	assimilation efficiency of chemical (dimensionless)
α_f	assimilation efficiency of food (dimensionless)
γ	fish's specific growth rate (day^{-1}) = $W^{-1}\ dW/dt$
η	solution viscosity (poise)
ν	molar volume (cm^3/mol)
ρ	lamellar density (lamellae/mm)

Figure 1. Application of Eq.(2-51) to describe the temperature dependence of the maximum daily consumption of brown trout (*Salmo trutta*) based on Elliott (1976b, Tables 2 and 9).



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 of parameterizing the above equations are now discussed.

3.1. Parameterizing K_f

Superficially, estimation of a fish's thermodynamic bioconcentration factor K_f via Eq. (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 Eq.(2-53)), it is a straightforward matter to calculate the fish's aqueous fraction using Eq. (2-54). Having done so, one can then immediately calculate the fish's non-lipid organic fraction since the sum of P_a, P_l, and P_o must be unity (i.e., Eq. (2-55)).

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 lipid of fish and it would seem reasonable to estimate K_l using a triglyceride/water partition coefficient, BASS assumes that K_l identically 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 organic carbon/water partition coefficients (K_{oc}), and K_{ow} to estimate this parameter. Specifically,

$$K_o = K_{oc} = 0.411\, K_{ow} \qquad (3\text{-}1)$$

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 given above. For example, whereas the K_{ow} of methylmercury at physiological pH's is on the order of 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. 1999a, 1999b). O'Loughlin et al. (2000) report similar discrepancies for organotin compounds. In general distribution coefficients for metals into fecal matter should be assigned values comparable to those used to model the environmental fate and transport of metals whereas metal distribution coefficients for metals into the non-lipid organic matter of fish should be assigned values up to an order of magnitude 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, mean interlamellar distance, and mean lamellar length must be specified. In general, each of these morphological variables is dependent on the fish' s body size according to the allometric functions,

$$S_g = s_1 W^{s_2} \qquad (3\text{-}2)$$

$$d = d_1 W^{d_2} \qquad (3\text{-}3)$$

$$l = l_1 W^{l_2} \qquad (3\text{-}4)$$

Although many authors have reported allometric coefficients and exponents for total gill surface areas, parameters for the latter are seldom available. Parameters for 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.,

$$\rho = \rho_1 W^{\rho_2} \qquad (3\text{-}5)$$

is known. Fortunately, lamellar densities, like total gill areas, are generally available in the literature. See Tables 2-4. BASS estimates d_1 and d_2 from ρ_1 and ρ_2 using the inter-specific regression (n=28, r=-0.92)

$$d = 0.118\rho^{-1.19} \qquad (3\text{-}6)$$

To overcome the scarcity of published morphometric relationships for lamellar lengths (see Table 5), BASS uses the default inter-specific regression (n=90, r=0.92)

$$l = 0.0188\, W^{0.294} \qquad (3\text{-}7)$$

Both of the preceding regressions are functional regressions rather than simple linear regressions (Rayner 1985; Jensen 1986); the data used for their calculation were drawn 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,

$$D = 2.101\times10^{-7}\,\eta^{-1.4}\,\nu^{-0.589} \qquad (3\text{-}8)$$

where ν (cm^3/mol) is the chemical's molar volume (Hayduk and Laudie 1974). The diffusivity of chemicals through the gill membrane which is needed to estimate the membrane's permeability k_m is then assumed to equal one 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 water-blood barrier. Based on the studies summarized in Table 6, BASS assumes a default water-blood barrier thickness of approximately 0.0029 cm for all fish species and then calculates k_m as the ratio of the chemical's membrane diffusivity to the thickness of the gill's water-blood barrier. These assumptions imply that

$$N_{Sh} = 0.0116^{-1}\, d \qquad (3\text{-}9)$$

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 Eq.(2-12)). Perfusion rates (ml/hr) are estimated using

$$Q_p = (0.23\,T - 0.78)\ 1.862\ W^{0.9} \qquad (3\text{-}10)$$

as the default for all species. Although this expression, in units of L/kg/kr, 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 Eq.(2-28) are interpolated internally by BASS from matrices of tabulated eigenvalues and mixing cup coefficients which encompass the range of Sherwood numbers (i.e., $1 < N_{Sh} < 10$) and ventilation/perfusion ratios (i.e., $1 < Q_v / Q_p < 20$) that are typical for fish (Hanson and Johansen 1970; Barron 1990; McKim et al. 1994; Sijm et al. 1994). See Figures 2-5.

3.3. Bioenergetic and Growth Parameters

In general parameterization of the physiological processes used by BASS to simulate fish growth poses no special problems since the literature abounds with studies that can be used for this purpose. Table 7 presents a very brief and cursory survey of data sources that can be used to parameterize BASS for a number of common and important fish species. The database that is distributed with the Wisconsin Bioenergetics Fish Model (Hanson et al. 1997) can also be used for this purpose. In addition to these sources, however, the reader should become familiar with Carlander's classic three volume work that summarizes allometric, growth, and natural history data for hundreds of North American fish species. See Carlander (1969, 1977, 1997). For oxygen consumption data the reader should also be aware of the computerized OXYREF database that has been complied by Thurston and Gerke (1993) . This database can be downloaded from the USEPA Center for Exposure Assessment Modeling web site at **http://www.epa.gov/ceampubl/oxyref.htm**.

Table 2. Summary of allometric coefficients and exponents for gill area and lamellar density for freshwater bony fishes and agnatha.

species	s_1	s_2	f_1	f_2	source
Acipenser transmontanus	3.50	0.849	15.3	-0.0475	Burggren et al. (1979)
Botia dario	10.5	0.716	41.0	-0.0460	Singh et al. (1988)
Botia lohachata	9.13	0.700	39.0	-0.0055	Sharma et al. (1982)
Catostomus commersoni	11.2	0.587	25.2	-0.109	Saunders (1962)
Cirrhinus mrigala	11.8	0.816	63.2	-0.129	Roy and Munshi (1986)
Comephorus dyoowski	2.15	0.675	--	--	Jakubowski (1993)
Cottocomephorus grewingki	6.56	0.91	24.6	-0.150	Jakubowski et al. (1995)
Cottocomephorus inermis	7.42	0.918	22.6	-0.110	Jakubowski et al. (1995)
Cottus gobio	7.20	0.849	--	--	Jakubowski et al. (1995)
Cottus gobio	1.35	1.29	21.8	-0.126	Liszka (1969) and Starmach (1971)
Ctenopharyngodon idella	9.44	0.774	33.0	-0.0513	Jakubowski (1982)
Cyprinus carpio	8.46	0.794	32.2	-0.0787	Oikawa and Itazawa (1985)
Esox lucius	0.274	1.24	78.6	-0.222	de Jager et al. (1977) and
Fundulus chrysotus	--	1.18	--	--	Burnside (1976)
Gambusia affinis	2.47	0.842	--	--	Murphy and Murphy (1971)
Glossogobius giuris	12.6	0.516	--	--	Singh and Munshi (1985)
Hoplias lacerdae	4.92	0.81	29.0	-0.06	Fernandes et al. (1994)
Hoplias malabaricus	1.26	1.14	35.0	-0.090	Fernandes et al. (1994)
Hoplias malabaricus	0.731	1.25	29.5	-0.0600	Fernandes and Rantin (1985)
Ictalurus nebulosus	4.98	0.728	15.9	-0.0917	Saunders (1962)
Ictalurus punctatus	--	--	10.2	-0.056	Barber (2000)
Lampetra fluviatilis	24.1	1.03	31.0	-0.123	Lewis and Potter (1976)
Lampetra planeri	23.9	0.689	28.3	-0.117	Lewis and Potter (1976)
Leiopotherapon unicolor	4.68	1.04	20.6	-0.0870	Gehrke (1987)
Lepomis macrochirus	--	--	20.1	-0.098	Barber (2000)
Macrognathus aculeatum	2.17	0.733	41.9	-0.0690	Ojha and Munshi (1974)
Micropterus dolomieui	7.36	0.819	30.0	-0.0615	Price (1931)
Mystus cavasius	6.17	0.915	40.2	-0.0970	Ojha et al. (1985)
Oncorhynchus mykiss	1.84	1.13	--	--	Niimi and Morgan (1980)
Oncorhynchus mykiss	3.15	0.932	27.5	-0.0639	Hughes (1984)
Oncorhynchus tshawytscha	7.13	0.922	--	--	Romough and Moroz (1990)

Orechromis alcalicus	11.1	0.789	38.4	-0.143	Hughes (1995)
Orechromis niloticus	6.35	0.777	32.9	-0.0545	Kisia and Hughes (1992)
Oryzias latipes	4.65	0.446	43.5	0.0	Umezawa and Watanabe (1973)
Piaractus mesopotamicus	5.65	0.769	40.2	-0.033	Severi et al. (1997)
Plagioscion squamosissimus	12.0	0.70	37.0	-0.07	Mazon et al. (1998)
Pomoxis nigromaculatus	--	--	18.4	-.074	Barber (2000)
Prochilodus scrofa	16.2	0.72	43.0	-0.12	Mazon et al. (1998)
Stizostedion vitreum	0.796	1.13	--	--	Niimi and Morgan (1980)
Tinca tinca	28.5	0.522	20.3	0.0160	Hughes (1972)
Tinca tinca	8.67	0.698	25.5	-0.0300	Hughes (1972)

Table 3. Summary of allometric coefficients and exponents for gill area and lamellar density for cartilaginous and marine boney fishes.

species	s_1	s_2	f_1	f_2	source
Acanthopagrus australis	2.40	0.788	--	--	Roubal (1987)
Alopias vulpinus	2512.	0.410	229.	-0.340	Emery and Szczepanski (1986)
Blennius pholis	7.63	0.849	28.3	-0.139	Milton (1971)
Carcharodon carcharias	42.7	0.770	27.5	-0.150	Emery and Szczepanski (1986)
Carcharhinus obscurus	6.17	0.880	33.8	-0.160	Emery and Szczepanski (1986)
Carcharhinus plumbeus	24.5	0.740	23.4	-0.130	Emery and Szczepanski (1986)
Coryphaena hippurus	52.1	0.713	33.8	-0.0360	Hughes (1972)
Fundulus similis	--	0.850	--	--	Burnside (1976)
Isurus oxyrinchus	57.5	0.740	50.0	-0.200	Emery and Szczepanski (1986)
Katsuwonus pelamis	52.2	0.850	59.0	-0.0759	Muir and Hughes (1969)
Morone saxatilis	--	--	17.0	-0.069	Barber (2000)
Opsanus tau	5.61	0.790	16.0	-0.0750	Hughes and Gray (1972)
Platichthys flesus	6.36	0.824	--	--	Hughes and Al-Kadhomiy (1986)
Prionace glauca	5.50	0.880	12.9	-0.0900	Emery and Szczepanski (1986)
Scomber scombrus	4.24	0.997	27.1	0.0230	Hughes (1972)
Scyliorhinus canicula	2.62	0.961	17.1	-0.0710	Hughes (1972)
Scyliorhinus stellaris	6.21	0.779	30.3	-0.167	Hughes et al. (1986)
Seriola quinqueradiata	22.9	0.686	38.5	-0.0419	Kobayashi et al. (1988)
Thunnus thynnus	24.4	0.901	63.2	-0.0938	Muir and Hughes (1969)
Torpedo marmorata	1.17	0.937	34.2	-0.167	Hughes (1978)

Table 4. Summary of allometric coefficients and exponents for gill area and lamellar density for air-breathing fishes.

species	s_1	s_2	f_1	f_2	source
Anabas testudineus	5.56	0.615	36.5	-0.152	Hughes et al. (1973)
Boleophthalmus boddaerti	2.81	0.709	24.6	-0.0830	Niva et al. (1981)
Boleophthalmus boddaerti	0.927	1.05	26.6	-0.229	Hughes and Al-Kadhomiy (1986)
Boleophthalmus boddaerti	6.79	0.481	23.1	-0.0307	Low et al. (1990)
Channa punctata	4.70	0.592	36.0	-0.138	Hakim et al. (1978)
Clarias batrachus	2.28	0.781	25.4	-0.0830	Munshi et al. (1980)
Clarias mossambicus	0.958	0.971	30.7	0.0909	Maina and Maloiy (1986)
Cobitis taenia	4.67	0.864	45.5	0.0	Robotham (1978)
Hoplerythrinus unitaeniatus	5.99	0.66	48.0	-0.16	Fernandes et al. (1994)
Hypostomus plecostomus	4.36	0.666	17.3	0.081	Perna and Fernandes (1996)
Lepidocephalichthys guntea	4.94	0.745	45.0	-0.221	Singh et al. (1981)
Lepisosteus oculatus	3.35	0.753	18.1	-0.0476	Landolt and Hill (1975)
Lepisosteus osseus	4.77	0.699	20.9	-0.0691	Landolt and Hill (1975)
Lepisosteus platostomus	3.01	0.793	15.3	-0.0236	Landolt and Hill (1975)
Noemacheilus barbatulus	3.60	0.577	36.4	0.0	Robotham (1978)
Periophthalmodon schlosseri	3.00	0.934	27.0	-0.0484	Yadav et al. (1990)
Periophthalmodon schlosseri	1.00	0.931	47.9	-0.0518	Low et al. (1990)
Periophthalmus chrysospilos	0.976	0.958	30.2	-0.237	Low et al. (1990)
Rhinelepis strigosa	6.25	0.757	12.3	0.020	Santos et al. (1994)
Saccobranchus fossilis	1.86	0.746	31.6	-0.0950	Hughes (1972)

Table 5. Summary of coefficients and exponents for lamellar lengths.

species	l_1	l_2	source
Hoplias lacerdae	0.012	0.23	Fernandes et al (1994)
Hoplias malabaricus	0.006	0.36	Fernandes et al (1994)
Hoplerythrinus unitaeniatus	0.014	0.22	Fernandes et al. (1994)
Ictalurus punctatus	0.00465	0.265	Barber (2000)
Lepomis macrochirus	0.00364	0.234	Barber (2000)
Morone saxatilis	0.00474	0.202	Barber (2000)
Piaractus mesopotamicus	0.0069	0.223	Severi et al. (1997)
Pomoxis nigromaculatus	0.00255	0.257	Barber (2000)
Rhinelepis strigosa	0.0422	0.231	Santos et al. (1994)

Table 6. Summary of studies reporting water-blood barrier thickness for freshwater and marine fishes.

source	species
Dube and Munshi (1974)	*Anabas testudineus*
Hughes (1972)	*Tinca tinca*
Hughes and Morgan (1973)	various species
Hughes and Umezawa (1983)	*Phrynelox tridens, Seriola quinqueradiata*
Hughes et al. (1986)	*Scyliorhinus stellaris*
Kobayashi et al. (1988)	*Seriola quinqueradiata*
Munshi et al. (1980)	*Clarias batrachus*
Ojha and Munshi (1974, 1976)	*Macrognathus aculeatum*
Ojha et al. (1982)	*Garra lamta*
Ojha et al. (1985)	*Mystus cavasius*
Piiper et al. (1986)	*Scyliorhinus stellaris*
Roy and Munshi (1987)	*Cirrhinus mrigala*
Sharma et al. (1982)	*Botia lohachata*
Singh and Munshi (1985)	*Glossogobius giuris*
Singh et al. (1981)	*Lepidocephalichthys guntea*
Singh et al. (1988)	*Botia dario*
Steen and Berg (1966)	various species
Stevens (1992)	*Sciaenops ocellatus*
Tuurala et al. (1998)	*Anguilla anguilla*

Table 7. Sources of bioenergetic and growth for selected fish species.

species	source
Alosa pseudoharengus	Stewart and Binkowski (1986)
Ambloplites rupestris	Roell and Orth (1993)
Ameiurus sp.	Glass (1969), Campbell and Branson (1978)
Ctenopharyngodon idella	Wiley and Wike (1986)
Cyprinodon sp.	Nordlie et al. (1991), Jordan et al. (1993)
Cyprinus carpio	Glass (1969), Oikawa and Itazawa (1984), Garcia and Adelman (1985)
Dorosoma cepedianum	Pierce et al. (1981), Drenner et al. (1982)
Esox lucius	Diana (1982a, 1982b), Salam and Davies (1994)
Gambusia affinis	Murphy and Murphy (1971), Shakuntala and Reddy (1977), Mitz and Newman (1989)
Lepomis sp.	Wohlschlag and Juliano (1959), O'Hara (1968), Pierce and Wissing (1974), El-Shamy (1976), Evans (1984)
Micropterus salmoides	Beamish (1970, 1974), Niimi and Beamish (1974), Tandler and Beamish (1981)
Micropterus dolomieu	Roell and Orth (1993)
Morone saxatilis	Hartman and Brandt (1995a)
Oncorhynchus mykiss	Kutty (1968), Rao (1968), Staples and Nomura (1976), Muller-Feuga et al. (1978), Grove et al. (1978), Rand et al. (1993)
Oncorhynchus nerka	Brett (1971), Beauchamp et al. (1989), Stewart and Ibarra (1991)
Oncorhynchus tshawytscha	Stewart and Ibarra (1991)
Osmerus mordax	Lantry and Stewart (1993)
Perca flavescens	Norstrom et al. (1976), Kitchell et al. (1977), Post (1990), Rose et al. (1999), Schaeffer et al. (1999)
Phoxinus phoxinus	Wootton et al. (1980), Cui and Wootton (1988)
Pimephales promelas	Wares and Igram (1979), Duffy (1998)
Ptychocheilus oregonensis	Petersen and Ward (1999)
Pungitius pungitius	Cameron et al. (1973)
Pylodictis olivaris	Roell and Orth (1993)
Salmo trutta	Glass (1969), Elliott (1972, 1975a, 1975b, 1976b)
Salvelinus namaycush	Stewart et al. (1983), Thomann and Connolly (1984)
Stizostedion canadense	Minton and McLean (1982)
Stizostedion vitreum vitreum	Kitchell et al. (1977), Tarby (1980), Madon and Culver (1993), Rose et al. (1999)

Figure 2. First eigenvalue for Eq.(2-28) as a function of gill Sherwood number and ventilation/perfusion ratio.

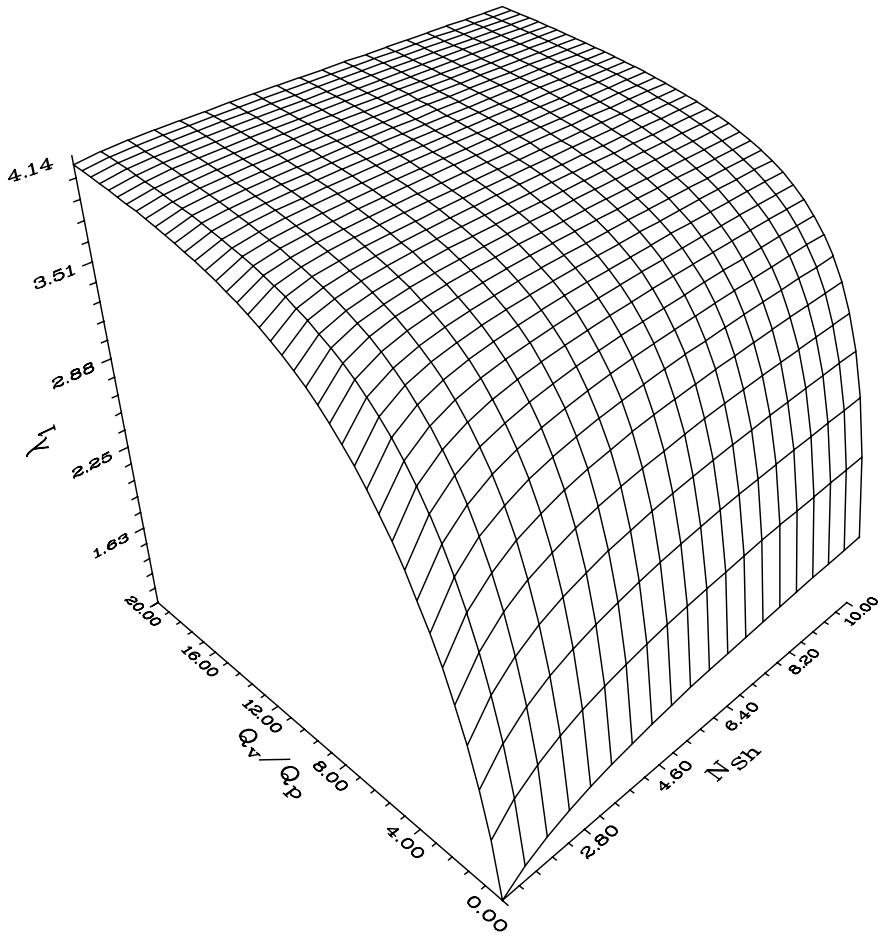


Figure 3. Second eigenvalue for Eq.(2-28) as a function of gill Sherwood number and ventilation/perfusion ratio.

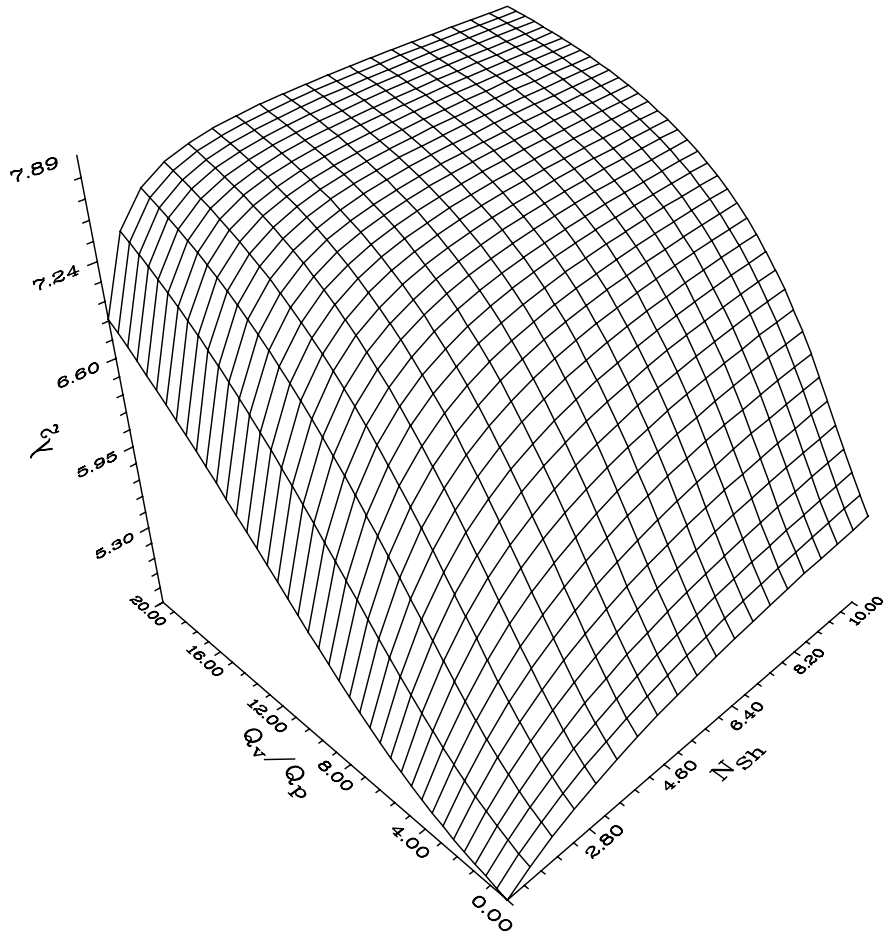


Figure 4. First bulk mixing cup coefficient for Eq.(2-28) as a function of gill Sherwood number and ventilation/perfusion ratio.

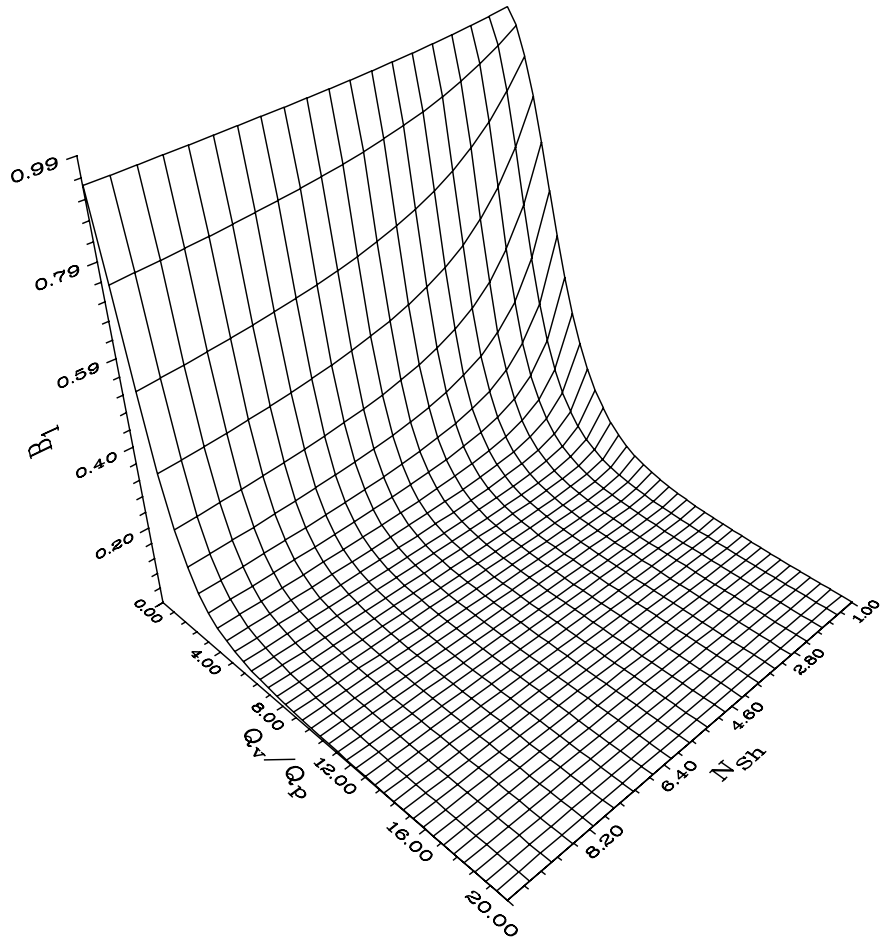
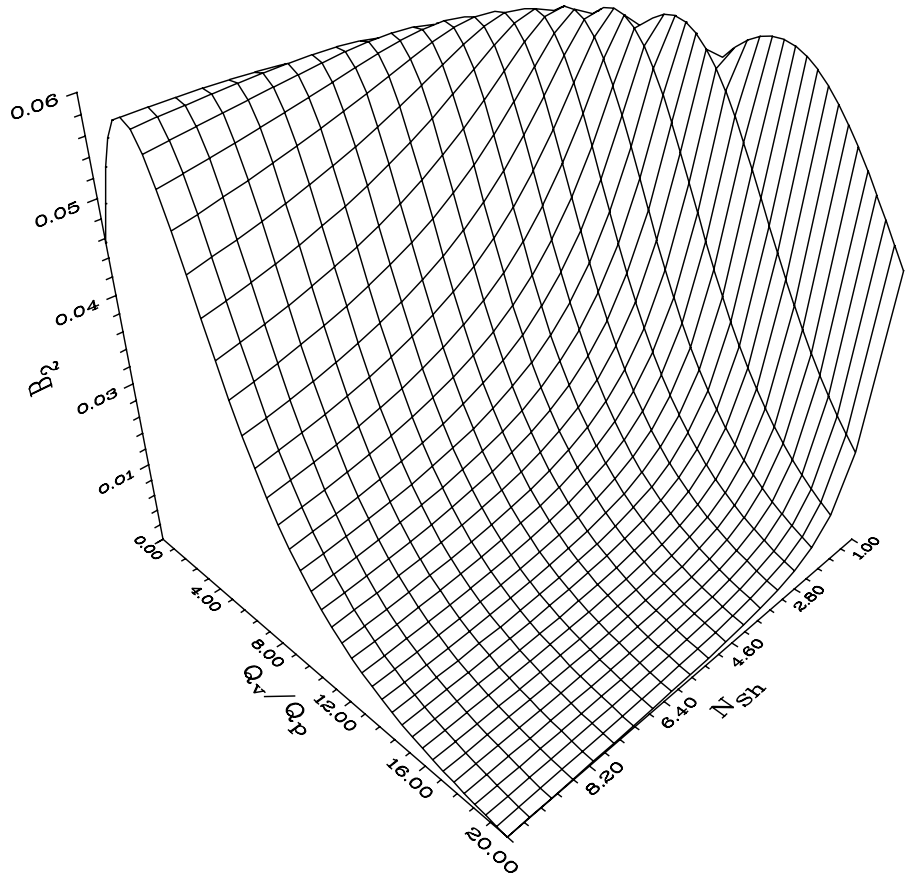


Figure 5. Second bulk mixing cup coefficient for Eq.(2-28) as a function of gill Sherwood number and ventilation/perfusion ratio.



4. BASS User Guide

Although BASS versions 1.0 and 1.1 were written in Fortran 77, BASS version 2.0 and higher is coded in Fortran 95. The model enables users to simulate the population and bioaccumulation dynamics of age-structured fish communities using a temporal and spatial scale of resolution of a day and a hectare, respectively. BASS currently ignores the migration of fish into and out of this simulated hectare. The duration of any species' age class can be specified as either a month or a year. This flexibility enables users to simulate small, short-lived species such as daces, live bearers, and minnows 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 either body weight, body length, or age. The user then specifies the dietary composition of each of these foraging classes as a combination of benthos, incidental terrestrial insects, periphyton, phytoplankton, zooplankton, and/or other fish species including its own. Presently the standing stocks of all nonfish prey are handled only as external forcing functions rather than as simulated state variables.

Although BASS was developed to simulate the bioaccumulation of chemical pollutants within a community or ecosystem context, it can also be used to 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 for the 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.
- Plotted annual dynamics of selected model variables as requested by the user.

BASS version 2.1 is still a beta test version. Please report any comments, criticisms, problems, or suggestions regarding the model software or user manual to

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4.1. Summary of New Features Available in BASS version 2.1

The following features that were unavailable in BASS versions 1.x are now active:

- There are now no restrictions to the number of chemicals that can be simulated.
- There are now no restrictions to the number of fish species that can be simulated.
- There are now no restrictions to the number of cohorts that fish species may have.
- There are now no restrictions to the number of feeding classes that fish species may have (see the command / FEEDING_OPTIONS).
- There are now no restrictions to the number of foraging classes that fish species may have (see the command / ECOLOGICAL_PARAMETERS).
- Improved 3-dimensional and 2-dimensional plots of selected state variables are available using the software package DISLIN.

BASS's output tabulations have also been reformatted, and several input commands have been given new syntax.

New features of BASS version 2.1 that were unavailable in version 2.0 include:

- The ability to integrate BASS's differential equations using either a simple Euler method or a fifth-order Runge-Kutta method with adaptive step sizing. In BASS version 2.1 the default method of integration is the Runge-Kutta method.

- The ability to simulate biotransformation of chemicals with or without daughter products.

Regarding BASS's Euler and Runge-Kutta integrators, the user should realize that these methods offer the user two distinctly different options with respect to software performance and execution. Although Euler methods often allow for fast model execution, these methods cannot assess the accuracy of their integration. Runge-Kutta methods, on the other hand, can monitor the accuracy of their integration but at the cost of increased execution time. Fortunately, however, this additional computational burden can often be significantly reduced by employing adaptive step sizing. BASS's Runge-Kutta integrator is patterned on the fifth-order Cash-Karp Runge-Kutta algorithm outlined by Press et. al. (1992).

4.2. Input File Structure

The general structure of a BASS' s input file is as follows

/ 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 (e.g., 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. Argument may be an integer (e.g., 7), a real number (e.g., 0, 3.7e-2, 1.3, etc.), or a character string. If a command allows multiple arguments, each argument must be separated by a semicolon. Commands may be continued by appending an ampersand (&) to the line, e.g., the following two commands lines 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 lower case before being decoded, the case of the input file is not significant. Likewise, spacing within a command is not significant because consecutive blanks or tabs are collapse into a single blank. The maximum length of a command line, including continuation lines, is 1024 characters.

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

Commands are broadly classified into three categories: simulation control parameters, chemical parameters, and fish 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, nonfish standing stocks, and output options. Chemical parameters specify not only the chemical's physico-chemical properties (e.g., the chemical's molecular weight, molecular volume, n-octanol/water partition coefficient, etc.) but also exposure concentrations in the environment (i.e., in water, sediment, benthos, insects, etc.). Fish parameters identify the fish's taxonomy (i.e., genus and species), feeding and metabolic demands, dietary composition, predator-prey relationships, gill morphometrics, body composition, initial weight, initial whole body concentrations for each chemical, and initial population sizes. In the following sections, these commands are described alphabetically by class.

The last command in any BASS input file must be /END. This command terminates program input and any text/commands following it will be 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.

To facilitate easier data management when analyzing multiple simulations of similar scenarios, a user can also specify blocks of BASS input commands using include statements of the form

include '*filename*'

For example, a BASS input file that has all of its chemical and fish data stored in separate files might appear as follows

```
!
! file: example file with include statements
!
/simulation_control
/ command   argument! simulation control command 1
/ command   argument! simulation control command 2
/ command   argument! simulation control command 3
# 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'
/ end
```

Users are strongly recommended to make use of BASS's include file capabilities. A recommended file and subdirectory structure for using and managing BASS include files is discussed in detail in Section 4.4.

4.2.1. Simulation Control Commands

These commands establish the length of the simulation and BASS's integration step, the ambient water temperature, the availability of benthos, incidental terrestrial insects and plankton, the community's water level, and various output options. These data are specified by the following block of twelve commands

```
/ SIMULATION_CONTROL
/ HEADER                  string
/ LENGTH_OF_SIMULATION    string
/ MONTH_T0                string
/ NSTEPS                  integer
/ TEMPERATURE             string
/ WATER_LEVEL             string
/ BIOTA                   string_1; ... ;string_n
/ ANNUAL_OUTPUTS          integer
/ ANNUAL_PLOTS            string_1; ...; string_n
/ SUMMARY_PLOTS           string_1; ...; string_n
/ FGETS
```

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, however, is not significant. The use of these commands will now be described in alphabetical order. See Appendix D for an example of the use of these commands.

■ **/ANNUAL_OUTPUTS *integer***

This command specifies the time interval, in years, between BASS's annual tabulated and plotted outputs. This number must be an non-negative integer. BASS assumes a default value of zero which signifies that no annual outputs will be generated. This command is optional.

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

This command specifies the variables whose annual dynamics will be plotted for the years specified by command /ANNUAL_OUTPUTS. The options may be specified one per card, or all in one card, separated by semicolons. Valid options are:

afish(*string*) to generate plots of each species' total aqueous phase chemical activity as a function of time (day of year) and the species' age, length, or weight class;

baf(*string*) to generate plots of each species' bioaccumulation factor (i.e., the ratio C_f / C_w) for each chemical as a function of time (day of year) and the species' age, length, or weight class;

bmf(*string*) to generate plots of each species' biomagnification factor (i.e., the ratio C_f / C_{prey}) for each chemical as a function of time (day of year) and the species' age, length, or weight class;

cfish(*string*) to generate plots of each species' whole body concentration (ppm) for each chemical as a function of time (day of year) and the species' age, length, or weight class;

pop(*string*) to generate plots of each species' population density (ind./ha) as a function of time (day of year) and the species' age, length, or weight class;

wt(*string*) to generate plots of each species' whole body weight (g(FW)/fish) as a function of time (day of year) and the species' age, length, or weight class;

where ***string*** equals "age", "length" or "weight". Each age class or cohort of the species is assigned to one of five size classes that are defined by BASS based on the species' largest/oldest and smallest/youngest individuals.

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

This command specifies nonfish standing stocks that are prey for the simulated fish assemblage. Valid options are:

benthos[*yunits*] = *string* to generate benthic standing stocks according to the function ***string*** whose units ***yunits*** must be dimensionally equivalent to g(DW)/m^2.

insects[*yunits*] = *string* to generate incidental terrestrial insect standing stocks according to the function ***string*** whose units ***yunits*** must be dimensionally equivalent to g(DW)/m^2.

periphyton[*yunits*] = *string* to generate periphyton standing stocks according to the function ***string*** whose units ***yunits*** must be dimensionally equivalent to g(DW)/m^2.

phytoplankton[*yunits*] = *string* to generate phytoplankton standing stocks according to the function ***string*** whose units

yunits must be dimensionally equivalent to g(DW)/L.

zooplankton[*yunits*] = *string* to generate zooplankton standing stocks according to the function ***string*** whose units ***yunits*** must be dimensionally equivalent to g(DW)/L.

Valid specifications for these biotic resource functions are

***function_name*[*yunits*] = α** to generate the a constant prey standing stock of α (*yunits*) for the simulation.

***function_name*[*yunits*] = α + β*sin(ω + ϕ*t[*xunits*])** to generate a sinusoidal prey 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 ϕ = 2π/period is its frequency (1/*xunits*).

function_name*[*yunits*] = file(*filename*)** to read and interpolate the specified prey standing stock from the file ***filename.

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

■ **/FGETS**

This command enables a user to run BASS without simulating the assemblage's population dynamics, i.e., only the growth and bioaccumulation of individual fish are simulated.

■ **/HEADER *string***

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

■ **/LENGTH_OF_SIMULATION *string***

This command specifies the ending time of the simulation. The valid syntax for *string* is

α[*units*]

where α is non-negative real value. The time unit specified with brackets is converted into days for internal use and subsequent model output.

■ **/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.

■ **/NSTEPS *number***

This command specifies the number of steps per day used by BASS's Euler numerical integrator and is optional since BASS's default integrator is a fifth-order Runge-Kutta method with adaptive step sizing. When used, the specified number should be greater than or equal to one.

■ **/SIMULATION_CONTROL**

This command specifies the beginning of input data that will apply to the simulation at large, i.e., the length of the simulation and its integration step, the ambient water temperature, the availability of benthos, incidental terrestrial insects and plankton, the community's water level, and various output options.

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

This command specifies the variables whose temporal dynamics will be plotted at the completion of the simulation. The options may be specified one per card, or all in one card, separated by semicolons. Valid options are:

afish(*string*) to generate plots of each species' total aqueous phase chemical activity as a function of time (day of simulation) and the species' age, length, or weight class;

baf(*string*) to generate plots of each species' bioaccumulation factor (i.e., the ratio C_f / C_w) for each chemical as a function of time (day of simulation) and the species' age, length, or weight class;

bmf(*string*) to generate plots of each species' biomagnification factor (i.e., the ratio C_f / C_{prey}) for each chemical as a function of time (day of simulation) and the species' age, length, or weight class;

cfish(*string*) to generate plots of each species' whole body concentration (ppm) for each chemical as a function of time (day of simulation) and the species' age, length, or weight class;

pop(*string*) to generate plots of each species' population density (ind./ha) as a function of time (day of simulation) and the species' age, length, or weight class;

where ***string*** equals "age", "length" or "weight". Each cohort of the species is assigned to one of five size classes that are defined by BASS based on the species' largest/oldest and smallest/youngest individuals.

■ **/TEMPERATURE *string***

The command specifies the ambient' s water temperature. Valid options for this command are:

temp[celsius] = α to generate a constant ambient water temperature for the simulation.

temp[celsius] = α + β*sin(ω + ϕ*t[*xunits*]) to generate 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***.

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***

For shallow water communities, this command specifies a community's actual water level. For deep water communities, however, this command specifies the depth of the community's productive plankton layer. Valid options for this command are:

depth[meter] = α to generate a constant water level for the simulation.

depth[meter] = α + β*sin(ω + ϕ*t[*xunits*]) to generate 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***.

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.

4.2.2. Chemical Input Commands

The physico-chemical properties and exposure concentrations of each chemical of interest are specified by a block of eleven 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*
/METABOLISM	$string_1$; ... ; $string_n$
/MOLAR_WEIGHT	*real number*
/MOLAR_VOLUME	*real number*
/MELTING_POINT	*real number*

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. See Appendix D for an example of the use of these commands.

■ **/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 by 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 data base.

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

This command enables the user to specify the temporal dynamics of chemical exposures to fish via the 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 which include particle-bound chemical. If multiple options are selected, each option must be separated by a semicolon. Valid options are:

cbnths[*yunits*] = *string* to generate potential dietary exposures to fish via benthic organisms according to the function ***string***.

cinsct[*yunits*] = *string* to generate potential dietary exposures to fish via incidental terrestrial insects according to the function ***string***.

cphytn[*yunits*] = *string* to generate potential dietary exposures to fish via periphyton according to the function ***string***.

cpplnk[*yunits*] = *string* to generate potential dietary exposures to fish via phytoplankton according to the function ***string***.

csdmnt[*yunits*] = *string* to generate sediment exposure concentrations according to the function ***string***.

cwater[*yunits*] = *string* to generate aqueous exposure concentrations according to the function ***string***.

czplnk[*yunits*] = *string* to generate potential dietary exposures to fish via zooplankton according to the function ***string***.

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 the time dependent exposure functions discussed below. 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:

***function_name*[*yunits*] = α** to generate a constant concentration of toxicant in benthos, periphyton, phytoplankton, sediment, or zooplankton.

***function_name*[*yunits*] = α*cwater[*xunits*]** to generate 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 the product of the component's dry organic fraction and the chemical's K_{ow}.

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

Valid expressions for insect dietary exposures are:

cinsct[*yunits*]= α to generate a constant concentrations of the toxicant in incidental terrestrial insects.

cinsct[*yunits*] = file(*filename*) to read and interpolate the concentration of the toxicant in incidental terrestrial insects from the file ***filename***.

Valid expressions for direct aqueous exposures are:

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

cwater[*yunits*] = α*csdmnt[*xunits*] to generate 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*]) to generate 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*]) to generate a sinusoidal dissolved chemical water concentrations 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***. This option is currently inactive.

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

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

This optional command specifies species specific LC_{50}'s for the chemicals of concern. Valid string options are:

LC50[units](*fish_name*) = α

LC50[units](*fish_name*) = α*Kow[-]^γ

where Kow[-] is the chemical's n-octanol/water partition coefficient and *fish_name* is the common name of the fish species to be simulated. BASS converts these user supplied 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 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 simple but 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 metal's binding constant for non-lipid organic matter (see Eq.(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 organometals.

■ **/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***

The 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. Valid strings options are:

BT[units](*fish_name, chemical_name*) = α

BT[units](*fish_name, chemical_name*) = α*Kow[-]^γ

BT[units](*fish_name*, none) = α

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

where BT is the whole body referenced biotransformation rate k_m in Eq.(2-46); Kow[-] is the chemical's n-octanol/water partition coefficient; and *fish_name* is the common name of the fish species that can metabolize the chemical of concern, and *chemical_name* is the name of the daughter product generated by the metabolism of chemical. 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 physical chemical properties of the identified by-product in the same way that the physical chemicals properties of the parent compound are specified.

■ **/MOLAR_VOLUME *real number***

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

$$D = \frac{2.101\times10^{-7}}{\eta^{1.4}\ \nu^{0.589}} \qquad (4\text{-}1)$$

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

$$\mathrm{Log}_{10}\left(\frac{\eta_{20}}{\eta_T}\right) = \frac{1.37(T-20) + 8.36\times10^{-4}(T-20)^2}{109+T} \qquad (4\text{-}2)$$

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

■ **/MOLAR_WEIGHT *real number***

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

4.2.3. Fish Input Commands

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

/COMMON_NAME *string*
/SPECIES *string*
/AGE_CLASS_DURATION *string*
/SPAWNING_PERIOD *string*
/FEEDING_OPTIONS $string_1$; ...; $string_n$
/INITIAL_CONDITIONS $string_1$; ...; $string_n$
/ECOLOGICAL_PARAMETERS $string_1$; ...; $string_n$
/COMPOSITIONAL_PARAMETERS $string_1$; ...; $string_n$
/MORPHOMETRIC_PARAMETERS $string_1$; ...; $string_n$
/PHYSIOLOGICAL_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. See Appendix D for examples of the commands described below.

■ **/AGE_CLASS_DURATION *string***

This command is used to specify the duration of each age class. Two character strings, i.e., "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 which must be separated by semicolons are:

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

pl[-] = α*W[*xunits*]^β which 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 integer or real numbers.

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

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

diet(α< *string* <β) = {$string_1 = \epsilon_1$, ... , $string_n = \epsilon_n$} which specifies the dietary composition for fish of the age or size range (α[*xunits*],β[*xunits*]) where[*xunits*] must be dimensionally equivalent to either yr, g(FW), or cm. The right hand side of the option specifies the prey items (***$string_n$***) and their contribution (**ϵ_n**) to the fish's diet. Each ***$string_n$*** is either the common name of one of the fish species to be simulated, "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 $1<\epsilon_n<100$, 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 $-1<\epsilon_n<1$, then ϵ_n is considered a prey electivity (see Eq.(2-71)). For any given foraging class, a user can specify both constant dietary percentages and prey electivities. Valid syntax for specifying the size or age range of the fish are

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

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

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

Although for a given species all range types must be the same (i.e., age, length, or weight), the range types between species may be different. The **diet(·)={·}**option can be repeated as many times as needed in order to define a complete lifetime sequence of diets for the fish.

lp[*yunits*] = α + β*L[*xunits*] which specifies the average length of prey consumed by a fish whose body length is L[***xunits***]. If a fish's average prey size is independent of its body length (i.e., β equals zero), however, this parameter can be specified simply as **lp[*yunits*] = α** .

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

nm[*yunits*] = α*W[*xunits*]^β which specifies a non-predatory mortality rate for fish whose body weight is W[*xunits*]; ***yunits*** must be dimensionally equivalent to 1/year. If the mortality rate of fish is independent of their body weight (i.e., β equals zero), however, this parameter can be specified simply as **nm[*yunits*] = α** .

tl_ro[*yunits*] = α which specifies the species' minimum total length when it reaches sexual maturity or its first reproduction.

rbi[-] = α which specifies the species' reproductive biomass investment, i.e., grams gametes per gram spawning fish.

wl[*yunits*] = α*L[*xunits*]^β which specifies the fish' s live weight as an allometric function of its total length.

yoy[*yunits*] = α which specifies the live weight of fish recruited into the population as age class 0.

■ **/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(α< *string* <β) to model expected feeding using Eq.(2-56).

clearance(α< *string* <β) to model expected feeding using Eq.(2-62).

holling(α< *string* <β) to model expected feeding using Eqs.(2-57).

linear(α< *string* <β) to model expected feeding using Eq.(2-63).

where α and β are integer or real numbers and ***string*** equals one of the following

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

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

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

Although for a given species all range types must be the same type (i.e., age, length, or weight), the range types between species may be different. The parameters for these models are specified using the /PHYSIOLOGICAL_PARAMETERS command.

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

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

age[*units*] = {n_1 , ... , n_{age_class}} to initialize the age of each cohort with the specified vector. The units which are delineated by brackets must be dimensionally equivalent to days.

***chemical_name*[*units*] = {n_1 , ... , n_{age_class}}** 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 of measurement which must be enclosed by brackets must be dimensionally equivalent to μg/ g(FW).

wt[*units*] = {n_1 , ... , n_{age_class}} to initialize the body size of each age class with the specified vector. The units which are delineated by brackets must be dimensionally equivalent to g(FW).

pop[*units*] = {n_1 , ... , n_{age_class}} to initialize the population density of each age class with the specified vector. The units which are delineated by brackets must be dimensionally equivalent to inds/ ha.

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

This command specifies the species' morphometric parameters that 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 which specifies the fish's total gill surface area. ***yunits*** must be dimensionally equivalent to cm^2 or cm^2/g(FW).

id[*yunits*] = α*W[*xunits*]^β which specifies the interlamellar distance between adjacent lamellae.

ld[*yunits*] = α*W[*xunits*]^β which specifies the density of secondary lamellae on the primary gill filaments, i.e., number of lamellae per mm gill filament.

ll[*yunits*] = α*W[*xunits*]^β which specifies the fish's lamellar length. ***yunits*** must be dimensionally equivalent to cm or cm /g(FW).

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 its 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 which specifies the fish's assimilation efficiency for periphyton and phytoplankton.

ae_invert[-] = α which specifies the fish's assimilation efficiency for benthos, insects, and zooplankton.

ae_fish[-] = α which specifies the fish's assimilation efficiency for fish.

ge[*yunits*] = α*G[*xunits*]^β *exp(γ*(T[celsius]-T_0))*h(T_0,T_1,T_2) which specifies the fish's gastric evacuation where **G** is the mass of food resident in the intestine. ***yunits*** must be dimensionally equivalent to g(DW)/day. In general, γ = ½, ⅔, or 1 (Jobling 1981). This parameter is required only if the feeding option **holling(·)** is selected.

mf[*yunits*] = α*W[*xunits*]^β*exp(γ*(T[celsius]-T_0))*h(T_0,T_1,T_2) which specifies the fish's maximum filtering rate. ***yunits*** must be dimensionally equivalent to L/day. Required only if the feeding option **clearance(·)** is selected.

mi[*yunits*]=α*W[*xunits*]^β*exp(γ*(T[celsius]-T_0))*h(T_0,T_1,T_2) which specifies the fish's maximum ingestion. ***yunits*** must be dimensionally equivalent to g(DW)/day. Required only if the feeding option **allometric(·)** is selected.

rq[-] = α which specifies the fish's respiratory quotient; rq = L(CO_2) respired / L(O_2) consumed.

rt:std[-] = α which specifies the ratio of a fish's routine respiration to its standard respiration; rt:std = (routine O_2 consumption) / (standard O_2 consumption). BASS assumes a default value equal 2.

sda:in[-] = α which specifies the ratio of a fish's SDA to its ingestion. BASS assumes a default value equal 0.17.

sg[*yunits*] = α*W[*xunits*]^β *exp(γ*(T[celsius]-T_0))*h(T_0,T_1,T_2) which specifies the fish's specific growth rate. ***yunits*** must be dimensionally equivalent to day^{-1}. Required only if the feeding option **linear(·)** is selected.

sm[*yunits*] = α*W[*xunits*]^β *exp(γ*(T[celsius]-T_0))*h(T_0,T_1,T_2) which specifies the size of the satiation meal consumed during the interval (0, st]. See option "st[·]" below. Required only if the feeding option **holling(·)** is selected.

so[*yunits*] = α*W[*xunits*]^β *exp(γ*(T[celsius]-T_0))*h(T_0,T_1,T_2) which specifies the fish's standard oxygen consumption. ***yunits*** must be dimensionally equivalent to mg(O_2)/ hr or mg(O_2)· g(FW)$^{-1}$· hr^{-1}.

st[*yunits*] = α*W[*xunits*]^β *exp(γ*(T[celsius]-T_0))*h(T_0,T_1,T_2) which specifies the time to satiation when feeding with an initially empty stomach. See option **sm[·]** above. Required only if the feeding option **holling(·)** is selected.

where

$$h(T_0, T_1, T_2) = \left(\frac{T_2 - T}{T_2 - T_0} \right)^{\gamma (T_2 - T_1)} \qquad (4\text{-}3)$$

where T_1 is the temperature at which each particular process's rate is maximal, T_2 is the upper temperature at which the process is no longer operative, and T_0 is the low end reference temperature that is used to specify the process's Q_{10} response. Specification of the hyperbolic function $h(T_0,T_1,T_2)$ is optional in which case the specification of the reference temperature T_0 is also optional. Consequently, all of the above temperature dependent power functions can also be specified simply 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 parameters identified as being allometric power functions, the resulting term **W[*xunits*]^0** does not have to be specified. If a required parameter is not specified, the program will terminate with an appropriate message.

■ **/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 command specifies the scientific name (genus and species)

of the fish to be modeled. When this command is encountered, BASS uses the specified scientific name to assign default ecological, morphological, and physiological parameters for the species of interest. These default parameters are then updated with the data that the user inputs via the /ECOLOGICAL_PARAMETERS, /MORPHOMETRIC_PARAMETERS, and /PHYSIOLOGICAL_PARAMETERS commands. This option, however, is not implemented in BASS version 2.1.

4.2.4. Units Recognized by BASS

The many 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 supplied units to those actually used by BASS is accomplished by referencing all units to the MKS system (i.e., meter, kilogram, second). Tables 8 and 9 summarize prefixes and fundamental units, respectively, that are recognized by BASS's unit conversion subroutines. Table 9 also summarizes the dimensionality and the conversion factor to the MKS system of each unit. Table 10 summarizes units that are recognized by BASS's unit conversion subroutines for specifying ecological, morphometric, and physiological units.

Units and their prefixes may be specified in either upper or lower case. If prefixes are used, there must be no embedded blanks between the prefix and the unit name, e.g., "milligrams" is correct, "milli grams" is incorrect. Only those units and their plural form presented in Tables 9 and 10 are valid. The circumflex (^) is used to denote exponentiation (e.g., cm^{-2} is presented as cm^-2). The slash (/) is used to denote 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" are "mg g^-1 day^-1" are equivalent. The unit conversion factor (Tables 9 and 10) converts from the given unit to the MKS system, e.g., 1 calorie $\times 2.388\times10^{-1} \equiv 1$ $meter^2$ kilogram $second^{-2}$.

4.2.5. Syntax for 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) = $\alpha+\beta$*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 independent power functions may be specified by their $\log_{10}$ or ln transforms. For example, the following options are valid

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

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

- 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*exp(β*(T[celsius]-20))*W[*xunits*]^γ

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

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

- If the temperature dependency is unknown, temperature-dependent power functions can be input for a specific temperature, β° 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*](β) = α*W[*xunits*]^γ

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

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

- If either the slope of a linear function or the exponent of a power functions is zero, the function can be input as a constant function 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(FW)]^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(FW)]^-0.2

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

The correct syntax for these options would be

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

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

4.2.6. User Supplied Exposure Files

If the user specifies the file option for the /BIOTA, /TEMPERATURE, /WATER_LEVEL, or /EXPOSURE 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,NV     ! comment
```

The 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, NV 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 specified as the first column of any user-supplied exposure file.

Valid character strings for specifying the remaining data columns include:

cbnths[*units*](*chemical name*) to input the concentration of ***chemical name*** in benthic invertebrates;

cinsct[*units*](*chemical name*) to input the concentration of ***chemical name*** in incidental terrestrial insects;

cphytn[*units*](*chemical name*) to input the concentration of ***chemical name*** in periphyton;

cpplnk[*units*](*chemical name*) to input the concentration of ***chemical name*** in phytoplankton;

csdmnt[*units*](*chemical name*) to input the sediment concentration of ***chemical name***;

cwater[*units*](*chemical name*) to input the unbound, aqueous concentration of ***chemical name***;

czplnk[*units*](*chemical name*) to input the whole body concentration of ***chemical name*** in zooplankton;

benthos[*units*] to input the standing stock of benthic invertebrates;

insects[*units*] to input the standing stock of incidental terrestrial insects;

periphyton[*units*] to input the standing stock of periphyton or grazable algae;

phytoplankton[*units*] to input the standing stock of phytoplankton;

zooplankton[*units*] to input the standing stock of zooplankton;

temperature[*units*] to input ambient water temperature.

depth[*units*] to input water depth.

If column names other than those listed above are specified BASS simply ignores them. Data records may be continued by appending an ampersand (&) to the line, e.g., the following data records are equivalent.

$v_{i,1}$ $v_{i,2}$ ... $v_{i,j}$ $v_{i,j+1}$ ... $v_{i,MV}$

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

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

4.3. Output Files Generated by BASS

Given a user's input BASS generates the following three output files

- an output file that summarizes the user's input parameters, input errors detected by BASS, and warnings/errors encountered during the actual simulation. This file will have the name of the user' s input command file, with extension "MSG"; e.g., INPUT.DAT will generate the file INPUT.MSG. If the file already exists, it will be silently overwritten. See Appendix E (page 95) for an example.

- an output file that tabulates selected results of the simulation. Tabulated summaries include 1) annual bioenergetic fluxes and growth statistics (i.e., mean body weight, mean growth rate) of individual fish by species and age class, 2) annual bioaccumulation fluxes and statistics (i.e., mean whole body concentrations, BAF, and BMF) of individual fish by species and age class, and 3) annual community fluxes and statistics (i.e., mean population densities and biomasses) of each fish species by age class. This file will have the name of the user' s input command file, with extension "BSS"; e.g., INPUT.DAT will generate the file INPUT.BSS. If the file already exists, it will be silently overwritten. See Appendix F (page 112) for an example.

- a Post-script file that contains the plots that were requested by the user. The file will have the name of the user' s input command file, with extension "PLX"; e.g., INPUT.DAT will generate the file INPUT.PLX. If the file already exists, it will be silently overwritten. See Appendix G (page 122) for an example.

4.4. Include Files and General File Management

As mentioned previously BASS enables the user to construct BASS simulation files using include files. Although the use of include files was introduced in Section 4.1 as simply a matter of user convenience, the installation software for BASS version 2.1 actually creates a specific subdirectory structure to help construct and maintain user input files. Although users do not have to use this subdirectory structure to run BASS, its use is strongly recommended since the graphical interface (GUI) that is currently being developed for BASS uses this directory structure. Using the installation procedures outlined in Section 5.1, the BASS installation software INSTBASS.EXE creates the directory structure below

```
C:\BASS --+-- INSTBASS.EXE
          |
          +-- BASS_V2.EXE
          |
          +-- \DISLIN
          |
          +-- \FISH -- *.FHS
          |
          +-- \COMUNITY -- *.CMM
          |
          +-- \PROPERTY -- *.PRP
          |
          +-- \PROJECTS --+ \project1 --+ *.PRJ
                          |             + *.CHM
                          |             + *.DAT
                          |             + *.BSS
                          |             + *.MSG
                          |             + *.PLX
                          + \project2
                          :
```

Files within the subdirectory \FISH are all assigned the extension FSH. These files specify the compositional, ecological, morphological, and physiological parameters of a fish species and are intended to be used as include files for constructing fish community files which are discussed next. The general structure of a *.FSH file is

```
! file: name.fsh
! date: june 20, 2000
!
! notes: structure of BASS fish file
!
/COMMON_NAME  <string>
/SPECIES  <string>
/AGE_CLASS_DURATION <string>
/SPAWNING_PERIOD <string>
/FEEDING_OPTIONS allometric(a<x[units]<b); &
                 clearance(a<x[units]<b); &
                 holling(a<x[units]<b); &
                 linear(a<x[units]<b)
/COMPOSITIONAL_PARAMETERS pa[-]=a*pl[-]+b; &
                          pl[-]=a*w[g]^b
/ECOLOGICAL_PARAMETERS lp[cm]=a*l[cm]+b; &
                       wl[g]=a*l[cm]^b; &
                       tl_r0[cm]=a; &
                       rbi[-]=a; &
                       yoy[g]=a; &
                       mls[yr]=a; &
                       nm[1/yr]=a*w[g]^b
/MORPHOMETRIC_PARAMETERS ga[cm^2]=a*w[g]^b; &
                         id[cm]=a*w[g]^b; &
                         ld[cm]=a*w[g]^b; &
```

```
                        ll[cm]=a*w[g]^b
/PHYSIOLOGICAL_PARAMETERS &
          ge[g/d]=a*w[g]^b*exp(c*t[celsius]); &
          mf[l/d]=a*w[g]^b*exp(c*t[celsius]); &
          mi[g/d]=a*w[g]^b*exp(c*t[celsius]); &
          sg[1/d]=a*w[g]^b*exp(c*t[celsius]); &
          sm[g]=a*w[g]^b*exp(c*t[celsius]); &
          so[mg(O2)/h]=a*w[g]^b*exp(c*t[celsius]); &
          st[min]=a*w[g]^b*exp(c*t[celsius]); &
          ae_fish[-]=a; &
          ae_invert[-]=a; &
          ae_plant[-]=a; &
          sda:in[-]=a; &
          rq[-]=a; &
          rt:std[-]=a
! end c:\bass\fish\name.fsh
```

Files within the \COMUNITY subdirectory are all assigned the extension CMM. These files specify the composition, trophic structure, and initial conditions of a particular fish community. These files will generally use FSH files from the \FISH subdirectory as include files and are themselves used as include files by PROJECTS files. The general form of a *.CMM file is

```
! file:c:\bass\comunity\name.cmm
! date: june 20,2000
!
! notes: structure of BASS community file
!
#include 'name1.fsh'
/ECOLOGICAL_PARAMETERS &
       diet(a<x[units]<b)={benthos=a,…,name1=b,…}; &
       diet(a<x[units]<b)={benthos=a,…,name1=b,…}; &
       diet(a<x[units]<b)={benthos=a,…,name1=b,…}; &
       diet(a<x[units]<b)={benthos=a,…,name1=b,…}
/INITIAL_CONDITIONS age[yr]={a,…,b}; &
                    wt[g]={a,…,b}; &
                    pop[inds/ha]={a,…,b}
!
! repeat above fish data block as needed
!
!
! end c:\bass\comunity\name.cmm
```

Files within the PROPERTY subdirectory are all assigned the extension PRP and specify the physico-chemical properties of individual chemicals. These files serve as include files for chemical exposure files. The general structure of *.PRP files is

```
! file: name.prp
! date: june 20, 2000
!
! notes: structure of BASS chemical 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 c:\bass\chemical\name.prp
```

The PROJECTS directory contains subdirectories that are created by the user for a particular model application. In general, each application should be assigned to its own subdirectory. For example, the BASS distribution example EVERGLD1.PRJ that simulates mercury bioaccumulation in a deep-water Florida Everglades community is assigned to the subdirectory C:\BASS\PROJECTS\EXAMPLE1. Six types of files will reside in each PROJECTS subdirectory. These file types are: 1) *. PRJ files that specify the simulation control parameters and chemical and fish/community include files to be used for this particular application, 2) *.CHM files that specify chemical exposures and properties, 3) *.DAT files which specify actual chemical exposures, nonfish standing stocks, water temperature, or water depth when these functions supplied by the 'file' option, 4) *.BSS which are the tabular output files generated by BASS, 5) *.MSG which are the message output files generated by BASS, and 6) *.PLX which are the Post Scrip plot files generated by BASS. The recommended structure of a PRJ file is

```
! file: name.prj
! date: june 20, 2000
!
! notes: structure of BASS project file
!
/SIMULATION_CONTROL
/HEADER <string>
/MONTH_T0 <string>
/LENGTH_OF_SIMULATION <number>[year]
/TEMPERATURE temp[celsius]=<string>
/WATER_LEVEL depth[meter]=<string>
/BIOTA  benthos[g/m^2]=<string>; &
        insects[g/m^2]=<string>; &
        periphyton[g/m^2]=<string>; &
        phytoplankton[mg/l]=<string>; &
        zooplankton[mg/l]=<string>
/ANNUAL_OUTPUTS <integer number>
/SUMMARY_PLOTS pop(length); cfish(length)
!
! specify chemical properties and exposures
!
#include 'name1.chm'
!
! specify fish community
!
#include 'name2.cmm'
/END
```

The chemical exposures and properties file NAME1.CHM specified in the preceding project file has the following general form

```
! file: name1.chm
! date: june 20, 2000
!
! notes: structure of chemical exposures
!        and properties file
!
! specify physico-chemical parameters
!
#include 'chem_1.prp'
/EXPOSURE cwater[ppm]=<string>; &
          cbnths[ppm]=<string>; &
          cinsct[ppm]=<string>; &
          cphytn[ppm]=<string>; &
          cpplnk[ppm]=<string>; &
          czplnk[ppm]=<string>
/LETHALITY    lc50[units](fish_1) = a; ....
/METABOLISM   bt[units](fish_1,chem_n) = a; ...
!
! repeat above data block as needed
! for other chemicals of concern
:
! end name1.chm
```

The *.FSH, *.CMM, and *.PRP files within the subdirectories \FISH, \COMUNITY, and \PROPERTY should be considered by the user to be canonical "databases" for the construction of new project files. If the user wishes to make changes to any of these files, the user should either 1) edit the files as desired and save the changes as a new *.FSH, *.CMM, and *.PRP file within the subdirectories \FISH, \COMUNITY, and \PROPERTY or 2) copy the desired files to a working project subdirectory. Unless identified with an absolute path, any file designated by an include command is assumed by default to specify a path and file name relative to the project file specified by the command line option "-i" when BASS is invoked. If a specified *.FSH, *.CMM, or *.PRP file can not be found in the subdirectory containing the user's project file, BASS then uses the extension of the specified file to search the subdirectories \FISH, \COMUNITY, or \PROPERTY.

4.5. Command Line Options

To run a BASS simulation which is specified by an input/project file INPUT.PRJ, the BASS software is invoked using the UNIX like command line shown below

C:\BASS21> bass_v21 -i input.prj

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

-a => print abbreviated tabular output with minimal flux summaries
-c => print distribution of cpu time in major subroutines
-e => integrate by Euler method
-h => print this help list and stop (also see -?)
-i filename => specify BASS input file (REQUIRED)
-l => turn off lethal effects
-o filename => specify BASS_V21 output file
-p => print messages associated with prey switching/limitation
-r => integrate by Runge-Kutta method (DEFAULT)
-t => run test of BASS Runge-Kutta integrator and stop
-? => print this help list and stop (also see -h)

For example, the command line

C:\BASS21> bass_v21 -i input.prj -a -c

will execute the project file INPUT.PRJ and generate abbreviated summary tables and a distribution of cpu time spent within various key BASS subroutines.

4.6. Restrictions and Limitations

Commands may be presented in any order with the exceptions noted below.

- The /CHEMICAL command must precede the commands for any particular chemical since this command defines a new chemical and increments the total number of chemicals to be simulated.
- The /COMMON_NAME command must precede the commands for the particular fish, since this command essentially defines a (new) fish.
- Chemical commands must precede any fish commands.
- The /END command must be the last command. Any other text or commands following it will be ignored.

Table 8. 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 9. Valid Unit Names for Length, Area, Volume, Mass, Time, and Energy. This list is not exhaustive and summaries only commonly used unit names that BASS's units conversion program recognizes.

	Conversion	Dimensions			
Unit Name	Factor	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 9. Valid Unit Names (Continuation)

Unit Name	Conversion Factor	Dimensions Metre	Kg	Second	Description
month	3.858×10^{-07}	0	0	1	
nauticalmile	5.400×10^{-04}	1	0	0	1852 meter
ng	$1.000\times10^{+12}$	0	1	0	nanograms
ounce	$3.527\times10^{+01}$	0	1	0	
oz	$3.527\times10^{+01}$	0	1	0	ounce
pint	$2.113\times10^{+03}$	3	0	0	8 pint ≡ 1 gallon
pound	$2.205\times10^{+00}$	0	1	0	
ppb	$1.000\times10^{+06}$	-3	1	0	nanograms/mL
ppm	$1.000\times10^{+03}$	-3	1	0	µgrams/mL
ppq	$1.000\times10^{+12}$	-3	1	0	femtograms/mL
ppt	$1.000\times10^{+09}$	-3	1	0	parts per trillion, picogram/mL
quart	$1.057\times10^{+03}$	3	0	0	4 quarts ≡ 1 gallon
s	$1.000\times10^{+00}$	0	0	1	second
sec	$1.000\times10^{+00}$	0	0	1	second
second	$1.000\times10^{+00}$	0	0	1	
ton	1.102×10^{-03}	0	1	0	2000 pounds
tonne	1.000×10^{-03}	0	1	0	1000 kilograms
week	1.653×10^{-06}	0	0	1	
yard	$1.094\times10^{+00}$	1	0	0	
year	3.169×10^{-08}	0	0	1	

Table 10. Valid Ecological, Morphometric, and Physiological Unit Names

Unit Name	Conversion Factor	Dimensions Metre	Kg	Second	Description
fish	n.a.	0	0	0	treated as information as is byte
gram(O2)	7.370×10^{-05}	2	1	-2	gram of oxygen
g(O2)	7.370×10^{-05}	2	1	-2	gram of oxygen
ha	1.000×10^{-04}	2	0	0	hectare
individuals	n.a.	0	0	0	treated as information as is byte
inds	n.a.	0	0	0	treated as information as is byte
kcal	2.388×10^{-04}	2	1	-2	kilocalorie
l(O2)	5.159×10^{-05}	2	1	-2	22.4 liters STP = mole
lamellae	n.a.	0	0	0	treated as information as is byte
mg(O2)	7.370×10^{-02}	2	1	-2	milligram of oxygen = 3.24 calorie
ml(O2)	5.159×10^{-02}	2	1	-2	milliliter of oxygen
mmole(O2)	2.303×10^{-03}	2	1	-2	millimole of oxygen
mole(O2)	2.303×10^{-06}	2	1	-2	mole of oxygen

Note: For purposes of units conversion, units used to report oxygen consumption are treated dimensionally as joules.

5. Software Installation and Management

5.1. MS-DOS Installation

The microcomputer ms-dos BASS 2.1 software is distributed with 1) a readme file, 2) the BASS 2.1 software, and 3) three example project simulations. The BASS 2.1 executable and example simulation files are compressed into a self extracting executable, INSTBASS.EXE, using PKZIP and must be decompressed before use. See instructions below.

BASS 2.1 is coded in Fortran 95 and its executable, BASS_V21, has been created using the Lahey/Fujitsu Fortran 95 5.60 compiler. Although BASS's source code is not included on its software distribution diskette, it is available to any interested party on request. Please note that there is a bug in the DISLIN graphics software that BASS uses to generate 3-dimensional plots of model results as a function of age or size class and time. In particular, there is a bug in DISLIN's hidden line removal algorithm. This bug has been reported and is being investigated.

INSTBASS.EXE not only installs the BASS 2.1 executable but also creates a subdirectory structure to organize and manage project files and their associated data files. Following the instructions given below, INSTBASS.EXE creates the following subdirectory structure

```
C:\BASS --+-- INSTBASS.EXE
          |
          +-- BASS_V21.EXE
          |
          +-- \DISLIN
          |
          +-- \FISH -- *.FHS
          |
          +-- \COMUNITY -- *.CMM
          |
          +-- \PROPERTY -- *.PRP
          |
          +-- \PROJECTS --+ \EXAMPLE1
                          |
                          + \EXAMPLE2
                          |
                          + \EXAMPLE3
```

The structure and use of the \FISH, \COMUNITY, \PROPERTY, and \PROJECTS subdirectories are described in Section 4.4 (page 43). The \DISLIN subdirectory contains the *.DLL file needed to execute the DISLIN graphing software.

Three example BASS projects are provided in the \PROJECTS subdirectory. Each example is allocated its own subdirectory. In \PROJECTS\EXAMPLE1 the project file EVERGLD1.PRJ simulates the bioaccumulation of methylmercury in a deep-water fish community in the Florida Everglades, USA. The major fish species in these communities are largemouth bass, Florida gar, yellow bullhead, bluegill and red ear sunfish, and *Gambusia*. EVERGLD1.PRJ uses the include file \COMUNITY\EVERGLD1.CMM to specify the ecological and physiological data for these species. The chemical exposures and properties of methylmercury are provide to EVERGLD1.PRJ using the include file MERCURY.CHM which in turn uses the include file \PROPERTY\METYL_HG.PRP. The community's water depth and the standing stocks of benthos, periphyton, and zooplankton are specified by NONFISH.DAT. This example is presented in Section 6 of this user's manual.

In the subdirectory \PROJECTS\EXAMPLE2 the project file EVERGLD2.PRJ also simulates the bioaccumulation of methylmercury in a deep-water fish community in the Florida Everglades, USA dominated by the same fish species. This example, however, uses BASS's "fgets" option to simulate only the growth and bioaccumulation of individual fish. The community's population dynamics are not simulated. The ecological and physiological data for this example are provided by the include file \COMUNITY\EVERGLD2.CMM. The chemical exposures and properties of methylmercury are provide to EVERGLD2.PRJ using the include file MERCURY.CHM which in turn uses the include file \PROPERTY\METYL_HG.PRP. The community's water depth and the standing stocks of benthos, periphyton, and zooplankton are specified by NONFISH.DAT. These files, however, are simply copies of those found in \PROJECTS\EXAMPLE1. Because the food web structure and dynamics specified and implied by \COMUNITY\EVERGLD2.CMM can not be made to coincide with that of \COMUNITY\EVERGLD1.CMM, the output of EVERGLD2.PRJ will not match that of EVERGLD1.PRJ.

In the subdirectory \PROJECTS\EXAMPLE3 the project file HARTWELL.PRJ simulates the bioaccumulation of tetra-, penta-, hexa-, and hepta-PCB in a largemouth/sunfish/catfish community of the Twelve Mile Creek region of Lake Hartwell, SC, USA which was a USEPA Superfund site. Because the structure of the Twelve Mile Creek fish community, like many other largemouth/sunfish/catfish communities throughout the southeastern USA, closely resembles an Everglades deep-water community, the project file HARTWELL.PRJ uses the community file \COMUNITY\EVERGLD1.CMM to model the community of concern. This example is intended only to demonstrate BASS's ability to simulate the bioaccumulation of arbitrary mixtures and not what is actually occurring Lake Hartwell fish communities. Despite this fact this simulation does

predict some interesting results regarding largemouth bass. In particular, largemouth bass are predicted to attain internal total chemical activities on the order of 10% of their expected lethal chemical activity threshold. As discussed earlier, one might suspect that such accumulations would begin to produce sublethal effects on these fish. Interestingly, biomarker studies on Twelve Mile Creek largemouth bass indeed suggest this to be the case.

To install the BASS software the user should first obtain a DOS prompt and follow the instructions below.

- Select a default drive into which the BASS software is to be installed (e.g., hard disk "C")

  C:\WINDOWS> CD C:\

b. Create a directory for BASS software and then move to that directory

  C:\> MKDIR BASS21
  C:\> CD BASS21\

c. Request verification of copy results

  C:\BASS21> VERIFY ON

d. Transfer the files from the distribution diskette (e.g., drive "A") to the hard disk

  C:\BASS21> COPY A:*.*

e. Execute the installation file INSTBASS.EXE to recover files from the ZIP archives using the option -d

  C:\BASS21> INSTBASS -d

f.. Edit your AUTOEXEC.BAT file as follows

  SET BASS=C:\BASS21
  SET PATH=%PATH%;%BASS%
  SET PATH=%PATH%;%BASS%\DISLIN

  to execute BASS from any directory and to enable the BASS executable to find DISDLL.DLL which is needed for DISLIN graphics.

g. To run one of the distribution examples move to the desired PROJECTS subdirectory and invoke BASS using the UNIX like command as shown in the example below

  C:\BASS21> CD PROJECTS\EXAMPLE1
  C:\BASS21\PROJECTS\EXAMPLE1> bass_v21 -i evergld1.prj

5.2. Auxiliary Software

To view and print BASS plot files the user will have to have some type of PostScript previewing software installed on their system. If the user does not have any such software, it is recommended that the user obtain a copy of the Ghostscript/Ghostview/GSview software. This freeware can be downloaded from the Ghostscript, Ghostview and Gsview homepage: http://www.cs.wisc.edu/~ghost/.

BASS's input files and non-PostScript output files can be viewed using a wide variety of editors. They can also be viewed using word processing software such as WordPerfect or Microsoft Word. When using a word processor, however, the user should select a non-true type font (e.g., Courier) for viewing so that the file's intended alignment is display properly. Using a word processor to view non-PostScript BASS, has the added advantage being able to compare similar files easily. For example, using WordPerfect's Document/Compare feature one a easily view any differences between two BASS output files resulting from a parameter change.

6. Example Application

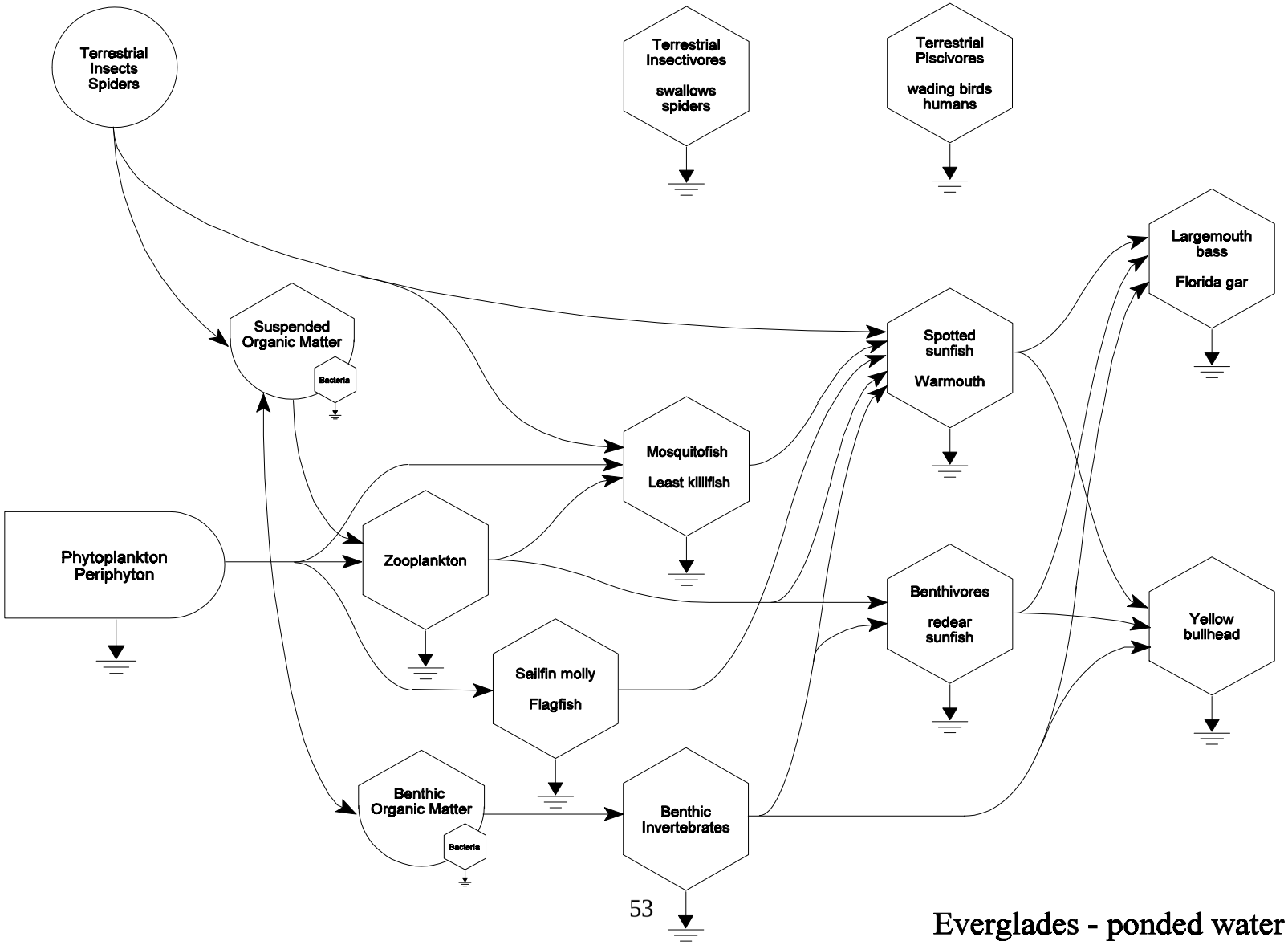
Appendix D presents an example BASS project file that simulates methyl mercury contamination in canals or open water habitats in the south Florida Everglades. This project file was constructed as outlined in Section 4.4 (page 43) and is supplied with the BASS distribution software as \EXAMPLE1. For this application largemouth bass (*Micropterus salmoides*), Florida gar (*Lepisosteus platyrhincus*), yellow bullheads (*Ameiurus natalis*), bluegills (*Lepomis macrochirus*), redear sunfish (*Lepomis microlophus*), and mosquito fish(*Gambusia holbrooki*) are assumed to be the dominate fish in the habitats of interest and a generalized food web of such assemblages is depicted in Figure 6. The sources of the ecological, morphological, and physiological parameters used for this example are documented by comment lines in the files presented in Appendix D. Total fish biomass in canal and open water Everglades habitats vary between 150 and 460 kg(FW)/ha (Frank Jordan unpublished data). Using Jordan's relative abundance data as guidelines, the initial standing stocks of the bass, gar, bullheads, bluegill, red ear sunfish, and mosquito fish were assigned to be 20, 10, 20, 200, 100, and 10 kg(FW)/ha, respectively, for a total community biomass of 360 kg(FW)/ha. Based on Loftus et al. (1998) the water concentration of methylmercury for the simulation was assigned to be a constant 0.444 ng/L and the BAF's for benthos and zooplankton were assigned to be $10^{6.17}$ and $10^{5.99}$, respectively.

Appendices D, E, and F present the resulting output files generated by BASS. At the end of the 10 year simulation the mean annual standing stocks of the bass, gar, bullheads, bluegill, red ear sunfish, and mosquito fish are 17.2, 12.7, 4.51, 191, 146, and 0 kg(FW)/ha, respectively, for a total community biomass of 371 kg(FW)/ha (see pages 120 and 121). Although the total elimination of mosquito fish during the simulation may not be particularly desirable, it is not unrealistic since bass and other piscivores often exert intense predatory pressures on mosquito fish and other small fishes in Everglades and other wetland or swallow water communities.

The simulated whole body concentrations of methyl mercury in these species agree also well with unpublished data collected by Ted Lange et al. and Loftus et al. (1998). The annual averaged concentrations of methylmercury in largemouth, gar, bullhead, bluegill and red ear weighted by cohort biomasses were 0.817, 0.694, 0.539, 0.495, and 0.416 mg Hg/kg(FW), respectively (see pages 113, 115, 116, 117, and 118). When weighted by cohort densities, the annual averaged concentrations of methylmercury in largemouth, gar, bullhead, bluegill and red ear were 0.671, 0.615, 0.467, 0.482, and 0.370 mg Hg/kg(FW), respectively (see pages 113, 115, 116, 117, and 118). Loftus et al. report whole body concentrations of methylmercury in largemouth, gar, bullhead, bluegill and red ear to be 0.967, 1.16, 0.443-0.755, 0.478, and 0.247 mg Hg/kg(FW), respectively.

As is typically observed under field conditions (Forrester et al. 1972; Scott and Armstrong 1972; Cross et al. 1973; Akielaszek and Haines 1981; Watling et al. 1981; Boush and Thieleke 1983a ,1983b; MacCrimmon et al.1983; Ueda and Takeda 1983; Wren and MacCrimmon 1986; Braune 1987; Luten et al. 1987; Moharram et al. 1987; Sprenger et al.1988; Grieb et al. 1990; Parks et al. 1991; Gutenmann et al. 1992; Lange et al. 1993; Tracey 1993; Joiris et al. 1995; Munn and Short 1997; Stafford and Haines 1997), BASS predicts a strong interdependence between the body sizes of fish and their mercury whole body mercury concentrations. For example, the mean annual mercury concentration of newly recruited largemouth whose average annual body weights is 86.9 g(FW) is 0.499 mg Hg/kg(FW). However, the mean annual mercury concentration of oldest largemouth whose average annual body weights is 1.09 kg(FW) is 1.03 mg Hg/kg(FW).

Figure 6. Conceptual model for the primary food web of Everglades open water fish assemblage.



7. Model Quality Assurance

Quality Assurance (QA) and Quality Control (QC) for the BASS simulation model has 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 which has been published in the peer reviewed literature (Barber et al. 1988, 1991). The bioenergetic modeling paradigm employed by BASS to simulate fish growth has been used 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). Moreover, since its construction FGETS has been included in numerous reviews bioaccumulation models that are applicable for ecological risk assessments and environmental management decisions (Barron et al. 1990; Jones et al. 1991; Barnthouse 1992; Chapra and Boyer 1992; Landrum et al. 1992; Olem et al. 1992; Dixon and Florian 1993; Cowan et al. 1995; Campfens and Mackay 1997; Feijtel et al. 1997; Howgate 1998; Wania and Mackay 1999; Mackay and Fraser 2000; Bartell et al. 2000).

Two criticisms have been lodged against FGETS in the literature. The fist of these is that it assumes or attempts to prove 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 as 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 which simply lumps all excretion pathways (i.e., gill, intestinal, urinary, and dermal) into one. What Madejian et al. are essentially 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 generally aimed at BASS's gill exchange model. As indicated by Tables 2 - 6, however, there is in fact an abundance of gill morphometric data available to estimate the parameters needed for this model.

7.1.2. How has the model or model algorithms been corroborated / validated?

BASS's bioconcentration and bioaccumulation algorithms have been validated by comparing its predicted uptake and elimination rates to published in the peer reviewed literature (Barber et al. 1988; Barber 2000). For organic chemicals these algorithms have also been validated by simulations of mixtures of PCBs in Lake Ontario salmonids and various laboratory studies (Barber et al. 1991). For sulfhydryl binding metals, BASS's bioconcentration algorithms have been validated by simulations of methylmercury bioaccumulation in Florida Everglades fish communities one of which is presented herein as a typical BASS application. For validation of BASS's bioenergetic growth algorithms the reader should refer to Barber et al. (1991) and the example herein.

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 class 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 term the following partial derivatives

$$\frac{\partial X_i}{\partial p_j} \; ; \qquad \frac{\partial X_i}{\partial Z_j} \; ; \qquad \frac{\partial X_i}{\partial X_j(0)}$$

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 which 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 model sensitivity as defined above is simply a mathematical characteristic of a model, model sensitivity in and of itself is neither good nor bad. Sensitivity is desirable if the 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 statistically variability associated with those components.

A generalized sensitivity analysis of BASS without explicit specification of a fish community of concern is undoable. 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 by the users of the software. Although procedures for enabling users to conduct a variety of structured sensitivity analyses are currently be developed, presently the onus of performing such analyses rests with the user. Users interested in issues and techniques related to model sensitivity and uncertainty should consult the following papers: Giersch (1991), Elston (1992), Summers et al. (1993), Håkanson (1995), Norton (1996), Loehle (1997), and Wallach and Genard (1998).

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 which summarizes all the input data that was 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 then on the user to verify that their input data has been properly processed. If not, the user's 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 is detected, an appropriate error message is written to the above *.MSG file and a error code is set to true. If this error code is true after all the user's input has been processed, BASS terminates without attempting further program execution.

7.2.2. Is the developer reasonably confident that program subroutines, functions, and procedures are transmitting and receiving the correct variables? Similarly, is the developer reasonably confident that program subroutines, functions, and procedures are not inadvertently changing variable assignments the shouldn't be changed?

All BASS subroutines and functions are accessed using implicit interface generated by the pertinent Fortran 95 compiler. Subroutines and functions are packaged together according to the function and degree of interaction. The BASS version 2.1 software is coded with one main program PROGRAM BASS_V21 (see BASS_V21.F90) and 25 procedure modules. These are

- 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_DEFINED - functions for determining whether program parameters and variables have been initialized or assigned (see BASS_DEFINED.F90).
- MODULE BASS_EXP - subroutines for calculating exposure conditions (see BASS_EXP.F90).
- MODULE BASS_INI - subroutines for initialization of program variables (see BASS_INI.F90).
- MODULE BASS_INPUT - subroutines for processing user input (see BASS_INPUT.F90).
- MODULE BASS_ODE - subroutines for the computational kernel of the BASS software (see BASS_ODE.F90).
- MODULE BASS_PLOTS - subroutines for generating BASS output plots (see BASS_PLOTS.F90).
- MODULE BASS_TABLES - subroutines for generating output tables (see BASS_TABLES.F90).
- MODULE DECODE_FUNCTIONS - subroutines for decoding constant, linear, and power functions from character strings (see UTL_DCOD_FNC.F90).
- MODULE DISLIN_PLOTS - general subroutines for generating 2 and 3-dimensional DISLIN plots (see UTL_PLOTS.F90).
- MODULE ERROR_MODULE - subroutines for printing error codes encountered with general utility modules (see UTL_ERRORS.F90).

- MODULE FILESTUFF - subroutines for parsing file names and obtaining version numbers or time stamps (see UTL_FILESTUFF.F90).
- 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.F90).
- MODULE MODULO_XFREAD - subroutines for reading files which contain comments, continuation lines, and include files (see UTL_XFREAD.F90).
- MODULE MSORT - subroutines for sorting and generating permutation vectors for lists and vectors (see UTL_MSORT.F90).
- MODULE MXGETARGS - subroutines for extracting arguments from a command line (see UTL_MXGETARGS.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 phase within a sorted list (see UTL_SEARCH2.F90).
- MODULE SEARCH_LISTS - subroutines for finding the location of a value within a sorted list (see UTL_SEARCH1.F90).
- MODULE STRINGS - subroutines for character string manipulations and printing multiline character text (see UTL_STRINGS.F90).
- 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).

In general these procedure modules are coded with minimal or no scoping units. Also 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 below), data exchanges between program procedures are performed via formal subroutine/function parameters whenever possible. The only notably exception to this coding policy are modules which must be used to supply auxiliary parameters to an "external" subroutine which is used as an argument to certain mathematical software packages. Working areas used by BASS are not used for data transfers between internal or external procedures.

To simplify the construction and maintenance of the formal parameter lists of many BASS subroutines and functions and to help prevent the inadvertent transposition subroutine or function formal parameters, BASS makes extensive use of derive type data structures. Each derived type definition is specified within its own module and all derive type definition modules are maintained in the file BASS_TYPES.F90. A good example of BASS's use of derive type data structures is the derive type variable used to store and transfer the ecological, physiological, and morphometric data for a particular fish species. This derived type is defined by following module

```
MODULE dt_fish_par
TYPE:: fish_par
   CHARACTER (LEN=80) :: ageclass, class_var, &
      genus_species, spawning_interval
   INTEGER :: classes=0, spawnings=0
   INTEGER, DIMENSION(:), POINTER :: &
      class_model=>NULL(), spawn_dates=>NULL()
   REAL :: ae_fish, ae_invert, ae_plant, &
      dry2live_ab, dry2live_aa, dry2live_bb, &
      dry2live_cc, gco2_d, la, longevity, &
      mgo2_s, rbi, rq, rt2std, sda2in, tl_r0, yoy
   REAL, DIMENSION(2) :: &
      ga, id, ld, ll, lp, nm, pa, pl, wl
   REAL, DIMENSION(6) :: ge, mf, mi, sg, sm, so, st
   REAL, DIMENSION(:), POINTER :: class_bnds=>NULL()
END TYPE fish_par
END MODULE dt_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 39). 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 live 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.

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_CONSTANTS.F90).
- MODULE CONSTANTS - constants used by utility subroutines (see UTL_CONSTANTS.F90).
- MODULE NOVALUE - specifies values for integer, real, and character variables that have been been initialized (see BASS_CONSTANTS.F90).
- MODULE SNGL_DBL_QUAD - specifies the precision of floating point variables as either single, double, or quad precision variables. This module also assigns certain associate floating point constants (see BASS_CONSTANTS.F90).
- MODULE WORKING_DIMENSIONS - specifies 'standard' sizes for character variable, input records, etc. (see BASS_CONSTANTS.F90).
- MODULE UNITS_PARAMETERS - specifies parameters used by the units conversion subroutines (see UTL_UPARAMS.F90)

7.2.4. Do all strictly mathematical algorithms do what they are suppose 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 live weight from its dry weight given an allometric relationship between its live body weight and its fraction lipid and linear relationships between its percent water, lipid, and non-lipid organic matter. 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).

As mentioned earlier, the BASS software allows the user to integrate BASS's differential equations using either a simple Euler method or a fifth-order Runge-Kutta method with adaptive step sizing. These methods offer the user two distinctly different options with respect to software performance and execution. Although Euler methods cannot assess the accuracy of their integration, such methods often allow for fast model execution. Runge-Kutta methods, on the other hand, can monitor the accuracy of their integration but at the cost of increased execution time. This additional computational burden, however, can often be significantly reduced by employing adaptive step sizing. BASS's Runge-Kutta 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.

$$
\begin{aligned}
dy_1/dx &= 1.0 \\
dy_2/dx &= x \\
dy_3/dx &= \cos(x) \\
dy_4/dx &= \cosh(x) \\
dy_5/dx &= \exp(x) \\
dy_6/dx &= 1.0/(1.0 + x) \\
dy_7/dx &= 1.0/(1.0 + x^2) \\
dy_8/dx &= 1.0/\sqrt{1.0 + x^2} \\
dy_9/dx &= -100\,(y_9 - \sin(x)) \qquad y_9(0) = 1 \\
du/dx &= 998\,u + 1998\,v \qquad u(0) = 1 \\
dv/dx &= -999\,u - 1999\,v \qquad v(0) = 0
\end{aligned}
$$

The analytical solution to this system of equations is

$$
\begin{aligned}
y_1 &= x - x_0 \\
y_2 &= 0.5\,(x^2 - x_0^2) \\
y_3 &= \sin(x) - \sin(x_0) \\
y_4 &= \sinh(x) - \sinh(x_0) \\
y_5 &= \exp(x) - \exp(x_0) \\
y_6 &= \ln(1 + x) - \ln(1 + x_0) \\
y_7 &= \arctan(x) - \arctan(x_0) \\
y_8 &= asinh(x) - asinh(x_0) \\
y_9 &= \frac{10101}{10001}\exp(-100\,x) - \frac{100}{10001}\cos(x) + \frac{10000}{10001}\sin(x) \\
u &= 2\exp(-x) - \exp(-1000\,x) \\
v &= -\exp(-x) + \exp(-1000\,x)
\end{aligned}
$$

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 $<10^{-6}$.

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. BASS, like many ecological models, utilizes threshold responses, absolute value functions, maximum and minimum functions, and linear interpolations between time series in its formulation and implementation. Although most of BASS's parameters are updated continuously, a few parameters (e.g., dietary compositions) which are computationally intensive to evaluate and which change very slowly are updated only daily and are

therefore step functions of time. 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 for 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 conditions 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 later case, BASS also recalculates the dietary compositions of the remaining fish which again 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 a simple reinitialization problem.

7.2.6. Are simulated results consistent with known mathematical constraint of the model? For example, if state variable are suppose to be non-negative, are they? Similarly, if the model is suppose to mass balance, does it?

BASS's state variables, like those of most physical or biological models, must be by definition non-negative. 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 which 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

$$y(t+h) = y(t) + h\, y'(t)$$

$$0 < y(t) + h\, y'(t)$$

$$\frac{-y(t)}{y'(t)} > h \qquad \text{where} \quad y'(t) < 0$$

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 types of situations that can occur during a BASS simulations that might necessitate this type of corrective action. The first of these occurs when a cohort experiences intense predation or other mortality that drives its population to extinction whereas the second situation might occur when there is the rapid excretion of a hydrophilic contaminant following the disappearance of an aqueous exposure. Regardless of the integration method used (i.e., Euler or Runge-Kutta), 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 not, BASS either executes a simple Euler step of the appropriate size or restarts the integration with the appropriate state variables initialized to zero.

When used it its full community mode (i.e., the non-FGETS option), BASS calculates and reports the mass balance between the community's total predicted predatory mortality and its total predicted piscivorous consumption as a mass balance check on its internal consistency and operation. For the example presented herein this mass balance is -1.953E-02 [g(DW)/ha/yr]. Since this community's total piscivory is calculated to be 2.778E+04 [g(DW)/ha/yr], this mass balance check would have a relative error of less than 10^{-6}. See page 121.

7.2.7. Are simulation results consistent across machines or compilers?

BASS was originally developed on a DEC 3000 work station using the DEC Fortran 90 compiler. It has also been ported to the Windows operating system on the DELL OptiPlex using the Lahey/Fujitsu Fortran 95 5.60 compiler. Although the results of these two implementations to 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.

7.2.8. Have test and reference/benchmark data sets been documented and archived?

At least three different test project files are maintained to tract changes in the operation of BASS associated with code maintenance and updates. These files are used as benchmarks to verify that code modifications that should not change BASS 's computational results in point of fact 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 specific real communities, its principal intended use is to predict and compare the outcomes of alterative management options that are associated with pollution control, fisheries management, and/or ecosystem restoration activities.

7.3.2. Does the User Guide provide the information needed to appropriate 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 one of the three example applications 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 will assign a few default 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's simulation. In general, these problem areas involve either the unsuccessfully resolution of a root of a nonlinear equation or the unsuccessfully 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 live weight is calculated to be less or equal to its dry weights. 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 any of these situations are encountered, BASS terminates execution and issues an appropriate error message to the current *.MSG file.

8. Planned Future Features

Presently, ten major program developments are planned for BASS. These include:

- Development of a graphical user interface (GUI) for easy construction of input files.
- Improved plotting capabilities including the generation of output files that users can input to their own graphic software.
- Development canonical fish and community databases (i.e., *.FSH and *.CMM files) to facilitate easier application of BASS.
- Software to perform model sensitivity analyses.
- Implementation of an option to read a simulated or measured time series of dissolved oxygen concentrations that are needed of calculate the fishes' ventilation volumes. See Eq.(2-12). Currently, BASS uses saturated dissolved oxygen concentrations that are calculated as a function of water temperature.
- Development of submodels for simulating the biomass dynamics of benthos, periphyton, phytoplankton, and zooplankton.
- Development of submodels for simulating the physiological tolerances of fish to water quality parameters other than toxic chemicals.
- Incorporation of quantitative structure activity relationships (QSAR's) to predict metabolism of organic chemicals.
- Development of migration algorithms for simulating the movement of fish into and out of the simulated community based on habitat parameters such as water depth, current velocity, availability of prey, etc.
- Development of subroutines to simulate sublethal, residue-based effects.

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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 which include 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 which include As, Cd, Co, Cr, Ni, Sn, and Zn bind not only to 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 is regulated by metallothioneins via sulfhydryl complexation reactions certainly 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 are the moles of metal bound to sulfhydryls; and RSH are the moles of free non-disassociated sulfhydryl. Metal complexation must be constrained by mass balances for both the metal and sulfhydryl binding sites. For the metal itself the following mass balance must hold

$$\begin{aligned} TM &= M + LM + RSM \\ &= [M^{+}] * P_a W + [M^{+}] K_{ow} P_l W + \frac{Kb\ RSH [M^{+}]}{[H^{+}]} \\ &= [M^{+}] \left(P_a W + P_l W K_{ow} + \frac{Kb\ RSH}{[H^{+}]} \right) \end{aligned} \tag{A-3}$$

$$[M^{+}] = \frac{TM}{W\ (P_a + P_l\ K_{ow}) + \frac{Kb\ RSH}{[H^{+}]}}$$

where TM are the total moles of metal; LM are the moles of metal that is partitioned into lipids; and W is the fish's volume in liters which is approximately equivalent to its kilogram live weight. The mass balance for the fish' s sulfhydryl content that must is satisfied is

$$\begin{aligned} TS &= RSH + RS^{-} + \sum_i RSM_i \\ &= RSH \left(1 + \frac{K_a}{[H^{+}]} \right) + \sum_i RSM_i \end{aligned} \tag{A-4}$$

where TS denotes the total moles of sulfhydryl ligands; RS^{-} are the moles of disassociated sulfhydryls; and $K_a = [RS^{-}][H^{+}]/[RSH]$ is the sulfhydryl's disassociation constant. In addition to the reaction specified in Eq. (A-1), mixtures of metals interact by competing for the same binding site, i.e.,

$$RSM_i + M_j^{+} \leftrightharpoons RSM_j + M_i^{+} \tag{A-5}$$

The stability constant for this reaction is

$$Kb_{ij} = \frac{[RSM_j]\ [M_i^{+}]}{[RSM_i]\ [M_j^{+}]} = \frac{Kb_j}{Kb_i} \tag{A-6}$$

From this expression it then follows

$$\begin{aligned} RSM_j\ [M_i^{+}]\ Kb_i &= RSM_i\ [M_j^{+}]\ Kb_j \\ \sum_i RSM_j\ [M_i^{+}]\ Kb_i &= \sum_i RSM_i\ [M_j^{+}]\ Kb_j \\ RSM_j \sum_i\ [M_i^{+}]\ Kb_i &= [M_j^{+}]\ Kb_j \sum_i RSM_i \\ \frac{RSM_j}{[M_j^{+}]\ Kb_j} \sum_i\ [M_i^{+}]\ Kb_i &= \sum_i RSM_i \\ \frac{RSH}{[H^{+}]} \sum_i\ [M_i^{+}]\ Kb_i &= \sum_i RSM_i \end{aligned} \tag{A-7}$$

If Eq.(A-3) is substituted in this equation, one then obtains

$$\begin{aligned} \sum_i\ RSM_i &= \frac{RSH}{[H^{+}]} \sum_i\ \frac{Kb_i\ TM_i}{P_a W + P_l W\ K_{ow_i} + Kb_i\ RSH/[H^{+}]} \\ &= RSH \sum_i\ \frac{Kb_i\ TM_i}{[H^{+}]\ W\ (P_a + P_l\ K_{ow_i}) + Kb_i\ RSH} \end{aligned} \tag{A-8}$$

This equation in turn can be substituted into Eq.(A-4) to obtain

$$TS = RSH\left(1 + \frac{K_a}{[H^+]}\right) + RSH\sum_i \frac{Kb_i\ TM_i}{[H^+]\ W\ (P_a + P_l\ K_{ow_i}) + Kb_i\ RSH} \quad \text{(A-9)}$$

For most metals, however,

$$[H^+]\,W(P_a + P_l K_{ow_i}) \ll Kb_i\ RSH \quad \text{(A-10)}$$

Therefore, the sulfhydryl balance equation is approximately equal to

$$TS = RSH\left(1 + \frac{K_a}{[H^+]}\right) + \sum_i TM_i \quad \text{(A-11)}$$

Thus,

$$RSH = \frac{TS - \sum_i TM_i}{1 + K_a/[H^+]} \quad \text{(A-12)}$$

If the metal's aqueous and organic phase concentrations (i.e., C_a and C_o) are expressed on a molar basis, then

$$RSM = C_o\ P_o\ W \quad \text{(A-13)}$$

$$[M^+] = C_a \quad \text{(A-14)}$$

When Eqs. (A-12), (A-13), and (A-14) are substituted into Eq.(A-2), one then obtains

$$Kb = \frac{P_o C_o W\ ([H^+] + K_a)}{C_a\ (TS - \sum_i TM_i)} \quad \text{(A-15)}$$

$$\frac{P_o C_o}{C_a} = \frac{Kb\ (TS - \sum_i TM_i)}{W\ ([H^+] + K_a)}$$

which can then be substituted into the equation

$$C_a = \frac{C_f}{P_a + P_l K_{ow} + \frac{P_o C_o}{C_a}} \quad \text{(A-16)}$$

to calculated the fish's aqueous phase concentrations.

To use the above complexation model one must specify both the metal's stability constant (see Eq.(A-2)) and the concentration of sulfhydryl binding sites (mol SH/g(DW)) 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. Despite this situation, however, a reasonable approximation of this parameter can still be made since data does exists 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 the 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 would be estimated to be 9.12 µmol(SH) / g(muscle) or 45.6 µmol(SH) / g(dry muscle). Opstevedt et al. (1984) reported the suldhydryl 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(dry 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(dry muscle) (Opstevedt et al. 1984) this value is equivalent to 73.2 µmol(SH) / g(dry muscle). Although few other studies have investigated the sulfhydryl content of whole fish muscle, several studies have reported on the sulfhydryl content 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), it would appear that the results of Itano and Sasaki (1983), Opstevedt et al. (1984), and Chung et al. (2000) can be applied to fish in general. Consequently, the sulfhydryl content of fish muscle can be assumed to be on the order of 45-70 µmol(SH) / g(dry muscle)

Although the sulfhydryl content of liver, kidney, gills, and intestine has not been measured directly, the sulfhydryl content of these tissues can be estimated from their metallothionein concentrations. Metallothioneins (MT) are sulfur-rich proteins which are responsible for the transport and storage of heavy and trace metals and which are also usually considered to be the principle 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 Ducan 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(dry liver). These values suggest that the hepatic sulfhydryl content of fish which would include both their baseline MT and cytoplasmic components that can be converted into MT, might be on the order of 40 µmol(SH) / g(dry liver). This 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(dry liver). Of these two possibilities the latter appears more likely.

Although gill, kidney, and intestine MTs have not been studied in the same detail that hepatic MTs have been, it appears that MT and hence sulfhydryl concentrations in gills and kidney are lower and not as inducible as hepatic concentrations (Klaverkamp and Ducan 1987; Hamilton et al. 1987a,b). 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 value agrees well 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 high for 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 such as those involved in fatty acid synthesis, glutathione, etc., it seems reasonable to assume that the sulfhydryl content of fish is approximately 70 µmol(SH) / g(DW). Because Davis and Boyd (1978) reported the mean sulfur content of 17 fish species to be 206 µmol(S) / g(DW), this assumption implies that almost 1/3 of a fish's sulfur pool exists as sulfhydryl groups.

The above complexation model was implemented within BASS using 70 µmol(SH) / g(DW) to calculate the total sulfhydryl content of fish and assuming that the mean dissociation constant for organic sulfhydryls is pKa=9.25 (i.e., the SPARC estimated pKa for cysteine). Using literature values for the stability constants of methylmercury, however, BASS overpredicted the bioammulation of methylmercury in fish by at least an order of magnitude. Consequently, a much simpler distribution coefficient algorithm was adapted.

APPENDIX B. Nondimensionalization of chemical exchange equations for fish gills.

Using the transformations

$$\Theta = \frac{C - C_a}{C_w - C_a} \tag{B-1}$$

$$X = \frac{x}{h} \tag{B-2}$$

$$Y = \frac{y\ D}{V\ h^2} \tag{B-3}$$

the PDE and boundary conditions

$$\frac{3}{2}\left(1 - x^2\right)\frac{\partial C}{\partial y} = D\ \frac{\partial^2 C}{\partial x^2} \tag{B-4}$$

$$\left.\frac{dC}{dx}\right|_{x=0} = 0 \tag{B-5}$$

$$D\left.\frac{\partial C}{\partial x}\right|_{x=h} = k_m\left(C(h,y) - C_a - \frac{2\,z\,D}{q_p}\int_y^l \left.\frac{\partial C}{\partial x}\right|_{x=h} dy\right) \tag{B-6}$$

can be nondimensionalized into

$$\frac{3}{2}\left(1 - X^2\right)\frac{\partial \Theta}{\partial Y} = \frac{\partial^2 \Theta}{\partial X^2} \tag{B-7}$$

$$\left.\frac{d\Theta}{dX}\right|_{X=0} = 0 \tag{B-8}$$

$$\left.\frac{\partial \Theta}{\partial X}\right|_{X=1} = -N_{Sh}\left(\Theta(1,Y) - \frac{2\,h\,z\,V}{q_p}\int_Y^{N_{Gz}} \left.\frac{\partial \Theta}{\partial X}\right|_{X=1} dY\right) \tag{B-9}$$

The boundary condition (B-9) that describes exchange across the secondary lamella, however, can be simplified by noting that the solution of Eq.(B-7) is separable, i.e., $\Theta(X, Y) = \Phi(X)\Psi(Y)$ and that $q_v = h\ z\ V$ is the ventilation volume of an individual interlamellar channel. Using these observations, one can then write

$$\Psi(Y)\left.\frac{d\Phi}{dX}\right|_{X=1} = N_{Sh}\left(\Phi(1)\,\Psi(Y) - \frac{2q_v}{q_p}\int_Y^{N_{Gz}} \Psi(Y)\left.\frac{d\Phi}{dX}\right|_{X=1} dY\right) \tag{B-10}$$

which can then be differentiated with respect to Y to obtain

$$\frac{d\Psi}{dY}\left.\frac{d\Phi}{dX}\right|_{X=1} = N_{Sh}\left(\Phi(1)\frac{d\Psi}{dY} - \frac{2q_v}{q_p}\Psi(Y)\left.\frac{d\Phi}{dX}\right|_{X=1}\right) \tag{B-11}$$

$$\frac{1}{\Psi(Y)}\frac{d\Psi}{dY}\left.\frac{d\Phi}{dX}\right|_{X=1} = N_{Sh}\left(\frac{\Phi(1)}{\Psi(Y)}\frac{d\Psi}{dY} - \frac{2q_v}{q_p}\left.\frac{d\Phi}{dX}\right|_{X=1}\right) \tag{B-12}$$

Because $\Psi(Y) = \exp(-\frac{2}{3}\lambda^2 Y)$ where $-\frac{2}{3}\lambda^2$ is the constant of separation for Eq.(B-7), the preceding equation is equivalent to

$$-\frac{2}{3}\lambda^2\left.\frac{d\Phi}{dX}\right|_{X=1} = -N_{Sh}\left(-\frac{2}{3}\lambda^2\Phi(1) + \frac{2q_v}{q_p}\left.\frac{d\Phi}{dX}\right|_{X=1}\right) \tag{B-13}$$

which can be manipulated to yield

$$\left.\frac{d\Phi}{dX}\right|_{x=1} = -\left(\frac{\frac{2}{3}\lambda^2 N_{Sh}}{\frac{2}{3}\lambda^2 - (2q_v/q_p)N_{Sh}}\right)\Phi(1) \tag{B-14}$$

Although this boundary condition is dependent on the eigenvalue λ, the eigenvalue expansion for the solution of Eq.(B-7) is still straightforward (Walter 1973; Fulton 1977). Note that as the fish's perfusion rate increases, this boundary condition converges to

$$\left.\frac{d\Phi}{dX}\right|_{x=1} = -N_{Sh}\,\Phi(1) \tag{B-15}$$

which is the boundary condition previously used by Barber et al. (1991).

APPENDIX C. Derivation of the consistency condition for feeding electivities.

To derive a self consistency condition on a fish's electivities and relative prey availabilities such that its calculate dietary frequencies will sum to unity, consider the following

$$e_i = \frac{d_i - f_i}{d_i + f_i} \qquad \text{(C-1)}$$

$$e_i\,(d_i + f_i) = d_i - f_i \qquad \text{(C-2)}$$

$$d_i = \left(\frac{1 + e_i}{1 - e_i}\right) f_i \qquad \text{(C-3)}$$

Summing Eq. (C-2) over all *i* then yields

$$\sum e_i\,(d_i + f_i) = \sum d_i - \sum f_i = 0 \qquad \text{(C-4)}$$

When Eq.(C-3) is substituted into this expression, one then obtains

$$\sum e_i \left(\frac{1+e_i}{1-e_i}\, f_f + f_i\right) = 0$$

$$\sum \frac{2\, e_i\, f_i}{1-e_i} = 0 \qquad \text{(C-5)}$$

$$\sum \frac{e_i\, f_i}{1-e_i} = 0$$

Adding $\sum f_i = 1$ to each side of the above equation one obtains the desired result, i.e.,

$$\sum \frac{e_i\, f_i}{1-e_i} + \sum f_i = 1$$

$$\sum \frac{e_i\, f_i}{1-e_i} + f_i = 1 \qquad \text{(C-6)}$$

$$\sum \frac{f_i}{1-e_i} = 1$$

APPENDIX D. Example project file constructed using include files as discussed in Section 4.4.

```
!
! file: evergld1.prj
! date: sept. 19, 2000
!
! notes: project file (*.prj) for BASS version 2.1. constructed to simulate
!        methylmercury bioaccumulation in a 'typical' deep-water fish community
!        of the Florida Everglades, USA.
!
! specify control parameters

/ SIMULATION_CONTROL
/ HEADER  methylmercury bioaccumulation in a "ponded" everglades community
/ MONTH_T0 april
/ LENGTH_OF_SIMULATION  10[year]
/ TEMPERATURE  temp[celsius]=25.0+10.0*sin(0.172142e-01*t[days]+6.02497)
/ WATER_LEVEL  depth[meter]=file(nonfish.dat)
/ BIOTA benthos[g/m^2]=file(nonfish.dat); &
        periphyton[g/m^2]=file(nonfish.dat); &
        zooplankton[mg/l]=file(nonfish.dat)
/ ANNUAL_OUTPUTS 10
/ SUMMARY_PLOTS  pop(length); cfish(length)

!
!  other available plots include:
!
!  / SUMMARY_PLOTS  afish(age); afish(length); afish(weight); &
!                   cfish(age); cfish(length); cfish(weight); &
!                   baf(age); baf(length); baf(weight); &
!                   bmf(age); bmf(length); bmf(weight); &
!                   pop(age); pop(length); pop(weight); &
!                   age(length); age(weight); tl(age); tl(weight); &
!                   wt(age); wt(length)

! specify chemical properties and exposures for methylmercury

#include 'mercury.chm'

! specify fish community; full community simulation

#include 'evergld1.cmm'

/ END
```

APPENDIX D. (cont.) Include file MERCURY.CHM for methylmercury properties and exposures.

```
!
! file: mercury.chm
! date: sept. 19, 2000
!
! notes: chemical properties and exposure file (*.chm) for BASS version 2.1. constructed
!        to simulate methylmercury bioaccumulation in a 'typical' deep-water fish community
!        in the Florida Everglades, USA.

#include 'methyl_hg.prp'

!
! refs:
!
! - Loftus, W.F., J.C. Trexler, and R.D. Jones. 1998. Mercury transfer through an
!   everglades aquatic food web. final report contrat SP-329. Florida Department
!   of Environmental Protection.
! - Stober, J., D. Scheidt, R. Jones, K. Thornton, L. Gandy, J. Trexler, and
!   S. Rathbun. 1998. South Florida ecosystem assessment. EPA-904-R-002
! - Watras, C. and N. Bloom. 1992. Mercury and methylmercury in individual
!   zooplankton: implications for bioaccumulation. Limnol. Oceanogr. 37:1313-1318.
!
! based on Loftus et al. (1998) total mercury concentrations are
!
! cwater[ng/l]     = 1.13         for total mercury
!                  = 0.15*1.13    for methymercury
! cphytn[ng/g(fw)] = 76.11
!                       57.85(n=4)   utricularia
!                    90.44(n=5)   diatoms
!                    76.58(n=3)   chlorophyta
! cinsct[ng/g(fw)] = 212.17
!                    258.04(n=9)  dolomedes
!                    148.95(n=6)  hydracarina
!                    304.29(n=12) tetragonids
!                    136.23(n=15) unid spiders
! czplnk[ng/g(fw)] = 54.60
!                    46.35(n=10)  cladocera
!                    62.90(n=12)  copepoda
!                    53.39(n=14)  ostracoda
! cbnths[ng/g(fw)] = 83.91
!                    38.03(n=18)  chironomids
!                    38.89(n=9)   gastropoda-littoridinops
!                    8.92(n=5)    gastropoda-melanoides
!                    50.05(n=12)  gastropoda-physella
!                    14.21(n=9)   gastropoda-planorbella
!                    14.76(n=2)   gastropoda-planorbella
!                    19.26(n=13)  gastropoda-pomacea
!                    126.55(n=20) hemiptera-belostoma
!                    95.98(n=22)  hemiptera-pelocoris
!                    44.85(n=23)  hyalella
!                    91.58(n=25)  odonata-libellulidae
!                    186.31(n=41) palaemonetes
!                    18.90(n=8)   pelycepoda-villosa
!                    64.33(n=24)  procambarus
!
! assume
!
! g(dw)/g(fw)   = 0.2 (Watras and Bloom 1992)
! mehg/total hg = 0.15 in water (Stober et al. 1998)
! mehg/total hg = 0.20 in phytoplankton (Watras and Bloom 1992)
! mehg/total hg = 0.60 in zooplankton (Watras and Bloom 1992)
! mehg/total hg > 0.90 in fish (Watras and Bloom 1992)
!
/ EXPOSURE cwater[ng/l]=0.444; cinsct[ppb]=212.17/0.2; &
           cphytn[ppb]=(0.2*16.74/0.2)/(1.13*0.15)*cwater[ng/l]; &
           czplnk[ppb]=(0.6*54.60/0.2)/(1.13*0.15)*cwater[ng/l]; &
           cbnths[ppb]=(0.6*83.91/0.2)/(1.13*0.15)*cwater[ng/l]
! end mercury.chm
```

APPENDIX D. (cont.) Include file METHYL_HG.PRP for methylmercury properties.

```
!
! file: methyl_hg.prp
! date: sept. 19, 2000
!
! specify chemical properties for methylmercury
!
! refs:
! - Arnold, A.P. and A.J. Canty. 1983. Methylmercury(II) sulfhydryl interactions.
!   Potentiometric determinations of the formation constants for complexation of
!   methylmercury(II) by sulfhydryl containing amino acids and related molecules
!   including gltathione. Can.J.Chem. 61:1428-1434.
! - Benoit, J.M., R.P. Mason, and  C.C. Gilmore. 1999a. Estimation of mercury-sulfid
!   speciation in sediment pore waters using octanol-water partitioning and implications
!   for availability to methylating bacteria. Environ. Toxicol. Chem. 18:2138-2141.
! - Benoit, J.M., C.C. Gilmore, R.P. Mason, and A. Heyes. 1999b. Sulfide controls on
!   mercury speciation and bioavailability to methylating bacteria in sediment pore
!   waters. Environ. Sci. Technol. 33:951-957.
! - Major, M.A., D.H. Rosenblatt, and K.A. Bostian. 1991. The octanol/water
!   partition coeffiecent of methylmercury chloride and methylmercury hydroxide
!   in pure water and salt solutions. Environ.Toxicol.Chem. 10:5-8.
! - Simpson, R.B. 1961. Association constants of methylmercury with sulfhydryl and
!   other bases. J.Am.Chem.Soc. 83:4711-4717.
!
! notes: Simpson (1961) reports that for cysteine log(kb)=log(k2)=7.1 and for
!        glutathione log(kb)=log(k2)=6.9. results of Arnold and Canty (1983),
!        however, estimate log(kb)=log(beta_110)-pka=16.46-8.22=8.24. therefore
!        assume log(kb)=(7.1+8.24)/2=7.67
!
/ CHEMICAL methylmercury
/ LOG_KB1 6.00 ! assumed
/ LOG_KB2 5.00 ! assumed
/ LOG_P -0.4 ! kow = 0.4 at physiological pH; see Major et al (1991)
/ MOLAR_VOLUME 51 ! calculated using liquid referenced molar volume of dimethylmercury
/ MOLAR_WEIGHT 215.6
/ MELTING_POINT 25

! end methyl_hg.prp
```

APPENDIX D. (cont.) Include file EVERGLD1.CMM for community structure parameters.

```
! file: evergld1.cmm
! date: sept. 19, 2000
!
! notes: community file (*.cmm) for BASS version 2.1. constructed to simulate methylmercury
!        bioaccumulation in a 'typical' deep-water fish community in the Florida Everglades,
!        USA.
!
! specify fish community
!

#include 'lgmouth.fsh'
/ ECOLOGICAL_PARAMETERS &
  diet(0<l[mm]<20)={zooplankton=100}; &
  diet(20<l[mm]<100)={zooplankton=35, benthos=35, bluegill=0, redear=0, gambusia=0}; &
  diet(100<l[mm]<200)={benthos=50, bass=0, bluegill=0, redear=0, gambusia=0}; &
  diet(200<l[mm]<600)={benthos=25, bass=0, bullhead=0, bluegill=0, redear=0}
/ INITIAL_CONDITIONS &
  age[day]={ 320., 685., 1050., 1415., 1780., 2145., 2510., 2875.}; &
  wt[g]={ 127., 294., 501., 740., 1008., 1302., 1618., 1957.}; &
  pop[fish/ha]={ 12.56, 6.70, 4.49, 3.35, 2.66, 2.19, 1.86, 1.62} ! 20.00[kg/ha]

#include 'gar.fsh'
/ ECOLOGICAL_PARAMETERS &
  diet(0<l[mm]<20)={zooplankton=100}; &
  diet(20<l[mm]<100)={zooplankton=25,benthos=25, bass=0, bluegill=0, redear=0, gambusia=0}; &
  diet(100<l[mm]<1000)={benthos=25, bass=0, bluegill=0, redear=0, gambusia=0}
/ INITIAL_CONDITIONS &
  age[day]={ 350., 715., 1080., 1445., 1810.}; &
  wt[g]={ 269., 511., 747., 980., 1210.}; &
  pop[fish/ha]={ 5.90, 3.65, 2.74, 2.24, 1.91} ! 10.00[kg/ha]

#include 'bullhead.fsh'
/ ECOLOGICAL_PARAMETERS &
  diet(0<l[mm]<50)={benthos=100}; &
  diet(50<l[mm]<500)={benthos=0, bullhead=0, redear=0}
/ INITIAL_CONDITIONS &
  age[day]={ 350., 715., 1080., 1445., 1810.}; &
  wt[g]={ 81., 219., 418., 674., 986.}; &
  pop[fish/ha]={ 33.53, 15.90, 9.80, 6.85, 5.15} ! 20.00[kg/ha]

#include 'bluegill.fsh'
/ ECOLOGICAL_PARAMETERS &
  diet(00<l[mm]<50)={zooplankton=100}; &
  diet(50<l[mm]<150)={zooplankton=0, gambusia=0, benthos=20}
/ INITIAL_CONDITIONS &
  age[day]={ 350., 715., 1080., 1445., 1810.}; &
  wt[g]={ 25., 55., 95., 143., 198.}; &
  pop[fish/ha]={ 1187.79, 643.79, 429.04, 316.59, 248.26} ! 200.00[kg/ha]

#include 'redear.fsh'
/ ECOLOGICAL_PARAMETERS &
  diet(00<l[mm]<50)={zooplankton=100}; &
  diet(50<l[mm]<60)={zooplankton=90, benthos=10}; &
  diet(60<l[mm]<70)={zooplankton=60, benthos=40}; &
  diet(70<l[mm]<80)={zooplankton=30, benthos=70}; &
  diet(80<l[mm]<150)={zooplankton=20, benthos=80}
/ INITIAL_CONDITIONS &
  age[day]={ 320., 685., 1050., 1415., 1780.}; &
  wt[g]={ 39., 91., 151., 218., 291.}; &
  pop[fish/ha]={ 375.86, 199.22, 135.84, 103.17, 83.23} ! 100.00[kg/ha]

#include 'gambusia.fsh'
/ ECOLOGICAL_PARAMETERS &
  diet(0<l[mm]<10)={zooplankton=100}; &
  diet(10<l[mm]<40)={zooplankton=0, gambusia=0}
/ INITIAL_CONDITIONS &
  age[day]={ 20., 170., 200., 230.}; &
  wt[g]={0.043, 0.260, 0.315, 0.374}; &
  pop[fish/ha]={39159.31, 10158.52, 8794.47, 7743.90} ! 10.00[kg/ha]

! end evergld1.cmm
```

APPENDIX D. (cont.) Include file LGMOUTH.FSH for basic largemouth bass parameters.

```
! file: lgmouth.fsh
! date: sept. 19, 2000
!
! notes: fish file (*.fsh) for BASS version 2.1
!
! refs:
! - Barber, M.C., L.A. Suarez, and R.R. Lassiter. 1991. Modelling bioaccumulation of organic
!   pollutants in fish with an application to PCBs in Lake Ontario salmonids.
!   Can.J.Fish.Aquat.Sci. 48:318-337.
! - Beamish, F.W.H. 1970. Oxygen consumption of largemouth bass, Micropterus salmoides, in
!   relation to swimming speed and temperature. Can.J.Zool. 48:1221-1228.
! - Beamish, F.W.H. 1974. Apparent specific dynamic action of largemouth bass, Micropterus
!   salmoides. J.Fish.Res.Bd.Can. 31:1763-1769.
! - Carlander, K.D. 1977. Handbook of Freshwater Fishery Biology, vol 2. Iowa State University
!   Press. Ames, IA.
! - Glass, N.R. 1969. Discussion of the calculation of power function with special reference to
!   respiratory metabolism in fish. J.Fish.Res.Bd Can. 26:2643-2650.
! - Lewis, W.M., R. Heidinger, W. Kirk, W. Chapman, and D. Johnson. 1974. Food intake of the
!   largemouth bass. Trans.Am.Fish.Soc. 103:277-280.
! - Lowe, T.P., T.W. May, W.G. Brumbaugh, and D.A. Kane. 1985. National Contaminant
!   Biomonitoring Program: concentrations of seven elements in freshwater fish, 1979-1981.
!   Arch.Environ.Contam.Toxicol. 14:363-388.
! - Niimi, A.J. and F.W.H. Beamish. 1974. Bioenergetics and growth of largemouth bass
!   (Micropterus salmoides) in relation to body weight and temperature. Can.J.Zool. 52:447-456.
! - Pandian, T.J. and F.J. Vernberg. 1987. Animal Energetis - v. 2. Bivalvia through Reptilia.
!   Academic Press.
! - Price, J.W. 1931. Growth and gill development in the small-mouthed black bass, Micropterus
!   dolomieu, Lacepede. Ohio State University, Franz Theodore Stone Laboratory 4:1-46.
! - Schmitt, C.J., and W.G. Brumbaugh. 1990. National Contaminant Biomonitoring Program:
!   Concentrations of arsenic, cadmium, lead, mercury, selenium, and zinc in U.S. freshwater
!   fish, 1976-1984. Arch.Environ.Contam.Toxicol. 19:731-747.
! - Schmitt, C.J.,  J.L. Zajicek, and P.H. Peterman. 1990. National Contaminant Biomonitoring
!   Program: Residues of organochlorine chemicals in U.S. freshwater fish, 1976-1984. Arch.
!   Environ.Contam.Toxicol. 19:748-781.
! - Tandler, A. and F.W.H. Beamish. 1981. Apparent specific dynamic action (SDA), fish weight,
!   and level of caloric intake in largemouth bass, Micropterus salmoides Lacepede.
!   Aquaculture 23:231-242.
! - Timmons, T.J. and W.L. Shelton. 1980. Differential growth of largemouth bass in West Point
!   Reservoir, Alabama-Georgia. Trans.Am.Fish.Soc. 109:176-186.

/ COMMON_NAME  bass
/ SPECIES  Micropterus salmoides
/ AGE_CLASS_DURATION  year
/ SPAWNING_PERIOD may-june
/ ECOLOGICAL_PARAMETERS &
  lp[cm]=0.6+0.27*L[cm]; & ! estimated from Timmons and Shelton (1980) for Lepomis
  wl[g]=0.0117*L[cm]^3.08; & ! Carlander (1977) 0.00543 adjusted such that  2.0kg = 50cm
  tl_r0[mm]= 150;  & ! Carlander (1977)
  yoy[g]=25.0; &
  mls[year]=8; &
  nm[1/day]=0.9*1.0*0.0814*W[g]^(-.675) ! see sg[] and assume exogenous mortality/total mortality = .9 and b=1
/ COMPOSITIONAL_PARAMETERS &
  pa[-]=0.80-1.57*pl[-]; & ! Lowe et al. (1985), Schmitt and Brumbaugh (1990), Schmitt et al. (1990)
  pl[-]=0.000121*W[g]^0.845 ! Lowe et al. (1985), Schmitt and Brumbaugh (1990), Schmitt et al. (1990)
/ MORPHOMETRIC_PARAMETERS &
  ga[cm^2]=7.32*W[g]^0.820; & ! Price (1931)
  ld[lamellae/mm_per_side]=31.28*W[g]^(-.072); & ! Price (1931)
  ll[cm]=0.0188*W[g]^0.294 ! assumed (see Barber et al. 1991)
/ FEEDING_OPTIONS linear(1<a[yr]<10)
/ PHYSIOLOGICAL_PARAMETERS &
  ae_fish[-]=0.89; & ! assumed (see Pandian and Verberg 1987)
  ae_invert[-]=0.66; & ! assumed (see Pandian and Verberg 1987)
  ae_plant[-]=0.44; & ! assumed (see Pandian and Verberg 1987)
  rq[-]=1.0; & ! assumed (see Barber et al. 1991)
  rt:std[-]=2.0; & ! BASS default
  sda:in[-]=0.127; & ! Beamish (1974), Tandler and Beamish (1981)
  sg[g/g/day](25)=0.0814*W[g]^(-.675); & ! Carlander (1977) assuming wt(yoy)=25 and wt(8)=2000
  so[mg(o2)/hr]=0.1187*EXP(0.0428*t[celsius])*W[g]^0.766 ! Glass (1969), Beamish (1970), Niimi and Beamish (1974)

! end lgmouth.fsh
```

APPENDIX D. (cont.) Include file GAR.FSH for basic Florida gar parameters.

```
! file: gar.fsh
! date: sept. 19, 2000
!
! notes: fish file (*.fsh) for BASS version 2.1
!
! refs:
! - Barber, M.C., L.A. Suarez, and R.R. Lassiter. 1991. Modelling bioaccumulation of organic
!   pollutants in fish with an application to PCBs in Lake Ontario salmonids.
!   Can.J.Fish.Aquat.Sci. 48:318-337.
! - Brim et al. 1993. Mercury concentrations in largemouth bass and other fishes of the
!   Loxahatchee National Wildlife Refuge. U.S. Fish and Wildlife Service publ.no. PCFO-EC 93-02.
! - Carlander, K.D. 1969. Handbook of Freshwater Fishery Biology, vol 1. Iowa State University
!   Press. Ames, IA.
! - Glass, N.R. 1969. Discussion of the calculation of power function with special reference to
!   respiratory metabolism in fish. J.Fish.Res.Bd Can. 26:2643-2650.
! - Landolt, J.C. and L.G. Hill. 1975. Observations on the gross structure and dimensions of the
!   gills of three species of gars (Lepisosteidae). Coepia 1975(3):470-475.
! - Pandian, T.J. and F.J. Vernberg. 1987. Animal Energetis - v. 2. Bivalvia through Reptilia.
!   Academic Press.
! - Rahn, H., K.B. Rahn, B.J. Howell, C. Gans, and S.M. Tenney. 1971. Air breathing of the
!   garfish (Lepisosteus osseus). Respir.Physiol. 11:285-307.
! - Smatresk, N.J. and J.N. Cameron. 1982. Respiration and acid-base physiology of the spotted
!   gar, a bimodel breather II. responces to temperature change and hypercapnia. J.Exp.Biol. 96:281-293.
! - Winger, P.V. and J.K. Andreasen. 1985. Contaminant residues in fish and sediments from
!   lakes in the Atchafalaya River Basin (Louisiana). Arch.Environ.Contam.Toxicol. 14:579-586.

/ COMMON_NAME gar
/ SPECIES  Lepisosteus platyrhincus
/ AGE_CLASS_DURATION  year
/ SPAWNING_PERIOD april-may
/ ECOLOGICAL_PARAMETERS &
  lp[cm]=0.15*L[cm]; & ! assumed
  wl[g]=0.00171*L[cm]^3.30; & ! Carlander (1969) for L. osseus 0.00065 adjusted such that 2.3 kg=720 cm
  tl_r0[mm]= 330;  & ! Carlander (1969)
  yoy[g]=25.0; &
  mls[year]=5; &
  nm[1/day]=1.0*0.882*W[g]^(-1.048) ! see sg[], assume exogenous mortality/total mortality = 1 and b=1.0
/ COMPOSITIONAL_PARAMETERS &
  pa[-] = 0.82-1.25*pl[-]; & ! assumed (see Barber et al. 1991)
  pl[-]=0.06 ! Winger and Andreasen (1985)
/ MORPHOMETRIC_PARAMETERS &
  ga[cm^2]=3.94*W[g]^0.738; & ! Landolt and Hill(1975)
  ld[lamellae/mm_per_side]=38.8*W[g]^(-.0603); & ! Landolt and Hill (1975)
  ll[cm]=0.0188*W[g]^0.294 ! assumed (see Barber et al. 1991)
/ FEEDING_OPTIONS linear(1<a[yr]<10)
/ PHYSIOLOGICAL_PARAMETERS &
  ae_fish[-]=0.89; & ! assumed (see Pandian and Verberg 1987)
  ae_invert[-]=0.66; & ! assumed (see Pandian and Verberg 1987)
  ae_plant[-]=0.44; & ! assumed (see Pandian and Verberg 1987)
  rq[-]=0.9; & ! Rahn et al. (1971) and Smatresk and Cameron (1982)
  rt:std[-]=2.0; & ! BASS default
  sda:in[-]=0.17; & ! assumed (see Barber et al. 1991)
  sg[g/g/day](25)=.882*W[g]^(-1.048); & ! Carlander (1969) and Hunt (1952) assuming wt(yoy)=25 and wt(5)=1219
  so[ml(o2)/kg/minute]=.43*exp(ln(.70/.43)/10*(t[celsius]-22)) ! Smatresk and Cameron (1982) for L. oculatus

! end gar.fsh
```

APPENDIX D. (cont.) Include file BULLHEAD.FSH for basic bullhead parameters.

```
! file: bullhead.fsh
! date: sept. 19, 2000
!
! notes: fish file (*.fsh) for BASS version 2.1
!
! refs:
! - Barber, M.C., L.A. Suarez, and R.R. Lassiter. 1991. Modelling bioaccumulation of organic
!   pollutants in fish with an application to PCBs in Lake Ontario salmonids.
!   Can.J.Fish.Aquat.Sci. 48:318-337.
! - Campbell, R.D. and B.A. Branson. 1978. Ecology and population dynamics of the black
!   bullhead, Ictalurus melas (Rafinesque), in central Kentucky. Tulane Studies in Zoology
!   and Botany 20:99-136.
! - Carlander, K.D. 1969. Handbook of Freshwater Fishery Biology, vol 1. Iowa State University
!   Press. Ames, IA.
! - Glass, N.R. 1969. Discussion of the calculation of power function with special reference to
!   respiratory metabolism in fish. J.Fish.Res.Bd.Can. 26:2643-2650.
! - Lowe, T.P., T.W. May, W.G. Brumbaugh, and D.A. Kane. 1985. National Contaminant
!   Biomonitoring Program: concentrations of seven elements in freshwater fish, 1979-1981.
!   Arch.Environ.Contam.Toxicol. 14:363-388.
! - Pandian, T.J. and F.J. Vernberg. 1987. Animal Energetis - v. 2. Bivalvia through Reptilia.
!   Academic Press.
! - Saunders, R.L. 1962. The irrigation of the gills in fishes II. Efficiency of oxygen uptake in
!   relation to respiratory flow, activity and concentrations of oxygen and carbon dioxide.
!   Can.J.Zool. 40:817-862.
! - Schmitt, C.J., and W.G. Brumbaugh. 1990. National Contaminant Biomonitoring Program:
!   Concentrations of arsenic, cadmium, lead, mercury, selenium, and zinc in U.S. freshwater
!   fish, 1976-1984. Arch.Environ.Contam.Toxicol. 19:731-747.
! - Schmitt, C.J., J.L. Zajicek, and P.H. Peterman. 1990. National Contaminant Biomonitoring
!   Program: Residues of organochlorine chemicals in U.S. freshwater fish, 1976-1984.
!   Arch.Environ.Contam.Toxicol. 19:748-781.

/ COMMON_NAME  bullhead ! yellow bullhead
/ SPECIES  Ameiurus natalis
/ AGE_CLASS_DURATION  year
/ SPAWNING_PERIOD march-april
/ ECOLOGICAL_PARAMETERS &
  lp[cm]=0.25*L[cm]; & ! assumed
  wl[g]=0.0304*L[cm]^2.82; & ! Carlander (1969) adjusted such that 1kg = 40cm
  tl_r0[mm] = 150; & ! Carlander (1969)
  yoy[g]=10.0; & ! assumed
  mls[year]=5; &
  nm[1/day]=0.90*0.0382*W[g]^(-.537) ! see sg[] and assume exogenous mortality/total mortality = 0.9 and b=1
/ COMPOSITIONAL_PARAMETERS &
  pa[-]=0.80-0.94*pl[-]; & ! Lowe et al. (1985), Schmitt and Brumbaugh (1990), Schmitt et al. (1990)
  pl[-]=0.08 ! Lowe et al. (1985), Schmitt and Brumbaugh (1990), Schmitt et al. (1990)
/ MORPHOMETRIC_PARAMETERS &
  ga[cm^2]=4.98*W[g]^0.728; & ! Saunders (1962) for brown bullhead
  id[cm]=9.26e-4*W[g]^0.200; & ! Brockway et al. for channel catfish
  ld[lamellae/mm_per_side]=15.9*W[g]^(-0.00917); & ! Saunders (1962) for brown bullhead
  ll[cm]=8.96e-3*W[g]^0.270  ! Brockway et al. for channel catfish
/ FEEDING_OPTIONS linear(1<a[yr]<5)
/ PHYSIOLOGICAL_PARAMETERS &
  ae_fish[-]=0.89; & ! assumed (see Pandian and Verberg 1987)
  ae_invert[-]=0.66; & ! assumed (see Pandian and Verberg 1987)
  ae_plant[-]=0.44; & ! assumed (see Pandian and Verberg 1987)
  rq[-]=1.0; & ! assumed (see Barber et al. 1991)
  rt:std[-]=2.0; & ! BASS default
  sda:in[-]=0.17; & ! assumed (see Barber et al. 1991)
  sg[g/g/day](25)=0.0382*W[g]^(-.537); & ! Carlander (1969) assuming wt(yoy)=10 and wt(5)=1000.0
  so[mg(o2)/hr]=0.0012*EXP(0.1838*t[celsius])*W[g]^1.02 ! Campbell and Branson (1978) Glass (1969)

! end bullhead.fsh
```

APPENDIX D. (cont.) Include file BLUEGILL.FSH for basic bluegill parameters.

```
! file: bluegill.fsh
! date: sept. 19, 2000
!
! notes: fish file (*.fsh) for BASS version 2.1
!
! refs:
! - Barber, M.C., L.A. Suarez, and R.R. Lassiter. 1991. Modelling bioaccumulation of organic
!   pollutants in fish with an application to PCBs in Lake Ontario salmonids.
!   Can.J.Fish.Aquat.Sci. 48:318-337.
! - Carlander, K.D. 1977. Handbook of Freshwater Fishery Biology, vol 2. Iowa State University
!   Press. Ames, IA.
! - Lowe, T.P., T.W. May, W.G. Brumbaugh, and D.A. Kane. 1985. National Contaminant
!   Biomonitoring Program: concentrations of seven elements in freshwater fish, 1979-1981.
!   Arch.Environ.Contam.Toxicol. 14:363-388.
! - O'Hara, J. The influence of weight and temperature on the metabolic rate of sunfish. Ecology
!   49:159-161.
! - Osenberg, C.W. M.H. Olson, and G.G. Mittelbach. 1994. Stage structure in fishes: Resource
!   productivity and competition gradients. In: D.J. Stouder, K.L. Fresh, R.J. Feller (eds);
!   M. Duke (ass.ed.). Theory and application in fish feeding ecology. University of South
!   Carolina Press. p 151-170.
! - Pandian, T.J. and F.J. Vernberg. 1987. Animal Energetis - v. 2. Bivalvia through Reptilia.
!   Academic Press.
! - Pierce, R.J. and T.E. Wissing. 1974. Energy cost of food utilization in the bluegill (Lepomis
!   macrochirus). Trans.Am.Fish.Soc. ??:38-44.
! - Price, J.W. 1931. Growth and gill development in the small-mouthed black bass, Micropterus
!   dolomieu, Lacepede. Ohio State University, Franz Theodore Stone Laboratory 4:1-46.
! - Schmitt, C.J., and W.G. Brumbaugh. 1990. National Contaminant Biomonitoring Program:
!   Concentrations of arsenic, cadmium, lead, mercury, selenium, and zinc in U.S. freshwater
!   fish, 1976-1984. Arch.Environ.Contam.Toxicol. 19:731-747.
! - Schmitt, C.J.,  J.L. Zajicek, and P.H. Peterman. 1990. National Contaminant Biomonitoring
!   Program: Residues of organochlorine chemicals in U.S. freshwater fish, 1976-1984.
!   Arch.Environ.Contam.Toxicol. 19:748-781.
! - Wohlschlag, D.E. and R.O. Juliano. Seasonal changes in bluegill metabolism. Limnog.
!   Oceanog. 4:195-209.

/ COMMON_NAME  bluegill
/ SPECIES  Lepomis macrochirus
/ AGE_CLASS_DURATION  year
/ SPAWNING_PERIOD april-june
/ ECOLOGICAL_PARAMETERS &
  lp[cm]=0.15*L[cm]; & ! assumed
  wl[g]=0.0209*L[cm]^3.06; & ! Carlander (1977) adjusted such that 200g = 20cm
  tl_r0[mm]= 80;  & ! Carlander (1977)
  yoy[g]=5.0; & ! assumed
  mls[year]=5; &
  nm[1/day]=0.1*0.75*0.0208*W[g]^(-.615) ! see sg[] and assume exogenous mortality/total mortality = 0.1
/ COMPOSITIONAL_PARAMETERS &
  pa[-]=0.781-0.94*pl[-]; & ! Lowe et al. (1985), Schmitt and Brumbaugh (1990), Schmitt et al. (1990)
  pl[-]=0.0597 ! Lowe et al. (1985), Schmitt and Brumbaugh (1990), Schmitt et al. (1990)
/ MORPHOMETRIC_PARAMETERS &
  ga[cm^2]=7.32*W[g]^0.820; & ! Price (1931)
  id[cm]=1.15e-3*W[g]^0.172; & ! Brockway et al.
  ll[cm]=6.55e-3*W[g]^0.259  ! Brockway et al.
/ FEEDING_OPTIONS linear(1<a[yr]<5)
/ PHYSIOLOGICAL_PARAMETERS &
  ae_fish[-]=0.89; & ! assumed (see Pandian and Verberg 1987)
  ae_invert[-]=0.66; & ! assumed (see Pandian and Verberg 1987)
  ae_plant[-]=0.44; & ! assumed (see Pandian and Verberg 1987)
  rq[-]=1.0; & ! assumed (see Barber et al. 1991)
  rt:std[-]=2.0; & ! BASS default
  sda:in[-]=0.127; &  ! Pierce and Wissing (1974)
  sg[g/g/day](25)=0.0208*W[g]^(-.615);& ! Carlander (1977) assuming wt(yoy)=5 and wt(5)=200
  so[mg(o2)/hr]=0.0243*EXP(0.1409*t[celsius])*W[g]^0.849 ! o'Hara (1968), Wohlschlag and Juliano (1959)

! end bluegill.fsh
```

APPENDIX D. (cont.) Include file REDEAR.FSH for basic redear sunfish (shell cracker) parameters.

```
! file: redear.fsh
! date: sept. 19, 2000
!
! notes: fish file (*.fsh) for BASS version 2.1
!
! refs:
! - Barber, M.C., L.A. Suarez, and R.R. Lassiter. 1991. Modelling bioaccumulation of organic
!   pollutants in fish with an application to PCBs in Lake Ontario salmonids.
!   Can.J.Fish.Aquat.Sci. 48:318-337.
! - Carlander, K.D. 1977. Handbook of Freshwater Fishery Biology, vol 2. Iowa State University
!   Press. Ames, IA.
! - Evans, D.O. 1984. Temperature independence of the annual cycle of standard metabolism in
!   the pumpkinseed. Trans.Amer.Fish.Soc. 113:494-512.
! - Lowe, T.P., T.W. May, W.G. Brumbaugh, and D.A. Kane. 1985. National Contaminant
!   Biomonitoring Program: concentrations of seven elements in freshwater fish, 1979-1981.
!   Arch.Environ.Contam.Toxicol. 14:363-388.
! - O'Hara, J. The influence of weight and temperature on the metabolic rate of sunfish. Ecology
!   49:159-161.
! - Osenberg, C.W. M.H. Olson, and G.G. Mittelbach. 1994. Stage structure in fishes: Resource
!   productivity and competition gradients. In: D.J. Stouder, K.L. Fresh, R.J. Feller (eds);
!   M. Duke (ass.ed.). Theory and application in fish feeding ecology. University of South
!   Carolina Press. p 151-170.
! - Pandian, T.J. and F.J. Vernberg. 1987. Animal Energetis - v. 2. Bivalvia through Reptilia.
!   Academic Press.
! - Pierce, R.J. and T.E. Wissing. 1974. Energy cost of food utilization in the bluegill (Lepomis
!   macrochirus). Trans.Am.Fish.Soc. ??:38-44.
! - Price, J.W. 1931. Growth and gill development in the small-mouthed black bass, Micropterus
!   dolomieu, Lacepede. Ohio State University, Franz Theodore Stone Laboratory 4:1-46.
! - Schmitt, C.J., and W.G. Brumbaugh. 1990. National Contaminant Biomonitoring Program:
!   Concentrations of arsenic, cadmium, lead, mercury, selenium, and zinc in U.S. freshwater
!   fish, 1976-1984. Arch.Environ.Contam.Toxicol. 19:731-747.
! - Schmitt, C.J.,  J.L. Zajicek, and P.H. Peterman. 1990. National Contaminant Biomonitoring
!   Program: Residues of organochlorine chemicals in U.S. freshwater fish, 1976-1984.
!   Arch.Environ.Contam.Toxicol. 19:748-781.
! - Wilbur, R.L. 1969. The redear sunfish in Florida. Florida Game and Fresh Water Fish
!   Commission. Fishery Bull no. 5.

/ COMMON_NAME redear ! shellcraker
/ SPECIES  Lepomis microlophus
/ AGE_CLASS_DURATION  year
/ SPAWNING_PERIOD may-june
/ ECOLOGICAL_PARAMETERS &
  wl[g]=0.0148*L[cm]^3.08; & ! Carlander (1977) adjusted such that 300g = 25cm
  tl_r0[mm]= 140;  & ! Wilbur (1969)
  yoy[g]=5.0; & ! assumed
  mls[year]=5; &
  nm[1/day]=0.3*0.75*0.0528*W[g]^(-.761) ! see sg[] and assume exogenous mortality/total mortality = 0.1
/ COMPOSITIONAL_PARAMETERS &
  pa[-]=0.781-0.941*pl[-]; & ! Lowe et al. (1985), Schmitt and Brumbaugh (1990), Schmitt et al. (1990)
  pl[-]=0.0597 ! Lowe et al. (1985), Schmitt and Brumbaugh (1990), Schmitt et al. (1990)
/ MORPHOMETRIC_PARAMETERS &
  ga[cm^2]=7.32*W[g]^0.820; & ! Price (1931)
  id[cm]=1.15e-3*W[g]^0.172; & ! Brockway et al.
  ll[cm]=6.55e-3*W[g]^0.259  ! Brockway et al.
/ FEEDING_OPTIONS linear(1<a[yr]<5)
/ PHYSIOLOGICAL_PARAMETERS &
  ae_fish[-]=0.89; & ! assumed (see Pandian and Verberg 1987)
  ae_invert[-]=0.66; & ! assumed (see Pandian and Verberg 1987)
  ae_plant[-]=0.44; & ! assumed (see Pandian and Verberg 1987)
  rq[-]=1.0; & ! assumed (see Barber et al. 1991)
  rt:std[-]=2.0; & ! BASS default
  sda:in[-]=0.127; &  ! Pierce and Wissing (1974)
  sg[g/g/day](25)=0.0528*W[g]^(-.761);& ! Carlander (1972) assuming wt(yoy)=5 and wt(5)=300
  so[mg(o2)/hr]=0.0474*EXP(0.0438*t[celsius])*W[g]^0.744 ! Evans (1984), o'Hara (1968)

! end redear.fsh
```

APPENDIX D. (cont.) Include file GAMBUSIA.FSH for basic *Gambusia* parameters.

```
! file: gambusi1.fsh
! date: sept. 19, 2000
!
! notes: fish file (*.fsh) for BASS version 2.1
!
! refs:
! - Barber, M.C., L.A. Suarez, and R.R. Lassiter. 1991. Modelling bioaccumulation of organic
!   pollutants in fish with an application to PCBs in Lake Ontario salmonids.
!   Can.J.Fish.Aquat.Sci. 48:318-337.
! - Haake, P.W. and J.M. Dean. 1983. Age and growth of four Everglades fishes using otolith
!   techniques. Everglades National Park. Tech. Rep. SFRC-83/03. pp 68.
! - Kushlan, J.A., S.A. Voorhees, W.F. Loftus, and P.C. Frohring. 1986. Length, mass, and
!   calorific relationships of Everglades animals. Fla. Sci. 49:65-79.
! - Meffe, G.K. and F.F. Snelson, jr. 1993. Lipid dynamics during reproduction in two
!   livebearing fishes, Gambusia holbrooki and Poecilia latipinna. Can.J.Fish.Aquat.Sci.
!   50:2185-2191.
! - Murphy, P.G. and J.V. Murphy. 1971. Correlations between respiration and direct uptake of
!   DDT in the mosquito fish Gambusia affinis. Bull.Environ.Contam.Toxicol. 6:581-588.
! - Pandian, T.J. and F.J. Vernberg. 1987. Animal Energetis - v. 2. Bivalvia through Reptilia.
!   Academic Press.

/ COMMON_NAME gambusia ! mosquitofish
/ SPECIES Gambusia affinis
/ AGE_CLASS_DURATION month
/ SPAWNING_PERIOD march-october
/ COMPOSITIONAL_PARAMETERS &
  pa[-] = 0.82-1.25*pl[-]; & ! assumed (see Barber et al. 1991)
  pl[-] = 0.125 ! Meffe and Snelson(1993)
/ ECOLOGICAL_PARAMETERS &
  lp[mm]= 0.2*L[mm]; & ! assumed
  log(wl[g])=-4.786+3.032*log(L[mm]); & ! std len Kushlan et al. (1986)
  tl_r0[mm] = 35; & ! Carlander (1969)
  yoy[g]=0.025; & ! assumed
  mls[day] = 240; &
  nm[1/day] = 0.1*0.75*0.0027*W[g]^(-0.693) ! see Haake and Dean below
/ MORPHOMETRIC_PARAMETERS &
  ga[cm^2] = 2.606*W[g]^0.883; & ! Murphy and Murphy (1971)
  ld[lamellae/mm_per_side] = 28.1*W[g]^(-0.0731); & ! interspecific geometric mean
  ll[cm] = 0.0188*W[g]^0.294 ! assumed (Barber et al. 1991)
/ FEEDING_OPTIONS linear(0<a[year]<1)
/ PHYSIOLOGICAL_PARAMETERS &
  ae_fish[-]=0.89; & ! assumed (see Pandian and Verberg 1987)
  ae_invert[-]=0.66; & ! assumed (see Pandian and Verberg 1987)
  ae_plant[-]=0.44; & ! assumed (see Pandian and Verberg 1987)
  rq[-]=1.0; & ! assumed (see Barber et al. 1991)
  rt:std[-]=2.0; & ! BASS default
  sda:in[-]=0.17; & ! assumed (see Barber et al. 1991)
  sg[g/g/day](25)=0.0027*W[g]^(-.693);& ! Haake and Dean (1983) assuming wt(yoy)=0.025 wt(8)=0.4
  so[mg(o2)/hr] = 0.0223*EXP(0.0552*t[celsius])*W[g]^0.695 ! Murphy and Murphy (1971)

! end gambusia.fsh
```

APPENDIX D. (cont.) Include file for nonfish prey and water level.

```
!
! file: nonfish.dat
! date: Tue Apr 11 13:49:08 2000
!
! notes: BASS 2.1 demonstration file showing the use and structure of
!        a BASS exposure file. this file is equivalent to the following
!        BASS commands
!
!        /BIOTA benthos[g/m^2]=5.0 ;&
!               periphyton[g/m^2]=0.0 ; &
!               zooplankton[mg/l]=0.2
!        /WATER_LEVEL depth[meter]=2.0
!
/001 time[day]
/002 benthos[g/m^2]
/003 periphyton[g/m^2]
/004 zooplankton[mg/l]
/005 depth[meter]
/start_data
1       5.0     0.0     0.2   2.0
5000    5.0     0.0     0.2   2.0
```

APPENDIX E. Example output file (filename.msg) that summarizes user input data, input data errors, and run time warnings and errors.

```
!  file       : evergld1.msg
!  input file  : evergld1.prj (Tue Dec 05 15:58:40 2000)
!  program file: C:\BASS\BASS_V21.EXE (Thu Jan 11 11:28:48 2001)
!
 GETINPT: summary of user commands in compressed format
         / simulation_control
         / header methylmercury bioaccumulation in a "ponded" everglades community
         / month_t0 april
         / length_of_simulation 10[year]
         / temperature temp[celsius]=25.0+10.0*sin(0.172142e-01*t[days]+6.02497)
         / water_level depth[meter]=file(nonfish.dat)
         / biota benthos[g/m^2]=file(nonfish.dat); periphyton[g/m^2]=file(nonfish.dat); zooplankton[mg/l]=file(nonfish.dat)
         / annual_outputs 10
         / summary_plots pop(length); cfish(length)
         / chemical methylmercury
         / log_kb1 6.00
         / log_kb2 5.00
         / log_p -0.4
         / molar_volume 51
         / molar_weight 215.6
         / melting_point 25
         / exposure cwater[ng/l]=0.444; cinsct[ppb]=212.17/0.2; cphytn[ppb]=(0.2*16.74/0.2)/(1.13*0.15)*cwater[ng/l];
          czplnk[ppb]=(0.6*54.60/0.2)/(1.13*0.15)*cwater[ng/l]; cbnths[ppb]=(0.6*83.91/0.2)/(1.13*0.15)*cwater[ng/l]
         / common_name bass
         / species micropterus salmoides
         / age_class_duration year
         / spawning_period may-june
         / ecological_parameters lp[cm]=0.6+0.27*l[cm]; wl[g]=0.0117*l[cm]^3.08; tl_r0[mm]= 150; yoy[g]=25.0; mls[year]=8;
          nm[1/day]=0.9*1.0*0.0814*w[g]^(-.675)
         / compositional_parameters pa[-]=0.80-1.57*pl[-]; pl[-]=0.000121*w[g]^0.845
         / morphometric_parameters ga[cm^2]=7.32*w[g]^0.820; ld[lamellae/mm_per_side]=31.28*w[g]^(-.072);
          ll[cm]=0.0188*w[g]^0.294
         / feeding_options linear(1<a[yr]<10)
         / physiological_parameters ae_fish[-]=0.89; ae_invert[-]=0.66; ae_plant[-]=0.44; rq[-]=1.0; rt:std[-]=2.0;
          sda:in[-]=0.127; sg[g/g/day](25)=0.0814*w[g]^(-.675); so[mg(o2)/hr]=0.1187*exp(0.0428*t[celsius])*w[g]^0.766
         / ecological_parameters diet(0<l[mm]<20)={zooplankton=100}; diet(20<l[mm]<100)={zooplankton=35, benthos=35,
          bluegill=0, redear=0, gambusia=0}; diet(100<l[mm]<200)={benthos=50, bass=0, bluegill=0, redear=0, gambusia=0};
          diet(200<l[mm]<600)={benthos=25, bass=0, bullhead=0, bluegill=0, redear=0}
         / initial_conditions age[day]={ 320., 685., 1050., 1415., 1780., 2145., 2510., 2875.}; wt[g]={ 127., 294., 501.,
          740., 1008., 1302., 1618., 1957.}; pop[fish/ha]={ 12.56, 6.70, 4.49, 3.35, 2.66, 2.19, 1.86, 1.62}
         / common_name gar
         / species lepisosteus platyrhincus
         / age_class_duration year
         / spawning_period april-may
         / ecological_parameters lp[cm]=0.15*l[cm]; wl[g]=0.00171*l[cm]^3.30; tl_r0[mm]= 330; yoy[g]=25.0; mls[year]=5;
          nm[1/day]=1.0*0.882*w[g]^(-1.048)
         / compositional_parameters pa[-] = 0.82-1.25*pl[-]; pl[-]=0.06
         / morphometric_parameters ga[cm^2]=3.94*w[g]^0.738; ld[lamellae/mm_per_side]=38.8*w[g]^(-.0603);
          ll[cm]=0.0188*w[g]^0.294
         / feeding_options linear(1<a[yr]<10)
         / physiological_parameters ae_fish[-]=0.89; ae_invert[-]=0.66; ae_plant[-]=0.44; rq[-]=0.9; rt:std[-]=2.0;
          sda:in[-]=0.17; sg[g/g/day](25)=.882*w[g]^(-1.048); so[ml(o2)/kg/minute]=.43*exp(ln(.70/.43)/10*(t[celsius]-22))
         / ecological_parameters diet(0<l[mm]<20)={zooplankton=100}; diet(20<l[mm]<100)={zooplankton=25,benthos=25, bass=0,
          bluegill=0, redear=0, gambusia=0}; diet(100<l[mm]<1000)={benthos=25, bass=0, bluegill=0, redear=0, gambusia=0}
         / initial_conditions age[day]={ 350., 715., 1080., 1445., 1810.}; wt[g]={ 269., 511., 747., 980., 1210.};
          pop[fish/ha]={ 5.90, 3.65, 2.74, 2.24, 1.91}
         / common_name bullhead
         / species ameiurus natalis
         / age_class_duration year
         / spawning_period march-april
         / ecological_parameters lp[cm]=0.25*l[cm]; wl[g]=0.0304*l[cm]^2.82; tl_r0[mm] = 150; yoy[g]=10.0; mls[year]=5;
          nm[1/day]=0.90*0.0382*w[g]^(-.537)
         / compositional_parameters pa[-]=0.80-0.94*pl[-]; pl[-]=0.08
         / morphometric_parameters ga[cm^2]=4.98*w[g]^0.728; id[cm]=9.26e-4*w[g]^0.200;
          ld[lamellae/mm_per_side]=15.9*w[g]^(-0.00917); ll[cm]=8.96e-3*w[g]^0.270
         / feeding_options linear(1<a[yr]<5)
         / physiological_parameters ae_fish[-]=0.89; ae_invert[-]=0.66; ae_plant[-]=0.44; rq[-]=1.0; rt:std[-]=2.0;
          sda:in[-]=0.17; sg[g/g/day](25)=0.0382*w[g]^(-.537); so[mg(o2)/hr]=0.0012*exp(0.1838*t[celsius])*w[g]^1.02
         / ecological_parameters diet(0<l[mm]<50)={benthos=100}; diet(50<l[mm]<500)={benthos=0, bullhead=0, redear=0}
         / initial_conditions age[day]={ 350., 715., 1080., 1445., 1810.}; wt[g]={ 81., 219., 418., 674., 986.};
          pop[fish/ha]={ 33.53, 15.90, 9.80, 6.85, 5.15}
         / common_name bluegill
```

```
/ species lepomis macrochirus
/ age_class_duration year
/ spawning_period april-june
/ ecological_parameters lp[cm]=0.15*l[cm]; wl[g]=0.0209*l[cm]^3.06; tl_r0[mm]= 80; yoy[g]=5.0; mls[year]=5;
 nm[1/day]=0.1*0.75*0.0208*w[g]^(-.615)
/ compositional_parameters pa[-]=0.781-0.94*pl[-]; pl[-]=0.0597
/ morphometric_parameters ga[cm^2]=7.32*w[g]^0.820; id[cm]=1.15e-3*w[g]^0.172; ll[cm]=6.55e-3*w[g]^0.259
/ feeding_options linear(1<a[yr]<5)
/ physiological_parameters ae_fish[-]=0.89; ae_invert[-]=0.66; ae_plant[-]=0.44; rq[-]=1.0; rt:std[-]=2.0;
 sda:in[-]=0.127; sg[g/g/day](25)=0.0208*w[g]^(-.615);so[mg(o2)/hr]=0.0243*exp(0.1409*t[celsius])*w[g]^0.849
/ ecological_parameters diet(00<l[mm]<50)={zooplankton=100}; diet(50<l[mm]<150)={zooplankton=0, gambusia=0,
 benthos=20}
/ initial_conditions age[day]={ 350., 715., 1080., 1445., 1810.}; wt[g]={ 25., 55., 95., 143., 198.}; pop[fish/ha]={
 1187.79, 643.79, 429.04, 316.59, 248.26}
/ common_name redear
/ species lepomis microlophus
/ age_class_duration year
/ spawning_period may-june
/ ecological_parameters wl[g]=0.0148*l[cm]^3.08; tl_r0[mm]= 140; yoy[g]=5.0; mls[year]=5;
 nm[1/day]=0.3*0.75*0.0528*w[g]^(-.761)
/ compositional_parameters pa[-]=0.781-0.941*pl[-]; pl[-]=0.0597
/ morphometric_parameters ga[cm^2]=7.32*w[g]^0.820; id[cm]=1.15e-3*w[g]^0.172; ll[cm]=6.55e-3*w[g]^0.259
/ feeding_options linear(1<a[yr]<5)
/ physiological_parameters ae_fish[-]=0.89; ae_invert[-]=0.66; ae_plant[-]=0.44; rq[-]=1.0; rt:std[-]=2.0;
 sda:in[-]=0.127; sg[g/g/day](25)=0.0528*w[g]^(-.761);so[mg(o2)/hr]=0.0474*exp(0.0438*t[celsius])*w[g]^0.744
/ ecological_parameters diet(00<l[mm]<50)={zooplankton=100}; diet(50<l[mm]<60)={zooplankton=90, benthos=10};
 diet(60<l[mm]<70)={zooplankton=60, benthos=40}; diet(70<l[mm]<80)={zooplankton=30, benthos=70};
 diet(80<l[mm]<150)={zooplankton=20, benthos=80}
/ initial_conditions age[day]={ 320., 685., 1050., 1415., 1780.}; wt[g]={ 39., 91., 151., 218., 291.};
 pop[fish/ha]={ 375.86, 199.22, 135.84, 103.17, 83.23}
/ common_name gambusia
/ species gambusia affinis
/ age_class_duration month
/ spawning_period march-october
/ compositional_parameters pa[-] = 0.82-1.25*pl[-]; pl[-] = 0.125
/ ecological_parameters lp[mm]= 0.2*l[mm]; log(wl[g])=-4.786+3.032*log(l[mm]); tl_r0[mm] = 35; yoy[g]=0.025;
 mls[day] = 240; nm[1/day] = 0.1*0.75*0.0027*w[g]^(-0.693)
/ morphometric_parameters ga[cm^2] = 2.606*w[g]^0.883; ld[lamellae/mm_per_side] = 28.1*w[g]^(-0.0731); ll[cm] =
 0.0188*w[g]^0.294
/ feeding_options linear(0<a[year]<1)
/ physiological_parameters ae_fish[-]=0.89; ae_invert[-]=0.66; ae_plant[-]=0.44; rq[-]=1.0; rt:std[-]=2.0;
 sda:in[-]=0.17; sg[g/g/day](25)=0.0027*w[g]^(-.693);so[mg(o2)/hr] = 0.0223*exp(0.0552*t[celsius])*w[g]^0.695
/ ecological_parameters diet(0<l[mm]<10)={zooplankton=100}; diet(10<l[mm]<40)={zooplankton=0, gambusia=0}
/ initial_conditions age[day]={ 20., 170., 200., 230.}; wt[g]={0.043, 0.260, 0.315, 0.374}; pop[fish/ha]={39159.31,
 10158.52, 8794.47, 7743.90}
/ end
```

```
decoding and initializing exposure files as required
```

```
ckecking user supplied control commands
CHKCTRL WARNING: insect standing stock not specified
CHKCTRL WARNING: phytoplankton standing stock not specified
CHKCTRL: no errors detected
```

```
methylmercury bioaccumulation in a "ponded" everglades community

start time[day]................. april 1
end time[day]................... 3652.
integration steps per day.......   8

ambient water temperature....... temp[celsius] = 25.0+10.0*sin(6.02+1.721E-02*t[day])
water level..................... depth[meter] = C:\BASS\projects\example1\nonfish.dat,column5
benthos standing stock.......... bnths[g(DW)/m^2] = C:\BASS\projects\example1\nonfish.dat,column2
insect standing stock........... insct[g(DW)/m^2] = not_specified
periphyton standing stock....... phytn[g(DW)/m^2] = C:\BASS\projects\example1\nonfish.dat,column3
phytoplankton standing stock.... pplnk[g(DW)/l] = not_specified
zooplankton standing stock...... zplnk[g(DW)/l] = C:\BASS\projects\example1\nonfish.dat,column4
```

```
ckecking user supplied chemical commands
CHKCHEM WARNING: methylmercury - dietary exposure via phytoplankton not specified
CHKCHEM: no errors detected
```

methylmercury bioaccumulation in a "ponded" everglades community

chemical........ methylmercury

log_ac.......... -0.451
log_kb1.........   6.00
log_kb2.........   5.00
log_p........... -0.400
melting_point...   25.0
molar_volume....   51.0
molar_weight....   216.

biotransformation rate in bass....... bt[1/d]=0.00
biotransformation rate in gar........ bt[1/d]=0.00
biotransformation rate in bullhead... bt[1/d]=0.00
biotransformation rate in bluegill... bt[1/d]=0.00
biotransformation rate in redear..... bt[1/d]=0.00
biotransformation rate in gambusia... bt[1/d]=0.00

LC50 for bass....... LC50[molar]=0.135E-02*Kow^-0.871
LC50 for gar........ LC50[molar]=0.135E-02*Kow^-0.871
LC50 for bullhead... LC50[molar]=0.135E-02*Kow^-0.871
LC50 for bluegill... LC50[molar]=0.135E-02*Kow^-0.871
LC50 for redear..... LC50[molar]=0.135E-02*Kow^-0.871
LC50 for gambusia... LC50[molar]=0.135E-02*Kow^-0.871

benthos dietary exposure.......... cbnths[ppm] = 1.485E+06*cwater[ppm]
insect dietary exposure........... cinsct[ppm] = 1.06
periphytic dietary exposure....... cphytn[ppm] = 9.876E+04*cwater[ppm]
phytoplankton dietary exposure.... cpplnk[ppm] = not_specified
zooplankton dietary exposure...... czplnk[ppm] = 9.664E+05*cwater[ppm]
sedimentary exposure.............. csdmnt[ppm] = not_specified
aqueous exposure.................. cwater[ppm] = 4.440E-07

```
ckecking user supplied fish commands
CHKFISH WARNING: bass - default reproductive biomass investment assigned
CHKFISH WARNING: gar - default reproductive biomass investment assigned
CHKFISH WARNING: bullhead - default reproductive biomass investment assigned
CHKFISH WARNING: bluegill - default reproductive biomass investment assigned
CHKFISH WARNING: redear - default reproductive biomass investment assigned
CHKFISH WARNING: gambusia - default reproductive biomass investment assigned
CHKFISH: no errors detected
```

methylmercury bioaccumulation in a "ponded" everglades community

common name... bass

ecological, morphological, and physiological parameters:

```
  assimilation efficiency (fish)...... ae[-] = 0.890
  assimilation efficiency (inverts)... ae[-] = 0.660
  assimilation efficiency (plant)..... ae[-] = 0.440
  gill area........................... ga[cm^2] = 7.320*W[g]^0.820
  gastric evacuation.................. ge[g(DW)/day] = not_specified
  interlamellar distance.............. id[cm] = 0.002*W[g]^0.086
  lamellar density.................... ld[lamellae/mm] = 31.280*W[g]^-0.072
  lamellar length..................... ll[cm] = 0.019*W[g]^0.294
  length of prey...................... lp[cm] = 0.600+0.270*L[cm]
  maximum filtering................... mf[L/day] = not_specified
  maximum ingestion................... mi[g(DW)/day] = not_specified
  maximum longevity................... mls[day] = 2922.
  non-predatory mortality............. nm[1/yr] = 26.8*W[g]^-0.675
  fraction aqueous.................... pa[-] = 0.800-1.570*pl[-]
  fraction lipid...................... pl[-] = 0.000*W[g]^0.845
  reproductive biomass investment..... rbi[-] = 0.150
  respiratory quotient................ rq[-] = 1.000
  routine:standard VO_2............... rt:std[-] = 2.000
  SDA:ingestion ratio................. sda:in[-] = 0.127
  specific growth rate................ sg[1/day] = 0.014*W[g]^-0.675*exp(0.069*t[celsius])
  satiation meal size................. sm[g(DW)] = not_specified
  standard VO_2....................... so[mg o2/hr] = 0.119*W[g]^0.766*exp(0.043*t[celsius])
  time to satiation................... st[minutes] = not_specified
  weight:length....................... wl[g(FW)] = 0.012*L[cm]^3.080
  length at first reproduction........ tl_r0[cm] = 15.0
  weight of recruits.................. yoy[g(FW)] = 25.0
  spawning interval................... may-june => day(s) = 62,
```

selected feeding models as a function of age or size:

```
  A[year]< 10.0  linear
```

dietary composition as a function of age or size (entries between 1 and 100 represent relative frequencies whereas entries between -1 and 1 represent electivities. a -1 entry signifies that the item is not utilized):

age/size	bass	gar	bullhead	bluegill	redear	gambusia	benthos	insects	periphyton	phytoplankton	zooplankton
L[cm]< 2.0	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	100.00
L[cm]< 10.0	-1.00	-1.00	-1.00	0.00	0.00	0.00	35.00	-1.00	-1.00	-1.00	35.00
L[cm]< 20.0	0.00	-1.00	-1.00	0.00	0.00	0.00	50.00	-1.00	-1.00	-1.00	-1.00
L[cm]< 60.0	0.00	-1.00	0.00	0.00	0.00	-1.00	25.00	-1.00	-1.00	-1.00	-1.00

initial conditions:

age class	age [days]	body weight [g(FW)]	population density [#/ha]	methylmercury [ug/g(FW)]
1	320.	127.0	12.6	0.000
2	685.	294.0	6.7	0.000
3	1050.	501.0	4.5	0.000
4	1415.	740.0	3.3	0.000
5	1780.	1008.0	2.7	0.000
6	2145.	1302.0	2.2	0.000
7	2510.	1618.0	1.9	0.000
8	2875.	1957.0	1.6	0.000

```
  initial standing stock ...  20.01 [kg(FW)/ha]
```

ecotoxicological parameters:

```
  mean lethal activiy...... la[-] =  1.066E-03
```

methylmercury bioaccumulation in a "ponded" everglades community

common name... gar

ecological, morphological, and physiological parameters:

```
  assimilation efficiency (fish)...... ae[-] = 0.890
  assimilation efficiency (inverts)... ae[-] = 0.660
  assimilation efficiency (plant)..... ae[-] = 0.440
  gill area........................... ga[cm^2] = 3.940*W[g]^0.738
  gastric evacuation.................. ge[g(DW)/day] = not_specified
  interlamellar distance.............. id[cm] = 0.002*W[g]^0.072
  lamellar density.................... ld[lamellae/mm] = 38.800*W[g]^-0.060
  lamellar length..................... ll[cm] = 0.019*W[g]^0.294
  length of prey...................... lp[cm] = 0.000+0.150*L[cm]
  maximum filtering................... mf[L/day] = not_specified
  maximum ingestion................... mi[g(DW)/day] = not_specified
  maximum longevity................... mls[day] = 1826.
  non-predatory mortality............. nm[1/yr] = 322.*W[g]^-1.048
  fraction aqueous.................... pa[-] = 0.820-1.250*pl[-]
  fraction lipid...................... pl[-] = 0.060*W[g]^0.000
  reproductive biomass investment..... rbi[-] = 0.150
  respiratory quotient................ rq[-] = 0.900
  routine:standard VO_2............... rt:std[-] = 2.000
  SDA:ingestion ratio................. sda:in[-] = 0.170
  specific growth rate................ sg[1/day] = 0.156*W[g]^-1.048*exp(0.069*t[celsius])
  satiation meal size................. sm[g(DW)] = not_specified
  standard VO_2....................... so[mg o2/hr] = 0.013*W[g]^1.000*exp(0.049*t[celsius])
  time to satiation................... st[minutes] = not_specified
  weight:length....................... wl[g(FW)] = 0.002*L[cm]^3.300
  length at first reproduction........ tl_r0[cm] = 33.0
  weight of recruits.................. yoy[g(FW)] = 25.0
  spawning interval................... april-may => day(s) = 31,
```

selected feeding models as a function of age or size:

```
  A[year]< 10.0  linear
```

dietary composition as a function of age or size (entries between 1 and 100 represent relative frequencies whereas entries between -1 and 1 represent electivities. a -1 entry signifies that the item is not utilized):

age/size	bass	gar	bullhead	bluegill	redear	gambusia	benthos	insects	periphyton	phytoplankton	zooplankton
L[cm]< 2.0	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	100.00
L[cm]< 10.0	0.00	-1.00	-1.00	0.00	0.00	0.00	25.00	-1.00	-1.00	-1.00	25.00
L[cm]< 100.0	0.00	-1.00	-1.00	0.00	0.00	0.00	25.00	-1.00	-1.00	-1.00	-1.00

initial conditions:

age class	age [days]	body weight [g(FW)]	population density [#/ha]	methylmercury [ug/g(FW)]
1	350.	269.0	5.9	0.000
2	715.	511.0	3.7	0.000
3	1080.	747.0	2.7	0.000
4	1445.	980.0	2.2	0.000
5	1810.	1210.0	1.9	0.000

initial standing stock ... 10.01 [kg(FW)/ha]

ecotoxicological parameters:

```
  mean lethal activiy...... la[-] =  1.066E-03
```

methylmercury bioaccumulation in a "ponded" everglades community

common name... bullhead

ecological, morphological, and physiological parameters:

```
  assimilation efficiency (fish)...... ae[-] = 0.890
  assimilation efficiency (inverts)... ae[-] = 0.660
  assimilation efficiency (plant)..... ae[-] = 0.440
  gill area........................... ga[cm^2] = 4.980*W[g]^0.728
  gastric evacuation.................. ge[g(DW)/day] = not_specified
  interlamellar distance.............. id[cm] = 0.001*W[g]^0.200
  lamellar density.................... ld[lamellae/mm] = 15.900*W[g]^-0.009
  lamellar length..................... ll[cm] = 0.009*W[g]^0.270
  length of prey...................... lp[cm] = 0.000+0.250*L[cm]
  maximum filtering................... mf[L/day] = not_specified
  maximum ingestion................... mi[g(DW)/day] = not_specified
  maximum longevity................... mls[day] = 1826.
  non-predatory mortality............. nm[1/yr] = 12.6*W[g]^-0.537
  fraction aqueous.................... pa[-] = 0.800-0.940*pl[-]
  fraction lipid...................... pl[-] = 0.080*W[g]^0.000
  reproductive biomass investment..... rbi[-] = 0.150
  respiratory quotient................ rq[-] = 1.000
  routine:standard VO_2............... rt:std[-] = 2.000
  SDA:ingestion ratio................. sda:in[-] = 0.170
  specific growth rate................ sg[1/day] = 0.007*W[g]^-0.537*exp(0.069*t[celsius])
  satiation meal size................. sm[g(DW)] = not_specified
  standard VO_2....................... so[mg o2/hr] = 0.001*W[g]^1.020*exp(0.184*t[celsius])
  time to satiation................... st[minutes] = not_specified
  weight:length....................... wl[g(FW)] = 0.030*L[cm]^2.820
  length at first reproduction........ tl_r0[cm] = 15.0
  weight of recruits.................. yoy[g(FW)] = 10.0
  spawning interval................... march-april => day(s) = 1,
```

selected feeding models as a function of age or size:

```
  A[year]< 5.0   linear
```

dietary composition as a function of age or size (entries between 1 and 100 represent relative frequencies
whereas entries between -1 and 1 represent electivities. a -1 entry signifies that the item is not utilized):

age/size	bass	gar	bullhead	bluegill	redear	gambusia	benthos	insects	periphyton	phytoplankton	zooplankton
L[cm]< 5.0	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	100.00	-1.00	-1.00	-1.00	-1.00
L[cm]< 50.0	-1.00	-1.00	0.00	-1.00	0.00	-1.00	0.00	-1.00	-1.00	-1.00	-1.00

initial conditions:

age class	age [days]	body weight [g(FW)]	population density [#/ha]	methylmercury [ug/g(FW)]
1	350.	81.0	33.5	0.000
2	715.	219.0	15.9	*******
3	1080.	418.0	9.8	0.000
4	1445.	674.0	6.8	0.000
5	1810.	986.0	5.2	0.000

initial standing stock ... 19.99 [kg(FW)/ha]

ecotoxicological parameters:

```
  mean lethal activiy...... la[-] =  1.066E-03
```

methylmercury bioaccumulation in a "ponded" everglades community

common name... bluegill

ecological, morphological, and physiological parameters:

```
  assimilation efficiency (fish)...... ae[-] = 0.890
  assimilation efficiency (inverts)... ae[-] = 0.660
  assimilation efficiency (plant)..... ae[-] = 0.440
  gill area........................... ga[cm^2] = 7.320*W[g]^0.820
  gastric evacuation.................. ge[g(DW)/day] = not_specified
  interlamellar distance.............. id[cm] = 0.001*W[g]^0.172
  lamellar density.................... ld[lamellae/mm] = not_specified
  lamellar length..................... ll[cm] = 0.007*W[g]^0.259
  length of prey...................... lp[cm] = 0.000+0.150*L[cm]
  maximum filtering................... mf[L/day] = not_specified
  maximum ingestion................... mi[g(DW)/day] = not_specified
  maximum longevity................... mls[day] = 1826.
  non-predatory mortality............. nm[1/yr] = 0.570*W[g]^-0.615
  fraction aqueous.................... pa[-] = 0.781-0.940*pl[-]
  fraction lipid...................... pl[-] = 0.060*W[g]^0.000
  reproductive biomass investment..... rbi[-] = 0.150
  respiratory quotient................ rq[-] = 1.000
  routine:standard VO_2............... rt:std[-] = 2.000
  SDA:ingestion ratio................. sda:in[-] = 0.127
  specific growth rate................ sg[1/day] = 0.004*W[g]^-0.615*exp(0.069*t[celsius])
  satiation meal size................. sm[g(DW)] = not_specified
  standard VO_2....................... so[mg o2/hr] = 0.024*W[g]^0.849*exp(0.141*t[celsius])
  time to satiation................... st[minutes] = not_specified
  weight:length....................... wl[g(FW)] = 0.021*L[cm]^3.060
  length at first reproduction........ tl_r0[cm] = 8.000
  weight of recruits.................. yoy[g(FW)] = 5.000
  spawning interval................... april-june => day(s) = 47,
```

selected feeding models as a function of age or size:

```
  A[year]< 5.0   linear
```

dietary composition as a function of age or size (entries between 1 and 100 represent relative frequencies whereas entries between -1 and 1 represent electivities. a -1 entry signifies that the item is not utilized):

age/size	bass	gar	bullhead	bluegill	redear	gambusia	benthos	insects	periphyton	phytoplankton	zooplankton
L[cm]< 5.0	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	100.00
L[cm]< 15.0	-1.00	-1.00	-1.00	-1.00	-1.00	0.00	20.00	-1.00	-1.00	-1.00	0.00

initial conditions:

age class	age [days]	body weight [g(FW)]	population density [#/ha]	methylmercury [ug/g(FW)]
1	350.	25.0	1187.8	0.000
2	715.	55.0	643.8	0.000
3	1080.	95.0	429.0	0.000
4	1445.	143.0	316.6	0.000
5	1810.	198.0	248.3	0.000

```
  initial standing stock ... 200.29 [kg(FW)/ha]
```

ecotoxicological parameters:

```
  mean lethal activiy...... la[-] =  1.066E-03
```

methylmercury bioaccumulation in a "ponded" everglades community

common name... redear

ecological, morphological, and physiological parameters:

```
  assimilation efficiency (fish)...... ae[-] = 0.890
  assimilation efficiency (inverts)... ae[-] = 0.660
  assimilation efficiency (plant)..... ae[-] = 0.440
  gill area........................... ga[cm^2] = 7.320*W[g]^0.820
  gastric evacuation.................. ge[g(DW)/day] = not_specified
  interlamellar distance.............. id[cm] = 0.001*W[g]^0.172
  lamellar density.................... ld[lamellae/mm] = not_specified
  lamellar length..................... ll[cm] = 0.007*W[g]^0.259
  length of prey...................... lp[cm] = not_specified
  maximum filtering................... mf[L/day] = not_specified
  maximum ingestion................... mi[g(DW)/day] = not_specified
  maximum longevity................... mls[day] = 1826.
  non-predatory mortality............. nm[1/yr] = 4.34*W[g]^-0.761
  fraction aqueous.................... pa[-] = 0.781-0.941*pl[-]
  fraction lipid...................... pl[-] = 0.060*W[g]^0.000
  reproductive biomass investment..... rbi[-] = 0.150
  respiratory quotient................ rq[-] = 1.000
  routine:standard VO_2............... rt:std[-] = 2.000
  SDA:ingestion ratio................. sda:in[-] = 0.127
  specific growth rate................ sg[1/day] = 0.009*W[g]^-0.761*exp(0.069*t[celsius])
  satiation meal size................. sm[g(DW)] = not_specified
  standard VO_2....................... so[mg o2/hr] = 0.047*W[g]^0.744*exp(0.044*t[celsius])
  time to satiation................... st[minutes] = not_specified
  weight:length....................... wl[g(FW)] = 0.015*L[cm]^3.080
  length at first reproduction........ tl_r0[cm] = 14.0
  weight of recruits.................. yoy[g(FW)] = 5.000
  spawning interval................... may-june => day(s) = 62,
```

selected feeding models as a function of age or size:

```
  A[year]< 5.0   linear
```

dietary composition as a function of age or size (entries between 1 and 100 represent relative frequencies whereas entries between -1 and 1 represent electivities. a -1 entry signifies that the item is not utilized):

age/size	bass	gar	bullhead	bluegill	redear	gambusia	benthos	insects	periphyton	phytoplankton	zooplankton
L[cm]< 5.0	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	100.00
L[cm]< 6.0	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	10.00	-1.00	-1.00	-1.00	90.00
L[cm]< 7.0	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	40.00	-1.00	-1.00	-1.00	60.00
L[cm]< 8.0	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	70.00	-1.00	-1.00	-1.00	30.00
L[cm]< 15.0	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	80.00	-1.00	-1.00	-1.00	20.00

initial conditions:

age class	age [days]	body weight [g(FW)]	population density [#/ha]	methylmercury [ug/g(FW)]
1	320.	39.0	375.9	0.000
2	685.	91.0	199.2	0.000
3	1050.	151.0	135.8	0.000
4	1415.	218.0	103.2	0.000
5	1780.	291.0	83.2	0.000

```
  initial standing stock ... 100.01 [kg(FW)/ha]
```

ecotoxicological parameters:

```
  mean lethal activiy...... la[-] =  1.066E-03
```

methylmercury bioaccumulation in a "ponded" everglades community

common name... gambusia

ecological, morphological, and physiological parameters:

```
  assimilation efficiency (fish)...... ae[-] = 0.890
  assimilation efficiency (inverts)... ae[-] = 0.660
  assimilation efficiency (plant)..... ae[-] = 0.440
  gill area........................... ga[cm^2] = 2.606*W[g]^0.883
  gastric evacuation.................. ge[g(DW)/day] = not_specified
  interlamellar distance.............. id[cm] = 0.002*W[g]^0.087
  lamellar density.................... ld[lamellae/mm] = 28.100*W[g]^-0.073
  lamellar length..................... ll[cm] = 0.019*W[g]^0.294
  length of prey...................... lp[cm] = 0.000+0.200*L[cm]
  maximum filtering................... mf[L/day] = not_specified
  maximum ingestion................... mi[g(DW)/day] = not_specified
  maximum longevity................... mls[day] = 240.
  non-predatory mortality............. nm[1/yr] = 0.740E-01*W[g]^-0.693
  fraction aqueous.................... pa[-] = 0.820-1.250*pl[-]
  fraction lipid...................... pl[-] = 0.125*W[g]^0.000
  reproductive biomass investment..... rbi[-] = 0.150
  respiratory quotient................ rq[-] = 1.000
  routine:standard VO_2............... rt:std[-] = 2.000
  SDA:ingestion ratio................. sda:in[-] = 0.170
  specific growth rate................ sg[1/day] = 0.000*W[g]^-0.693*exp(0.069*t[celsius])
  satiation meal size................. sm[g(DW)] = not_specified
  standard VO_2....................... so[mg o2/hr] = 0.022*W[g]^0.695*exp(0.055*t[celsius])
  time to satiation................... st[minutes] = not_specified
  weight:length....................... wl[g(FW)] = 0.018*L[cm]^3.032
  length at first reproduction........ tl_r0[cm] = 3.500
  weight of recruits.................. yoy[g(FW)] = 0.025
  spawning interval................... march-october => day(s) = 15, 45, 75, 105, 135, 165, 195, 345,
```

selected feeding models as a function of age or size:

```
  A[year]< 1.0   linear
```

dietary composition as a function of age or size (entries between 1 and 100 represent relative frequencies whereas entries between -1 and 1 represent electivities. a -1 entry signifies that the item is not utilized):

age/size	bass	gar	bullhead	bluegill	redear	gambusia	benthos	insects	periphyton	phytoplankton	zooplankton
L[cm]< 1.0	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	-1.00	100.00
L[cm]< 4.0	-1.00	-1.00	-1.00	-1.00	-1.00	0.00	-1.00	-1.00	-1.00	-1.00	0.00

initial conditions:

age class	age [days]	body weight [g(FW)]	population density [#/ha]	methylmercury [ug/g(FW)]
1	20.	0.0	39159.3	0.000
2	170.	0.3	10158.5	0.000
3	200.	0.3	8794.5	0.000
4	230.	0.4	7743.9	0.000

```
  initial standing stock ...   9.99 [kg(FW)/ha]
```

ecotoxicological parameters:

```
  mean lethal activiy...... la[-] =  1.066E-03
```

```
summary of special conditions during the simulation:


RKINT_RESTART: euler step taken at t=  4.50
RKINT_RESTART: euler step taken at t=  4.62
RKINT_RESTART: euler step taken at t=  4.63
RKINT_RESTART: euler step taken at t=  4.63
RKINT_RESTART: euler step taken at t=  4.63
RKINT_RESTART: dn/dt for species  6 cohort  1 approximates a step function for t=  4.63     solution restarted
RKINT_RESTART: euler step taken at t=  7.50
RKINT_RESTART: euler step taken at t=  7.91
RKINT_RESTART: euler step taken at t=  7.98
RKINT_RESTART: euler step taken at t=  7.99
RKINT_RESTART: euler step taken at t=  7.99
RKINT_RESTART: euler step taken at t=  7.99
RKINT_RESTART: dn/dt for species  6 cohort  2 approximates a step function for t=  7.99     solution restarted
RKINT_RESTART: euler step taken at t=  9.50
RKINT_RESTART: euler step taken at t=  10.0
RKINT_RESTART: dn/dt for species  6 cohort  3 approximates a step function for t=  10.0     solution restarted
BASS_ODESOLVR: species 6 cohort 4 dies on day=  12.0     due to exceeding maximum longevity
BASS_ODESOLVR: species 2 cohort 5 dies on day=  18.0     due to exceeding maximum longevity
BASS_ODESOLVR: species 3 cohort 5 dies on day=  18.0     due to exceeding maximum longevity
BASS_ODESOLVR: species 4 cohort 5 dies on day=  18.0     due to exceeding maximum longevity
BASS_ODESOLVR: species 1 cohort 8 dies on day=  48.0     due to exceeding maximum longevity
BASS_ODESOLVR: species 5 cohort 5 dies on day=  48.0     due to exceeding maximum longevity
RKINT_RESTART: euler step taken at t=  350.
RKINT_RESTART: euler step taken at t=  350.
RKINT_RESTART: euler step taken at t=  350.
RKINT_RESTART: euler step taken at t=  350.
RKINT_RESTART: euler step taken at t=  350.
RKINT_RESTART: dn/dt for species  5 cohort  6 approximates a step function for t=  350.     solution restarted
BASS_ODESOLVR: species 2 cohort 4 dies on day=  383.     due to exceeding maximum longevity
BASS_ODESOLVR: species 3 cohort 4 dies on day=  383.     due to exceeding maximum longevity
BASS_ODESOLVR: species 4 cohort 4 dies on day=  383.     due to exceeding maximum longevity
BASS_ODESOLVR: species 1 cohort 7 dies on day=  413.     due to exceeding maximum longevity
BASS_ODESOLVR: species 5 cohort 4 dies on day=  413.     due to exceeding maximum longevity
BASS_ODESOLVR: species 2 cohort 3 dies on day=  748.     due to exceeding maximum longevity
BASS_ODESOLVR: species 3 cohort 3 dies on day=  748.     due to exceeding maximum longevity
BASS_ODESOLVR: species 4 cohort 3 dies on day=  748.     due to exceeding maximum longevity
BASS_ODESOLVR: species 1 cohort 6 dies on day=  778.     due to exceeding maximum longevity
BASS_ODESOLVR: species 5 cohort 3 dies on day=  778.     due to exceeding maximum longevity
BASS_ODESOLVR: species 2 cohort 2 dies on day= 0.111E+04 due to exceeding maximum longevity
BASS_ODESOLVR: species 3 cohort 2 dies on day= 0.111E+04 due to exceeding maximum longevity
BASS_ODESOLVR: species 4 cohort 2 dies on day= 0.111E+04 due to exceeding maximum longevity
BASS_ODESOLVR: species 1 cohort 5 dies on day= 0.114E+04 due to exceeding maximum longevity
BASS_ODESOLVR: species 5 cohort 2 dies on day= 0.114E+04 due to exceeding maximum longevity
BASS_ODESOLVR: species 2 cohort 1 dies on day= 0.148E+04 due to exceeding maximum longevity
BASS_ODESOLVR: species 3 cohort 1 dies on day= 0.148E+04 due to exceeding maximum longevity
BASS_ODESOLVR: species 4 cohort 1 dies on day= 0.148E+04 due to exceeding maximum longevity
BASS_ODESOLVR: species 1 cohort 4 dies on day= 0.151E+04 due to exceeding maximum longevity
BASS_ODESOLVR: species 5 cohort 1 dies on day= 0.151E+04 due to exceeding maximum longevity
RKINT_RESTART: euler step taken at t= 0.156E+04
RKINT_RESTART: euler step taken at t= 0.156E+04
RKINT_RESTART: euler step taken at t= 0.156E+04
RKINT_RESTART: euler step taken at t= 0.156E+04
RKINT_RESTART: euler step taken at t= 0.156E+04
RKINT_RESTART: dn/dt for species  4 cohort  2 approximates a step function for t= 0.156E+04 solution restarted
BASS_ODESOLVR: species 3 cohort 1 dies on day= 0.183E+04 due to exceeding maximum longevity
BASS_ODESOLVR: species 2 cohort 1 dies on day= 0.186E+04 due to exceeding maximum longevity
BASS_ODESOLVR: species 1 cohort 3 dies on day= 0.187E+04 due to exceeding maximum longevity
BASS_ODESOLVR: species 3 cohort 1 dies on day= 0.219E+04 due to exceeding maximum longevity
BASS_ODESOLVR: species 2 cohort 1 dies on day= 0.222E+04 due to exceeding maximum longevity
BASS_ODESOLVR: species 1 cohort 2 dies on day= 0.224E+04 due to exceeding maximum longevity
BASS_ODESOLVR: species 4 cohort 1 dies on day= 0.224E+04 due to exceeding maximum longevity
BASS_ODESOLVR: species 5 cohort 1 dies on day= 0.226E+04 due to exceeding maximum longevity
RKINT_RESTART: euler step taken at t= 0.226E+04
RKINT_RESTART: euler step taken at t= 0.226E+04
RKINT_RESTART: euler step taken at t= 0.226E+04
RKINT_RESTART: euler step taken at t= 0.226E+04
RKINT_RESTART: dn/dt for species  4 cohort  2 approximates a step function for t= 0.226E+04 solution restarted
BASS_ODESOLVR: species 3 cohort 1 dies on day= 0.256E+04 due to exceeding maximum longevity
BASS_ODESOLVR: species 2 cohort 1 dies on day= 0.259E+04 due to exceeding maximum longevity
BASS_ODESOLVR: species 1 cohort 1 dies on day= 0.260E+04 due to exceeding maximum longevity
BASS_ODESOLVR: species 5 cohort 1 dies on day= 0.262E+04 due to exceeding maximum longevity
BASS_ODESOLVR: species 3 cohort 1 dies on day= 0.292E+04 due to exceeding maximum longevity
BASS_ODESOLVR: species 2 cohort 1 dies on day= 0.295E+04 due to exceeding maximum longevity
```

```
BASS_ODESOLVR: species 4 cohort 1 dies on day= 0.297E+04 due to exceeding maximum longevity
BASS_ODESOLVR: species 1 cohort 1 dies on day= 0.299E+04 due to exceeding maximum longevity
BASS_ODESOLVR: species 5 cohort 1 dies on day= 0.299E+04 due to exceeding maximum longevity
BASS_ODESOLVR: species 3 cohort 1 dies on day= 0.329E+04 due to exceeding maximum longevity
BASS_ODESOLVR: species 2 cohort 1 dies on day= 0.332E+04 due to exceeding maximum longevity
BASS_ODESOLVR: species 4 cohort 1 dies on day= 0.334E+04 due to exceeding maximum longevity
BASS_ODESOLVR: species 1 cohort 1 dies on day= 0.335E+04 due to exceeding maximum longevity
BASS_ODESOLVR: species 5 cohort 1 dies on day= 0.335E+04 due to exceeding maximum longevity
```

```
         total cpu =   511.
 bass_odesolvr cpu =   503.
     bass_dydt cpu =   473.
       dwdtflx cpu =   126.
       dbdtflx cpu =   108.
 bass_foodweb1 cpu =   116.
 bass_foodweb0 cpu =   57.4
        ee_adj cpu =   28.9
      dry2live cpu =   46.3
R-K integrator cpu =   490.
   load/unload cpu =   70.4
  bass_restart cpu =   1.80
            mean h =  0.491    (n= 7445)
```

APPENDIX F. Example output file (filename.bss) that tabulates annual bioenergetic and contaminant fluxes.

```
!                                                                                                                    page   1
!  file        : evergld1.bss
!  input file  : evergld1.prj (Tue Dec 05 15:58:40 2000)
!  program file: C:\BASS\BASS_V21.EXE (Thu Jan 11 11:28:48 2001)
!
```

*** SUMMARY FOR YEAR 10 ***

bioenergetics of a representative individual bass:

cohort	residence time [days]	mean body weight [g(FW)]	mean body weight [g(DW)]	mean growth rate [1/day]	weight gain/loss [g(DW)/yr]	ingestion [g(DW)/yr]	assimilation [g(DW)/yr]	metabolism [g(DW)/yr]
1	303.	86.9	18.2	5.541E-03	22.1	145.	111.	88.4
2	365.	208.	45.4	2.696E-03	39.4	314.	259.	220.
3	365.	355.	80.8	1.814E-03	49.6	464.	384.	334.
4	365.	501.	118.	1.418E-03	58.0	597.	495.	437.
5	365.	639.	156.	1.194E-03	65.2	715.	593.	528.
6	365.	768.	194.	1.051E-03	71.5	819.	680.	608.
7	365.	885.	229.	9.519E-04	77.0	910.	756.	679.
8	365.	992.	263.	8.798E-04	81.8	990.	823.	741.
9	64.0	1.088E+03	294.	8.769E-04	16.5	205.	170.	154.

exchange of methylmercury by a representative individual bass:

cohort	residence time [days]	mean body conc. [ug/g(FW)]	mean log(BAF)	mean log(BMF)	gill uptake [ug/yr]	ingested [ug/yr]	metabolically generated [ug/yr]	egested & excreted [ug/yr]	metabolically degraded [ug/yr]
1	303.	0.499	6.05	0.326	13.0	158.	0.00	78.3	0.00
2	365.	0.758	6.23	0.415	33.7	423.	0.00	295.	0.00
3	365.	0.837	6.28	0.429	51.9	634.	0.00	494.	0.00
4	365.	0.883	6.30	0.432	68.2	824.	0.00	676.	0.00
5	365.	0.918	6.32	0.431	82.7	995.	0.00	841.	0.00
6	365.	0.940	6.33	0.429	95.5	1.136E+03	0.00	983.	0.00
7	365.	0.962	6.34	0.426	107.	1.268E+03	0.00	1.113E+03	0.00
8	365.	0.983	6.35	0.424	117.	1.387E+03	0.00	1.231E+03	0.00
9	64.0	1.03	6.37	0.420	24.7	299.	0.00	270.	0.00

mean body conc. weighted by cohort biomasses = 0.817
mean body conc. weighted by cohort densities = 0.671
log mean BAF weighted by cohort biomasses = 6.26
log mean BAF weighted by cohort densities = 6.18

*** SUMMARY FOR YEAR 10 ***

total aqueous phase chemical activity in a representative individual bass:

cohort	as a fraction of lethal narcotic activity
1	9.307E-04
2	1.424E-03
3	1.586E-03
4	1.686E-03
5	1.764E-03
6	1.819E-03
7	1.872E-03
8	1.922E-03
9	2.028E-03

*** SUMMARY FOR YEAR 10 ***

bioenergetics of a representative individual gar:

cohort	residence time [days]	mean body weight [g(FW)]	mean body weight [g(DW)]	mean growth rate [1/day]	weight gain/loss [g(DW)/yr]	ingestion [g(DW)/yr]	assimilation [g(DW)/yr]	metabolism [g(DW)/yr]
1	334.	190.	48.4	7.322E-03	67.2	188.	155.	88.0
2	365.	409.	104.	2.026E-03	69.2	317.	263.	194.
3	365.	599.	153.	1.292E-03	67.9	417.	347.	279.
4	365.	758.	193.	9.932E-04	67.0	501.	417.	350.
5	365.	890.	227.	8.319E-04	66.5	572.	476.	409.
6	33.0	985.	251.	6.485E-04	5.36	54.8	45.4	40.0

exchange of methylmercury by a representative individual gar:

cohort	residence time [days]	mean body conc. [ug/g(FW)]	mean log(BAF)	mean log(BMF)	gill uptake [ug/yr]	ingested [ug/yr]	metabolically generated [ug/yr]	egested & excreted [ug/yr]	metabolically degraded [ug/yr]
1	334.	0.517	6.07	0.174	11.1	254.	0.00	76.9	0.00
2	365.	0.680	6.18	0.288	28.8	433.	0.00	243.	0.00
3	365.	0.742	6.22	0.319	43.3	579.	0.00	395.	0.00
4	365.	0.781	6.25	0.338	55.2	703.	0.00	530.	0.00
5	365.	0.804	6.26	0.349	65.2	806.	0.00	644.	0.00
6	33.0	0.838	6.28	0.346	6.19	81.1	0.00	64.0	0.00

mean body conc. weighted by cohort biomasses = 0.694
mean body conc. weighted by cohort densities = 0.615
log mean BAF weighted by cohort biomasses = 6.19
log mean BAF weighted by cohort densities = 6.14

total aqueous phase chemical activity in a representative individual gar:

cohort	as a fraction of lethal narcotic activity
1	9.945E-04
2	1.309E-03
3	1.429E-03
4	1.503E-03
5	1.548E-03
6	1.614E-03

*** SUMMARY FOR YEAR 10 ***

bioenergetics of a representative individual bullhead:

cohort	residence time [days]	mean body weight [g(FW)]	mean body weight [g(DW)]	mean growth rate [1/day]	weight gain/loss [g(DW)/yr]	ingestion [g(DW)/yr]	assimilation [g(DW)/yr]	metabolism [g(DW)/yr]
1	364.	56.4	15.5	6.277E-03	24.3	210.	139.	114.
2	365.	172.	47.3	2.923E-03	43.8	679.	466.	422.
3	365.	330.	90.8	1.986E-03	60.4	1.331E+03	927.	866.
4	365.	516.	142.	1.538E-03	75.1	2.047E+03	1.479E+03	1.404E+03
5	365.	720.	198.	1.275E-03	88.0	2.865E+03	2.092E+03	2.004E+03
6	3.00	774.	213.	7.992E-04	0.509	9.65	7.06	6.55

exchange of methylmercury by a representative individual bullhead:

cohort	residence time [days]	mean body conc. [ug/g(FW)]	mean log(BAF)	mean log(BMF)	gill uptake [ug/yr]	ingested [ug/yr]	metabolically generated [ug/yr]	egested & excreted [ug/yr]	metabolically degraded [ug/yr]
1	364.	0.429	5.98	0.373	17.3	139.	0.00	109.	0.00
2	365.	0.520	6.07	0.432	66.6	473.	0.00	447.	0.00
3	365.	0.548	6.09	0.421	139.	956.	0.00	951.	0.00
4	365.	0.584	6.12	0.411	226.	1.573E+03	0.00	1.609E+03	0.00
5	365.	0.609	6.14	0.412	324.	2.306E+03	0.00	2.394E+03	0.00
6	3.00	0.635	6.16	0.404	0.871	8.80	0.00	7.23	0.00

mean body conc. weighted by cohort biomasses = 0.539
mean body conc. weighted by cohort densities = 0.467
log mean BAF weighted by cohort biomasses = 6.08
log mean BAF weighted by cohort densities = 6.02

total aqueous phase chemical activity in a representative individual bullhead:

cohort	as a fraction of lethal narcotic activity
1	8.380E-04
2	1.017E-03
3	1.071E-03
4	1.141E-03
5	1.191E-03
6	1.242E-03

*** SUMMARY FOR YEAR 10 ***

bioenergetics of a representative individual bluegill:

cohort	residence time [days]	mean body weight [g(FW)]	mean body weight [g(DW)]	mean growth rate [1/day]	weight gain/loss [g(DW)/yr]	ingestion [g(DW)/yr]	assimilation [g(DW)/yr]	metabolism [g(DW)/yr]
1	318.	16.4	4.50	5.023E-03	5.42	150.	98.9	93.5
2	365.	16.4	4.52	-2.006E-04	-0.285	196.	129.	130.
3	365.	23.1	6.36	2.252E-04	0.694	290.	191.	191.
4	365.	32.2	8.87	1.823E-03	5.54	366.	242.	236.
5	365.	50.8	14.0	1.475E-03	7.14	527.	348.	341.
6	49.0	60.4	16.6	3.520E-04	0.277	75.6	49.9	49.7

exchange of methylmercury by a representative individual bluegill:

cohort	residence time [days]	mean body conc. [ug/g(FW)]	mean log(BAF)	mean log(BMF)	gill uptake [ug/yr]	ingested [ug/yr]	metabolically generated [ug/yr]	egested & excreted [ug/yr]	metabolically degraded [ug/yr]
1	318.	0.452	6.01	0.494	15.7	79.0	0.00	82.3	0.00
2	365.	0.486	6.04	0.517	22.2	106.	0.00	129.	0.00
3	365.	0.512	6.06	0.520	33.0	176.	0.00	208.	0.00
4	365.	0.519	6.07	0.520	40.5	226.	0.00	255.	0.00
5	365.	0.528	6.08	0.524	58.3	327.	0.00	371.	0.00
6	49.0	0.526	6.07	0.526	7.93	44.2	0.00	50.1	0.00

mean body conc. weighted by cohort biomasses = 0.495
mean body conc. weighted by cohort densities = 0.482
log mean BAF weighted by cohort biomasses = 6.05
log mean BAF weighted by cohort densities = 6.04

total aqueous phase chemical activity in a representative individual bluegill:

cohort	as a fraction of lethal narcotic activity
1	8.893E-04
2	9.553E-04
3	1.007E-03
4	1.020E-03
5	1.038E-03
6	1.034E-03

*** SUMMARY FOR YEAR 10 ***

bioenergetics of a representative individual redear:

cohort	residence time [days]	mean body weight [g(FW)]	mean body weight [g(DW)]	mean growth rate [1/day]	weight gain/loss [g(DW)/yr]	ingestion [g(DW)/yr]	assimilation [g(DW)/yr]	metabolism [g(DW)/yr]
1	303.	26.4	7.27	6.921E-03	9.83	37.0	24.4	14.6
2	365.	68.0	18.7	2.645E-03	15.9	79.7	52.6	36.7
3	365.	117.	32.2	1.668E-03	18.3	111.	73.2	54.9
4	365.	165.	45.5	1.261E-03	20.0	137.	90.7	70.8
5	365.	211.	58.1	1.039E-03	21.2	160.	106.	84.6
6	64.0	243.	66.9	9.883E-04	4.24	34.1	22.5	18.2

exchange of methylmercury by a representative individual redear:

cohort	residence time [days]	mean body conc. [ug/g(FW)]	mean log(BAF)	mean log(BMF)	gill uptake [ug/yr]	ingested [ug/yr]	metabolically generated [ug/yr]	egested & excreted [ug/yr]	metabolically degraded [ug/yr]
1	303.	0.320	5.86	0.279	1.95	22.6	0.00	8.37	0.00
2	365.	0.409	5.96	0.385	5.34	48.9	0.00	27.8	0.00
3	365.	0.435	5.99	0.411	8.21	68.0	0.00	44.8	0.00
4	365.	0.450	6.01	0.426	10.7	84.3	0.00	60.0	0.00
5	365.	0.460	6.02	0.435	12.9	98.4	0.00	73.7	0.00
6	64.0	0.473	6.03	0.447	2.85	20.9	0.00	16.6	0.00

mean body conc. weighted by cohort biomasses = 0.416
mean body conc. weighted by cohort densities = 0.370
log mean BAF weighted by cohort biomasses = 5.97
log mean BAF weighted by cohort densities = 5.92

total aqueous phase chemical activity in a representative individual redear:

cohort	as a fraction of lethal narcotic activity
1	6.298E-04
2	8.051E-04
3	8.562E-04
4	8.850E-04
5	9.045E-04
6	9.296E-04

*** SUMMARY FOR YEAR 10 ***

all cohorts of gambusia have been exterminated

*** SUMMARY FOR YEAR 10 ***

community level fluxes for bass:

cohort	prey consumption [g(DW)/ha/yr]	endogenous predatory mortality [g(DW)/ha/yr] / [#/ha/yr]	exogenous mortality [g(DW)/ha/yr] / [#/ha/yr]	productivity [g(DW)/ha/yr]	mean standing stock [g(DW)/ha] / [g(FW)/ha]	mean population [#/ha]
1	6.853E+03	118. / 10.1	848. / 63.3	1.141E+03	600. / 2.879E+03	38.4
2	5.058E+03	17.8 / 0.514	510. / 12.4	656.	683. / 3.141E+03	15.9
3	3.542E+03	1.70 / 2.583E-02	304. / 3.92	387.	592. / 2.605E+03	7.50
4	2.698E+03	0.00 / 0.00	210. / 1.81	266.	519. / 2.195E+03	4.44
5	2.177E+03	0.00 / 0.00	159. / 1.03	201.	464. / 1.898E+03	2.99
6	1.747E+03	0.00 / 0.00	122. / 0.638	154.	404. / 1.604E+03	2.10
7	1.483E+03	0.00 / 0.00	101. / 0.442	127.	366. / 1.415E+03	1.61
8	1.271E+03	0.00 / 0.00	84.2 / 0.323	106.	331. / 1.251E+03	1.26
9	240.	0.00 / 0.00	14.4 / 4.894E-02	19.2	60.2 / 223.	0.205
total	2.507E+04	138. / 10.7	2.353E+03 / 83.9	3.056E+03	4.019E+03 / 1.721E+04	74.3

community level fluxes for gar:

cohort	prey consumption [g(DW)/ha/yr]	endogenous predatory mortality [g(DW)/ha/yr] / [#/ha/yr]	exogenous mortality [g(DW)/ha/yr] / [#/ha/yr]	productivity [g(DW)/ha/yr]	mean standing stock [g(DW)/ha] / [g(FW)/ha]	mean population [#/ha]
1	4.259E+03	0.00 / 0.00	1.303E+03 / 58.3	1.703E+03	778. / 3.050E+03	20.0
2	2.466E+03	0.00 / 0.00	470. / 4.90	556.	767. / 3.007E+03	7.62
3	1.836E+03	0.00 / 0.00	261. / 1.76	304.	651. / 2.553E+03	4.32
4	1.454E+03	0.00 / 0.00	171. / 0.898	197.	547. / 2.145E+03	2.85
5	1.188E+03	0.00 / 0.00	122. / 0.542	140.	463. / 1.814E+03	2.05
6	81.4	0.00 / 0.00	7.93 / 3.160E-02	7.96	33.7 / 132.	0.134
total	1.128E+04	0.00 / 0.00	2.335E+03 / 66.4	2.907E+03	3.239E+03 / 1.270E+04	36.9

community level fluxes for bullhead:

cohort	prey consumption [g(DW)/ha/yr]	endogenous predatory mortality [g(DW)/ha/yr] / [#/ha/yr]	exogenous mortality [g(DW)/ha/yr] / [#/ha/yr]	productivity [g(DW)/ha/yr]	mean standing stock [g(DW)/ha] / [g(FW)/ha]	mean population [#/ha]
1	4.863E+03	90.2 / 11.4	409. / 50.6	541.	249. / 905.	23.1
2	4.261E+03	1.69 / 5.952E-02	207. / 5.00	262.	254. / 924.	5.79
3	4.131E+03	0.00 / 0.00	143. / 1.68	180.	253. / 919.	2.89
4	3.876E+03	0.00 / 0.00	109. / 0.802	137.	248. / 900.	1.78
5	3.631E+03	0.00 / 0.00	86.5 / 0.449	108.	234. / 852.	1.20
6	11.6	0.00 / 0.00	0.741 / 3.489E-03	0.611	2.10 / 7.64	9.866E-03
total	2.077E+04	91.9 / 11.5	955. / 58.6	1.228E+03	1.241E+03 / 4.508E+03	34.8

*** SUMMARY FOR YEAR 10 ***

community level fluxes for bluegill:

cohort	prey consumption [g(DW)/ha/yr]	endogenous predatory mortality [g(DW)/ha/yr] / [#/ha/yr]	exogenous mortality [g(DW)/ha/yr] / [#/ha/yr]	productivity [g(DW)/ha/yr]	mean standing stock [g(DW)/ha] / [g(FW)/ha]	mean population [#/ha]
1	7.052E+05	6.218E+03 / 2.086E+03	1.708E+03 / 458.	2.478E+04	1.655E+04 / 6.015E+04	3.883E+03
2	5.618E+05	4.009E+03 / 977.	1.192E+03 / 281.	-2.684E+03	1.201E+04 / 4.365E+04	2.609E+03
3	4.029E+05	3.111E+03 / 499.	673. / 107.	447.	8.228E+03 / 2.991E+04	1.283E+03
4	3.538E+05	2.343E+03 / 282.	547. / 63.6	5.235E+03	8.066E+03 / 2.932E+04	924.
5	2.734E+05	1.722E+03 / 133.	353. / 25.9	3.564E+03	6.897E+03 / 2.507E+04	500.
6	2.693E+04	221. / 13.3	36.5 / 2.20	101.	797. / 2.895E+03	48.0
total	2.324E+06	1.762E+04 / 3.990E+03	4.508E+03 / 938.	3.144E+04	5.255E+04 / 1.910E+05	9.246E+03

community level fluxes for redear:

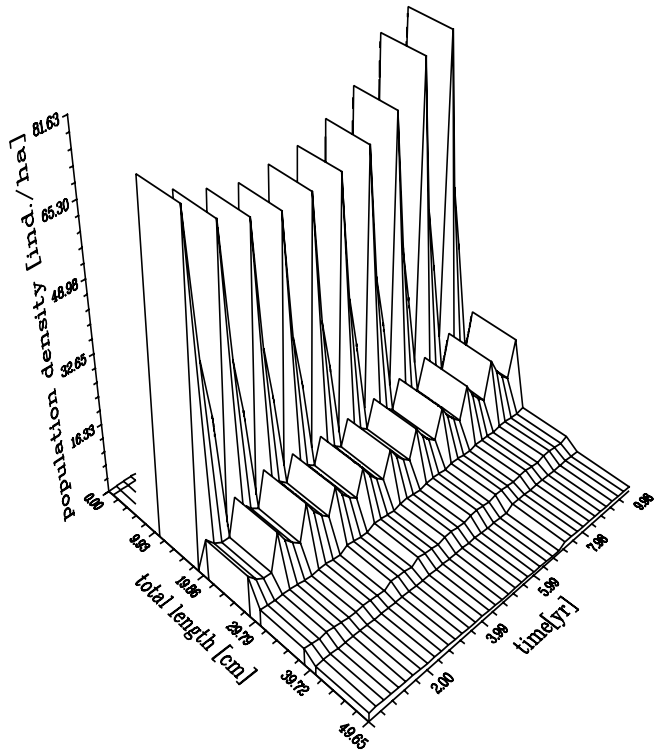
cohort	prey consumption [g(DW)/ha/yr]	endogenous predatory mortality [g(DW)/ha/yr] / [#/ha/yr]	exogenous mortality [g(DW)/ha/yr] / [#/ha/yr]	productivity [g(DW)/ha/yr]	mean standing stock [g(DW)/ha] / [g(FW)/ha]	mean population [#/ha]
1	6.110E+04	6.717E+03 / 1.600E+03	3.268E+03 / 676.	1.734E+04	8.406E+03 / 3.055E+04	1.331E+03
2	3.648E+04	2.231E+03 / 147.	1.461E+03 / 85.0	7.399E+03	8.198E+03 / 2.979E+04	453.
3	2.917E+04	606. / 20.4	968. / 30.8	4.844E+03	8.341E+03 / 3.031E+04	261.
4	2.707E+04	241. / 5.54	791. / 17.6	3.946E+03	8.879E+03 / 3.227E+04	196.
5	1.701E+04	118. / 2.08	452. / 7.84	2.256E+03	6.119E+03 / 2.223E+04	105.
6	349.	15.0 / 0.224	7.97 / 0.119	43.3	120. / 437.	1.80
total	1.712E+05	9.929E+03 / 1.776E+03	6.949E+03 / 817.	3.583E+04	4.006E+04 / 1.456E+05	2.347E+03

all cohorts of gambusia have been exterminated

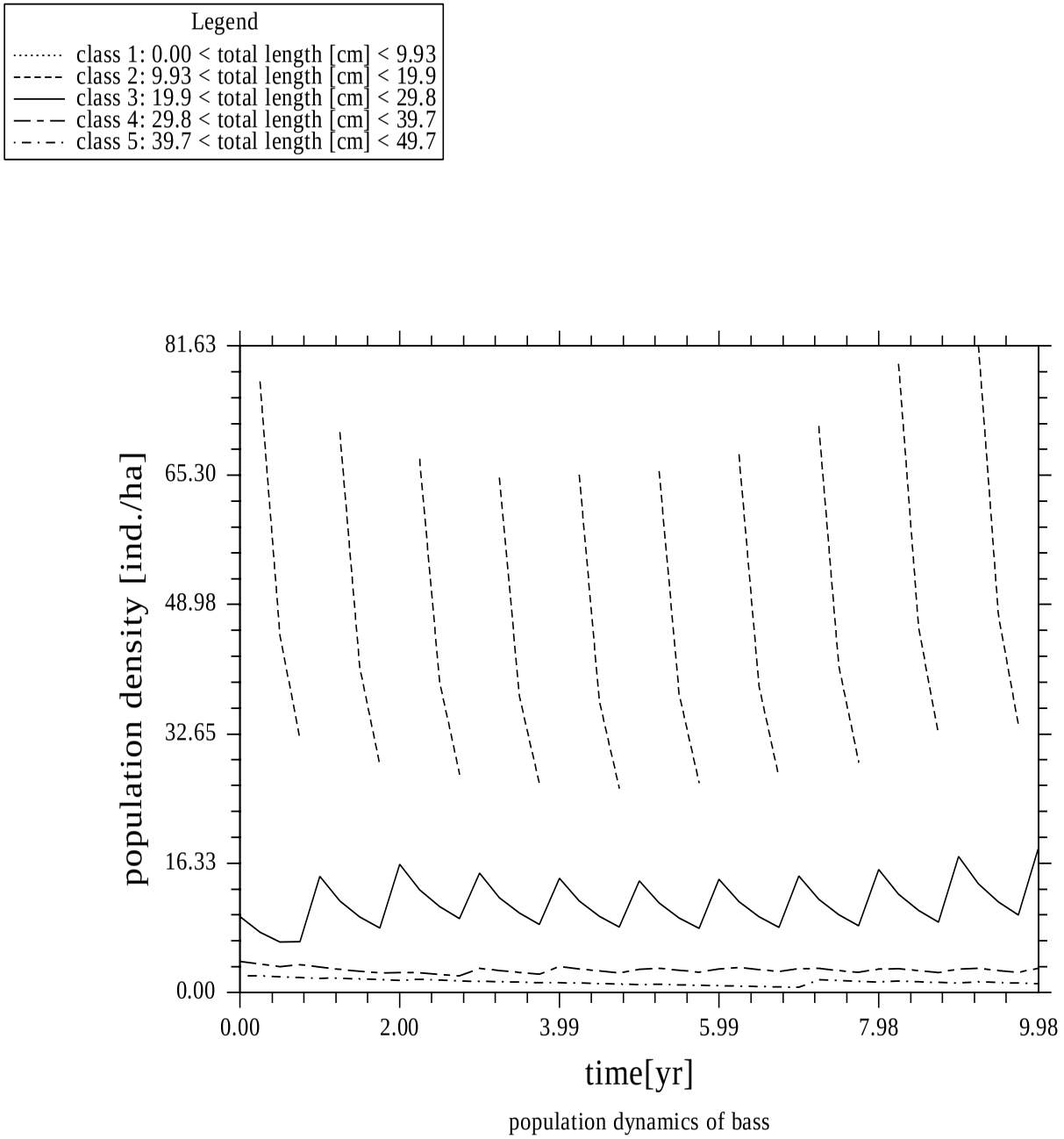
community consumption [g(DW)/ha/yr] of benthos..... 1.566E+06 (0.61 of total consumption)
community consumption [g(DW)/ha/yr] of insects..... 0.00 (0.00 of total consumption)
community consumption [g(DW)/ha/yr] of periphyton..... 0.00 (0.00 of total consumption)
community consumption [g(DW)/ha/yr] of phytoplankton... 0.00 (0.00 of total consumption)
community consumption [g(DW)/ha/yr] of zooplankton..... 9.588E+05 (0.38 of total consumption)
community consumption [g(DW)/ha/yr] of fish..... 2.778E+04 (0.01 of total consumption)

community mass balances
piscivory - predatory mortality [g(DW)/ha/yr].....-1.953E-02

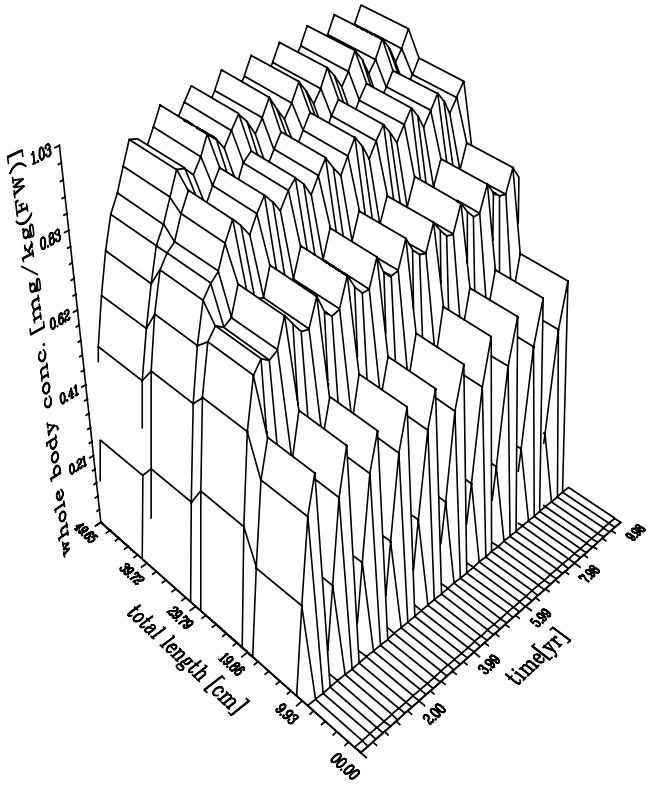
APPENDIX G. Example output file (filename.plx) that plots the variables requested by the user.



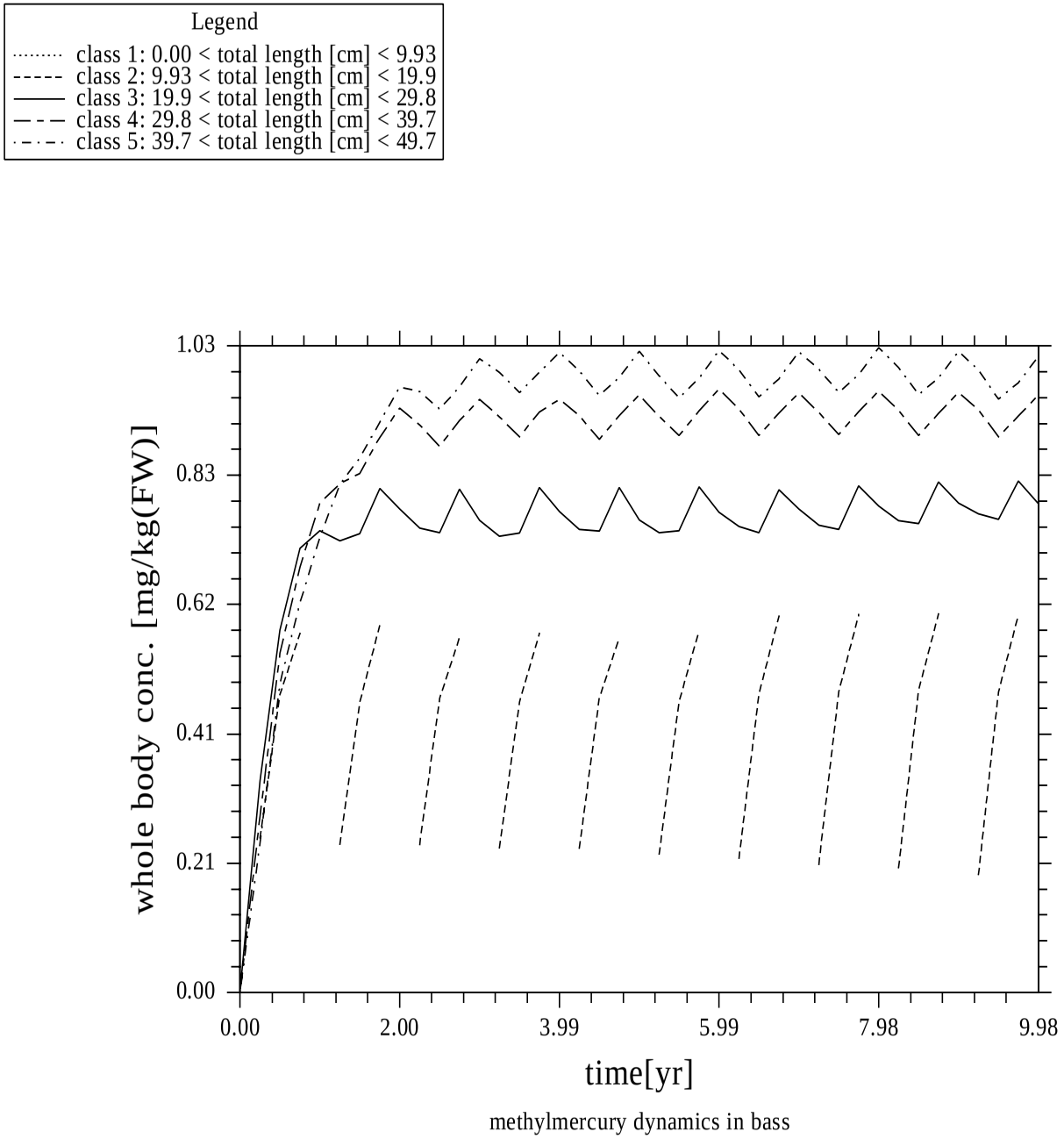
population dynamics of bass

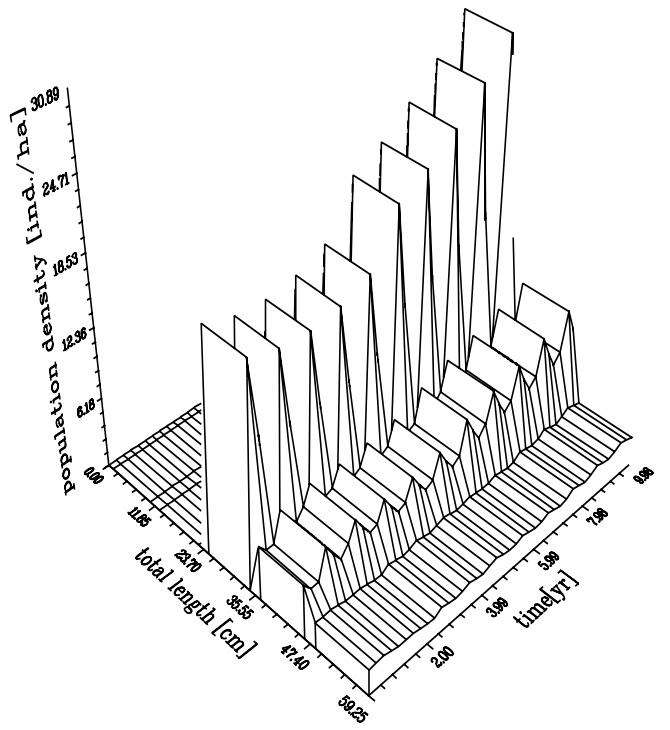


population dynamics of bass

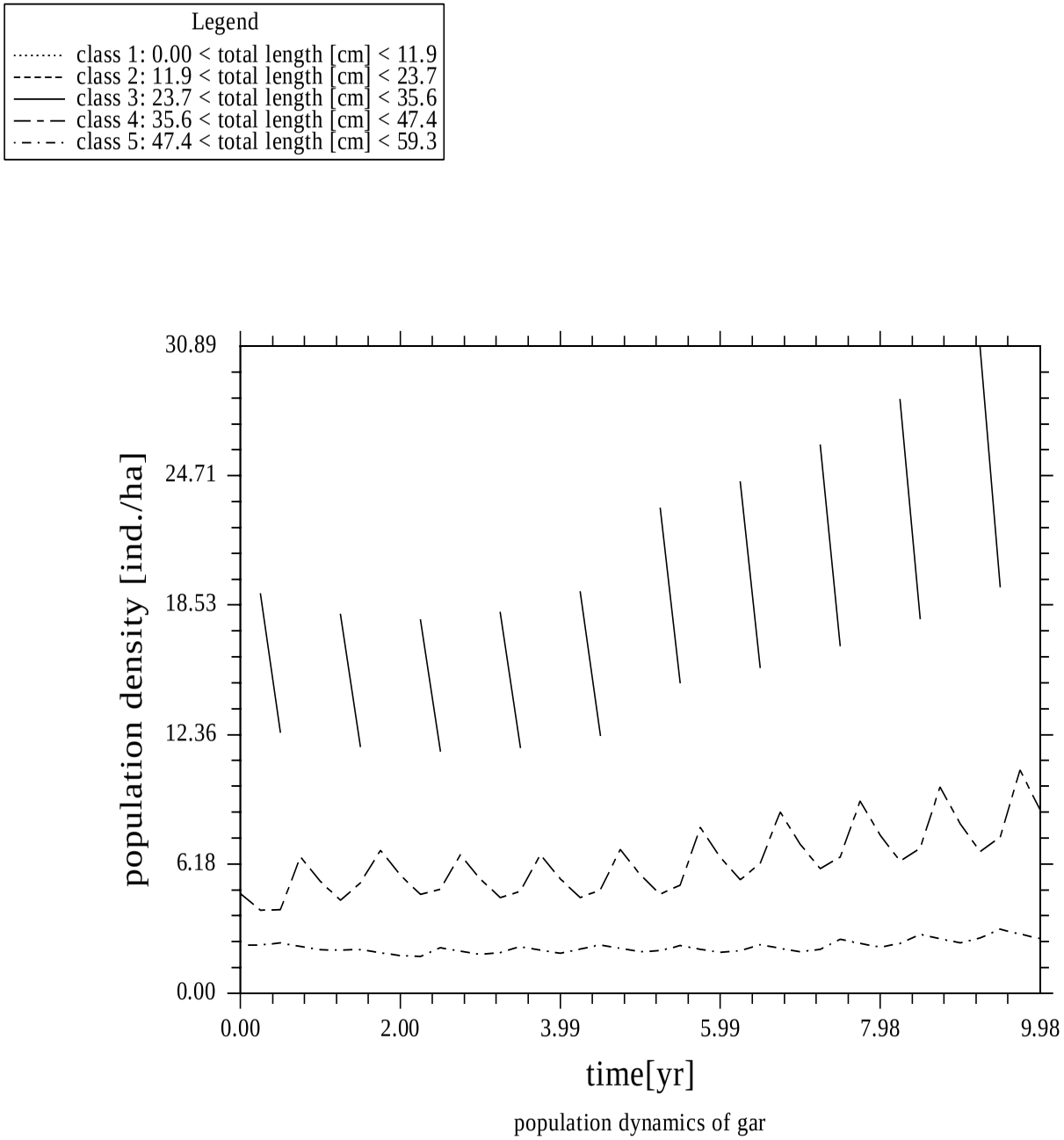


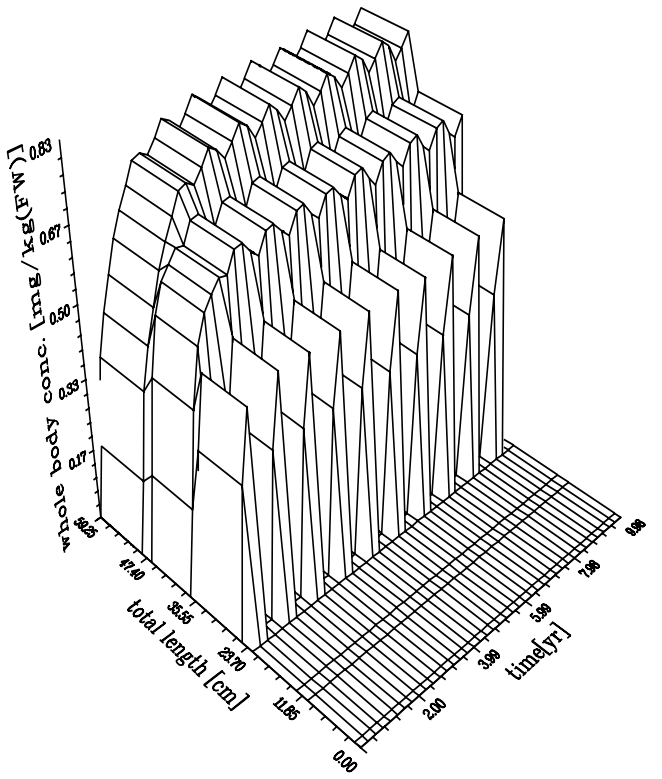
methylmercury dynamics in bass


Legend
class 1: 0.00 < total length [cm] < 9.93
class 2: 9.93 < total length [cm] < 19.9
class 3: 19.9 < total length [cm] < 29.8
class 4: 29.8 < total length [cm] < 39.7
class 5: 39.7 < total length [cm] < 49.7
whole body conc. [mg/kg(FW)]
1.03
0.83
0.62
0.41
0.21
0.00
0.00
2.00
3.99
5.99
7.98
9.98
time[yr]
methylmercury dynamics in bass

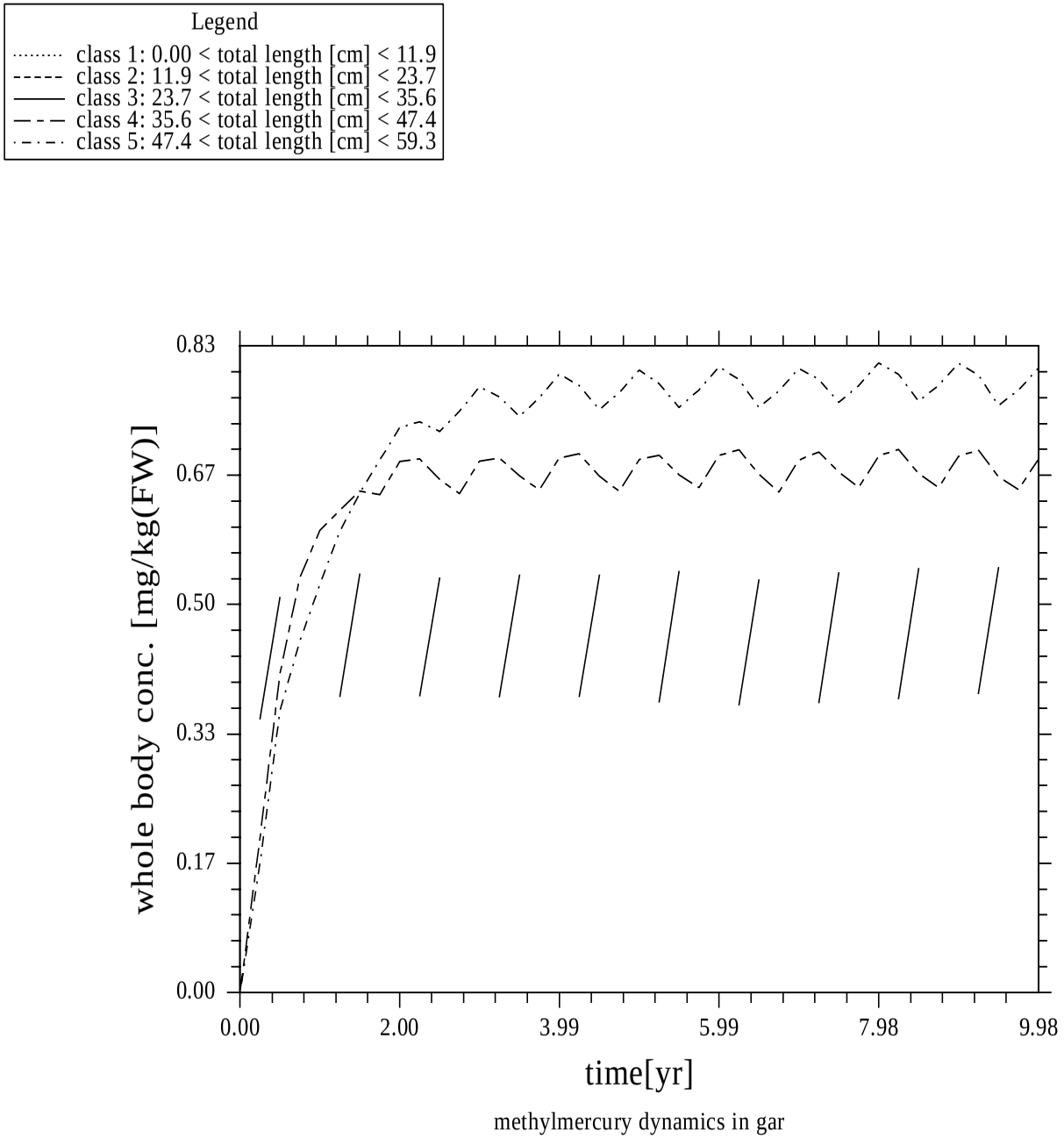


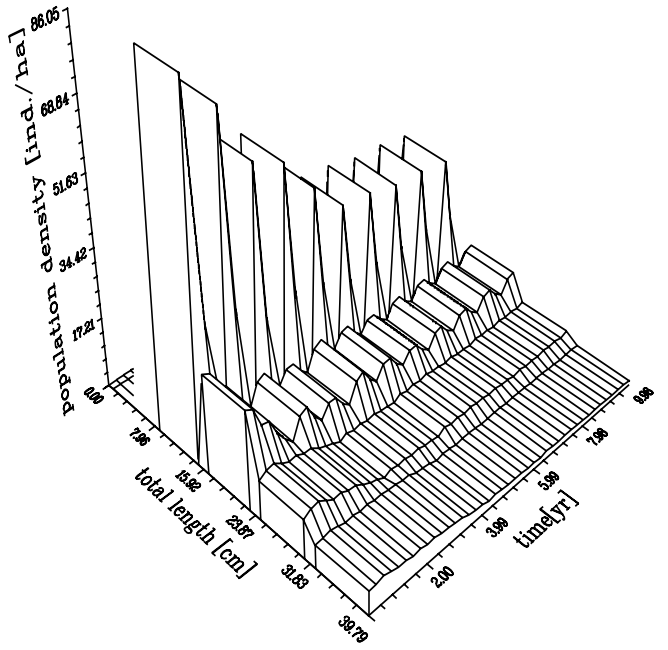
population dynamics of gar


Legend
class 1: 0.00 < total length [cm] < 11.9
class 2: 11.9 < total length [cm] < 23.7
class 3: 23.7 < total length [cm] < 35.6
class 4: 35.6 < total length [cm] < 47.4
class 5: 47.4 < total length [cm] < 59.3
30.89
24.71
18.53
12.36
6.18
0.00
population density [ind./ha]
0.00
2.00
3.99
5.99
7.98
9.98
time[yr]
population dynamics of gar

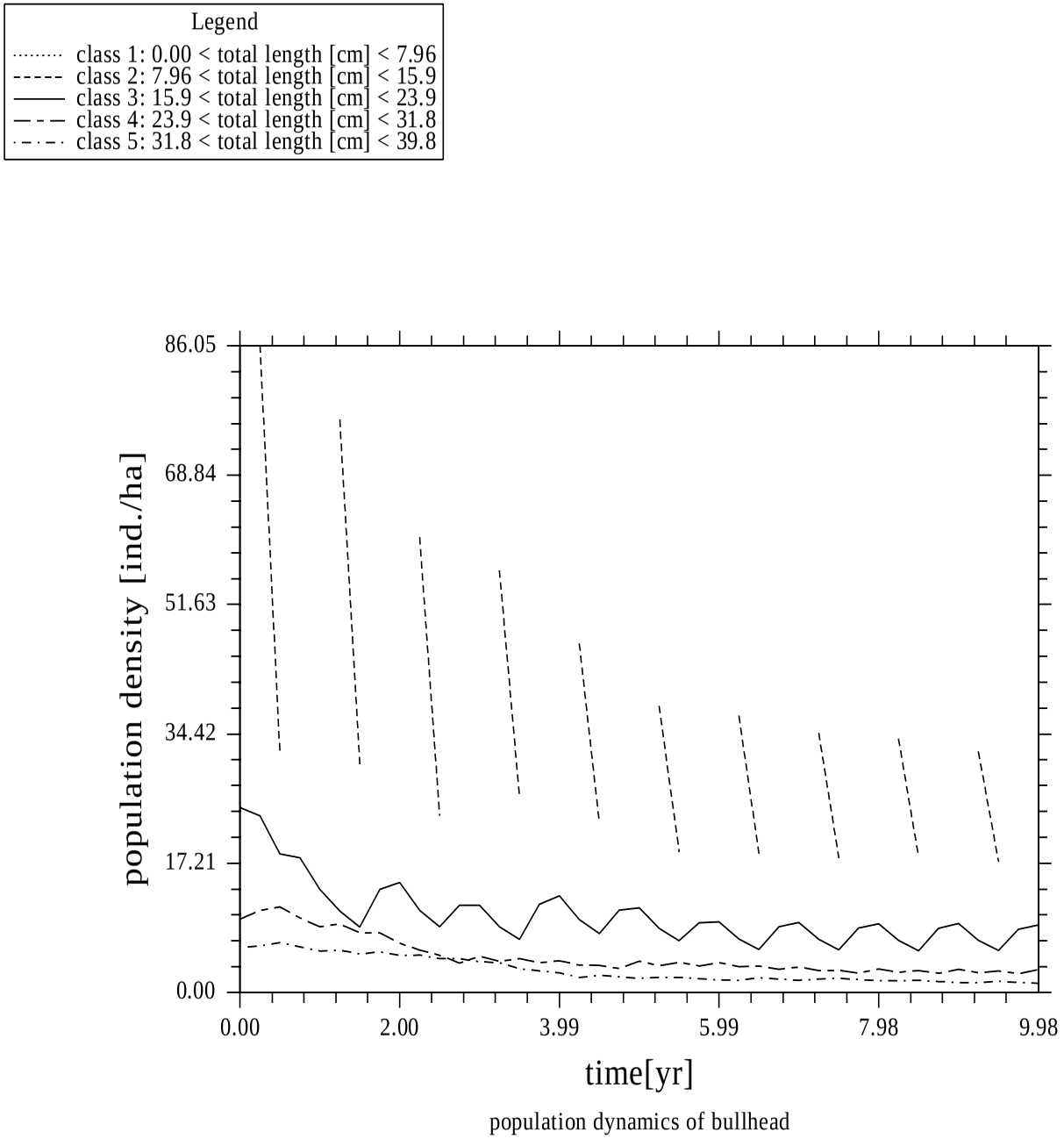


methylmercury dynamics in gar


Legend
class 1: 0.00 < total length [cm] < 11.9
class 2: 11.9 < total length [cm] < 23.7
class 3: 23.7 < total length [cm] < 35.6
class 4: 35.6 < total length [cm] < 47.4
class 5: 47.4 < total length [cm] < 59.3
whole body conc. [mg/kg(FW)]
0.83
0.67
0.50
0.33
0.17
0.00
0.00
2.00
3.99
5.99
7.98
9.98
time[yr]
methylmercury dynamics in gar



population dynamics of bullhead


Legend
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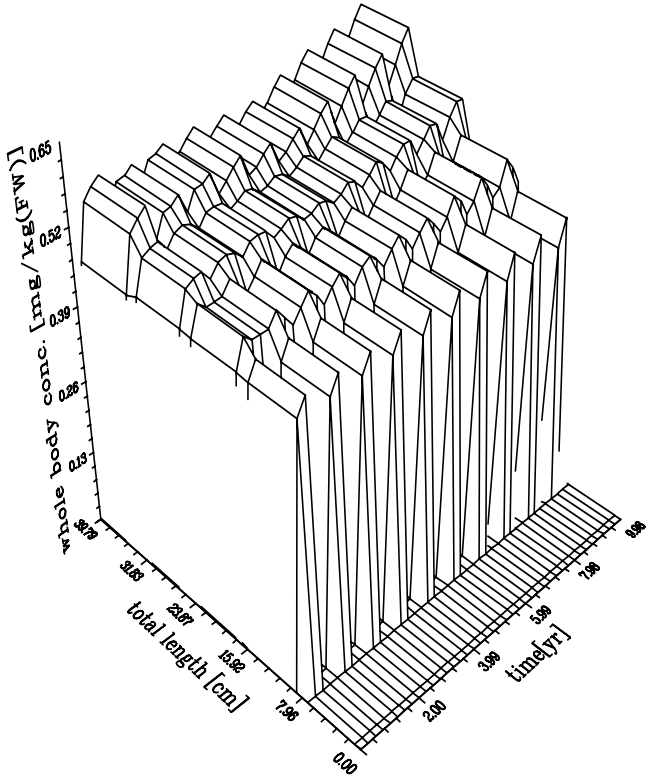
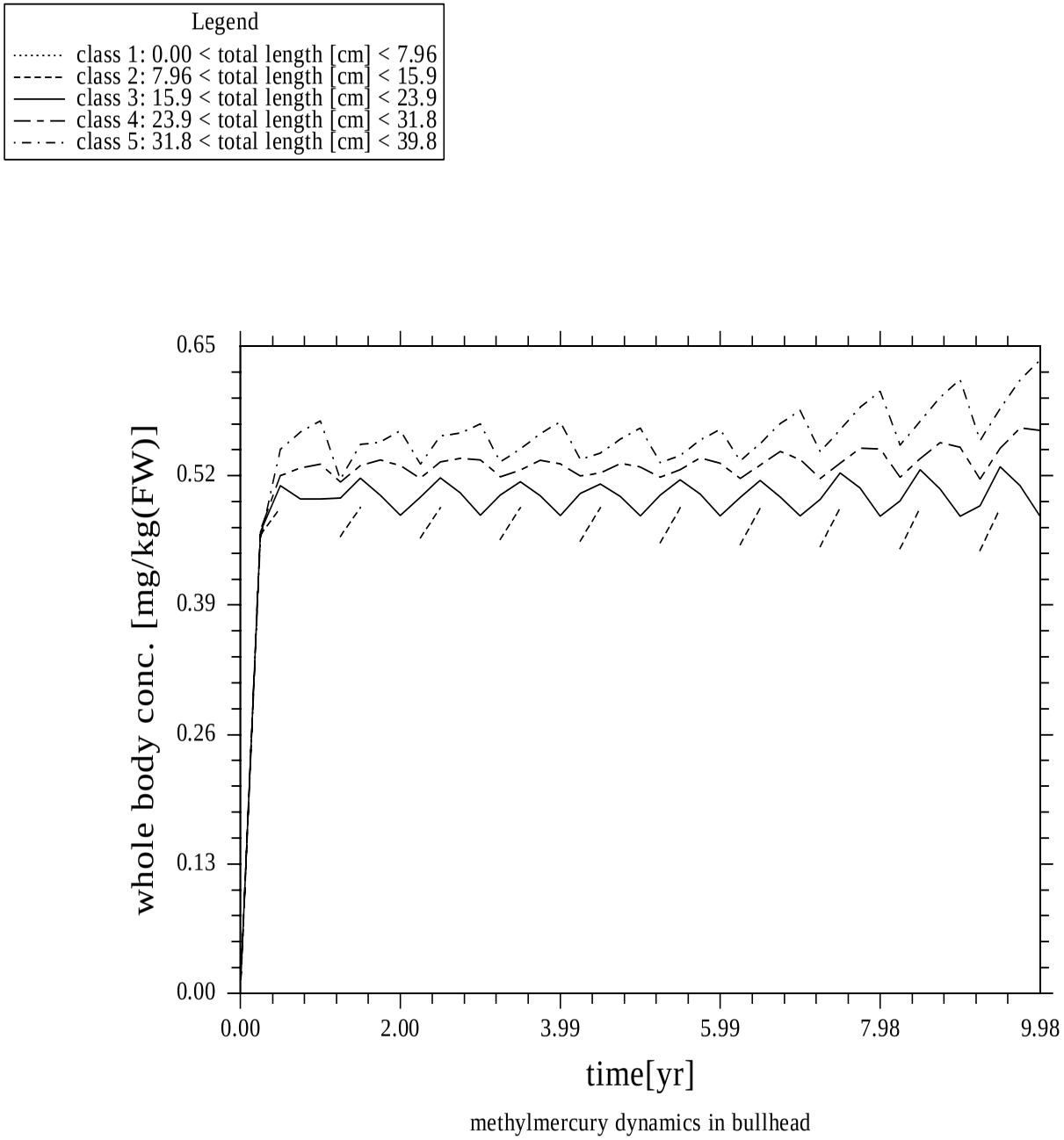
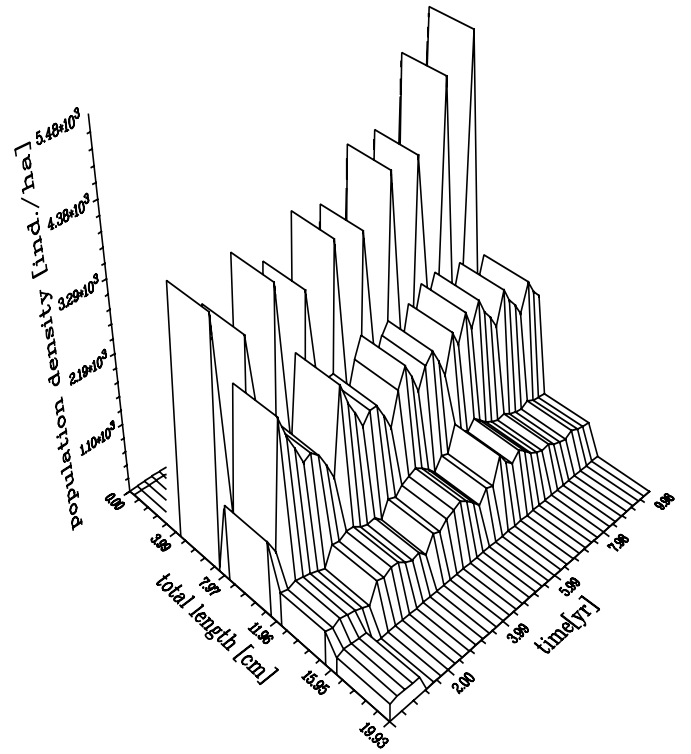
class 2: 7.96 < total length [cm] < 15.9
class 3: 15.9 < total length [cm] < 23.9
class 4: 23.9 < total length [cm] < 31.8
class 5: 31.8 < total length [cm] < 39.8
86.05
68.84
51.63
34.42
17.21
0.00
population density [ind./ha]
0.00
2.00
3.99
5.99
7.98
9.98
time[yr]
population dynamics of bullhead

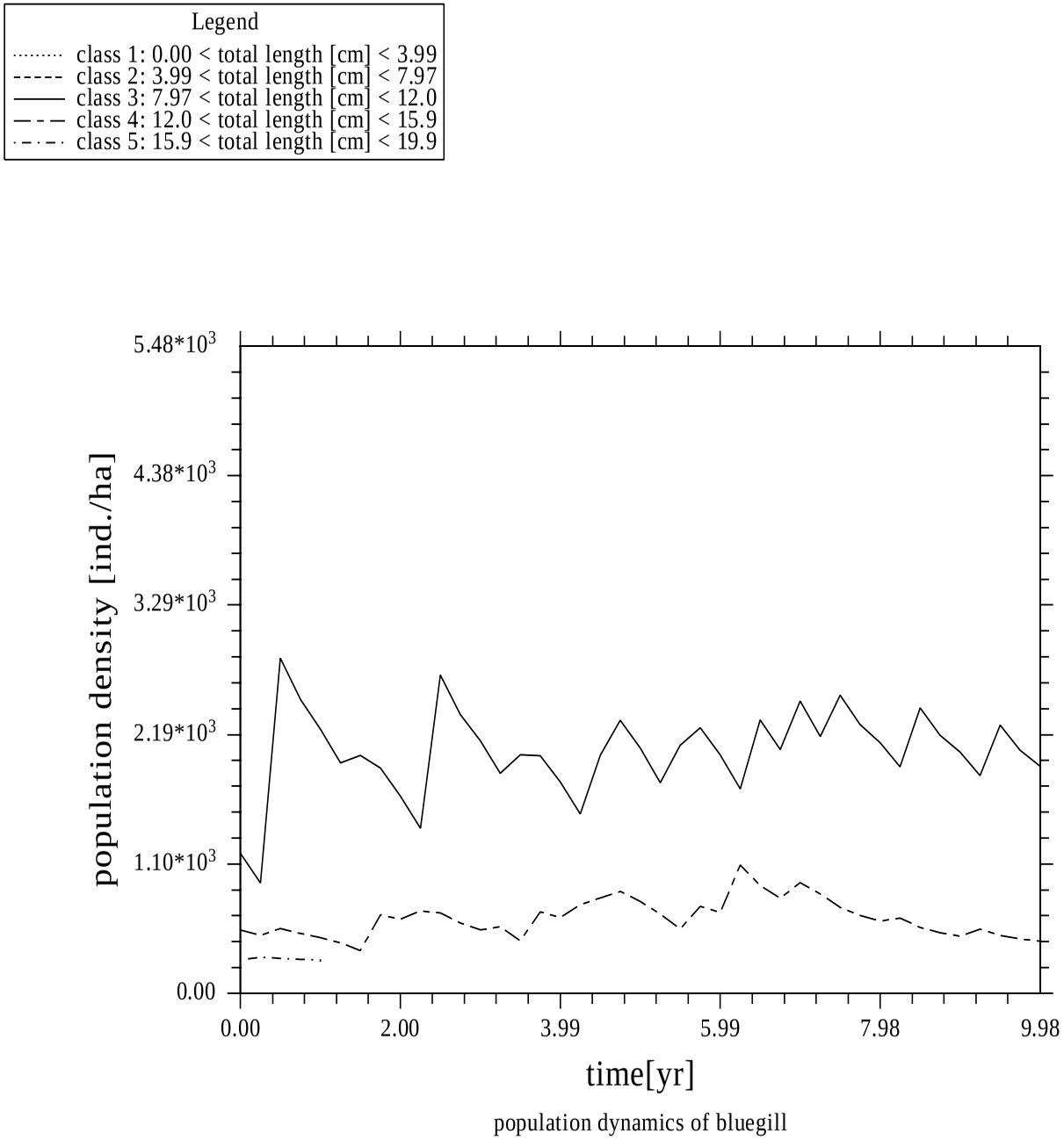


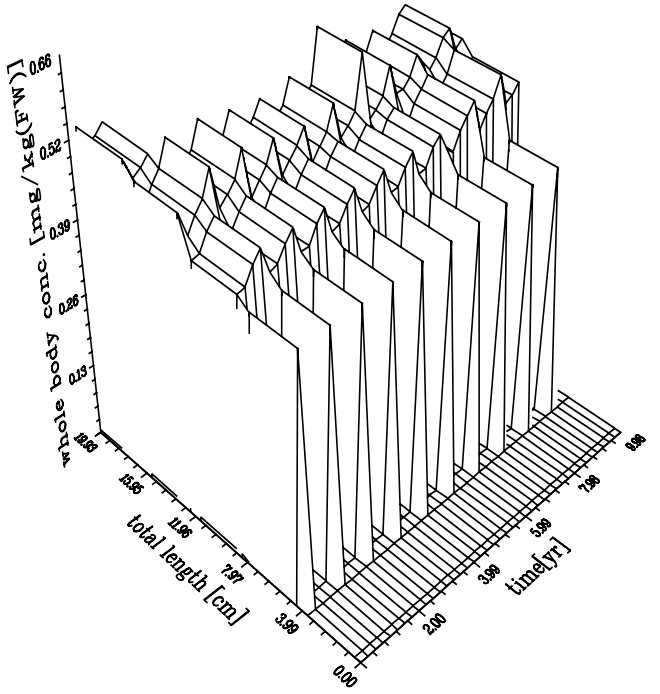
methylmercury dynamics in bullhead


Legend
class 1: 0.00 < total length [cm] < 7.96
class 2: 7.96 < total length [cm] < 15.9
class 3: 15.9 < total length [cm] < 23.9
class 4: 23.9 < total length [cm] < 31.8
class 5: 31.8 < total length [cm] < 39.8
whole body conc. [mg/kg(FW)]
0.65
0.52
0.39
0.26
0.13
0.00
0.00
2.00
3.99
5.99
7.98
9.98
time[yr]
methylmercury dynamics in bullhead

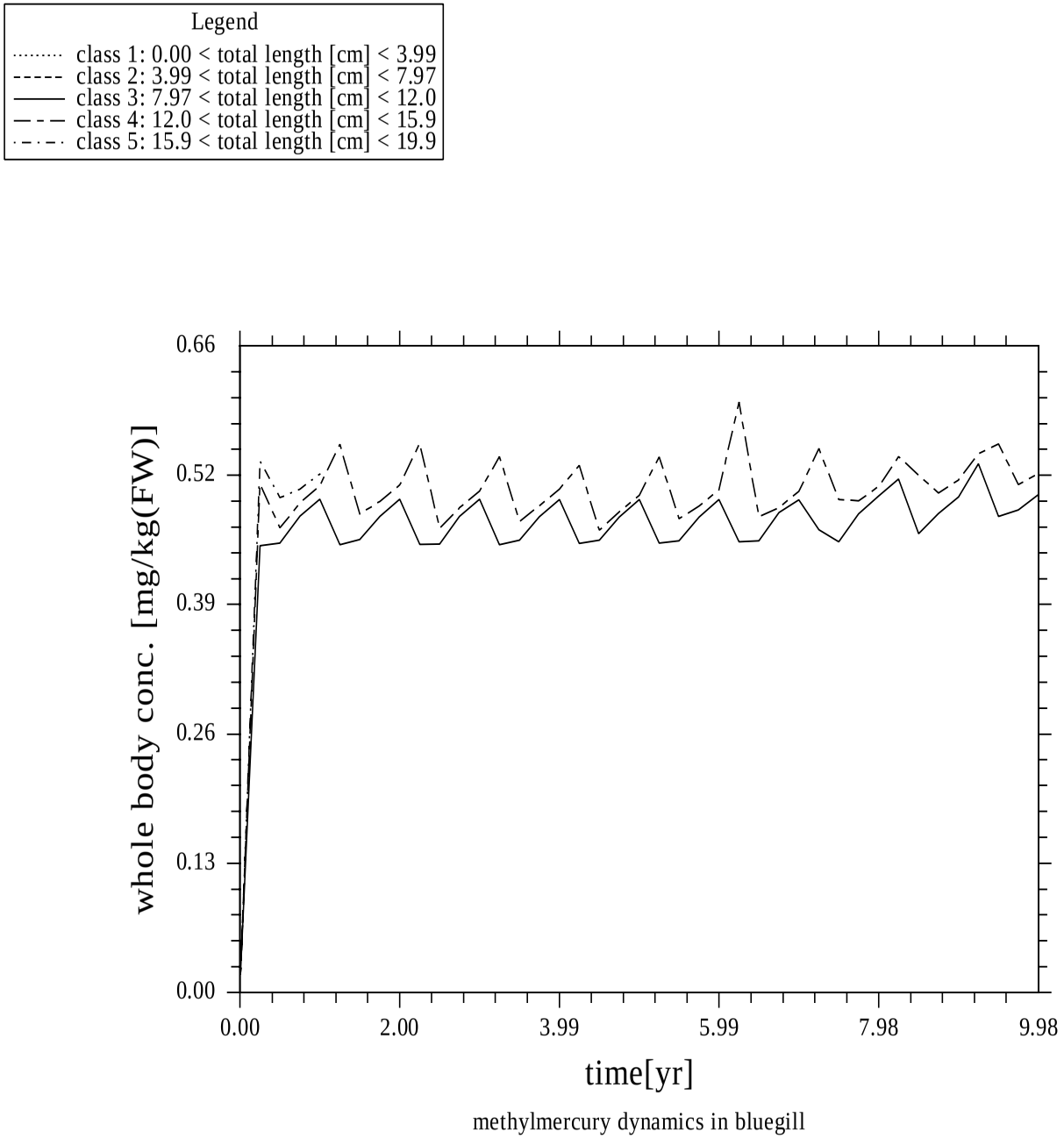


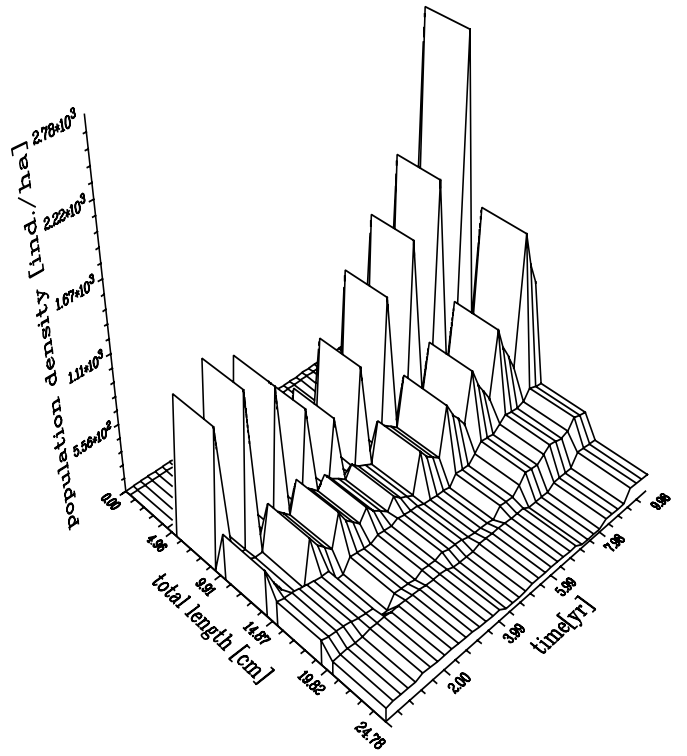
population dynamics of bluegill


Legend
class 1: 0.00 < total length [cm] < 3.99
class 2: 3.99 < total length [cm] < 7.97
class 3: 7.97 < total length [cm] < 12.0
class 4: 12.0 < total length [cm] < 15.9
class 5: 15.9 < total length [cm] < 19.9
5.48*10^3
4.38*10^3
3.29*10^3
2.19*10^3
1.10*10^3
0.00
population density [ind./ha]
0.00
2.00
3.99
5.99
7.98
9.98
time[yr]
population dynamics of bluegill

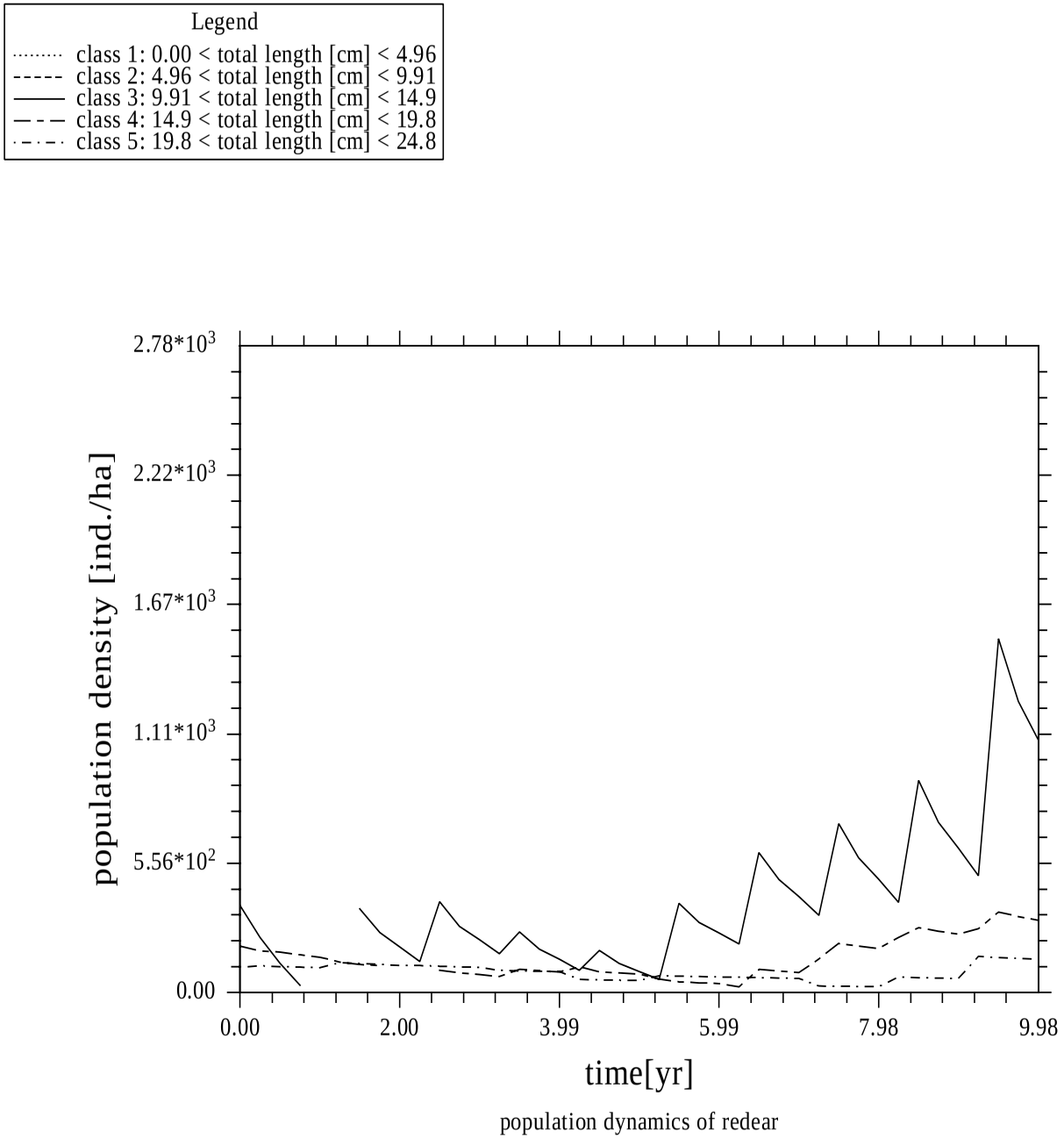


methylmercury dynamics in bluegill

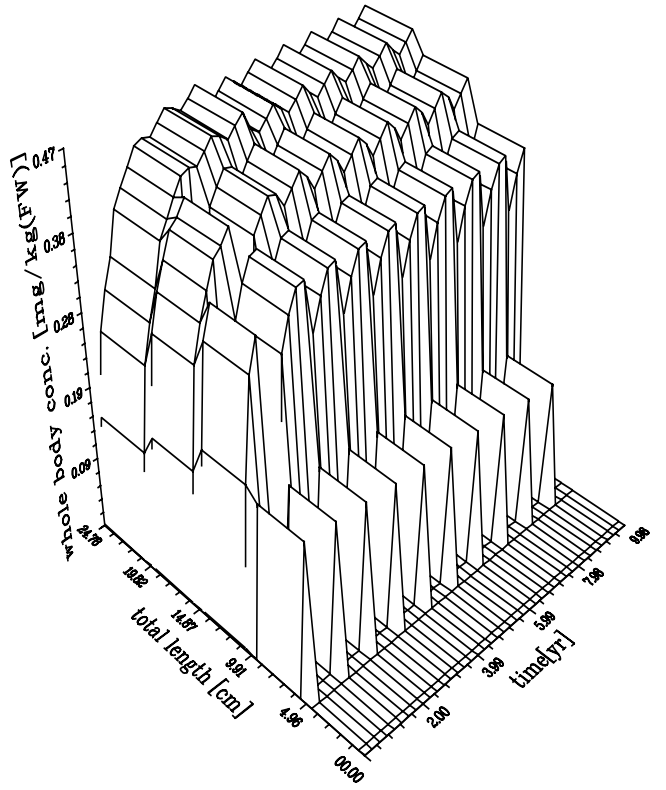

Legend
class 1: 0.00 < total length [cm] < 3.99
class 2: 3.99 < total length [cm] < 7.97
class 3: 7.97 < total length [cm] < 12.0
class 4: 12.0 < total length [cm] < 15.9
class 5: 15.9 < total length [cm] < 19.9
whole body conc. [mg/kg(FW)]
0.66
0.52
0.39
0.26
0.13
0.00
0.00
2.00
3.99
5.99
7.98
9.98
time[yr]
methylmercury dynamics in bluegill



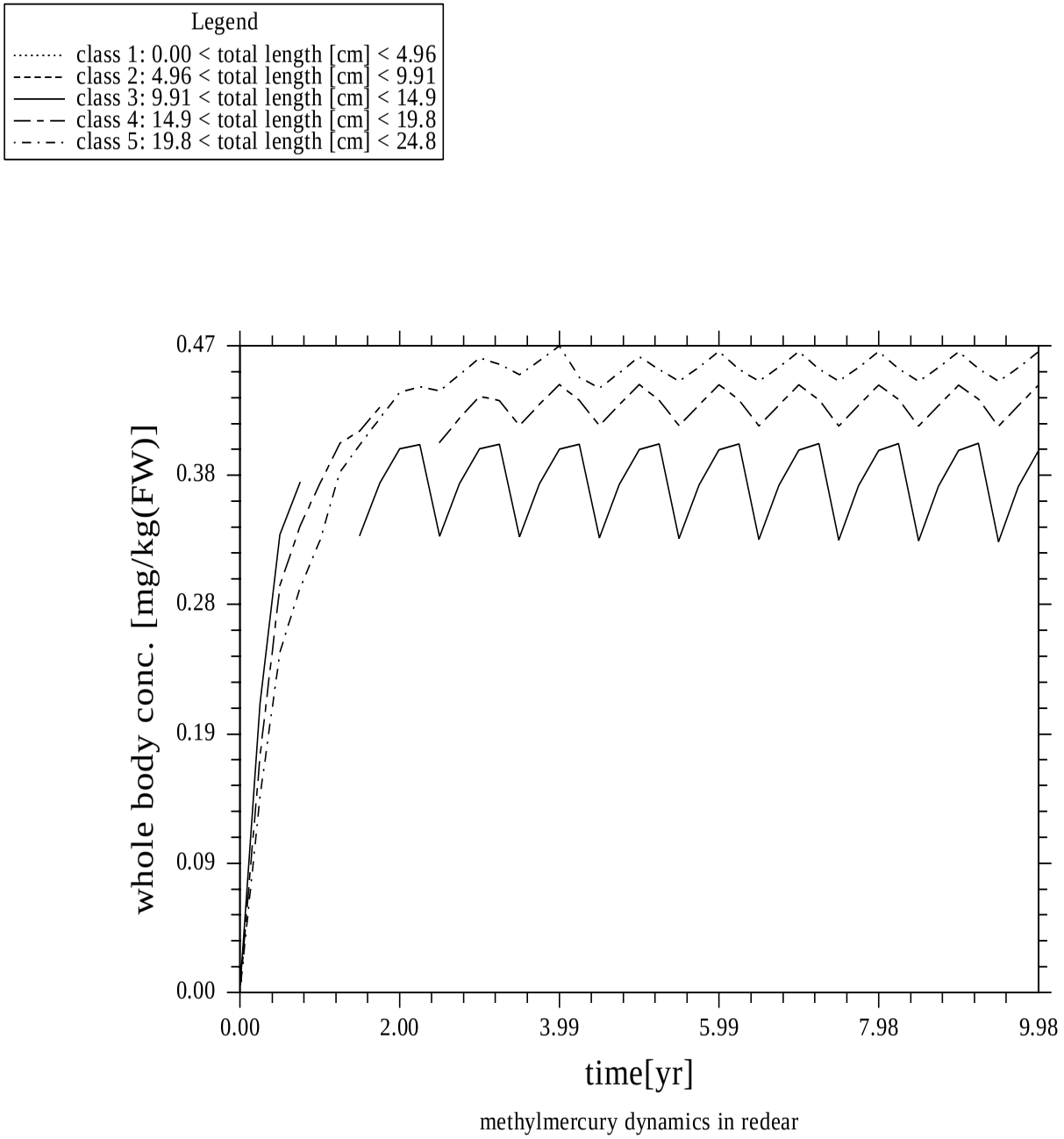
population dynamics of redear

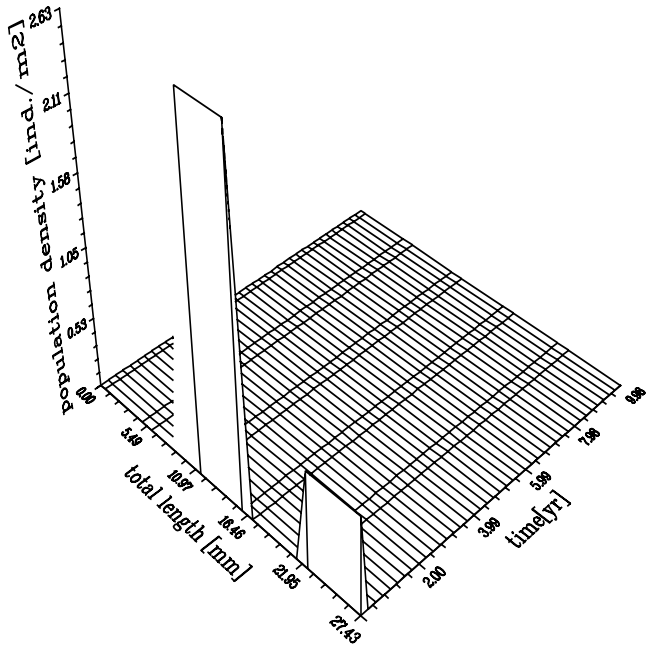


population dynamics of redear

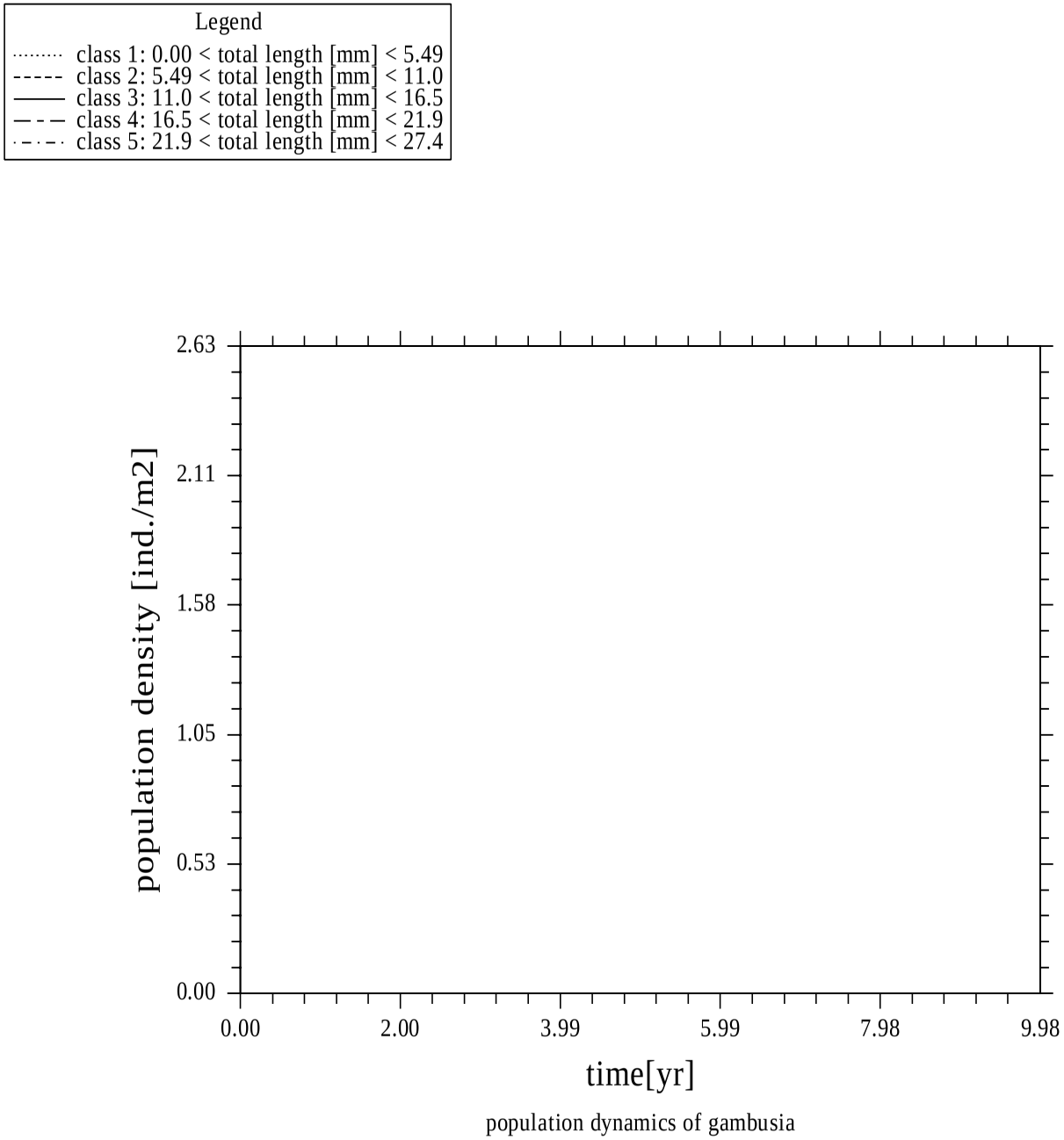


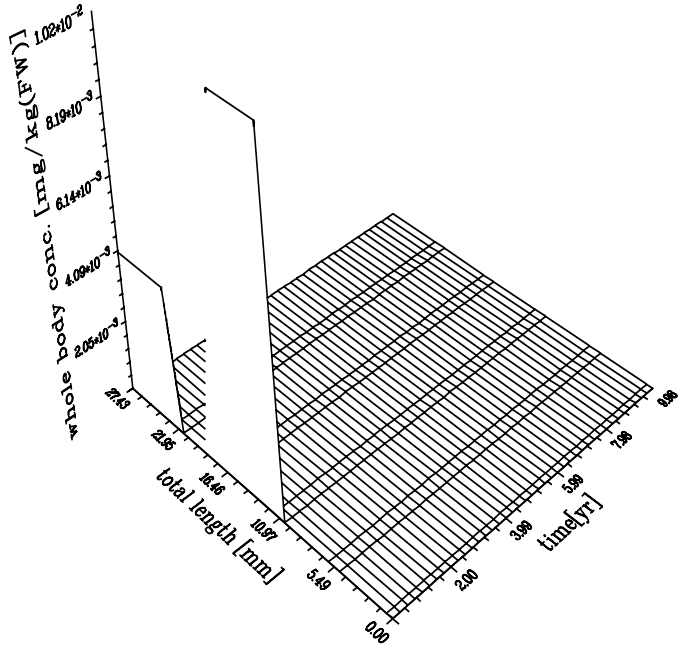
methylmercury dynamics in redear


Legend
class 1: 0.00 < total length [cm] < 4.96
class 2: 4.96 < total length [cm] < 9.91
class 3: 9.91 < total length [cm] < 14.9
class 4: 14.9 < total length [cm] < 19.8
class 5: 19.8 < total length [cm] < 24.8
whole body conc. [mg/kg(FW)]
0.47
0.38
0.28
0.19
0.09
0.00
0.00
2.00
3.99
5.99
7.98
9.98
time[yr]
methylmercury dynamics in redear

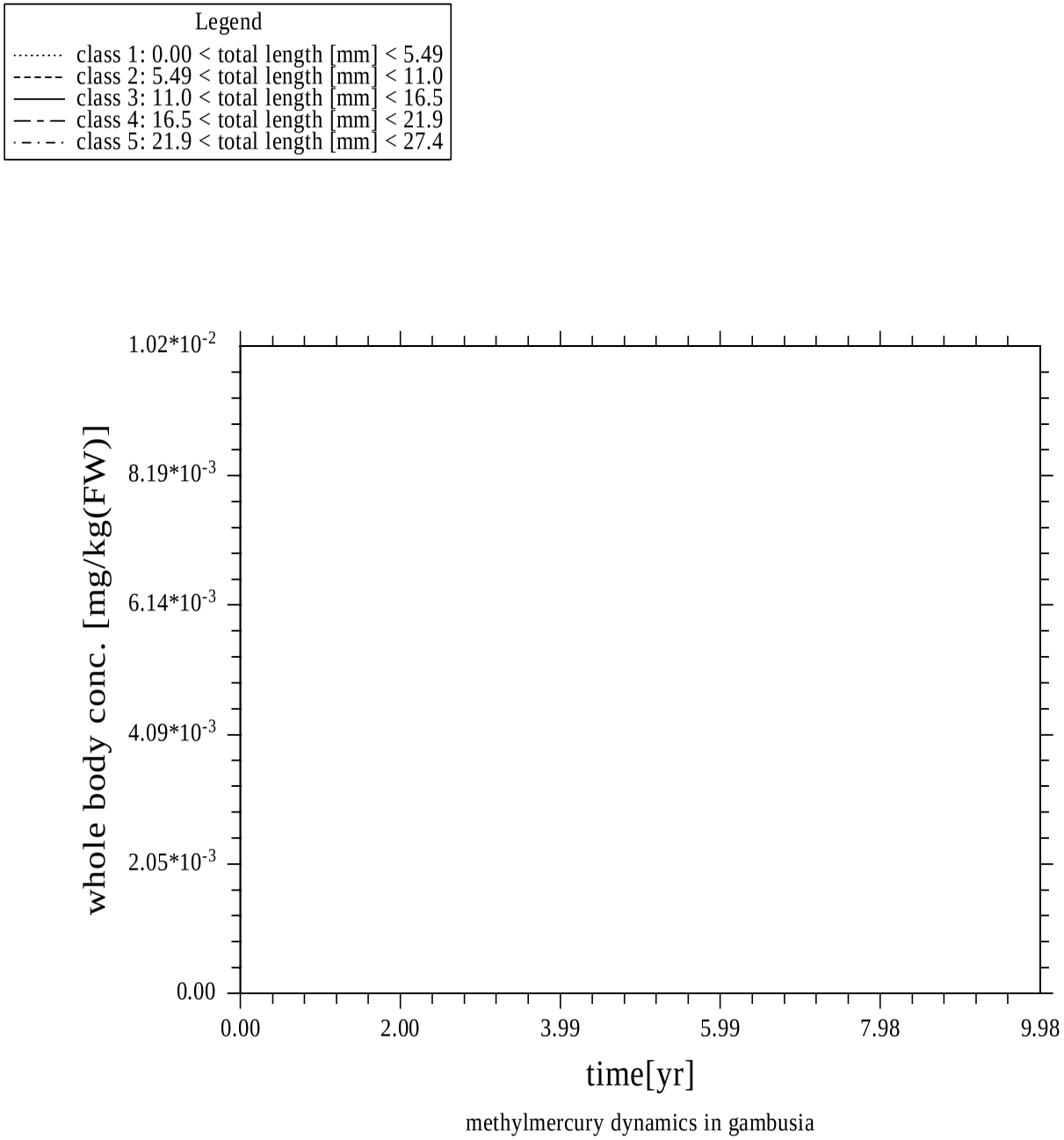


population dynamics of gambusia


Legend
class 1: 0.00 < total length [mm] < 5.49
class 2: 5.49 < total length [mm] < 11.0
class 3: 11.0 < total length [mm] < 16.5
class 4: 16.5 < total length [mm] < 21.9
class 5: 21.9 < total length [mm] < 27.4
population density [ind./m2]
2.63
2.11
1.58
1.05
0.53
0.00
0.00
2.00
3.99
5.99
7.98
9.98
time[yr]
population dynamics of gambusia



methylmercury dynamics in gambusia


Legend
class 1: 0.00 < total length [mm] < 5.49
class 2: 5.49 < total length [mm] < 11.0
class 3: 11.0 < total length [mm] < 16.5
class 4: 16.5 < total length [mm] < 21.9
class 5: 21.9 < total length [mm] < 27.4
whole body conc. [mg/kg(FW)]
1.02*10-2
8.19*10-3
6.14*10-3
4.09*10-3
2.05*10-3
0.00
0.00
2.00
3.99
5.99
7.98
9.98
time[yr]
methylmercury dynamics in gambusia

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