PB88-133558

EPA/600/3-87/038
December 1987

FGETS (FOOD AND GILL EXCHANGE OF TOXIC SUBSTANCES): A Simulation Model for Predicting Bioaccumulation of Nonpolar Organic Pollutants by Fish

by

M.C. Barber, L.A. Suarez, and R.R. Lassiter
Biology Branch
Environmental Research Laboratory
Athens, GA 30613

ENVIRONMENTAL RESEARCH LABORATORY
OFFICE OF RESEARCH AND DEVELOPMENT
U.S. ENVIRONMENTAL PROTECTION AGENCY
ATHENS, GA 30613

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FOREWORD

As environmental controls become more expensive and penalties for judgment errors become more severe, environmental management requires more precise assessment tools based on greater knowledge of relevant phenomena. As part of this Laboratory's research on the occurrence, movement, transformation, impact, and control of environmental contaminants, the Biology Branch conducts research to predict the rate, extent, and products of biological processes that control pollutant fate in soil and water and develops methods for forecasting ecosystem level effects suitable for exposure and risk assessment.

The Athens Environmental Research Laboratory, along with Office of Research and Development laboratories in Corvallis, OR, Duluth, MN, and Gulf Breeze, FL, is developing a system to assess ecological risks from exposure to environmental toxicants. This system will provide the capability to assess risk associated with different uses of chemicals resulting from various options for regulating pesticides and toxic chemicals to protect organisms in their natural environment. This report describes a component of that system, the Food and Gill Exchange of Toxic Substances (FGETS) model.

The authors wish to acknowledge Drs. Gilman Veith and James McKim of Duluth ERL whose personal communications and research regarding fish toxicity and toxicokinetics motivated this research. The authors also acknowledge the invaluable assistance of Dr. Samuel Karickhoff of Athens ERL in the development of the model presented herein.

Rosemarie C. Russo
Director
Environmental Research Laboratory
Athens, GA

ABSTRACT

A model for the bioaccumulation of nonpolar, nonmetabolized organic chemicals by fish is described. This model, FGETS, simulates thermodynamically driven chemical exchange by fish assuming either aqueous exposure only or joint aqueous and food chain exposure. Parameterization of the model incorporates allometric relationships between the fish's body weight and its gill and intestinal surface areas, lipid content of the fish, and physico-chemical properties of the chemical (i.e., molecular weight, melting point, and n-octanol/water partition coefficient). The model is validated by comparing predicted and observed depuration rates of organic chemicals by rainbow trout (Salmo gairdneri). An application of the model describing the bioaccumulation of polychlorinated biphenyls by Lake Michigan lake trout (Salvelinus namaycush) also is presented.

This report covers a period from October 1, 1986, to September 30, 1987, and work was completed as of September 30, 1987.

I. INTRODUCTION

When aquatic ecosystems are polluted with organic chemicals, fish in those systems will bioaccumulate the xenobiotics directly both from the water and from prey that have become contaminated with the chemicals. For benthic species, chemicals also may be accumulated by dermal contact with contaminated sediments. If these chemicals are not metabolized, their ultimate concentrations in fish should be predictable based on principles of thermodynamic partitioning. The purpose of this work is to present a dynamic model, FGETS (Food and Gill Exchange of Toxic Substances), that describes thermodynamically driven bioaccumulation of nonmetabolized organic toxicants by fish. This work is an extension of a previously published model (Barber et al. 1987, Suárez et al. 1987) which describes the uptake and depuration of organic toxicants across fish gills.

FGETS is a FORTRAN simulation model that predicts temporal dynamics of a fish's whole body concentration [i.e., ppm = microgram of chemical per gram (live weight fish)] of a nonmetabolized, organic chemical that is bioaccumulated either from water only, which is probably the predominant exchange route for acute exposures, or from water and food jointly, which is more characteristic of chronic exposure. These dynamics are calculated algebraically from the fish's predicted total body burden and live weight. Additionally, FGETS calculates time to death assuming that the chemical's mode of action is simple narcosis.

II. MODEL FORMULATION

The following discussion is a brief overview of the formulations used in FGETS to predict a fish's total body burden, B_f (B_f = micrograms of chemical per fish), live body weight, W (W = grams of live weight), and time to death.

II.1. Modeling B_f Assuming Only Water Exposure

Because the exchange of nonpolar organic chemicals across the gills of fish apparently occurs by simple diffusion (Opperhuizen et al. 1985, Opperhuizen and Scharp 1987), Fick's first law of diffusion can be used to model this process. Several models of diffusive exchange in fish have been proposed (e.g., Yalkowsky et al. 1973, Mackay 1982, Mackay and Hughes 1984, Gobas et al. 1986, Gobas and Mackay 1987). Barber et al. 1987, however, modeled the total body burden of nonmetabolized, organic chemicals in fish starting with the differential equation,

$$dB_f/dt = S_g J_g = S_g k_w (C_w - C_a) \qquad (1)$$

where S_g is the fish's total gill area (cm^2), J_g is the net diffusive flux (microgram/cm^2/day) across the fish's gills, k_w is the chemical's mass conductance (cm/day) through the interlamellar water of the gills, and C_w and C_a are the chemical's concentration (ppm) in the environmental water and the fish's aqueous blood, respectively. Note that while the total resistance (i.e., the reciprocal for conductance) to mass exchange across gills actually depends on individual resistances in both the interlamellar water and the gill epithelium, Equation 1 assumes that all resistance to exchange of a nonpolar organic is in the water. For chemicals that have n-octanol/water partition coefficients, K_{ow}, on the order of log K_{ow}>2, however, this assumption is reasonable (see Barber et al. 1987).

To apply Equation 1, however, a functional relationship between the fish's total body burden, B_f, and aqueous blood concentration, C_a, must be specified. To this end, Barber et al. (1987) noted that a fish's whole body concentration, $C_f = B_f / W$, could be expressed as

$$C_f = B_f / W = P_a C_a + P_l C_l + P_s C_s, \qquad (2)$$

where P_a, P_l, and P_s are the fractions of the whole fish that are water, lipid,

and structural organic material, respectively, and C_l and C_s are the chemical's concentrations (ppm) in the fish's lipid and structural organics, respectively. Since the depuration rates of organic chemicals from different tissues within a fish apparently do not differ significantly (Grzenda et al. 1970, van Veld et al. 1984, Branson et al. 1985, Norheim and Roald 1985), internal equilibration between the aqueous, lipid, and structural organic phases can be assumed to be rapid in comparison with exchange across the gills. Consequently, Equation 2 can be rewritten as

$$C_f = B_f / W = (P_a + P_l K_l + P_s K_s) C_a \qquad (3)$$

where K_l and K_s are thermodynamic partition coefficients between lipid and water and between organic carbon and water, respectively. Because C_w equals C_a at equilibrium (see Equation 1), it follows from Equation 3 that a fish's ultimate biomagnification factor, $BCF = C_f/C_w$, assuming only gill exchange, is simply

$$BCF = (P_a + P_l K_l + P_s K_s) \qquad (4)$$

Therefore, using Equations 3 and 4, Equation 1 can be rewritten as

$$dB_f/d_t = S_g k_w (C_w - C_f/BCF) = S_g k_w (C_w - B_f/(W BCF)) \qquad (5)$$

II.2. Modeling B_f Assuming Food and Water Exposure

To model the dynamics of a fish's total body burden that is accumulated from both water and food, Equation 5 simply needs to be modified as

$$dB_f/d_t = S_g k_w (C_w - C_f/BCF) + J_i \qquad (6)$$

where J_i is the net mass exchange (micrograms/day) across the fish's intestine from food. Although this modification is straightforward, the selection of a formulation to model J_i is not. Consequently, FGETS has three different optional formulations for this flux.

The crudest formulation of J_i assumes that fish can assimilate a constant fraction of the chemical it ingests, i.e.,

$$J_i = \beta\ C_p\ F \qquad (7)$$

where β is an assimilation efficiency (dimensionless) for the chemical, C_p is the chemical's concentration (microgram/gram prey) in the ingested prey, and F is the fish's daily feeding flux (gram prey/day). Since the exchange of nonpolar organic chemicals across the intestines of fish also is driven by diffusive gradients (Vetter et al. 1985), the assimilation efficiency, β, should be a decreasing function of the fish's total body concentration, C_f. Consequently, Equation 7 generally will overestimate a fish's body burden. FGETS allows for this nonthermodynamic formulation, however, because 1) food exposure has been previously modeled in this way (Norstrom et al. 1976, Jensen et al. 1982, Thomann and Connolly 1984), and 2) when β = 1.0, i.e., the fish is assumed to assimilate all the ingested chemical, an absolute upper bound to bioaccumulation can be estimated. Importantly, however, this upper bound will exceed the thermodynamic limit to bioaccumulation.

A second candidate formulation for J_i is

$$J_i = C_p\ F - C_e\ E \qquad (8)$$

where C_e is the chemical's concentration (microgram/gram) in the fish's daily egestive/fecal flux, E (gram/day). If the transit time through the gastrointestinal tract is relatively slow, it might be reasonable to assume that the concentration of the chemical in the fish's aqueous blood, intestinal fluids, and fecal matter have equilibrated with one another. In this case,

$$C_e = P_{OC}\ K_{OC}\ C_a \qquad (9)$$

where P_{OC} is the fraction of the fish's feces that is organic carbon and K_{OC} is a thermodynamic partition coefficient between water and refractory organic

matter (see for example Karickhoff 1981, Briggs 1981, and Chiou et al. 1986). Therefore, using Equations 3, 4, and 9, Equation 8 can be rewritten as

$$J_i = C_p F - (P_{oc} K_{oc} C_f/BCF) E \quad (10)$$

If on the other hand the feces do not equilibrate with the fish's aqueous blood, then J_i should be modeled kinetically and, in particular,

$$J_i = S_i k_i (C_{ia} - C_a) \quad (11)$$

where S_i (cm^2) is the surface area of the intestine, k_i is the mass conductance (cm/day) of the chemical through the intestinal fluids, and C_{ia} is the concentration of the chemical in the intestinal fluids or the aqueous portion of the food resident in the intestine. To use Equation 11, C_{ia} must be expressed as a function of the prey's total body concentration, C_p. Therefore, in a manner similar to Equations 2 and 3, the total concentration, C_i, of chemical in the intestinal food is formulated as

$$C_i = B_i / I = P_{ia} C_{ia} + P_{io} C_{io}$$

where B_i is the total burden (microgram) of chemical in the intestinal food, I is the wet mass of the intestinal food, P_{ia} and P_{io} are the fractions of the intestinal food that are water and dry organic matter, respectively, and C_{ia} and C_{io} are the chemical's concentration in these two phases. Because enzymatic and mechanical processes transform food in a fish's intestine into a more or less mixed suspension, it seems reasonable to assume that C_{ia} and C_{io} maybe equilibrated and hence

$$C_i = B_i / I = (P_{ia} + P_{io} K_{oc}) C_{ia} \quad (12)$$

Because C_i can be calculated from the solutions of the differential equations,

$$dB_i/dt = C_p F - S_i k_i (C_{ia} - C_a) - C_i E \text{ and} \quad (13)$$

$$dI/dt = F - A - E \quad (14)$$

where F, A, and E are the fish's mass fluxes (grams/day) of feeding,

assimilation, and egestion, respectively, the system of Equations 6 and 11 - 14 constitute a kinetic model for joint gill and food exchange of organic toxicants by fish.

II.3. Modeling the Growth of Fish

A fish's growth can be modeled straightforwardly by the mass balance equation,

$$dW/dt = F - E - R - SDA \qquad (12)$$

where F, E, R and SDA are the fish's mass fluxes (grams/day) of feeding, egestion, routine respiration, and specific dynamic action, respectively.

Traditionally, a fish's maximal feeding flux, F, has been described empirically by the allometric function,

$$F = f_1 W^{f_2} \qquad (13)$$

where the coefficient, f_1, is generally a function of water temperature (see Paloheimo and Dickie 1965). An alternative expression for F, however, is

$$F = \phi \ (S_{max} - S), \qquad (14)$$

where ϕ is the fish's ad libitum feeding rate, S_{max} is the fish's maximum stomach/gut capacity, and S is the amount of food resident in the gut. S, in turn, is modeled by

$$dS/d_t = F - G \qquad (15)$$

where $G = g_1 S^{g2}$ represents gastric evacuation (Holling 1966, Ware 1972, Jobling 1986). FGETS allows the user to specify either the allometric type (i.e. Equation 13) or the Holling type (i.e., Equations 14 and 15) model to simulate fish ad libitum feeding. Simulating a fish's growth for long time intervals assuming continuous ad libitum consumption, however, is ecologically unrealistic because prey availability usually limits feeding to submaximal levels. In general, therefore, a fish's feeding, F, predicted by either the allometric type or the

Holling type models should be adjusted as

$$F = f() F \tag{16}$$

where f() describes the fish's functional response to available prey. Although f() eventually will be modeled, presently FGETS assumes f() = 0.5.

The proportion of F that a fish egests or defecates as nonassimilated matter, E, depends on ration size and quality. Presently, however, FGETS assumes that E is simply some constant fraction of F, i.e.,

$$E = (1 - a) F \tag{17}$$

where a is an assimilation efficiency.

Like the allometric expression for F, the respiratory expenditure, R, of fish associated with routine maintenance and activity traditionally has been described by a power function of the form,

$$R = r_1 W^{r_2} \tag{18}$$

where the coefficient, r_1, is generally a function of water temperature, T. In particular,

$$r_1 = r_1(T_{opt}) \exp (q (T-T_{opt})) \tag{19}$$

where $r_1(T_{opt})$ is the fish's respiratory coefficient at temperature T_{opt} (Paloheimo and Dickie 1965, Ursin 1967). On the other hand, the specific dynamic action of fish, which is the additional metabolic expenditure in excess of R required to assimilate food (Jobling 1981), often has been described simply as a constant fraction, σ, of the fish's assimilated food, i.e.,

$$SDA = \sigma a F \tag{20}$$

FGETS presently assumes that σ equals 0.2 for all fish (see Stewart et al. 1983, Stewart and Binkowski 1986, and Yarzhombek et al. 1984).

II.4. Predicting Narcotic Toxicity in Fish

Although Quantitative Structure Activity Response (QSAR) models that correlate lethal water concentrations for acute, predetermined periods of exposure with chemical properties (e.g., Konemann 1981, Veith et al. 1983) are ultimately required to predict fish mortality due to environmental exposures, these regression models have tended to neglect the fact that fish are killed not by the water concentration of chemicals per se but by the accumulated internal body concentrations of chemicals that result from such exposures. Neely (1984), Friant and Henry (1985), McCarty et al. (1985), and McCarty (1986) have discussed the importance of this distinction.

For chemicals whose mode of action is narcosis, i.e., a nonspecific and reversible physiological intoxication, the relationship between internal body concentrations and observed effects is apparently quite simple. In particular, if two chemicals are narcotics and their thermodynamic chemical activities in an animal's blood (or any phase when the assumption of internal equilibrium, i.e., Equation 3, is valid) are equal, then they will produce the same level of physiological effect (Ferguson 1939, Mullins 1954). Therefore, if LA denotes chemical activity of a narcotic in a fish's aqueous blood that causes death, the question we now want to address is what is the relationship between LA and LC50(t)'s determined by acute toxicity tests of duration t days.

Let LC50(t)'s denote the molar LC50 of a narcotic chemical for an acute aqueous exposure that lasts for t days and assume that during this exposure period the biological characteristic of the fish, i.e., its body weight, gill surface area, lipid content, etc., and the physico-chemical properties of the chemical, i.e. its log K_{ow}, (see Equations 3 - 5) are such that the fish's aqueous blood concentration equilibrates to within at least 99% of the water

concentration. If there are now two consecutive water concentrations, NC and LC, such that at NC no fish are killed whereas at LC all fish are killed, then clearly the lethal internal blood concentration and hence LA can be estimated from some measure of central tendency of these two concentrations. Moreover, since Stephan (1977) argues that the geometric mean of NC and LC is a valid estimator of LC50(t), in general LA can be estimated from any calculated LC50(t) provided the fish essentially can equilibrate with the water and in particular

$$LA = a_w \, v_w \, LC50(t) \qquad (21)$$

where a_w is the activity coefficient of the chemical in water and v_w is the molar volume of water (0.018 l/ mole).

Using data reported by Chiou (1985), we can estimate the aqueous activity coefficient of an organic chemical, which is the reciprocal of its super cooled liquid solubility, by the functional regression (see for details Jensen 1986 or Rayner 1985),

$$\log(a_w) = 1.131 \log(K_{ow}) + 1.053 \quad (n=37;\ r=0.98) \qquad (22)$$

This result is consistent with analogous linear regressions between aqueous solubilities and K_{ow} reported elsewhere, e.g., Chiou and Schmedding (1982) and Miller et al. (1985), but is significantly different from the regression

$$\log(a_w) = 0.944 \log(K_{ow}) + 1.422 \quad (n=??;\ r=0.98) \qquad (23)$$

reported by Yalkowsky et al. (1983). This difference, however, is due to the fact that Equation 22 uses measured logP's whereas Equation 23 was obtained using calculated logP's.

Since Equations 21 - 23 predict that

$$\log(LC50(t)) = m \log(K_{ow}) + b, \qquad (24)$$

where $-1.131 < m < -0.944$ and this result agrees with Veith et al. (1983) (see section III.4 below), FGETS predicts the narcotic death of fish as soon as the toxicant's chemical activity in the aqueous blood attains a predetermined threshold.

III. MODEL PARAMETERIZATION

Since reliable application of a model depends ultimately on its assumptions and parameterization, important assumptions used to parameterize the above equations follow.

III.1. Equation 1

Parameterization of Equation 1 depends on the fish's gill morphometry not only via the total gill surface area, S_g, but also by way of the conductance, k_w, which depends on both the spacing, d (cm), between lamellae and the mean length, l (cm), of individual lamellae. In general, each of these gill dimensions is dependent on the fish's body size according to the allometric functions, S_2

$$S_g = s_1 W^{d_2} \quad (25)$$

$$d = d_1 W^{i_2} \quad \text{and} \quad (26)$$

$$l = l_1 W \quad (27)$$

Although allometric coefficients and exponents for total gill surface areas are readily available in the literature and have been tabulated by Hughes (1972, 1984), de Jager and Dekkers (1976) and in Table I herein, allometric parameters for interlamellar distances and lamellar lengths seldom are reported. Fortunately, however, estimates of d_1 and d_2 often can be made using the relationship,

$$d = 0.102\ \rho^{-1.142} \quad (28)$$

where ρ is the density of secondary lamellae on one side of the fish's gill filament (i.e., number of lamellae/mm of gill filament), since many gill morphometric studies do report parameter values for the allometric function,

$$\rho = \rho_1 W^{\rho_2} \quad (29)$$

Equation 28 was exercised for 18 species of fish reported by Saunders (1962)

and Hughes (1966) and tabulated values for p_1 and p_2 are reported by Hughes (1972, 1984) and in Table 1. Finally, since allometric regressions for lamellar lengths virtually are unreported in the literature (for exceptions see Hughes 1984 and Stevens and Lightfoot 1986), a generalized allometric relationship for this gill dimension can be calculated again using data from Saunders (1962) and Hughes (1966) as

$$l = 0.0187\ w^{0.208} \qquad (30)$$

Since characterization of chemical uptake and excretion across a fish's gill can be formalized as a problem dealing with mass exchange from laminar water flow between adjacent secondary lamellae that form 'lamellar channels', methods that have been used traditionally to analyze convective mass transfer within arbitrarily shaped channels should provide the means to estimate the interlamellar conductances, k_w. In general, both analytical and numerical solutions to problems concerning such transport phenomena have been expressed as functions of dimensionless variables known as the Sherwood number, which can be defined as

$$N_{Sh} = D / (h\ k) \qquad (31)$$

where D is diffusivity (cm^2/sec) of the chemical being transported, k is the chemical's conductance (cm/sec) to and from the walls of the channel, and h is the channel's hydraulic radius (cm) (see Kays 1966). Clearly, given any three quantities in this equation, it is simple to calculate the fourth and, in fact, this is precisely how the interlamellar conductance can be estimated. To make such calculations, however, a fixed geometry and set of relevant boundary conditions for the lamellar channels must be specified. Although lamellar channels have been considered analogous to rectangular ducts (see Hughes 1966), because they generally have very high aspect ratios (i.e., mean lamellar height/ interlamellar distance), they can also be considered without loss of generality

to be essentially parallel plates. This assumed geometry means not only that the hydraulic radius of the lamellar channels is simply the interlamellar distance, d(cm), but also that Sherwood numbers for lamellar chemical exchange can be estimated using previously published results for convective mass transfer between permeable flat plates (Colton et al. 1971, Ingham 1984). Since chemicals are exchanged across fish gills by a counter current mechanism, a constant diffusion gradient is probably maintained between the interlamellar water and the capillary blood along the length of the secondary lamellae (see Layton 1987). Consequently the relevant boundary condition for estimating lamellar Sherwood numbers would be that of constant flux.

Local Sherwood numbers at any distance, z, from the entrance of a lamellar channel can be expressed as functions of the dimensionless length,

$$x(z) = z\ D_{..} / (d^2\ v), \tag{32}$$

where v is the mean flow velocity (cm/sec) between the lamellae, and in particular

$$N_{Sh}(z) = \begin{cases} 1.1829\ x(z)^{-1/3}, & \text{if } x(z)<0.1 \\ 3.7704 & \text{otherwise} \end{cases} \tag{33}$$

(see Colton et al. 1971). Chemical exchange along the entire length of the lamellar channels can be characterized with the mean Sherwood number,

$$N_{Sh} = \frac{1}{1} \int_0^1 N_{Sh}(z)dz \tag{34}$$

Depending on the magnitude of the channel's dimensionless length, the mean lamellar Sherwood number assumes one of two distinct forms. That is, when $x(1) < 0.1$, then

$$N_{Sh} = 1.7744\ x(1)^{-1/3}, \tag{35}$$

whereas if $x(1) > 0.1$, then

$$N_{Sh} = 3.7704 + 0.005232/x(1). \tag{36}$$

In either case, if the hydrodynamics of lamellar flow is then modeled as Poisuellian slit flow and in particular if

$$v = (0.5\ d)^2\ \Delta\ P/(3\ \mu\ l) \qquad (37)$$

where Δ P is the pressure drop across the gill (i.e., approximately 500 dynes/cm^2), and μ is the dynamic viscosity of water (i.e., 0.01 poise) (Hughes 1966, Lauder 1984, Stevens and Lightfoot 1986, Barber et al. 1987), then the lamellar Sherwood number given by Equations 35 and 36 can be expressed as a function of only chemical diffusivity, interlamellar distance, and lamellar length.

The actual interlamellar conductance for Equation 1 can now be estimated by substituting either Equation 35 or 36 into Equation 31, setting d equal to h, and solving for $k = k_w$. Since the units of this conductance will be cm/sec, it must be time-scaled appropriately for use in Equation 1.

III.2. Equation 3

Reasonable choices for the partition coefficients, K_l and K_s, are assumed to be the triolein/water partition coefficient, K_{tw}, and a organic carbon/water partition coefficient, K_{oc}, respectively. Since both K_{tw} and K_{oc} are collinear with the n-octanol/water partition coefficient, K_{ow}, however, Equation 3 is effectively parameterized by K_{ow} according to the relationships,

$$K_l = K_{tw} = 1.44\ K_{ow} \quad \text{and} \qquad (38)$$

$$K_s = K_{oc} = 0.40\ K_{ow} \qquad (39)$$

(Karickhoff 1981, Patton et al. 1984, Chiou 1985). If K_{oc} is equated to K_s, Equation 3 must be modified slightly, i.e.,

$$C_f = B_f\ /\ W = (P_a + P_l\ K_l + P_s\ P_{oc}\ K_{oc})\ C_a, \qquad (40)$$

where P_{oc} is the fraction of the structural organic matter that is organic carbon. FGETS assumes that P_{oc} equals 0.55.

Because a fish's lipid fraction, P_l, is generally a user input to FGETS (see Section IV.1 regarding "$p_l$fish" below), it is important for the parameterization of Equations 3 and 4 to know empirical or functional relationships between P_l and the fish's aqueous and structural fractions, P_a and P_s, since P_l is being treated essentially as an independent variable. In general, the empirical relation between P_l and P_a can be described adequately by

$$P_a = a_0 - a_1 P_l \tag{41}$$

where a_0 and a_1 are positive constants (Eschmeyer and Philips 1965, Love 1970, Elliott 1976, Craig 1977, Shubina and Rychagova 1982, Beamish and Legrow 1983, Gill and Weatherley 1983, Weatherley and Gill 1983). Since of the sum of P_a, P_l, and P_s must be unity, this relationship consequently demands that

$$P_s = (1 - a_0) - (1 - a_1) P_l. \tag{42}$$

For salmonid fishes, means for a_0 and a_1 are approximately 0.85 and 1.5, respectively, and presently these values are used to parameterize FGETS. Consequently, using these assumed values of a_0 and a_1 and Equations 38 and 39 FGETS estimates a fish's bioconcentration factor (approximately) as

$$BCF = (1.33\ Pl + 0.033)\ K_{OW}. \tag{43}$$

III.3. Equations 11 and 12

A fish's total intestinal surface area, S_i, like its gill surface area should depend allometrically on its body weight. Unlike gill morphometric studies, however, only a handful of studies have reported such morphometric relationships for fish intestine. These are summarized by Pauly (1981) and Kapoor et al. (1975). The parameterization of S_i is further complicated by the uncertainty of what particular anatomical surface area most closely corresponds to the intestine's effective surface area. For example, results of Wilson and Dietschy (1974) indicate that the intestine's effective surface is greater than

the outside surface area of the intestinal serosa but much less than the internal surface area of the intestinal mucosa. Allometric regressions for these two surface areas are summarized in Table 2. Because it is unclear whether the differences between the coefficients in Table 2 are due to type of surface area measured or to the food habits of the fish, FGETS arbitrarily uses the surface area of the outer intestine to parameterize S_i.

Because the movement of food through the gastrointestinal tract is so slow, an expression for intestinal conductance, k_i, does not require a term like a Sherwood number to account for forced convection of the intestinal contents. Consequently, this conductance can be defined simply as

$$k_i = D/b \qquad (44)$$

where D is again the chemical's aqueous diffusivity (cm^2/sec) and b is the barrier thickness (cm) associated with intestinal transport. This conductance must be scaled to cm^2/day for use in Equation 11. Presently, FGETS assumes a constant barrier thickness for all fish and chemicals equal to 50 micrometers (see Wilson and Dietschy 1974).

III.4. Equation 21

Recall that to estimate accurately the lethal chemical activity, LA, by equation 20, it is essential that the fish essentially be equilibrated with the water. Using the formalism of the gill exchange model summarized in section II.1, this requires that

$$C_a/C_w = 1 - e = (1 - \exp(-(k_1\ t)/BCF) \qquad (45)$$

where $k_1 = (S_g\ k_w)/W$ is the fish's first order uptake rate for the chemical. Since the only physio-chemical property that these uptake rates depend upon is chemical diffusivity, which varies only slightly between chemicals, k_1 is essentially a constant for a given size of fish (see for example Opperhuizen

1986) and consequently Equation 45 essentially depends only on the fish's lipid fraction and the chemical's K_{OW} via BCF. If ε equals 0.01 (i.e., the fish is 99% equilibrated), then for 30-day-old fathead minnows like those used by Veith et al. (1983), LA should be estimated using only LC50 (96 hr)'s for chemical's with log K_{OW}<4. In particular, because 30-day-old fathead minnows typically have lipid fractions (p_1) and daily uptake rates (k_1) approximately equal to 0.04 and 1000, respectively (Call et al. 1980, Eaton et al. 1983), for a 96-hour exposure Equation 45 becomes

$$K_{OW} = - 4000/(0.11\ ln(\varepsilon)) \qquad (46)$$

(see Equation 43). Therefore, if ε equals 0.01, chemical concentrations in fish and water will be equilibrated only for chemicals whose logP is less than 3.89.

IV. MODEL VALIDATION

Aqueous uptake and elimination of organic chemicals by fish generally have been described using the linear, first order model

$$dC_f/d_t = k_1\ C_w - k_2\ C_f, \qquad (47)$$

where k_1 and k_2 are rate constants with dimensions of reciprocal time. Since chemical concentrations in fish may decrease due to 1) growth of the fish (i.e., biodilution); 2) branchial, fecal, or urinary excretion; and 3) metabolic transformation, k_2 is, in general, the sum of at least five individual transfer rates, i.e.,

$$k_2 = \gamma + \varepsilon_g + \varepsilon_f + \varepsilon_u + \mu \qquad (48)$$

where γ is the fish's specific growth rate ($W^{-1}\ dW/dt$); $\varepsilon_g + \varepsilon_f + \varepsilon_u$ are the fish's excretion rates via the gills, feces, and urine, respectively; and μ is the chemical's rate of metabolic transformation. If for the moment the gills are assumed to be the principle excretory organ for the elimination

of nonpolar, nonmetabolized organic chemicals, then this equation can be simplified and rewritten as

$$\varepsilon_g = k_2 - \gamma \qquad (49)$$

Since the gill exchange component of FGETS predicts that ε_g equals $(S_g\ k_w)/(W\ BCF)$, FGETS could be validated initially by comparing these predicted rates to $(k_2 - \gamma)$ that can be calculated from the literature. Using published data for rainbow trout, Salmo gairdneri, (Branson et al. 1975; Neely 1979; Niimi and Cho 1981; Niimi and Oliver 1983; Oliver and Niimi 1983, 1984, 1985; Niimi and Palazzo 1985; Branson et al. 1975, 1985; Niimi 1986) the following functional regression was calculated

$$\log(k_2 - \gamma) = 0.919\ \log(S_g\ k_w)/(W\ BCF) - 0.429\ (n=68;\ r=0.75) \qquad (50)$$

Because the 95% confidence interval for this regression's slope is (1.15, 0.74), the predicted gill excretion rates are directly proportional to $(k_2 - \gamma)$ and in particular

$$k_2 - \gamma = (0.37\ S_g\ k_w)/(W\ BCF) \qquad (51)$$

This result is quite remarkable because, under nominal conditions, the functional surface area of fish gills has been estimated to be approximately 36% of their anatomical area which S_g measures (Booth 1978, Duthie and Hughes 1987, Gehrke 1987).

Clearly, if the majority of a fish's excretion is not branchial, the foregoing analysis would be fortuitous. There are, however, theoretical considerations to support the assumption that the gills are indeed a fish's principle excretory organ for such chemicals. The relative contribution of branchial and fecal excretion can be estimated by the ratio of the mass flux (E_g = mass chemical/day) across the gills to the fecal excretory flux (E_f = mass chemical/day) when contaminated trout are placed in clean water and fed clean food

ad libitum. If fecal excretion is modeled kinetically (i.e., Equation 11), the following inequality can be calculated

$$E_g/E_f = (S_g\ k_w\ C_a)/(S_i\ k_i\ C_a) = (S_g\ N_{Sh}\ b)/(S_i\ d) > (S_g\ 3.77\ b)/(S_i\ d) \quad (52)$$

For trout this inequality becomes

$$E_g/E_f > 19.23\ W^{0.339} \quad (53)$$

If this relationship is adjusted for the trout's functional gill area, i.e., 0.36 S_g, then, for 1 kg trout like those studied by Niimi and Oliver (1983), branchial excretion would be estimated to be at least 70 times greater than the trout's fecal excretion. Although this calculation supports the assumed importance of gill excretion, it is at odds with results reported by McKim and Heath (1983) and McKim et al. (1986).

Qualitative validation of FGETS was established by simulating the bioaccumulation of Aroclor 1254 by Lake Michigan lake trout (Salvelinus namaycush) assuming first gill exchange only and then joint gill and food exchange. Appendix C presents the FGETS user file used for this model application. Inspection of the simulation results presented in Appendix D shows that FGETS accurately reproduced the bioaccumulation of Aroclor 1254 by lake trout for fish up to 6 years old when joint kinetic exchange is assumed. The observed whole body concentrations of PCB's indicated in these FGETS plots are data for fish collected in 1971 (see Thomann and Connolly 1984). The failure of FGETS to predict whole body concentration of PCB's in older lake trout is probably due to the fact that these older 1971 trout were exposed to water concentrations that were historically higher than 8.5 ng/l.

Thomann and Connolly (1984) also constructed a bioaccumulation model of PCB's by Lake Michigan lake trout. Although their model also fits observed

data, their model indicates that gill uptake is insignificant when compared with PCB accumulation via the food chain. In particular, Thomann and Connolly concluded that 99% of the total body burden of PCB was accumulated through food. This conclusion conflicts with FGETS's prediction that the ratio of gill uptake to food uptake is approximately 1:3. Acknowledgment of this difference is important if heterogeneous, time varying exposures, instead of constant PCB exposure scenarios, are simulated.

V. CONCLUSION AND PROSPECTUS

Initial analysis indicates that FGETS can simulate observed patterns of bioaccumulation and depuration of a single, nonpolar, slowly or nonmetabolized organic pollutant by individual fish quite well. Extensions planned for FGETS include:

A. Simulation of the bioaccumulation of mixtures of two or more nonpolar, nonmetabolized chemicals simultaneously.

B. Integration of FGETS to realistic predator-prey models to more accurately describe food chain exposure.

C. Incorporation of models for the metabolic transformation of organic pollutants.

D. Modification of FGETS to model kinetic exchange of polar or charged organics.

E. Consideration of nonkinetic mechanisms that affect whole body concentrations of organic chemical -- such as the rapid catabolism or depuration the lipid reserves associated with reproduction.

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Table 1. Summary of allometric parameters for gill surface area and lamellar density.

	s_1	s_2	ρ_1	ρ_2	source
Anabas testudineus	5.56	0.615	36.5	-0.152	Hughes (1972)
baracuda	0.274	1.281	-999*	-999	Hughes (1980)
Blennius pholis	7.63	0.849	28.3	-0.139	Milton (1971)
Boleophthalmus boddarti	0.93	1.050	53.1	-0.229	Hughes and Al-Kadhomiy (1986)
Botia lohachata	9.13	0.700	78.0	-0.005	Sharma et al. (1982)
Catostomus commersonii	7.98	0.639	-999	-999	de Jager and Dekkers (1976)
Catostomus commersonii	11.17	0.587	25.0	-0.107	Saunders (1962)
Channa punctata	4.70	0.592	-999	-999	Hakim et al. (1978)
Cobitis taenia	4.67	0.864	45.5	0.000	Robotham (1978)
Coryphaena hippurus	52.08	0.713	33.8	-0.036	Hughes (1972)
Cyprinus carpio	8.46	0.794	32.2	-0.079	Oikawa and Itazawa (1985)
Gambusia affinis	2.33	0.873	-999	-999	Murphy and Murphy (1971)
Ictalurus nebulosa	2.65	0.845	-999	-999	de Jager and Dekkers (1976)
Ictalurus nebulosa	4.98	0.728	15.8	-0.091	Saunders (1962)
Katsuwonus pelamis	56.75	0.841	59.0	-0.076	Muir and Hughes (1969)
Leiopotherapon unicolor	4.68	1.040	41.2	-0.087	Gehrke (1987)
Lepidocephalichthys guntea	4.94	0.745	45.0	-0.221	Singh et al. (1981)
Lepisosteus sp.	3.94	0.738	38.8	-0.060	Landolt and Hill (1975)
Micropterus dolomieu	7.31	0.820	30.0	-0.062	Price (1931)

Table 1. continued

Noemachceilus barbatulus	3.60	0.577	36.4	0.000	Robotham (1978)
Opsanus tau	5.60	0.790	16.0	-0.075	Hughes and Gray (1972)
Platichthys flesus	6.36	0.824	-999	-999	Hughes and Al-Kadhomiy (1986)
Raja clavata	-999	0.970	-999	-0.154	Hughes et al. (1986)
Saccobranchus fossilis	1.86	0.746	31.6	-0.095	Hughes et al. (1974)
Salmo gairdneri	3.90	0.900	-999	-999	de Jager and Dekkers (1976)
Salmo gairdneri	1.84	1.125	-999	-999	Niimi and Morgan (1980)
Salmo gairdneri	3.14	0.932	27.5	-0.064	Hughes (1984)
Scomber scomber	4.42	0.997	27.1	0.023	Hughes (1972)
Scyliorhinus canicula	2.62	0.961	17.2	-0.071	Hughes (1972)
Scyliorhinus stellaris	-999	0.779	-999	-0.167	Hughes et al. (1986)
Stizostedion vitreum	0.80	1.129	-999	-999	Niimi and Morgan (1980)
Thunnus thynnus	24.43	0.901	60.9	-0.089	Muir and Hughes (1969)
Tinca tinca	12.20	0.657	-999	-999	de Jager and Dekkers (1976)
Tinca tinca	8.67	0.698	25.5	-0.030	Hughes (1972)
Torpedo marmorata	1.18	0.937	34.2	-0.167	hughes (1978)
geometric mean	5.50	0.816	33.7	-0.092	

* "-999" indicates that the parameter was not available.

Table 2. Summary of allometric paramters intestinal surface areas of fish. Parenthetic letters signify the parameters are for mucosal surface areas, (m), or serosal surface area, (s).

	s_1	s_2	
Gobio gogio(m)	6.339	0.591	Pauly (1981)
Rutilus rutilus (m)	6.223	0.580	Pauly (1981)
Salmo trutta (s)	1.198	0.571	Burnstock (1959)
Solea solea (s)	2.12	0.57	Ursin (1967)
various species (m)	1.83	0.92	Al-Hussaini (1949) Unnithan (1965) Gohar and Latiff (1959) Montgomery (1976))

Appendix A. Definition the variables appearing the the text.

b = barrier thickness for diffusion across the intestine (cm);
BCF= (P_a + P_l K_l + P_s K_s) = bioconcentration factor in whole fish assuming gill exchange only (dimensionless);
B_i = total burden of a chemical in food residing in the intestine (micro g);
B_f = total body burden of a chemical (micro g / fish);
C_a = concentration of a chemical in the aqueous fraction of the fish (ppm);
C_l = concentration of a chemical in the lipid fraction of the fish (ppm);
C_f = whole body concentration of a chemical (ppm = micro g / g live fish);
C_s = concentration of a chemical in the structural fraction of the fish (ppm);
C_w = concentration of a chemical in water (ppm);
d = mean interlamellar distance (cm);
D = aqueous diffusivity (cm^2/sec);
E = egestive flux (g /day);
F = ad libitum feeding flux (g /day);
h = hydraulic radius of a channel (cm) = 2 (channel cross section area)/ (channel perimeter);
I = mass of food resident in the intestine (g);
J_g = diffusive flux of chemical across the gills (microgram/cm^2/day);
k_w = chemical conductance through interlamellar water (cm /day or cm / sec);
K_l = partition coefficient between lipid and water (dimensionless);
K_{oc}= partition coefficient between bulk organic carbon and water (dimensionless);
K_{ow}= partition coefficient between n-octanol and water matter (dimensionless);
K_s = partition coefficient between structural matter and water (dimensionless);
l = mean length of lamellae (cm);
P_a = fraction of whole fish that is aqueous water (dimensionless);
P_l = fraction of whole fish that is lipid(dimensionless);
P_s = fraction of whole fish that is structural organic matter (dimensionless);
R = routine respiratory flux (g /day);
SDA= respiratory flux due to specific dynamic action (g /day);
S_i = total intestinal surface area (cm^2);
S_g = total gill surface area (cm^2);
v = mean velocity of lamellar flow (cm/sec)
W = live body weight of fish (g);
α = assimilation efficiency of food (dimensionless);
β = assimilation efficiency of chemical from food (dimensionless);
μ = dynamic viscosity (poises);
ρ = density of secondary lamellae on gill filaments (# lamellae/mm);

Appendix B. Abbreviated User Guide to FGETS.

B.1 User Input

FGETS requires a user input file which has the following general format:

```
c
c file  :  FGETS.DAT
c
      / toxlab          string
      / molwt           number
      / logp            number
      / mp              number
      / spplab          string
      / famlab          string
      / liflab          string
      / act-gill        number
      / wt              number
      / wtunits         string
      / mod$opt         string1 string2 string3
      / plfish          string number1 number2
      / cfish           number
      / cfunits         string
      / cwater          string1 string2 number1 number2 number3 number4
      / cwunits         string
      / temp            string1 string2 number1 number2 number3 number4
      / cprey           number1
      / plprey          number1
      / bmf             number1
      / time            number1 number2
      / tunits          string
/ end.
```

FGETS treats all records that begin with a "c" or "!" in column 1 as comments. The exclamation symbol "!" can also be used anywhere in the record field to start an end-of-line comment. Therefore users can document FGETS input file in as much detail as desired. All records that begin with "/" are considered to define model input and may appear in any order. Blanks before or after the input slash delimiter are not significant. Each input slash is followed by a keyword or phrase, as indicated above, which identifies record's data. Keywords must be spelled in full without any embedded blanks and must be separated from the record's remaining information by at least one blank character. Letter case is not significant since each record is transliterated to lower case. A brief description of each of these input records follows.

RECORD: "/ toxlab string"

This record simply specifies the name of the chemical whose exchange kinetics is being simulated and is used for output purposes only.

RECORD: "/ logp number"

This record specifies the chemical's log Kow, where Kow is the chemical n-octanol/water partition coefficient.

RECORD: "/ molwt number"

This record specifies the chemical's molecular weight(i.e., g/mole).

RECORD: "/ mp number"

This record specifies the chemical's melting point(i.e., Celsius). This data together with the chemical's logp is used by PGETS to calculate the toxicant's chemical activity.

RECORD: "/ spplab string"

This record specifies the scientific name of the fish being modeled by PGETS. For example, rainbow trout must be specified as Salmo gairdneri. This record and records, "/ famlab ..." and "/ liflab ...", are used to extract appropriate gill morphometric parameters from the data base file, MORPHO.DAT, for the simulation.

RECORD: "/ famlab string"

This record specifies the family of the fish being modeled by PGETS.

RECORD: "/ liflab string"

This record specifies the life form of the fish being by PGETS. Presently, the only recognized input for string is "freshwater" or "marine".

RECORD: "/ act-gill number"

This record specifies the fraction of the fish's anatomical gill that is physiologically active. Typical values for the variable range between 1/3 and 1/2 (Booth 1978, Piiper et al. 1986, Duthie and Hughes 1987). This value is used to adjust the kinetic exchange rates predicted by PGETS (see Barber et al. 1987).

RECORD: "/ wt number"

This record specifies the initial live weight of the fish being modeled by PGETS. The units wt (i.e., g, kg, pounds, oz, etc.) are specified by the record, "/ wtunits string".

RECORD: "/ wtunits string"

See RECORD: "/ wt number" above.

RECORD: "/ mod$opt string1 string2 string3"

This record specifies various modeling options and maybe input in any order.

String="growth(arg)" specifies the function, g, that FGETS will use to model the fish's growth, i.e., dW/dt = g, where W is the fish's gram live weight and t is time in days. Presently, there are three different options. If arg="linear, number", then linear growth, i.e.,

$$dW/dt = number * W \qquad (g.1)$$

is simulated. When arg="allometric", then fish growth essentially is modeled by

$$dW/dt = \alpha * F - R \qquad (g.2)$$

where alpha is the fish's assimilation efficiency, and F and R are the fish's daily feeding and respiratory fluxes, which are described by the allometric functions, F=f1*W**f2 and R=r1*W**r2, respectively. If arg="holling", fish growth also is modeled by (g.2) but with the modification that the fish's feeding is described by a Holling type formulation, i.e.,

$$F = \phi * (S_{max} - S) \qquad (g.3)$$

where S_{max} is the fish's maximum stomach/gut capacity and S is the amount of food presently resident in the gut, which is itself modeled by

$$dS/dt = F - G \qquad (g.4)$$

where G=g1*S**g2 represent gastric evacuation (Holling 1966, Ware 1972, Jobling 1986). When the fish's growth is modeled by either the "allometric" or "holling" option, FGETS attempts to retrieve all the required physiological parameters form the data file, PHYSIO.DAT, based on either the fish's family or species. If parameters do not exists in the data file, then FGETS terminates with an appropriate error message.

String="gill" specifies that FGETS will simulate bioaccumulation assuming there is only gill exchange of the toxicant.

String="joint(arg)" specifies that FGETS will simulate bioaccumulation assuming there is joint gill and food exchange of the toxicant. Both options, "joint" and "gill", can be specified concurrently.

RECORD: "/ plfish string number1 number2"

This record specifies the fraction of the fish's live weight that is lipid. If string equals "database", FGETS estimates the fish's lipid

fraction using an allometric function,

$$plfish = p_1 * W(g\ live)^{**} p_2$$

that is retrieved from the FGETS database and no number needs to be specified. Alternatively, users can input their own allometric function by specifying "/ plfish allometric f_1 f_2 ". If this option is selected, FGETS assumes that

$$plfish = f_1 * W^{**} f_2$$

where Wt has units of wt$units below. There are two other valid options for string. If "/ plfish constant p_1" is input, the fish's lipid is held constant during the simulation while if "/plfish exp f_1 f_2 " is input, the fish's lipid fraction is generated dynamically as

$$plfish = f_1 * exp\ (f_2 * t)$$

where the unit of t are specified by t$units below.

RECORD: "/ cfish number"

This record specifies the fish's initial whole body concentration on a live weight basis of the chemical. The units of cfish are specified by "/ cfunits ...."

RECORD: "/ cfunits string"

This record specifies the units of cfish. FGETS converts cfish from cfunits to ppm for internal calculation and model output.

RECORD: "/ plprey number"

This record specifies the fractional lipid content of the fish's prey (also see "RECORD: "/ plfish number" above). FGETS attempts to assign a default value for this variable if it is not input or is specified as a negative number. Presently, default values are available only for salmonids, which are assumed to be piscivores. These defaults are assigned by SUBROUTINE FODWEB.

RECORD: "/ cprey number"

This record specifies the toxicant's concentration in the fish's prey (also see "RECORD: "/ cfish number" above). The units of this record are assumed to be the same as those specified for record, "/cfish ...". FGETS attempts to assign a default value for this variable if it is not input or is specified as a negative number. This default is assigned by SUBROUTINE FODWEB assuming that the prey is thermodynamically equilibrated with the water. This default can be adjusted by record, "/bmf ...." See below.

RECORD: "/ bmf number"

This record specifies the bio-agnification factor (bmf) for the fish's prey and is required only if the default option for cprey is used. The default value for this record is bmf=1. If the user wants the prey to be biomagnified above thermodynamic equilibrium, then bmf>1. On the other hand, if the user assumes that the prey has not yet equilibrated with the water, bmf<1. Based on preliminary analysis (Barber et al. 1987) typically 0<bmf<5.

RECORD: "/ cwater string1 string2 number1 number2 number3 number4

This record specifies the temporal dynamics of the chemical's dissolved water concentration. Valid expressions for string1 are either "file" or "function." If string1 equals "file", then FGETS will read time series data for the chemical's dissolved water concentration from the file whose name is string2. If string1 equals "function," then FGETS will generate dynamic dissolved water concentrations of the chemical according to the time function specified by string2. In this case, there are presently only three valid expressions for string2 , i.e., "constant," "sin," or "exp."

To illustrate these alternative inputs let cw(t) denotes the chemical's water concentration at time t. When the record "/ cwater ..." is specified as "/ cwater file abc.dat," FGETS will read time series of chemical concentrations from the file abc.dat using a FORTRAN free formated read statement that is equivalent to:

```
READ (JTABLE, *, END=1120) t, cw(t)
```

where file abc.dat is attached to unit JTABLE. FGETS requires that the records of this file be ordered according to ascending time, i.e., t(i) < t(i+1) for all i-th records, since FGETS linearly interpolates chemical concentrations between consecutive times, t(i) and t(i+1). See RECORD: "/ temp string1 string2 number1 number2 number3 number4" for special exception to this usage.

If "/ cwater function constant number1 " is specified, then FGETS will generate dissolved water concentrations as

$$cw(t) = number1$$

where number1 has units of cwunits. If "/cwater ..." is specified as "/ cwater function sin number1 number2 number3 number4," then FGETS will generate dissolved water concentrations as

$$cw(t) = number1 * \sin(number2 * t + number3) + number4$$

where number1 and number4 have units of cwunits and number2 has units of 1/tunits. Finally, if "/ cwater function exp number1 number2 number3 " is input, then FGETS generates dissolved water concentrations as

$$cw(t) = number1 * \exp(number2 * t) + number3$$

where number1 and number3 have units of cwunits and number2 has units of 1/tunits.

The units of cw(t) (e.g., ppm, mg/l, etc.) and of t (e.g., days, years, etc.) are specified by the records, "/ cwunits string" and "/tunits string", respectively. FGETS converts cw(t) from cwunits to ppm for internal calculations and model output by appropriately converting either time series data from file abc.dat or the parameters, number1,..., number4. The values, number1,...,number4, must be separated by one or more blanks.

RECORD: "/ temp string1 string2 number1 number2 number3 number4"

This record specifies the temporal dynamics of water temperature (Celsius). Data specified on this record is processed like record "/ cwater ...." For example, if temp(t) is the ambient water temperature at time t, and if "/ temp file xyz.dat" is specified, then FGETS will read time series of water temperatures from the file xyz.dat using a FORTRAN free formated read statement that is equivalent to

```
READ (JTABLE, *, END=1120) t, temp(t)
```

where file xyz.dat is attached to unit JTABLE. Again FGETS requires that the records of this file be ordered according to ascending time, i.e., t(i) < t(i+1) for all i-th records, since FGETS linearly interpolates water temperatures between all consecutive times, t(i) and t(i+1).

When a user has concomitant data for chemical concentration and water temperature, the files abc.dat and xyz.dat, specified by records, "/ cwater file ..." and "/ temp file ...", respectively, may be assigned to be the same. In this case FGETS will read time series of chemical concentrations and ambient water temperatures from the specified file using a FORTRAN free formated read statement that is equivalent to

```
READ (JTABLE, *, END=1120) t, cw(t), temp(t).
```

As before, if "/ temp function constant number1 " is specified, then FGETS will generate ambient water temperatures as

```
temp(t) = number1
```

where number1 has units of Celsius. If "/temp ..." is specified as "/ temp function sin number1 number2 number3 number4", then FGETS will generate ambient water temperatures as

```
temp(t) = number1*sin(number2*t+number3) + number4
```

where number1 and number4 have units of Celsius and number2 has units of 1/tunits. Finally, if "/ temp function exp number1 number2 number3 " is input, then FGETS generates ambient water temperatures as

```
temp(t) = number1*exp(number2*t) + number3
```

where number1 and number3 have units of Celsius and number2 has units of 1/tunits.

RECORD: "/ time number1 number2"

This record specifies the beginning time, number1, and ending time, number2, for the FGETS's simulation. The units of these times are specified by the record, "/ tunits string." FGETS converts these times into days for internal usage and subsequent model output. If the user does not specify number2, the the simulation's beginning time is assumed to be t=0 and number1 is assigned as the simulation's ending time.

RECORD: "/ tunits string"

This record specifies the time units (e.g., hours, days, years, etc.) associated with the user input records, "/ time ...," "/ cwater ...," and "/ temp ...." The time units associate with these three data records must be the same! The user must be careful to verify that the time units associated with these three records and any associated exposure files (see RECORD: "/ cwater ..." and RECORD: "/ temp ..." above) are indeed the same.

RECORD: "/ end."

This record specifies the end of a user input sequence.

B.2 Required Database Files

DATA FILE: MORPHO.DAT

This file contains morphometric data for the allometric functions:

s = gill area (cm**2) = s_1 * wt ** s_2;
ρ = # lamellae / mm gill filament = ρ_1 * wt ** ρ_2;
l = lamellar length (cm) = l_1 * wt ** l_2.

Data is organized in this file in sets of three records each. Each set represents morphological data for one species. The XXX-th set of MORPHO.DAT contains the following information:

XXX.1 species/family/lifeform
XXX.2 reference
XXX.3 s1 s2 ρ_1 ρ_2 l_1 l_2

A value of -999 designates that the parameter was not reported.

DATA FILE: PHYSIO.DAT

This file contains physiological data for the allometric functions:

cmax = maximum observed ingestion (gram/day) = cmax1 * wt ** cmax2;
gmax = maximum capacity of stomach (gram) = gmax1 * wt ** gmax2;
fsat = size of satiation meal consumed during (0, tsat), gram
= fsat1 * wt ** fsat2;
tsat = time (min) to satiation when feeding with an initially empty stomach;
= tsat1 * wt ** tsat2 + tsat3;
evac = stomach evacuation (gram/day) = evac1 * g ** evac2 ;
in general evac2 = 1/2, 2/3, or 1.0 (see jobling 1981);
imax = maximum intestinal capacity (gram) = imax1 * wt ** imax2;
o2 = routine respiration (mg o2 consumed/ hr) at temperature tref
= o2$1 * wt ** o2$2;
pl = fraction fat = p_{1_1} * wt ** p_{1_2} ;

as well as constant parameters:

alpha = assimilation efficiency;
rq = respiratory quotient 1 co2 respired/ 1 o2 consumed;
tref = physiological reference temperature (c);
q10 = q10 for temperature deviation from tref.

Data are organized in this file in sets of five records each. Each set represents physiological data for one species. The XXX-th set of MORPHO.DAT contains the following information:

XXX.1 species/family
XXX.2 reference
XXX.3 cmax1 cmax2 gmax1 gmax2 fsat1 fsat2 tsat1 tsat2 tsat3
XXX.4 imax1 imax2 evac1 evac2 alpha o2$1 o2$2 rq q10 tref
XXX.5 p_{1_1} p_{1_2}

A value of -999 designates that the parameter was not reported.

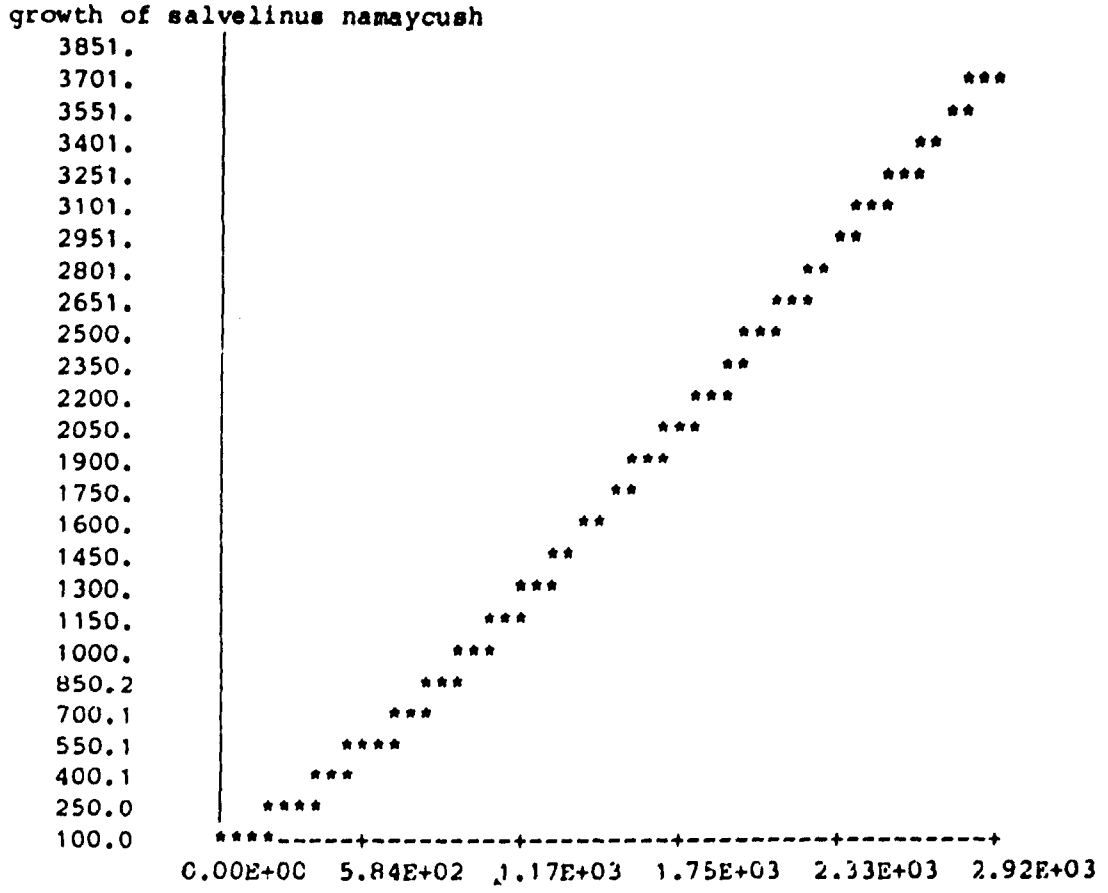
Appendix C. Example FGETS user input sequence.

```
c
c file  : lake_trout.dat
c update: 20-aug-1987 09:13:48
c
c notes concerning parameters:
c
c i. assume cw = (13+12.4+2.9+5.7)/4 = 8.5 ng/l based on:
c    cw = 13 ng/l (veith (1972) see weininger (1978));
c       = 12.4 ng/l calculated by weininger (1978)) assuming 60% of total
c         pcb reported by haile (1977) is particulate bound;
c       = 2.9 ng/l mean of 8 samples for aug 1979 (range 1.1-11.2) reported
c         by rice et al. (1982);
c       = 5.7 ng/l mean of 4 samples for apr 1980 (range 4.7-7.1) reported
c         by rice et al. (1982);
c
c     note that neely (1977) and jensen et al. (1982) assumed cw = 10 ng/l
c     while thomann and connolly (1984) assumed cw = 5 ng/l;
c     note also that doskey and andren (1981) report 2.6e-11 molar aroclor 1254
c     in lake michigan which converts to 8.48 n/l (see ii.1 below).
c
c ii. physico-chemical properties of aroclor 1254: aroclor 1254 is by weight
c     54% chlorine. since tetra-, penta-, and hexa-pcb's are 48.6%, 54.3%,
c     and 59.0% chlorine, respectively, assume aroclor 1254 is essentially
c     a penta-pcb. therefore:
c     1) molwt = 326.25 g/mole.
c     2) mp    = 102.6 celsius, i.e., mean of 5 penta-pcb's from mackay
c        et al. (1982);
c     3) logp  = 6.62 based on the following considerations:
c        mean solubility of aroclor 1254 1.825e-2 mg/l (schnoor et al. 1987),
c        which converts to 5.594e-8 molar (assuming 326 g/mole). consequently,
c
c        log(5.594e-8)=-0.944*logp - 0.01*102.6 + 0.323 ==> logp = 6.94
c
c                                or
c
c        logp=-0.862(log(5.5948e-8) + 0.01*(102.6-25)) + 0.710 = 6.29,
c
c        see yalkowsky et al. (1983) and chiou and schmedding (1982),
c        respectively. therefore assume logp=(6.94+6.29)/2=6.62. note
c        a mean calculated logp for penta-pcb is 7.47 (n=5 see yalkowsky
c        et al. 1983) while a mean measured logp for penta-pcb's is 6.11
c        (n=3 see miller et al. (1985) and chiou (1985)).therefore logp
c        equals (7.47+6.11)/2 = 6.79.
c
c references:
c  -chiou 1985. environ.sci.technol. 19:57-62.
c  -doskey and arden 1981. environ.sci.technol. 15:705-710.
c  -haile 1977.
c  -jensen et al. 1982. can.j.fish.aquat.sci. 39:700-709.
c  -mackay et al. 1980. chemosphere 9:257-264.
c  -miller et al. 1985. environ.sci.technol. 19:522-529.
c  -neely 1977. sci. total environ. 7:117-129
c  -rice et al. 1982. j. great lake res. 8:265-270.
c  -schnoor et al. 1987. epa/600/3-87/015.
c  -stewart et al. 1983. can.j.fish.aquat.sci. 40:681-698.
c  -thomann and connolly 1984. environ.sci.technol. 18:65-71.
c  -veith 1972.
c  -weininger 1978.
c  -yalkowsky et al. 1983. residue reviews 85:43-55.
```

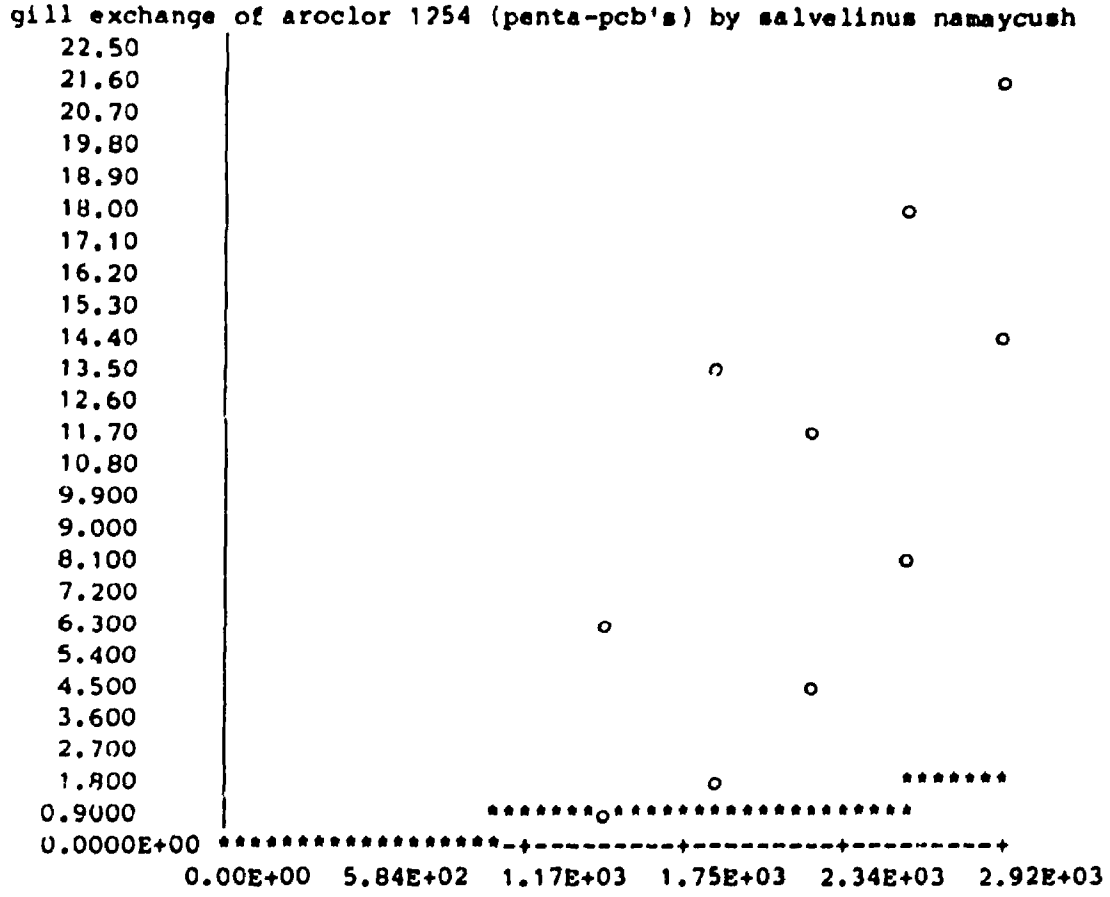
```
      / toxlab      aroclor 1254 (penta-pcb's)
      / molwt       326.25
      / logp        6.62
      / mp          100.0
      / spplab      salvelinus namaycush
      / famlab      salmonidae
      / liflab      freshwater
      / wt          100.0
      / wtunits     g
      / mod$opt     growth(holling, 0.5) gill joint(kinetic)
      / plfish      database
      / cfish       0.0
      / cfunits     ppm
      / cwater      function  constant 8.5
      / cwunits     ng / l
      / time        8
      / tunits      year
      / temp        function  sin 4.0 6.283185 0.0 8.0  ! frequency in year**-1
      / act-gill    0.37
      / cprey       5.0
      / plprey      0.07
      / bmf         1.0
c
c data as reported by thoman and connoly (1984) and stewart et al.(1983)
c     yr         cf(ppm)       wt(g live)
c
      4         4.0 +- 3.0    1710 +- 0.0
      5         8.0 +- 5.5    2800 +- 0.0
      6         8.5 +- 3.5    3590 +- 0.0
      7        13.5 +- 5.0    4310 +- 0.0
      8        18.5 +- 4.0    5180 +- 0.0
      / end.
```

Appendix D. Example FGETS output for user input presented in Appendix C.

```
***summary of user input specifications***

input           toxicant: aroclor 1254 (penta-pcb's)
input              molwt:    326.
input               logp:    6.62
input                 mp:    100.
input             cwater: cw(ppm) = 8.500E-06
input               temp: celsius = 4.00 * sin( 1.720E-02 * t(days) + 0.000E+00) + 8.
input             tstart:   0.000E+00 days
input               tend:   2.922E+03 days
input             fishid: salvelinus namaycush
input                wt0:    100.     live weight, g
input             growth: holling; c/cmax= 0.500
input             plfish: database function, pl = 2.158E-03 * w(g) ** 0.497
input              cfish:   0.000E+00 ppm
input       active$gill:   0.370
input              joint: kinetic
input             plprey:   7.000E-02
input                bmf:    1.00
input              cprey:    5.00

***parameters for narcotic toxicity***

model               lc50: 8.544E-04 ppm = 2.619E-09 molar = 1.508E-02 activity
model   water solubility: 1.708E-02 ppm = 5.236E-08 molar

***summary of parameters for fish growth***

model             mean temperature:    8.00      c
model       growth rate (g/ g/day):   0.270      * w(g) ** -0.787      (  1.250E-03)
model   ingestion rate (g/ g/ day):   0.263      * w(g) ** -0.602
model respiration rate (g/ g/ day):   9.886E-03 * w(g) ** -0.319

***summary of parameters for gill only exchange***

model    gill surface area (cm**2):    2.86      * w(g) **  0.983
model  interlamellar distance (cm):   2.343E-03 * w(g) **  7.306E-02
model          lamellar length(cm):   1.870E-02 * w(g) **  0.208
model      uptake rate, k1(1/ day):    512.      * w(g) ** -0.104      (   245.     )
model    excretion rate, k2(1/day):   1.087E-02 * w(g) ** -0.445      (  4.886E-04)

***summary of parameters for food exchange***

model       uptake rate, k1(1/day):   3.605E-03 * w(g) ** -0.136      (  1.396E-03)
model  elimination rate, k2(1/day):   1.537E-03 * w(g) ** -0.785      (  7.236E-06)
```



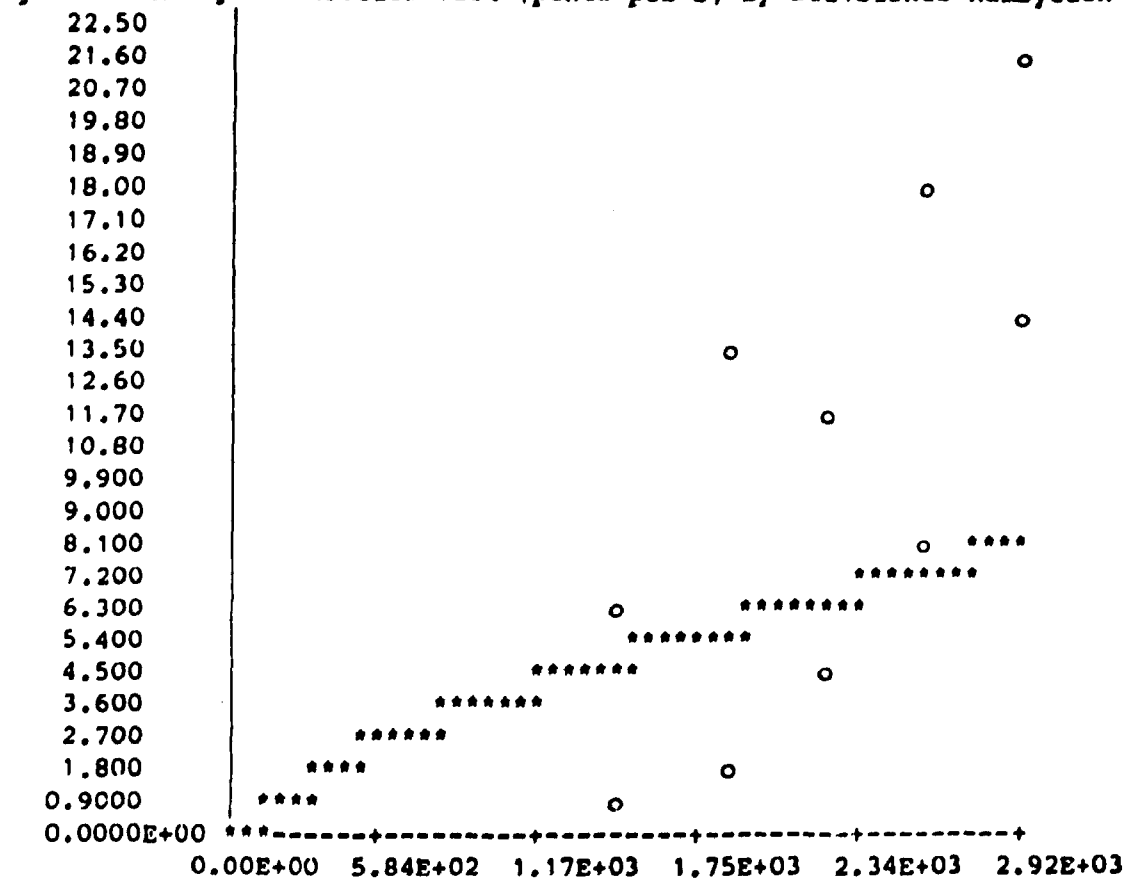
model	mean temperature:	8.00	c
model	total ingestion:	1.451E+04	g
model	total evacuation:	1.425E+04	g
model	total assimilation:	1.053E+04	g
model	total egestion:	3.699E+03	g
model	total respiration:	4.665E+03	g



x-axis: days
y-axis: whole body concentration (ppm)

model	mean water conc.:	8.500E-06	ppm
model	mean temperature:	8.00	c
model	total gill uptake:	1.048E+04	micro g
model	total gill excretion:	2.651E+03	micro g

joint exchange of aroclor 1254 (penta-pcb's) by salvelinus namaycush



x-axis: days
y-axis: whole body concentration (ppm)

model	mean water conc.:	8.500E-06	ppm
model	mean prey conc.:	5.00	ppm
model	prey bmf:	1.00	
model	mean temperature:	8.00	c
model	joint gill uptake:	1.048E+04	micro g
model	joint gill excretion:	1.156E+04	micro g
model	joint gut uptake:	3.369E+04	micro g
model	joint gut excretion:	118.	micro g