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Project Summary

FGETS (Food and Gill Exchange of Toxic Substances): A Simulation Model for Predicting Bioaccumulation of Nonpolar Organic Pollutants by Fish

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A FORTRAN program that *simulates the kinetic exchange of a* nonpolar, nonmetabolized organic chemical across fish gills and from contaminant food is described. The program is based on a set of diffusion and forced convection differential equations. Gill morphometric and physiological parameters are estimated by the program via two internal databases. The database of gill morphometry spans approximately 30 species, whereas the physiological database presently is complete only for salmonid fishes and rainbow trout (*Salmo gairdneri*).

This Project Summary was developed by EPA's Environmental Research Laboratory, Athens, GA, to announce key findings of the research project that is fully documented in a separate report (see Project Report ordering information at back).

Introduction

When aquatic ecosystems are polluted with organic chemicals, fish in those systems will bioaccumulate such substances both directly from the water and from their prey, which have likewise 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, then 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, GETS, which describes the uptake and depuration of organic toxicants across fish gills.

Development of the FGETS model is part of a four-laboratory ecological risk assessment research program. Contributing to the research program are scientists at EPA's Environmental Research Laboratories in Athens, GA, Corvallis, OR, Duluth, MN, and Gulf Breeze, FL.

FGETS itself is a FORTRAN simulation model that predicts temporal dynamics of a fish's whole body concentration, C_f (ppm = μg chemical/g live weight fish), of a nonmetabolized, organic chemical. The chemical is bioaccumulated either from water only, which is, perhaps, the predominant route of exchange during acute exposures,or

from water and food jointly, which is the more characteristic route for chronic exposures. These dynamics are calculated algebraically as the ratio of the fish's predicted total body burden, B_f = µg chemical/fish, to its live weight, W = g live/fish. The dynamics are simulated by a system of coupled differential equations.

In particular, fish growth is modeled using the mass balance equation,

$$dW/dt = F - E - R - SDA \quad (1)$$

where:

F = fish's feeding fluxes (g/day)
E = fish's egestive fluxes (g/day)
R = fish's respiratory fluxes (g/day)
SDA = fish's specific dynamic action (g/day)

The total body burden of a fish is modeled by

$$dB_f/dt = S_g J_g + J_1 = S_g k_w (C_w - C_a) + J_1 \quad (2)$$

where:

S_g = the fish's total gill area (cm^2)
J_g = the net diffusive flux across the gills (µg/cm^2/day)
J_1 = the net mass exchange across the fish's intestine from food (µg/day)
k_w = the chemical's mass conductance through the interlamellar water of the gills (cm/day)
C_w = the chemical's concentration in the environmental water (ppm)
C_a = the chemical's concentration in the fish's aqueous blood (ppm)

The gill exchange portion of equation 2 is simply a direct application of Fick's first law of diffusion FGETS allows a user to select one of three possible model formulations to represent chemical exchange from food. In particular, J_1 can be modeled assuming either a constant toxicant assimilation efficiency, in which the fish's feces and whole body are thermodynamically equilibrated, or a kinetic expression of Fick's first law of diffusion.

To use equation 2, a functional relationship between a chemical's concentration in whole fish and its aqueous fraction must be specified. To this end, fish are treated conceptually as a three-phase solvent consisting of water, lipid, and structural organic matter. It is further assumed that equilibration between these phases is rapid in comparison to exchange across the fish's gills and intestine. Consequently, the fish's whole body concentration of the chemical can be written as

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

where:

P_a = the aqueous fraction of the whole fish
P_l = the lipid fraction of the whole fish
K_l = partition coefficient between lipid and water (e.g., K_{ow})
P_s = the structural organic fraction of the whole fish
K_s = partition coefficient between lipid and structural organic matter(e.g., $K_{oc} = 0.4 K_{ow}$)

Note that if only gill exchange is considered, then the fish's bioconcentration factor, BCF = C_f/C_w is given by the weighted sum

$$BCF = P_a + P_l K_l + P_s K_s$$

Consequently, equation 2 can be rewritten as

$$dB_f/dt = S_g k_w (C_w - C_f/BCF) + J_1 = S_g k_w (C_w - B_f/(W\,BCF)) = J_1 \quad (2.a)$$

which shows explicitly how equations 1 and 2 are coupled.

Model Application

To use FGETS, a user must specify several input parameters:

1. the scientific name of the fish to be analyzed (e.g., *Salmo gairdneri*) the fish's family (e.g., Salmonidae), and the fish's life form (i.e. freshwater or marine),
2. the chemical molecular weight, molar volume, melting point, and log K_{OW} (i.e., logP),
3. the fish's initial live weight (g),
4. the fish's lipid content as a proportion of its total body weight (g lipid/g live weight),
5. the fish's initial whole body concentration of the chemical (i.e., µg chemical/g live weight fish, and
6. an exposure scenario, i.e., the chemical's aqueous concentration as well as the chemical's concentration in the fish's prey.

The fish's species name, family, and life form are used to assign the gill morphometric parameters that FGETS's subroutine, GILL$KW, uses to estimate the fish's net exchange rate (S k_w). These assignments are made by FGETS using a model data file, MORPHO.DAT. This file, which is supplied with FGETS contains coefficients and exponents f the allometric functions

S = total gill area, cm^2 = $s_1 W^{s2}$ an
ρ = # lamellae (mm gill filament)-1 = $r_1 W^{r2}$

where W is the fish's live weight (g).

From this data file, five geometri means are calculated by FGETS for eac of the values, s_1, s_2, r_1, and r_2. Fc example, FGETS calculates a geometri mean for s_1, first using all the dat reported in this file. Concurrently, FGET also calculates geometric means for s using only data records that have th same life form, family, genus, an species of the fish designated by th user. FGETS then attempts to assign s s_2, r_1, and r_2 using first the specie geometric means.

If, however, the species is nc represented in MORPHO.DAT, FGET then tries to assign the geometric mean that might have been calculated for th same genus as the desired species. I like fashion, if the genus is not found i the model data file, geometric means fc the fish's family are assigned. If thes assignments are not possible, th geometric means for the same life forr (i.e., freshwater versus marine) as th desired fish are used. The fish's specie name, family, and life form also are use to assign the physiological parameter (i.e., feeding and respiration rates assimilation efficiencies, etc.) that FGET retrieves from its physiological database PHYSIO.DAT.

FGETS is parameterized for particular chemical of concern b specifying the chemical's log K_{ov} molecular weight, molar volume, an melting point. The chemical's molecul volume is used to estimate its aqueou diffusivity, which is needed to estimat the conductance, k_w. The chemical's lo K_{ow} is used in the calculation of the fish' bioconcentration factor, BCF.

The physical characteristics of the fis that are required as input are the fish live weight (W) and lipid fraction (P_l). Th fish's aqueous and structural organ fractions (P_a and P_s), which also ar needed to calculate the fish's BCF, ar estimated internally by FGETS b empirical functions of P_l. The user als must specify an adjustment facto active$gill, which is used to calibrate th fish's predicted mass exchange of th chemical across the gill. In general, th value specified for this parameter shou be 0.33 < active$gill < 1. Importantl this calibration is expected based upc

the difference between a fish's physiological and anatomical surface areas.

Any initial whole body concentration, C_f, of the chemical in the fish may be specified by the user. The chemical's aqueous environmental concentration, C_w, can be input as either an arbitrary time series or as a constant, sinusoidal or exponential function of exposure time. Chemical concentrations in the prey (C_p) are assumed to be a fixed proportion of that predicted by thermodynamic equilibrium. This proportion can be either less than or greater than unity (i.e., biomagnification of prey can be specified). Consequently, the user can analyze a myriad of possible exposure scenarios.

Prospectus

FGETS has been preliminarily validated and appears capable of predicting dynamic internal body concentrations of organic chemicals in fish. This capability is important when chemical exchange between fish and their environment becomes kinetically limiting either by the physicochemical properties of the chemical (e.g., high logP or low water solubility) or by allometric propertie of the fish (e.g., dynamic surface to volume ratios) because it is actually the chemical's concentration within the fish at specific or nonspecific sites of action that elicit acute or chronic ecological/physiological effects.

Additionally, the ability of FGETS to predict dynamics of bioaccumulation of organic chemicals in fish offers a powerful tool to assess potential food chain exposure for terrestrial fish-eating organisms. For example, if the use of a particular chlorinated organic pesticide was banned within a river basin, one could determine when the pesticide's concentration might no longer pose a health risk to man or an environmental threat to bald eagles or other piscivorous birds in the region.

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The complete report, entitled "FGETS (Food and Gill Exchange of Toxic Substances): A Simulation Model for Predicting Bioaccumulation of Nonpolar Organic Pollutants by Fish," (Order No. PB 88-133 558/AS; Cost: $14.95, subject to change) will be available only from:

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