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Project Summary

GETS, A Simulation Model for Dynamic Bioaccumulation of Nonpolar Organics by Gill Exchange: A User's Guide

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A FORTRAN program that estimates the absorption and depuration of a chemical across fish gills is described. The program is based on a set of diffusion and forced convection differential equations. Gill morphometric parameters are computed by the program via its own internal database. This database spans approximately 20 species. The program requires that the user input 12 relatively easily obtainable parameters.

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 of the same title (see Project Report ordering information at back).

Introduction

When fish are exposed to dissolved organic chemicals, such substances are accumulated within the fish by diffusive transport across its gills. During acute exposures, chemical exchange across the gill is the fish's prevailing route of exposure. During chronic exposure in the environment, exposure through contaminated food can become increasingly important or even greatly exceed direct gill uptake. Nevertheless, gill exchange still reciprocally controls the fish's body concentrations by determining the fish's excretory rates of the chemical.

Ultimate levels of organic toxicants in aquatic organisms can be explained in large measure as thermodynamic partitioning between toxicant in the aqueous environment and hydrophobic components of the organisms (primarily lipid). Reports of exceptions to this simple rule are numerous, however, particularly for chemicals having high partition coefficients. The frequency with which these exceptions have been noted has often led to questions of the reliability and utility of the relationship between bioconcentration factors (BCF) and thermodynamic partitioning. Based on our review of reported results for both laboratory and field investigations of BCF, uptake, and depuration, we have concluded that such results are both expected and explainable on an essentially thermodynamic (but not equilibrium) basis. Furthermore, we have developed a thermodynamically based kinetic model called GETS, which predicts whole-body burdens and concentrations of organic chemicals in fish.

GETS (Gill Exchange of Toxic Substances) is a FORTRAN simulation model that predicts a fish's whole body concentration (i.e., ppm = μg chemical [g live weight fish]$^{-1}$) of a nonmetabolized, organic chemical which is exchanged across a fish's gill by thermodynamic concentration gradients. These concentration dynamics are calculated algebraically after simulating a fish's total body burden of the chemical, Bf = μg chemical fish^{-1}, and its live weight, W = g live weight fish^{-1}. The temporal dynamics of these two quantities are generated by the system of coupled differential equations

$$\frac{dBf}{dt} = S^{*}kw^{*}(Cw - [PL^{*}KL]^{-1}CF) \quad (1)$$

$$\frac{dW}{dt} = \text{gamma} * W \qquad (2)$$

where S is the fish's total gill area (i.e., cm^2), kw is the chemical mass conductance through the interlamellar gill water (i.e., cm/day), Cw is the chemical's environmental concentration (i.e., ppm = mg 1^{-1}), PL is the fish's lipid content as a fraction of its total live weight, KL is a lipid to water partition coefficient (i.e., [mole chemical/g lipid]/[mole chemical/g water]), Cf = Bf/W is the fish's whole body concentration of the chemical, and *gamma* is the fish's specific growth rate (i.e., g/g/day).

Scope of Model

To use GETS, a user must specify 12 relatively straightforward input parameters. These are:

1. the scientific name of the fish to be analyzed (e.g., *Salmo gairdneri*)
2. the fish's family (e. g. Salmonidae)
3. the fish life form (i.e., freshwater or marine)
4. the chemical's molecular weight
5. the chemical's log K_{ow} (i.e. log P)
6. the fish's initial live weight (g)
7. the fish's lipid content as a proportion of its total body weight (g lipid/g live weight)
8. the fish's specific growth rate (i.e., g/g/day)
9. the fish's initial whole body concentration of the chemical (i.e., μg (g live weight fish)$^{-1}$)
10. the chemical's environmental concentration as ppm = mg 1^{-1}
11. a kinetic adjustment factor that is discussed below (unitless)
12. the length of the desired simulation in days

The fish's species name, family, and life form are used to assign the gill morphometric parameters that the GETS's subroutine GILRAT uses to estimate the fish's net exchange rate (S*kw). These assignments are made by GETS using a model data file. This file, which is supplied with GETS, contains the coefficients and exponents of the allometric functions arranged by species,

$$S = \text{total gill area, } cm^2 = s1\ W^{e2} \text{ and}$$
$$RHO = \#\text{ lamellae (mm gill filament)}^{-1} = \rho^1\ W\rho^2$$

where W is the fish's live weight (g). From this data file five geometric means are calculated by GETS for each of the values, s1, s2, ρ1, and ρ2. For example, GETS calculates a geometric mean for s1, first using all the data reported in this file. Concurrently, GETS also calculates geometric means for s1, using only data records which have the same life form, family, genus, and species of the fish designated by the user. GETS then attempts to assign s1, s2, ρ1, and ρ2 using first the species geometric means. If, however, the species is not represented in MORPHO.DAT, GETS then tries to assign the geometric means that might have been calculated for the same genus as the desired species. In like fashion, if the genus is not found in the model data file, geometric means for the fish's family are assigned. If these assignments are not possible, the geometric means for the same life form (i.e., freshwater vs. marine) as the desired fish are used.

GETS is parameterized for a particular chemical of concern by specifying the chemical's molecular weight and log K_{ow}. The chemical's molecular weight is used to estimate its aqueous diffusivity, which is needed to estimate the conductance, kw. The chemical's log K_{ow} is used in the calculation of the fish's excretion rate, $k_2 = S*kw*(PL*KL)^{-1}$.

The physical characteristics of the fish that are required as input are the fish's live weight (W), its lipid fraction (PL) and its specific growth rate (gamma). The specific growth rate, gamma, specified as input should be nonnegative. Although negative growth is exhibited by organisms under stress in natural ecosystems, it is not known whether fish that are losing weight significantly alter their gill morphometry. Therefore, although negative growth rates, per se, can be input to GETS, the resulting simulations, which depend on gill morphometry, may not be meaningful.

Because the user can specify any initial whole body concentration, Cf, of the chemical in the fish as well as any environmental concentration, Cw, the user can analyze either absolute uptake (i.e., Cf = 0 and Cw $\neq$ 0), pure depuration (i.e., Cf $\neq$ 0 and Cw = 0) or any scenario between these two extremes.

The user-supplied adjustment factor, adjust, is used to calibrate the mass conductance of the chemical that is estimated by GETS. In general, the value specified for this parameter should be in the range of 0.1 > adjust > 0.05 since the estimated conductance, kw, is generally between 10 and 20 times higher than laboratory studies would indicate. Such overestimation, however, is expected.

Conclusion

GETS enables internal fish concentrations of an organic chemical to be related dynamically to the chemical's environmental concentration. This capability is important when chemical exchange between fish and their environment is kinetically limited either by the physicochemical properties of the chemical (e.g., high log P or low water solubility) or by allometric properties of the fish (e.g., dynamic surface to volume ratios) since it is actually the chemical's concentration within the fish at specific or nonspecific sites of action that elicit potentially adverse ecological or physiological responses.

Similarly, the ability of GETS to predict the 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 were banned within a river basin, when might the pesticide's concentration 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 "GETS, A Simulation Model for Dynamic Bioaccumulation of Nonpolar Organics by Gill Exchange," (Order No. PB 87-132 791/AS; Cost: $13.95, subject to change) will be available only from:

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