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Project Summary

WASTOX, A Framework for Modeling the Fate of Toxic Chemicals in Aquatic Environments: Part 2. Food Chain

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A food chain bioaccumulation mathematical framework was developed as part of a broader framework for modeling the fate of toxic chemicals in natural water systems, entitled WASTOX. A user's guide for WASTOX was published in August 1984 as Part 1 of this report (1).

The food chain component of WASTOX described here is a generalized model for estimating the uptake and elimination of toxic chemicals by aquatic organisms. Rates of uptake and elimination are related to the bioenergetic parameters of the species encompassed in either a linear food chain or a food web. Concentrations are calculated as a function of time and age for each species included. Exposure to the toxic chemical in food is based on a consumption rate and predator-prey relationships that are specified as a function of age. Exposure to the toxic chemical in water is functionally related to the respiration rate. Steady-state concentrations may also be calculated.

Food chain exposure to chemicals may be specified by the user of the model or may be taken directly from the values calculated by the exposure concentration component of WASTOX. Migratory species, as well as nonmigratory species, may be considered.

The model has been successfully used to model Kepone in the James River striped bass food chain and PCBs in the Lake Michigan lake trout food chain and Saginaw Bay, Lake Huron yellow perch food.

This Project Summary was developed by EPA's Environmental Research Laboratory, Gulf Breeze, FL, 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

The hazard posed to a natural water system by a toxic chemical is governed by the uptake of the chemical by the resident biota and subsequent acute and chronic health effects. Evaluation of the hazard involves three steps proceeding from the specification of the rate of chemical discharge to the system:

1) estimation of the chemical concentrations in the water and sediment
2) estimation of the rate of uptake of chemical by segments of the resident biota
3) estimation of the toxicity resulting from uptake of the chemical.

Execution of each step in this hazard assessment requires consideration of the transport, transfer, and reaction of the chemical and the dependence of these processes on properties of the affected natural water system and its biota. Based on experimentation and theoretical development, each process has been, or can be, described mathematically, specifying its functional dependence on specific properties. These expressions may be combined, using the principle of conservation of mass, to form a mathematical model that addresses one of the steps in the hazard assessment.

Steps 1 and 2 of this hazard assessment are addressed by the general modeling framework entitled WASTOX, an acronym for Water (Quality) Analysis Simulation for TOXics. This modeling framework is composed of two parts which may be termed the exposure concentration and food chain components, respectively.

The exposure concentration component is the computational structure for applying step 1 to a specific natural water system, as described in Part 1 of this report published in August, 1984 (1). The food chain component described in this report is the computational structure for applying step 2 to a specific natural water system. Both components were developed to determine the fate of toxic chemicals in estuaries (CR807827) and the Great Lakes (CR807853).

Model Framework

The concentration of a toxic substance that is observed in an aquatic organism is the result of several uptake and loss processes that include: transfer across the gills, surface sorption, ingestion of contaminated food, desorption, metabolism, excretion and growth. These processes are controlled by the bioenergetics of the organisms and the chemical and physical characteristics of the toxic substance. The equations used to describe these processes were formulated by Norstrom et al. (2) and Weininger (3) and for food chain by Thomann (4) and Thomann and Connolly (5).

For phytoplankton and detrital organic material representative of the base of the food chain, sorption-desorption controls toxic substance accumulation. Instantaneous equilibrium is assumed because the sorption rates are generally much faster than the uptake and excretion rates of higher levels of the food chain and the transport and transformation rates of the toxic substance. The concentration of chemical in phytoplankton detritus is computed as the product of a user specified partition coefficient and the dissolved chemical concentration.

For species above the phytoplankton/detritus level, uptake of toxicant due to ingestion of contaminated food must be considered. This uptake will depend on a) toxicant concentration in the food, b) rate of consumption of food, and c) the degree to which the ingested toxicant in the food is actually assimilated into the tissues.

The rate of consumption of food is computed from user specified respiration and growth rates and food assimilation efficiency. The uptake of toxicant from water by these species is determined by the rate of transfer of toxicant across the gills. This rate of transfer is calculated from the rate of transfer of oxygen from water to the blood of the fish.

The rate of loss of the toxicant from an organism is the sum of the excretion and detoxification or degradation rates of the chemical. If the organism is exposed to the toxicant in water only, this rate is related to the uptake rate by the bioconcentration factor.

In the model the excretion rate may be internally calculated from a specified bioconcentration factor or it may be specified. If it is specified directly, the equivalent bioconcentration factor will decrease during an age class. The uptake rate decreases as a function of weight because the respiration is dependent on weight. If the excretion rate is constant for an age class, the result is a decreasing bioconcentration factor.

The processes mentioned above are defined by bioenergetic and chemical related parameters. In addition, the variation of these parameters with age and the feeding habits of each species modeled must be specified.

Feeding habits are generally discontinuous functions of age. The prey size or prey species generally change as an organism grows. Life span is separated into age classes in which the predator-prey relationships are assumed to be constant.

Species at the lower end of the food chain tend to exhibit a concentration of chemical that does not vary with age. Their relatively rapid uptake and excretion rates, and the lack of a major diet change with age, cause them to achieve equilibrium with the chemical in a short time relative to their life span. This fact justifies the use of an equilibrium or steady-state modeling approach for these species. For each species in the model, the user may choose to calculate either a steady-state concentration or the concentration distribution with age.

The specific parameter requirements for each species in the model are listed in Table 1.

Table 1. *Input requirements for each species included in the food chain model*

Bioenergetic Related Parameters:
growth rate
respiration rate
assimilation efficiency of food
predator-prey relationships
Toxic Chemical Related Parameters:
assimilation efficiency of chemical in food; molecular diffusivity of the toxic chemical; bioconcentration factor or whole body excretion rate

If migratory species are modeled, then the spatial variability of the toxic chemical and the seasonal movement of the species must be considered. This is accomplished through the use of "spatial compartments." The water body or system is separated into compartments in which the toxic chemical concentration is assumed to be constant. Nonmigratory food chains are specified for each compartment reflecting the predator-prey relationships in that region of the system. The migratory species is exposed sequentially to each of these food chains in a pattern that reflects its seasonal movement.

To facilitate interfacing the food chain model with the exposure concentration component of WASTOX, the toxic chemical concentration in each spatial compartment is computed as the arithmetic average of the segments in the exposure concentration component that lie within the spatial compartment. Water column and sediment segments are averaged separately to provide concentrations for the pelagic and benthic components of the food chain.

Model Application

The food chain component of WAS-WASTOX has been applied to the following chemicals and food chains:

1) PCB—Lake Michigan lake trout food chain
2) Kepone—James River, VA, striped bass food chain

In the PCB-lake trout application, a single spatial compartment was considered and the model was calibrated for a single year, 1970. The model compared favorably with concentration in each level of the food chain and with the age distribution of concentration in alewife and lake trout.

In the Kepone-striped bass application two spatial compartments account for migration of atlantic croaker and striped bass. The model was calibrated to a seven-year time-history of data. The model reproduced the observed within-year and year-to-year concentration variations for all three fish species considered: white perch, atlantic croaker, and striped bass. The calibrated model was used to project the response of the food chain to reductions in water umn and sediment chemical concentrations for both applications.

Conclusions

WASTOX is a framework for modeling toxic chemicals in natural water system that is generally useful in development of a model for a specific application. The food chain component can simulate any food web configuration. The successful use of the food chain component in modeling both lake and estuarine food chains demonstrates its validity and wide-range applicability.

References

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3. Weininger, D. 1978. Accumulation of PCBs by lake trout in Lake Michigan. Ph.D. Thesis, The University of Wisconsin-Madison, 232 p.
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The complete report, entitled "WASTOX, A Framework for Modeling the Fate of Toxic Chemicals in Aquatic Environments: Part 2. Food Chain," (Order No. PB 85-214 435/AS; Cost: $10.00, subject to change) will be available only from:

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