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WASTOX, A FRAMEWORK FOR MODELING THE FATE OF TOXIC CHEMICALS IN AQUATIC ENVIRONMENTS
PART 2: FOOD CHAIN

by

John P. Connolly
Robert V. Thomann
Environmental Engineering & Science
Manhattan College
Bronx, N.Y. 10471

Project Officers

Parmely H. Pritchard
Environmental Research Laboratory
Gulf Breeze, Florida 32561
Cooperative Agreement No. R807827

William L. Richardson
Large Lakes Research Station-Grosse Ile, MI
Environmental Research Laboratory
Duluth, Minnesota 55804
Cooperative Agreement No. R807853

ENVIRONMENTAL RESEARCH LABORATORY
OFFICE OF RESEARCH AND DEVELOPMENT
U.S. ENVIRONMENTAL PROTECTION AGENCY
GULF BREEZE, FL 32561
AND
DULUTH, MN 55804

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FOREWORD

The protection of estuarine and freshwater ecosystems from damage caused by toxic organic pollutants requires that regulations restricting the introduction of these compounds into the environment be formulated on a sound scientific basis. Accurate information describing the potential exposure of indigenous organisms and their communities to these toxic chemicals under varying conditions is required. The Environmental Research Laboratory, Gulf Breeze, contributes to this information through research programs aimed at determining:

- the effects of toxic organic pollutants on individual species, communities of organisms, and ecosystem processes.
- the fate and transport of toxic organics in the ecosystem.
- the application of methodologies which integrate fate and effects information to predict environmental hazard.

The magnitude and significance of chemical contamination of aquatic environments are increasingly evident. The potential persistence and possible accumulation of those chemicals in aquatic food chains means that the impact on the health and activities of man is more direct. Therefore, the ability to predict exposure concentration, bioaccumulation, and chronic toxicity is critical to our efforts in hazard assessment. Mathematical models provide a basis for quantifying the inter-relationships among the various physical, chemical, and biological variables that affect fate, transport, and bioaccumulation of toxic chemicals. Such models also provide a mechanism for extrapolating laboratory information to the environment and a rationale and conceptually relevant basis for decision making.

This report presents the mathematical framework of a generalized model to estimate the uptake and elimination of toxic chemicals by aquatic organisms. The model is part of a broader framework called WASTOX which was supported by our EPA laboratories in Gulf Breeze, FL, and Duluth, MN. It provides a means of modeling the fate of toxic chemicals in natural water systems including fate due to food chain bioaccumulation. Part 1, a user's guide for WASTOX (EPA-600/3-84-077) was published in August 1984. Part 2 explains the use of the food chain component of WASTOX.

Henry F. Enos
Director
Environmental Research Laboratory
Gulf Breeze, Florida

N.A. Jaworski
Director
Environmental Research Laboratory
Duluth, Minnesota

PREFACE

WASTOX is a batch oriented computer program that solves the mass balance equations that define the fate of toxic chemicals in aquatic systems. This report documents the food chain component of the program which analyzes the uptake and elimination of chemicals by aquatic organisms. The exposure concentration component of the program which analyzes the time-variable or steady-state, physical-chemical behavior of chemicals is documented in a separate report (1). The model is generally applicable to all types of water bodies.

WASTOX was developed under cooperative agreements with the Environmental Research Laboratory, Gulf Breeze, Florida (CR807827) and the Large Lakes Research Station of the Environmental Research Laboratory, Duluth, Minnesota (CR807853). Application of the program to estuaries and to lakes is being conducted through the Gulf Breeze and Duluth cooperative agreements, respectively.

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ABSTRACT

This report describes a mathematical modeling framework for the analysis of toxic chemicals in aquatic biota. This framework is part of a broader framework for modeling the fate of toxic chemicals in natural water systems, entitled WASTOX, an acronym for Water quality Analysis Simulation for TOXics. WASTOX is composed of an exposure concentration component which computes the time-variable or steady-state concentrations of a toxic chemical in the water column and bed of a natural water system as well as the food chain component described in this report.

The food chain component is a generalized model of the uptake and elimination of toxic chemicals by aquatic organisms. It is a mass balance calculation in which the rates of uptake and elimination are related to the bioenergetic parameters of the species. A linear food chain or a food web may be specified. 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.

The concentrations of toxic chemical to which the food chain is exposed 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. Thus the food chain component may be executed as a separate model or as a post-processor to the exposure concentration component. Migratory species, as well as non-migratory species, may be considered. Separate non-migratory food chains may be specified and the migratory species is exposed sequentially to each based on its seasonal movements.

The model may be applied to any type of natural water system. It has been successfully used to model PCB in the Lake Michigan lake trout food chain and the Saginaw Bay, Lake Huron yellow perch food chain, and Kepone in the James River striped bass food chain.

ACKNOWLEDGEMENTS

The assistance of Rosella Tonelli in testing and applying a myriad of preliminary versions of this framework and the programming assistance of Paul Rontonini are greatly appreciated.

The support of the project officers involved in the food chain research of which this work is a result; Parmely H. Pritchard and William L. Richardson, was an important contribution to its successful completion.

The many and significant contributions of our colleagues at Manhattan College; Dominic M. Di Toro, Donald J. O'Connor, and Richard P. Winfield, are gratefully acknowledged.

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SECTION 1

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 of WASTOX is the computational structure for applying step 1 to a specific natural water system. The food chain component of WASTOX is the computational structure for applying step 2 to a specific natural water system.

The purpose of this report is to describe the theoretical basis, structure, and use of the food chain component. The exposure concentration component is described in a separate report (1). Both components of WASTOX were developed as part of projects to determine the fate of toxic chemicals in estuaries (CR807827) and the Great Lakes (CR807853).

SECTION 2

FUNDAMENTAL EQUATIONS

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 organism and the chemical and physical characteristics of the toxic substance. The equations used to describe these processes were formulated and applied for a single species by Norstrom, et al. (2) and Weininger (3) and for an entire 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 and the change in the concentration, ν_o (μg/g(w)) may be written as:

$$\frac{d\nu_o}{dt} = k_{uo}c_d - K_o\nu_o \tag{1}$$

in which k_{uo} is the rate of uptake directly from the water or the sorption rate (ℓ/d-g(w)), c_d is the concentration of dissolved toxicant (μg/ℓ), K_o is the loss rate or desorption rate (d^{-1}), and t is time (d). 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, instantaneous equilibrium may be assumed. Equation (1) then reduces to:

$$\nu_o = N_oc_d \tag{2}$$

in which N_o, the bioconcentration factor, is the ratio of the uptake to the loss rate.

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, C, (g/g-d) is dependent on metabolic requirements and growth rate. It may be written as:

$$C = \frac{R + G}{a} \tag{3}$$

in which R is the respiration rate (g/g-d), G is the growth rate (d^{-1}), and a is the fraction of ingested food that is assimilated.

The uptake of toxicant from water by these species, k_u is determined by the rate of transfer of toxicant across the gills. This rate of transfer can be calculated from the rate of transfer of oxygen from water to the blood of the fish.

The rate of mass transport of a substance by passive diffusion across the gills is given by:

$$M = \frac{DA}{\delta} (a_w - a_b) \tag{4}$$

where M is the mass transport [μg/d], D is the diffusivity of the substance [cm^2/s], δ is the effective thickness of the gill [cm], and a_w and a_b are the activities of the substance in the water and blood, respectively [μg/ℓ]. If the activity of the chemical in water is assumed to be equal to its concentration, c, and the transport across the gill from blood to water is parameterized into a whole body excretion term, equation (4) may be reduced to:

$$M = \frac{DA}{\delta} c \tag{5}$$

If it is assumed that the mechanism for uptake of the chemical is identical to oxygen uptake then:

$$\frac{M_C}{M_{O_2}} = \frac{D_C\ c_C}{D_{O_2} c_{O_2}} \tag{6}$$

where the subscripts C and O_2 are for the chemical and dissolved oxygen respectively. From (6),

$$M_C = (\beta \frac{M_{O_2}}{c_{O_2}})\ c_C \tag{7}$$

where $\beta = D_C/D_{O2}$, the ratio of the diffusivity of the chemical to that of oxygen. From (7),

$$M_C = k_u'\ c_C \tag{8}$$

where

$$k_u' = \beta\ M_{O_2}/c_{O_2} \tag{9}$$

The quantity k_u' represents the mass uptake for the whole fish and has units, ℓ/d. Dividing k_u' by the fish weight gives the uptake rate per unit weight, i.e.

$$k_u = \frac{k_u'}{w} = \beta\ \frac{M_{O_2}/w}{c_{O_2}} \tag{10}$$

The quantity M_{O_2}/w is the respiration rate, r, of the fish, i.e.

$$r = M_{O_2}/w$$

where r has units $[gO_2/g(w) - d]$. The uptake rate for the chemical is therefore related to the respiration rate of the organism by:

$$k_u = \beta\ \frac{r}{c_{O_2}} \tag{11}$$

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, N, as specified by Eq. (2). Assuming no significant weight change during the bioconcentration test, the loss rate, K, may be written as:

$$K = \frac{k_u}{N} \tag{12}$$

This rate incorporates several excretory processes including renal and hepatic excretion, diffusion from blood across the gill and diffusion from blood across the gut wall. The relative importance of each of these processes will vary depending on the metabolic rate of the animal, the route of exposure to the chemical and the characteristics of the chemical. Although the use of a single rate effectively lumps parameters from more fundamental processes, it is the only approach that is empirically justifiable given the current state of knowledge.

In the model the excretion rate may be internally calculated from a specified bioconcentration factor, as given by eq. 12 or it may be specified directly. 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 (see eq. 17). If the excretion rate is constant for an age class the result is a decreasing bioconcentration factor.

Combining the above uptake and loss rates, the general mass balance equation for the whole body burden, ν'(μg), may be written as:

$$\frac{d\nu'}{dt} = k_u w c_d + \alpha C w \nu_p - K\nu' \tag{13}$$

in which w is the weight of the organism (g(w)), α is the fraction of ingested toxicant that is assimilated, and ν_p is the toxicant concentration in the prey (μg/g(w)). Because the whole body burden is the product of the toxicant concentration and weight of the organism, the derivative in Eq. (13) may be written and expanded as:

$$\frac{d\nu'}{dt} = \frac{d(\nu w)}{dt} = \nu \frac{dw}{dt} + w \frac{d\nu}{dt} \tag{14}$$

Equation (13) may then be rewritten in terms of toxicant concentration as:

$$\frac{d\nu}{dt} = k_u c_d + \alpha C \nu_p - k'\nu \tag{15}$$

where:

$$k' = K + \frac{dw}{dt}/w = K + G$$

and G is the growth rate of the organism (g/g/d).

The growth rate term in Eq. (15) accounts for the dilution of toxicant caused by the increase in weight of the organism.

SECTION 3

MODELING FRAMEWORK

3.1 APPROACH

The analysis of toxic chemicals in aquatic food chains using Eq. (2) for phytoplankton and detrital organic material and Eq. (15) for higher trophic level species requires the bioenergetic and chemical related parameters included in Eqs. (3), (11) and (12). In addition, the variation of these parameters with age and the feeding habits of each species modeled must be known.

Feeding habits are generally discontinuous functions of age. The prey size or prey species generallly change as an organism grows. Thus, Eq. (15) may not be solved continuously over the life span of an organism. Instead the life span is separated into age classes over which the predator-prey relationships are assumed to be constant. Eq. (15) is then applied to each age class with the term representing uptake through feeding expanded to allow more than one prey for each predator age class.

The use of age classes also provides a convenient mechanism for computing concentrations in all life stages simultaneously, rather than the Lagrangian approach of following a single organism that results from the direct solution of Eq. (15). The criteria for age class size is the birth frequency of the organism, thus restarting the first age class of an organism at the proper interval.

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. The equation defining the equilibrium concentration is obtained from equation (15) by assuming the uptake and loss rates are constant and setting the derivative, $d\nu/dt$ to zero:

$$\nu = \frac{k_u c_d + \alpha C \nu_p}{K'} \qquad (16)$$

The use of equation (16) for appropriate species reduces the computation time of the model.

3.2 APPLICATION

Use of the model requires the determination of an appropriate food chain for the natural water system being considered and the specification of a number of bioenergetic and toxic chemical related parameters for each member of the food chain. In general the top component of the food chain is chosen first. The feeding habits of this species define additional species whose feeding habits, in turn, define still further species until the base of the food chain is reached. Because most species within a trophic level have similar growth and metabolic rates and carry similar body burdens of the toxic chemical being studied, a first-cut model may use a single species as representative of a class of species at a given trophic level.

The specific parameter requirements for each species in the model are listed in Table I. Growth rate may be obtained from the observed weight-age relationship of the species. Respiration rate is derived from laboratory studies of metabolic rate and its dependence on weight, temperature, and activity level (swimming speed). Species for which a steady-state concentration is appropriate require a single respiration value representative of an average across age and its dependence on temperature. Respiration is assumed to vary exponentially with temperature, T(°C), and the user must specify a coefficient, $\rho(°C^{-1})$, for each species. Species for which concentration is calculated in time for several age classes (i.e., age-dependent) also require specification of the dependence of respiration on body weight and swimming speed. The relationship between respiration R(g/g/d), body weight W(g) and swimming speed u(cm/s) is (6):

$$R = \beta W^{\gamma} e^{\rho T} e^{\nu u} \qquad (17)$$

where $$u = \omega W^{\delta} e^{\phi T}$$

Values for β, γ, ρ, ν, ω, δ, and ϕ must be specified by the user. The value of γ is generally believed to be constant across species at a value in the range of -0.2 to -0.3. The negative sign is inserted by the model and the user should specify the absolute value of γ. For salmonid fish, Stewart (6) reported values of ν(s/cm) ranging from 0.23 to 0.33 with a mean of 0.27, values of ω(cm/s) ranging from 9.7 to 12.4 with a mean of 11, values of δ ranging from 0.05 to 0.13 with a mean of 0.1, values of ρ ranging from 0.055 to 0.086 with a mean of 0.067, and $\phi(°C^{-1})$ constant at 0.0405.

To convert the respiration rate from units of g(w)/g(w)/d to the units of $g(O_2)$/g(w)/d used in the uptake rate calculation (eq. 11); (1) wet weight is converted to dry weight by a user supplied ratio, (2) dry weight is converted to carbon assuming a carbon to dry weight ratio of 0.4, and (3) carbon is stoichiometrically converted to oxygen.

The assimilation efficiency of food is dependent on the type of prey consumed as well as the consumption rate. As a general guide, values for carnivores and herbivores may be assumed to range between 0.7 and 0.8 and 0.3 and 0.5, respectively. The chemical assimilation efficiency and bioconcentration factor are estimated from laboratory tests in which aquatic species are exposed to the chemical in food or water. Bioconcentration factors are generally readily available. Excretion rates have been measured for many chemicals and aquatic species. However, little information is available for the larger fish. The chemical assimilation efficiency is difficult to determine and is rarely measured. Available data suggest that for many chemicals the assimilation efficiency is in the range of 0.5 to 0.9.

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. Non-migratory food chains are specified for each compartment reflecting the predatorprey relationships in that region of the system. The migratory species is exposed sequentially to each of these food chains in a pattern reflective of 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.

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

SECTION 4
STRUCTURE OF COMPUTER CODE

4.1 OVERVIEW

The food chain component of WASTOX is a general purpose computer program for modeling the accumulation of toxic chemicals in any aquatic food chain or food web. It is designed to be used as part of the overall WASTOX model, although it may be used separately or as a post-processor to other toxic chemical models.

Exposure concentrations can be inputted by the user or read from disk files created by the exposure concentration component of WASTOX. In both cases these concentrations are assumed to apply to segments of the spatial compartments used in the food chain calculation. The segment concentrations are averaged over the spatial compartment.

Chemical concentrations in the food chain are calculated at a user specified integration interval and outputted at a user specified print interval. The flow diagram for the model is shown in Fig. 1.

4.2 SUBROUTINES

FDCHAN

FDCHAN calls the input and computation subroutines. It prints results at a user specified time interval.

FCINPT

FCINPT reads the input for the species and spatial compartments of the model.

EXPOSE

EXPOSE reads the concentrations of dissolved and adsorbed chemical for the segments that comprise the spatial compartments. This subroutine is executed only if the food chain model is run separately from the exposure concentration model.

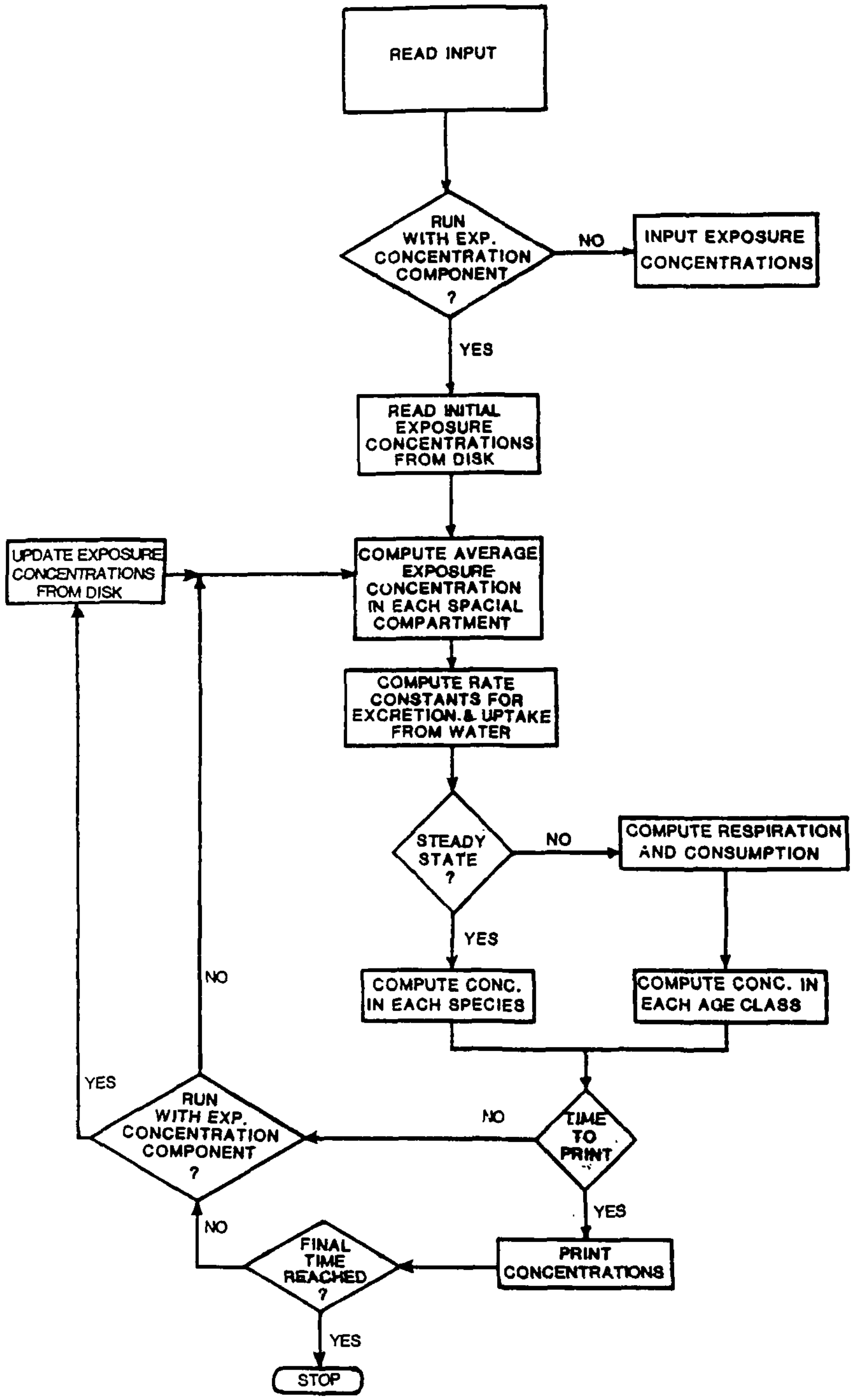

Figure 1. Flow diagram for the model

FDCHN

FDCHN is the main computation subroutine. It calls the other computation subroutines and calculates the concentrations in each age-dependent species. It also updates concentrations at the end of each year to initialize the concentration in each age class for the next year. Movement of migrating species between compartments is also performed.

SSCONC

SSCONC calculates the concentration in each species specified to be at steady-state.

KNETIC

KNETIC computes the rate constants for uptake from water and excretion for each steady-state species and each age class of the age-dependent species.

INTERP

INTERP reads chemical concentrations from the disk files set up by the exposure concentration component of WASTOX and linearly interpolates between the exposure concentration components print times to provide concentrations for each time step of the food chain calculation.

SECTION 5
PREPARATION OF DATA INPUT

5.1 INTRODUCTION

Data input includes information about the chemical, the species, and the spatial compartmentalization of the natural water system. The structure of the input varies slightly depending on the inclusion of benthic species and whether the model is run with or without the exposure concentration component of WASTOX. If run with the exposure concentration component, the food chain component uses the concentrations outputted to disk by the exposure concentration component. Linear interpolation is used to provide values between the outputting intervals. When the food chain component is run alone the user must input the exposure concentrations.

The input data should be structured as a card image file. The program expects the input data file to have the name "WASTOX.INP". Output is written to a file named "WASTOX.OUT". Depending on whether the food chain component is executed with or without the exposure concentration component, the input for the exposure concentration component must precede that for the food chain component. (See the exposure concentration component documentation (Connolly and Winfield, 1983) for the necessary additional input).

5.2 CARD GROUP A - NUMBER OF SPECIES

5.2.1 Number of Age-Dependent and Steady-State Species

5	10
NSP	NSPSS
FORMAT(2I5)	

NSP - number of species for which concentrations are calculated in relation to age.

NSPSS - number of species for which steady-state concentrations are calculated.

(maximum number of species, i.e., NSP + NSPSS, equals 20)

5.3 CARD GROUP B - COMPOUND RELATED PARAMETERS

5.3.1 Compound Characteristics

10	20
KP	DIFF
FORMAT(2F10.0)	

KP - partition coefficient (bioconcentration factor) of compound to plankton-detritus ($\mu g/g_w \div \mu g/\ell$)

DIFF - molecular diffusivity of compound (cm^2/s)

5.4 CARD GROUP C - STEADY-STATE SPECIES PARAMETERS

This card group is repeated NSPSS times; once for each steady-state species.

5.4.1 Identification

5	10	22
IFLG(I)	IFLG1(I)	TITLE
FORMAT(2I5, 3A4)		

IFLG(I) - flag indicating that species I is either a pelagic or a benthic species:

If IFLG(I) = 0, then species (I) is pelagic
If IFLG(I) = 1, then species (I) is benthic and consumes only detritus.

IFLG(I) - flag indicating whether excretion rate for species I will be entered or will be computed from a bioconcentration factor

If IFLG1(I) = 0, then a bioconcentration factor will be entered
If IFLG1(I) = 1, then an excretion rate will be entered

TITLE - name of steady-state species.

5.4.2 Bioenergetic Parameters

10	20	30	40	50	60	70
RESP(I)	GROW(I)	ASM(I)	BCF(I)	ASIM(I)	FDRY(I)	RHO(I)

FORMAT(8F10.0

RESP(I) - respiration rate of steady-state species I (g/g/day)

GROW(I) - growth rate of species I (d^{-1})

ASM(I) - toxicant assimilation efficiency of species I

BCF(I) - bioconcentration factor of species I ($\mu g/g_w \div \mu g/\ell$) or excretion rate (1/d) as specified in 5.4.1

ASIM(I) - food assimilation efficiency of species I

FDRY(I) - fraction dry weight of species I

RHO(I) - exponential coefficient for temperature dependence of species I respiration.

5.5 CARD GROUP D - AGE DEPENDENT SPECIES PARAMETERS

This card group is repeated NSP times; once for each age dependent species

5.5.1 Identification

5	10	22
IFLG(I)	IFLG1(I)	TITLE

FORMAT(2I5,3A4)

IFLG(I) - flag indicating that species I is either a pelagic or a benthic species;

If IFLG(I) = 0, then species (I) is pelagic

If IFLG(I) = 1, then species (I) is benthic and consumes only detritus

NOTE: the current structure assumes that all benthic species are steady-state. IFLG should always be 0.

IFLG1(I) - flag indicating whether excretion rate for species I will be entered or will be computed from a bioconcentration factor

If IFLG1(I) = 0, then a bioconcentration factor will be entered
If IFLG1(I) = 1, then an excretion rate will be entered

TITLE - name of the age-dependent species

5.5.2 Bioenergetic Parameters

5	15	25	35	45	55	65
NAC(I)	ACS(I)	ASM(I)	BETA(I)	GAMMA(I)	ASIM(I)	FDRY(I)

FORMAT(I5,6F10.0)

NAC(I) - number of age classes for age-dependent species I

ACS(I) - age class size of species I(d)
ASM(I) - toxicant assimilation efficiency of age-dependent species I
BETA(I) - respiration coefficient for age-dependent species I
GAMMA(I) - respiration weight exponent for age-dependent species I
ASIM(I) - food assimilation efficiency of age-dependent species I
FDRY(I) - fraction dry weight of age-dependent species I

10	20	30	40	50
RHO(I)	OMGA(I)	DLTA(I)	PHI(I)	XNU(I)

FORMAT(5F10.0)

RHO(I) = exponential coefficient for temperature dependence of species I respiration ($°C^{-1}$)
OMGA(I) = swimming speed coefficient (cm/s) for age-dependent species I
DLTA(I) = swimming speed weight exponent for age-dependent species I
PHI(I) = exponential coefficient for temperature dependence of species I swimming speed ($°C^{-1}$)
XNU(I) = exponential coefficient for swimming speed (s/cm)

5	15
MFLG(I)	SPBD(I)
FORMAT(I5,F10.0)	

MFLG(I) = flag indicating that this species is a continuation of the last species inputted. Used when a species is divided to separate non-migrating juveniles from migrating adults:

If MFLG(I) = 0 then species I is a different species than species I-1

If MFLG(I) = 1 then species I is a continuation of species I-1

SPBD(I) = numbers of julian days after start of calculation to the species birthdate.

10	20	30
WO(K)	GROW(K)	BCF(K)
FORMAT(3F10.0)		

WO(K) - weight of age class K at beginning of run (g_{wet})

GROW(K) - growth rate of age class K

BCF(K) - bioconcentration factor of age class K ($\mu g/g_w \div \mu g/\ell$) or excretion rate (1/d) as indicated by 5.5.1

This card is repeated NAC(I) times; once for each age-class of species I

5.6 CARD GROUP E - MIGRATING SPECIES PARAMETERS

5.6.1 Numer of Migrating Species

5
NMIG
FORMAT(I5)

NMIG - number of migrating species in model (maximum of 2)

5.6.2 Identification and Migrating Pattern

Card group 5.6.2 is repeated NMIG times; once for each migrating species

5
MIGSN(I)
FORMAT(I5)

MIGSN(I) - species number of Ith migrating species

5	15	20	30	35	80
NBRKS(I)	TIMEM(I,J)	COMPRT(I,J)	TIMEM(I,J)	COMPRT(I,J)	. . . . .
FORMAT(I5,5(F10.0,I5))					

NBRKS(I) - number of breaks describing the migratory pattern of the Ith migratory species.

TIMEM(I,J) - time of break J in the migratory pattern of the Ith migratory species (d).

COMPRT(I,J) - spatial compartment occupied by the Ith migratory species for the time up to TIMEM(I,J).

5.7 CARD GROUP F - SETUP OF SPATIAL COMPARTMENTS

5.7.1 Number of Compartments

5
NSC
FORMAT(I5)

NSC - number of spatial compartments included in the model. (Maximum = 12)

5.7.2 Compartment Characteristics

Card groups 5.7.2 through 5.7.4 are repeated NSC times; once for each spatial compartment

a. Annual temperature profile

5
NBRKS2(I)
FORMAT(I5)

10	20	30 80	
TIMET(I,J)	TEMP(I,J	TIMET(I,J)	TIME(I,J)

FORMAT(8F10.0)

NBRKS2(I) - number of breaks describing the annual temperature cycle in spatial compartment I (maximum of 14)

TIMET(I,J) - time of break J in the temperature cycle in compartment I(d)

TEMP(I,J) - temperature at break J in the temperature cycle in compartment I(°C)

b. Species in Compartment

5
NSPSI(I)

FORMAT(I5)

NSPSI(I) - number of species above the plankton level in compartment I

5.7.3 Characteristics of the Food Chain

Card group 5.7.3 is repeated NSPSI(I) times in each compartment I: once for each species in the compartment

a. Species Number

5
SPNO(I,J)

FORMAT(I5)

SPNO(I,J) - species number of the Jth species in compartment I. If species J is age-dependent or pelagic and steady-state skip to c.

b. Benthic Species Initial Concentration

10
CFC(I,J)

FORMAT(F10.0)

CFC(I,J) = concentration of chemical in species J in compartment I at the start of the calculation (μg/gw)

Skip to 5.7.4

c. Predator-Prey Relationships

i. Number of Prey

5
NPREY(I,J)
FORMAT(I5)

NPREY(I,J) - number of prey of species or age class J in compartment I. (maximum of 3)

ii. Consumption Split

5	15	20	30	75
PREY(I,J,L)	PREF(I,J,L)	PREY(I,J,L)	PREF(I,J,L)	. . . .
FORMAT(5(I5,F10.0))				

PREY(I,J,L) - step number of the Lth prey of step J in compartment I.

PREF(I,J,L) - fraction of step J's consumption that is on its Lth prey in compartment I.

Note: Steps are counted for each compartment from the first species above the plankton-detritus level and include the steady-state species and each age class of age dependent species.

For example, if a food chain consists of plankton, a steady-state invertebrate, and an age-dependent fish with 3 age classes the steps are as follows:

	Step
invertebrate	1
fish age 1	2
fish age 2	3
fish age 3	4

If fish age 2 preys on the invertebrate then for compartment I PREY(I,3,1) = 1 and PREF(I,3,1) = 1.0.

d. Initial Concentration

10
CFC(I,J)
FORMAT(F10.0)

CFC(I,J) - concentration of chemical in steady-state species or age-class J in compartment I at the start of the calculation (μg/gw)

(Note: For each age-dependent species, (c) and (d) are repeated for each class).

5.7.4 Interfacing Segments from Exposure Concentration Component With the Spatial Compartments

a. Number of segments

5	10
NSEG(I),	NBSEG(I)
FORMAT(2I5)	

NSEG(I) - number of water column segments from exposure concentration model included in spatial compartment I.

NBSEG(I)- number of bed segments from exposure concentration model included in spatial compartment I.

5	10	
SEGNO(I,1)	SEGNO(I,2) ...	SEGNO(I,NSEG(I))

FORMAT(16I5)

SEGNO(I,M) - segment number of the Mth water column segment included in spatial compartment I.

5	10	
BSEGNO(I,1)	BSEGNO(I,2) ...	BEGNO(I,NBSEG(I))

FORMAT(16I5)

BSEGNO(I,M) - segment number of the Mth sediment segment included in spatial compartment I.

Note: if executing the food chain with the exposure concentration component and it is desired to have a spatial compartment with no toxicant set SEGNO to 0.

5.8 CARD GROUP G - INTEGRATION INFORMATION

5.8.1 Printing and Integration Information

10	20	30	40
DT	TTIME	PRNT	TØ

FORMAT(4F10.0)

DT - time step (d)

TTIME - total run time (d)

PRNT - print interval for outputting concentrations (d)

TØ - julian date at beginning of run (typically 0 days)

5.9 CARD GROUP H - EXPOSURE CONCENTRATIONS

This card group read in only if the food chain component is executed separately from the exposure concentration component

This card group is repeated for each segment specified in card group 5.7.4 in sequence from segment 1 to segment N.

5.9.1 Number of values describing the temporal distribution of concentration

5
NCON

FORMAT(I5)

NCON - number of values of concentrations to be inputted

5.9.2 Concentration Profile

8	16	24	32	40	48
DCON(L,1)	PCON(L,1)	TCON(L,1)	DCON(L,2)	PCON(L,2)	TCON(L,2)...

FORMAT(9F8.0)

DCON(L,M) - dissolved chemical concentration in segment L up to time TCON(L,M) (μg/ℓ)

PCON(L,M) - adsorbed chemical concentration in segment L up to time TCON(L,M) (μg/ℓ)

TCON(L,M) - time of concentration change in segment L (days)

(a maximum of 15 times may be specified)

SECTION 6
EXAMPLE APPLICATIONS

6.1 PCB IN THE LAKE MICHIGAN LAKE TROUT FOOD CHAIN (5)

The accumulation of PCBs in the Lake Michigan food chain was modeled assuming a four species food chain consisting of phytoplankton, *Mysis relicta*, alewife (*Alosa pseudoharengus*), and lake trout (*Salvelinus namaycush*). This species linkage constitutes the major energy transport route to the lake trout. Both *Mysis* and alewife were viewed as representative species of the middle levels of the food chain acknowledging that other invertebrates and small fish also contribute to the observed PCB levels in lake trout. The phytoplankton component of the model was assumed to represent nonliving particulate organic material as well as living plankton.

Phytoplankton were represented by a single compartment that was assumed to be in dynamic equilibrium with water column dissolved PCB. The other species were separated into discrete age classes.

The food chain model was structured with four 4 month age classes of *Mysis* reflecting life span and birth frequency. All classes consumed phytoplankton exclusively. The alewife component was divided into 7 single year classes. The feeding structure reflected field observations of stomach contents, young-of-the-year alewife consuming phytoplankton and all other age classes consuming *Mysis* with a bias toward the larger *Mysis*.

The lake trout component of the model was divided into 13 single-year age classes. Reflecting stomach content, the first two age classes consumed *Mysis* exclusively, the next class consumed *Mysis* and first and second year alewife. Older trout consumed alewife exclusively, with an age class distribution commensurate with the stomach content data. Movement of the species was not considered and a single spatial compartment representing the open waters of Lake Michigan was used.

The final calibration was the result of a series of model runs that determined a consistent set of parameter values that were in agreement with observed values and reproduced the observed PCB concentrations in Lake Michigan lake trout and alewife. Data for 1971 were used in the calibration. A constant dissolved PCB concentration of 5 ng/ℓ was assumed. A constant value implies that the alewife and lake trout sampled in 1971 were exposed to a constant PCB concentration for their entire lives, which for the oldest trout represented is ten years. A time variable dissolved PCB concentration was not used because no accurate data history exists. The values assigned to the PCB assimilation efficiency were adjusted to reproduce the observed PCB distribution. This parameter was chosen as the calibration variable because of the uncertainty of its value relative to the other parameters in the model.

The comparison between observed data and calculated PCB concentrations in alewife and lake trout is shown in Fig. 2. The parameter values used in the model are summarized in Table 2. The model reproduces the observed data with the exception of the early age classes of lake trout. No combination of parameters was successful at reproducing the high PCB values in age class 2 and 3 lake trout while maintaining consistency with reported parameter values and reproducing the observed concentrations in the upper age classes.

6.2 KEPONE IN THE JAMES RIVER STRIPED BASS FOOD CHAIN (7)

Accumulation of Kepone in the striped bass food chain was modeled using four trophic levels. Phytoplankton-detritus is the base of the food chain. The invertebrate level is represented by _Neomysis_ and _Nereis_, reflecting the importance of both pelagic and benthic species to the higher levels. Atlantic croaker (_Micropogan undalatus_) and white perch (_Morone americana_) are the fish species representing the level immediately below the striped bass (_Morone saxatilis_).

Phytoplankton-detritus, _Neomysis_, and _Nereis_ were represented by single compartments that are assumed to be in dynamic equilibrium with

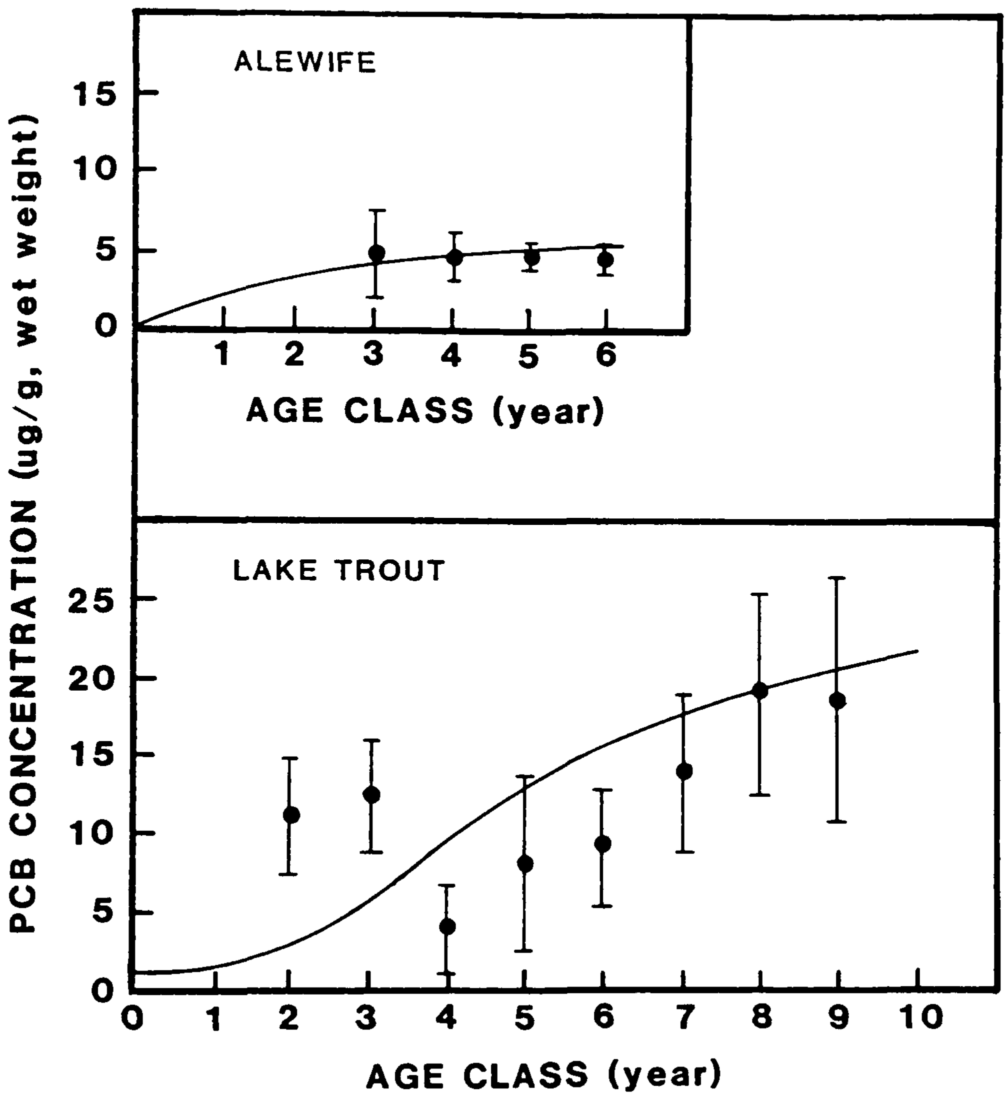

Figure 2. Comparison between observed and calculated PCB concentrations in alewife and lake trout

TABLE 2. PARAMETER VALUES USED FOR THE LAKE MICHIGAN LAKE TROUT FOOD CHAIN STUDY

Species	Growth		Respiration					Swimming Speed			BCF	Food Assim. Efficiency	Toxicant Assim. Efficiency	Fraction Dry Weight
	G	WO	R	BETA	GAMMA	RHO	XNU	OMGA	DLTA	PHI				
	d^{-1}	g_w	d^{-1}			$°C^{-1}$	s/cm			$°C^{-1}$	ℓ/g_w			
Phytoplankton	—	—	—	—	—	—	—	—	—	—	20	—	—	0.1
Mysis			-	0.0157	0.25	0	0	-	-	-	50	0.3	0.35	0.2
0-4 mo.	0.0193	0.00021												
4-8 mo.	0.0107	0.0022												
8-12 mo.	0.0073	0.0081												
12-16 mo.	0.0056	0.0198												
Alewife			-	0.047	0.2	0	0	-	-	-	100	0.8	0.7	0.25
0-3 yrs.	0.00245	2.5												
4-6 yrs.	0.00047	36.85												
Lake Trout			-	0.03	0.295	0	0.022	2.79	0.1285	0	100	0.8	0.8	0.25
0-1 yrs.	0.0058	2.2												
2-12 yrs.	0.0012	153.6												

Kepone in the water column and in their food. The white perch, the atlantic croaker and the striped bass were separated into year classes.

Neomysis americana is a mysid shrimp of considerable importance in the estuarine food chain linking organic detritus to fish. As a filter feeder it collects detritus and algae during diurnal migrations between the bed and the surface of the water column. In the model it was assumed to feed on the phytoplankton-detritus level only.

Nereis is an errant polychaete generally found in estuarine environments and may be classified as a deposit-feeder. Sediment particulate material was assumed to be the diet of *Nereis* in the model.

The atlantic croaker was divided into three single year classes. The first age class consumed photoplankton, the second age class consumed phytoplankton as well as *Neomysis* and *Nereis*, and the third age class consumed only *Neomysis* and *Nereis*. All age classes were assumed to be migratory entering the James River in March and leaving in October.

The white perch component of the model was divided into 10 single-year age classes. The first age class consumed phytoplankton, the second age class consumed phytoplankton and *Neomysis*, and the remaining age class fed on *Neomysis* and *Nereis*.

Eleven single-year age classes of striped bass were considered in the model. The first age class consumed phytoplankton, the next two consumed *Neomysis* and *Nereis*, and the older bass consumed the age classes of white perch and atlantic croaker consistent with observed prey size distributions. The first three age classes were assumed to permanently reside in the James River. Older striped bass were assumed to be migratory and present in the river from November to May. During the period from November to March when the atlantic croaker is not in the estuary the adult striped bass were assumed to prey on white perch only.

Kepone concentrations in the water column, sediment and fish of the James River have been monitored routinely by the Virginia State Water Control Board (SWCB) since 1976. These data provide a seven-year time history against which the model was compared and tested. The observed water column and sediment concentrations and the values used in the model are shown in Fig. 3. Spatially constant values were assumed because no consistent spatial gradient is evident from the data. During the portion of the year that atlantic croaker and striped bass were outside the James River they were assumed to be exposed to no Kepone. In the calibration procedure the Kepone assimilation efficiency and excretion rate were adjusted within their range of observed values to provide the best comparison of observed and computed Kepone concentrations. The parameters used in the model are shown in Table 3.

The comparisons between observed data and calculated Kepone concentrations in white perch, atlantic croaker, and striped bass are shown in Fig. 4. The data and calculated values are averages over all age classes. The model reproduces the observed within-year and year-to-year concentration variations for all species. The oscillation in atlantic croaker and striped bass concentrations reflects the migration of these species between the James River and the uncontaminated Chesapeake Bay and Atlantic Ocean.

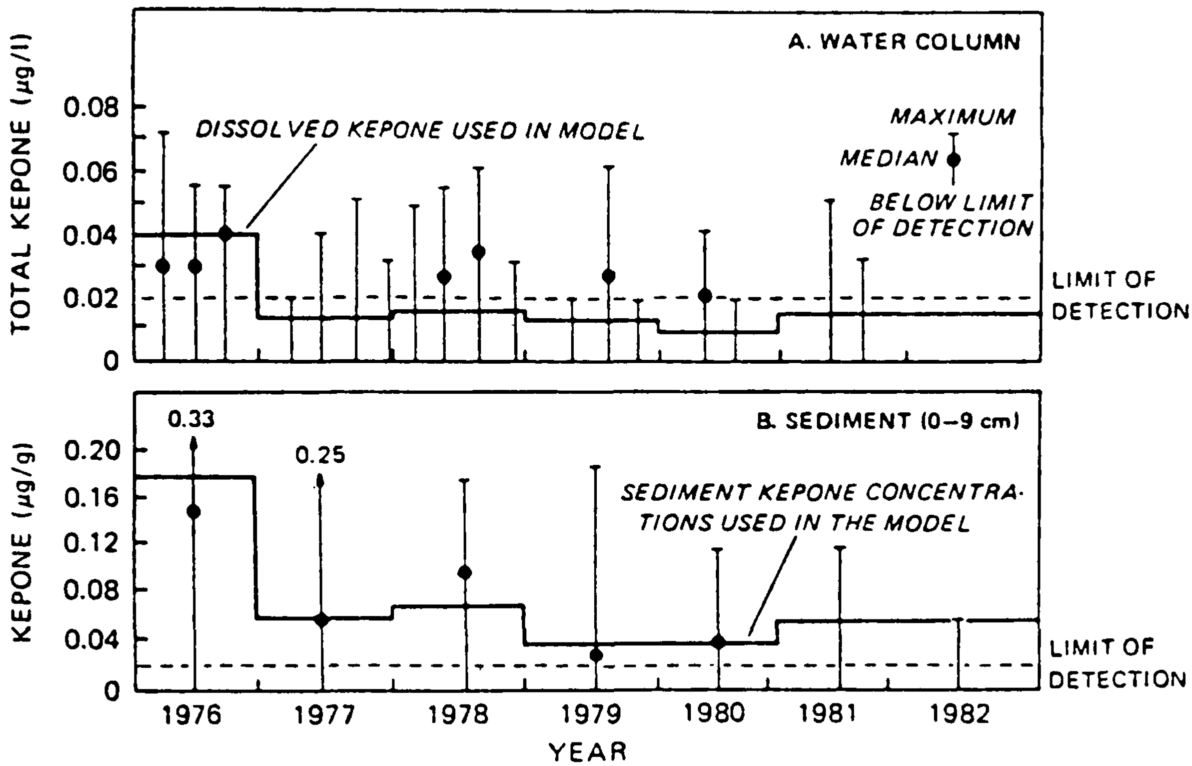

Figure 3. Kepone concentrations observed in the lower James River estuary (0-60 km) and the values used in the model for a) the water column, and b) the surface sediment

TABLE 3. PARAMETERS USED IN THE JAMES RIVER STRIPED BASS FOOD CHAIN STUDY

Species	Growth		Respiration					Swimming Speed			BCF	Food Assim. Efficiency	Toxicant Assim. Efficiency	Fraction Dry Weight
	G	WO	R	BETA	GAMMA	RHO	XNU	OMGA	DLTA	PHI				
	d^{-1}	g_w	d^{-1}			$°C^{-1}$	s/cm			$°C^{-1}$	ℓ/g_w			
Phytoplankton	—	—	—	—	—	—	—	—	—	—	6	—	—	0.1
Polychaete	0.007	-	0.02	-	-	0	-	-	-	-	6	0.3	0.3	0.2
Neomysis	0.01	-	0.102	-	-	0	-	-	-	-	6	0.3	0.3	0.2
Atlantic Croaker			-	0.038	0.2	0	0	-	-	-	6	0.8	0.72	0.25
0-1 yr.	0.0114	1.0												
1-2 yr.	0.0032	65.												
2-3 yr.	0.0026	210.												
White Perch			-	0.038	0.2	0	0	-	-	-	6	0.8	0.8	0.25
0-2 yr.	0.004	1.9												
2-5 yr.	0.0016	33.												
5-9 yr.	0.0007	140.												
Striped Bass			-	0.069	0.3	0	0.0176	1.19	0.32	0.0405	10	0.8	0.9	0.25
0-2 yr.	0.0069	2.												
2-3 yr.	0.0026	312.												
3-6 yr.	0.0014	808.												
6-9 yr.	0.00087	3759.												
9-11 yr.	0.00039	9770.												

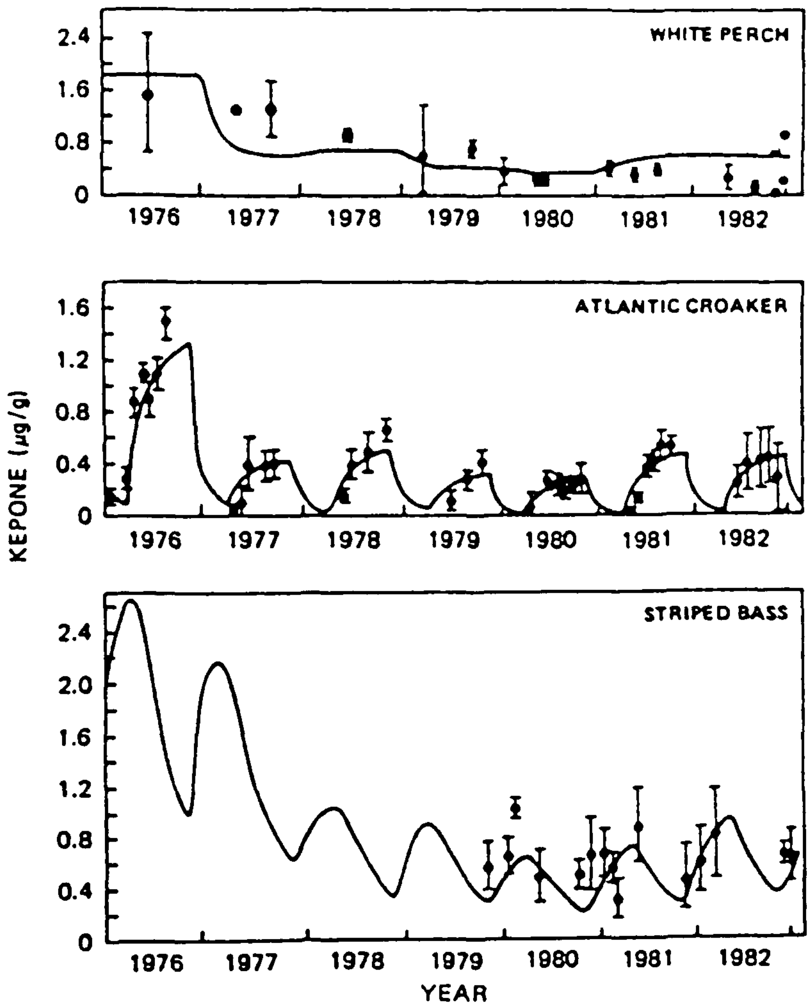

Figure 4. Comparison of observed and calculated Kepone concentrations in the atlantic croaker, white perch, and striped bass.

SECTION 7

OPERATIONAL CONSIDERATIONS

This chapter describes how to obtain the computer program WASTOX, how to install it on a DEC PDP mini computer, how to test the program with a sample dataset, and what machine limitations limit the program.

7.1 AQUISITION PROCEDURES

To obtain the program WASTOX along with a sample dataset and support software, write to:

Center for Water Quality Modeling
Environmental Research Laboratory
U.S. Environmental Protection Agency
College Station Road
Athens, GA 30613

A nine-track magnetic tape will be mailed to you. Please copy the contents and return the tape.

7.2 INSTALLATION PROCEDURES

The subroutines that comprise WASTOX must be compiled and linked into a task image. This is accomplished on the PDP IAS operating system by running the command file "WXTCMP.CTL." If the compilation succeeds, then linkage is automatically attempted with the command file "WXTLNK.CTL."

7.3 TESTING PROCEDURES

Once WASTOX is installed, the sample input dataset should be run and compared with the sample output dataset to verify that the program is calculating correctly. To perform a simulation on the PDP, submit the batch input sequence "WXTRUN.CTL."

7.4 MACHINE LIMITATIONS

Currently, WASTOX is set up for the following configuration:

	PDP 11/70 Hardware
	RSTS/E operating system
	FORTRAN IV
Physico-chemical component:	60 segments - steady-state
	75 segments - time-variable
	4 systems
Food Chain component:	20 species
	10 species in any spatial compartment
	2 migrating species
	12 spatial compartments
	10 physico-chemical model segments per spatial compartment
	150 age classes + steady-state species
	30 age classes + steady-state species in any spatial compartment

The PDP 11/70 computer utilizing RSTS/E operating system allocates a 32k word (64k byte) user area for execution of programs. WASTOX occupies at least 31k words of memory. Any enlargement of this program may result in an overflow of the user area.

REFERENCES

(1) Connolly, J.P. and R.P. Winfield. 1984. User's guide for WASTOX, a framework for modeling the fate of toxic chemicals in aquatic environments, Part 1: Exposure concentration. EPA-600/3-84-077.

(2) Norstrom, R.J., A.E. McKinnon, and A.S.W. DeFreitas. 1976. A bioenergetics based model for pollutant accumulation in fish: Simulation of PCB and methyl mercury residue levels in Ottawa River yellow perch (Perca Flavescens). J. Fish. Res. Board Can. 33:248-267.

(3) Weininger, D. 1978. Accumulation of PCBs by lake trout in Lake Michigan. Ph.D. Thesis, The University of Wisconsin-Madison, 232 p.

(4) Thomann, R.V. 1981. Equilibrium model of the fate of microcontaminants in diverse aquatic food chains. Can. J. Fish. Aquat. Sci., 38(3):280-296.

(5) Thomann, R.V. and J.P. Connolly. 1983. A model of PCB in the Lake Michigan lake trout food chain. Environ. Sci. Technol.

(6) Stewart, D.J. 1980. Salmonid Predators and their forage base in Lake Michigan: A bioenergetics-modeling synthesis Ph.D. Thesis, The University of Wisconsin-Madison. 225 p.

(7) Connolly, J.P. and R. Tonelli. 1985. A model of Kepone in the striped bass food chain of the James River Estuary. Estuarine, Coastal and Shelf Sci.

APPENDIX 1
GLOSSARY

I. Variables in Common Block MAIN

ACS(I)	- size in days of each age class of age-dependent species I
ASIM(I)	- food assimilation efficiency of species I
ASM(I)	- toxicant assimilation efficiency of species I
BCF(I)	- toxicant bioconcentration factor for species I (ℓ/gm)
BETA(I)	- respiration coefficient for age-dependent species I
BSEGNO(I,J)	- number of the J^{th} segment from the exposure concentration component included in the benthic region of compartment I
CFC(I,J)	- concentration of toxicant in the J^{th} step of the food chain in compartment I(μg/g). Steps are counted from the first species above the plankton-detritus level and include the steady state species and each age class of the age dependent species
CNSMP(I)	- consumption rate of the I^{th} step of the food chain (g/g/d)
DIFF	- molecular diffusivity of the toxicant (cm^2/s)
DLTA(I)	- swimming speed weight exponent for age-dependent species I
DT	- time step for the calculation (d)
FDRY(I)	- dry weight to wet weight ratio for species I
GAMMA(I)	- respiration weight exponent for age-dependent species I
GROW(I)	- growth rate for step I of the food chain (g/g/d)
IFLG(I)	- flag indicating that species I is either pelagic or benthic
KP	- phytoplankton-detritus bioconcentration factor (ℓ/g)
MFLG(I)	- flag specifying whether species I is a continuation of species I-1
NAC(I)	- number of age classes for age dependent species I

NBSEG(I) - number of bed segments included in compartment I

NPREY(I,J) - number of prey of the J^{th} step in compartment I

NSC - number of spatial compartments in the model

NSEG - number of water column segments included in compartment I

NSP - number of age-dependent species in the model

NSPI(I) - number of species in compartment I

NSPSS - number of steady-state species in the model

OMGA(I) - swimming speed coefficient for age-dependent species I

PHI(I) - exponential coefficient for temperature dependence of species I swimming speed ($°C^{-1}$)

PREF(I,J,L) - fraction of the consumption rate of step J in compartment I that is on step L

PREY(I,J,L) - step number of prey L for step J in compartment I

PRNT - outputting interval in days

RESP(I) - respiration rate of step I (g/g/d)

RHO(I) - exponential coefficient for temperature dependence of species I respiration ($°C^{-1}$)

SEGNO(I,J) - segment number of the J^{th} water column segment included in spatial compartment I

SPBD(I) - date of birth for species I (julian days from start of run)

SPNO(I,J) - species number of the J^{th} species in compartment I

TIME - current time during the run (d)

TTIME - final time of the run (d)

TO - julian date at the start of the run

W(I) - current weight of age class I in the food chain (counting from the first age-dependent species) (g_{wet})

WO(I) - initial weight of age class I (g_{wet})

XNU(I) - exponential coefficient for swimming speed (s/cm)

II. Variables in Common Block INIT

COMPRT(I,J) - spatial compartment occupied by the I^{th} migratory species for time up to TIMEM(I,J)

MIGSC(I) - compartment currently occupied by the I^{th} migratory species

MIGSN(I) - species number of the I^{th} migratory species

MINDX(J,I) - step number for the first age class of migrating species J when it is in compartment I

NBRKS(I) - number of breaks describing the migratory pattern of the I^{th} migratory species

NCNT(I) - counter for the migratory pattern arrays COMPRT and TIMEM for the I^{th} migratory species

NMIG - number of migratory species in the model

TIMEM(I,J) - time of break J in the migratory pattern of the I^{th} migratory species (d)

III. Variables in Common Block SYSTRN

ITCNT(I) - counter for the time variable temperature function for spatial compartment I

NBRKS2(I) - number of time-temperature pairs defining the I^{th} spatial compartments annual temperature cycle

TEMP(I,J) - temperature at break J in the temperature cycle of compartment I (°C)

TIMET(I,J) - time of break J in the temperature cycle of compartment I (d)

IV. Variables in Common Block PHOTO

DISTOX(I) - current dissolved toxicant concentration in segment I (μg/ℓ)

PARTOX(I) - current adsorbed toxicant concentration in segment I (μg/g)

V. Variables in Common Block JUNK

DCON(I,J) - dissolved toxicant concentration in segment I up to time TCON(I,J) (μg/ℓ)

MX(I) - counter for the concentration profile in segment I

PCON(I,J) - adsorbed chemical concentration in segment I up to time TCON(I,J) (μg/g)

TCON(I,J) - time of the J^{th} concentration change in segment I (d)

VI. Variables in Common Block MAINA

IN	- unit number assigned to the input file
ISYS	- variable used in exposure concentration component of WASTOX
IREC	- record counter used in reading the time output file of the exposure concentration component
IRECL(I)	- record counter used in reading the output file of the I^{th} system of the exposure concentration component
NOSEG	- number of segments in the exposure concentration component
NOSYS	- number of systems in the exposure concentration component
OUT	- unit number assigned to the output file
SYSEX(I)	- array used in the exposure concentration component

VII. Variables in Common Block OPTION

PRGOPT	- programming option specifying whether the exposure concentration component is run alone, the food chain is run alone, or they are run together
TYPE	- variable used in the exposure concentration component to indicate a time variable or steady state run

VIII. Variables in Common Block DUMP

MXDMP	- number of variables written to output for each system in the exposure concentration component
MXSEG	- maximum number of segments permitted in the exposure concentration component (75)

IX. Variables in Common Block UPTAKE

O2	- dissolved oxygen concentration (g/ℓ)
DRATIO	- ratio of the molecular diffusivity of oxygen to the molecular diffusivity of the toxicant

APPENDIX 2
TEST PROGRAM INPUT AND OUTPUT

To test that the computer code for the food chain component of WASTOX is working correctly on the user's computer, a simple test food chain problem is provided. Three species are considered; two steady state and one age-dependent. The steady state species are a pelagic invertebrate that consumes phytoplankton and a benthic invertebrate that consumes detritus. The age-dependent species is a fish divided into 3 single-year age classes, all of which prey equally on the two invertebrate species. A single spatial compartment is considered. The parameters used in the model are shown in Table A1.

TABLE A1. TEST PROGRAM INPUT PARAMETERS

Species	Growth		Respiration					Swimming Speed			BCF	Food Assim. Efficiency	Toxicant Assim. Efficiency	Fraction Dry Weight
	G	WO	R	BETA	GAMMA	RHO	XNU	OMGA	DLTA	PHI				
	d^{-1}	g_w	d^{-1}			$°C^{-1}$	s/cm			$°C^{-1}$	ℓ/g_w			
Phytoplankton	—	—	—	—	—	—	—	—	—	—	10	—	—	0.1
Pelagic Invertebrate	0.01	-	0.102	-	-	0.0	-	-	-	-	10	0.3	0.3	0.2
Benthic Invertebrate	0.01	-	0.02	-	-	0.0	-	-	-	-	10	0.3	0.3	0.2
Fish*			-	0.038	0.2	0.0	0.0176	11	0.1	0.045	10	0.8	0.8	0.25
0-1 yr.	0.007	1												
1-2 yr.	0.003	12.96												
2-3 yr.	0.001	38.86												

* Birth Date = 0.0

Compound Diffusivity = 4.55×10^{-6} cm^2/s
Water Column Concentration = 0.01 μg/ℓ
Bed Dissolved Concentration = 0.14 μg/ℓ
Bed Adsorbed Concentration = 0.277 μg/g
Water Temperature = 15°C

INPUT FILE

```
WASTOX.INP;17                        4-JAN-1985 16:13                Page 1

 2
    1    2
  10.      .00000455
    0    0  PLG INVT
    0.102      0.01       0.3       10.0       0.3       0.2       0.0
    1    0 BNTH INVT
     0.02      0.01       0.3       10.0       0.3       0.2       0.0
    0    0    FISH
    3 366.       0.8      0.038      0.2       0.8       0.25
      0.0      11.0       0.1     0.0405      0.01
        0        0.0
        1      0.007      10.0
    12.96      0.003      10.0
    38.86      0.001      10.0
    0
    1
    1
   9999.0      15.0
    3
    1
    1
    0 1.0
      0.0
    2
      0.0
    3
    2
    1       0.5    2      0.5
      0.0
    2
    1       0.5    2      0.5
      0.0
    2
    1       0.5    2      0.5
      0.0
    1    1
    1
    2
      2.0      366.0      30.0       0.0
    1
   0.01     0.0    366.0
    1
   0.14   0.277    366.0


12345678901234567890123456789012345678901234567890123456789012345678901234567890
         1         2         3         4         5         6         7         8
```

OUTPUT FILE

****

F O O D   C H A I N   I N P U T

****

1 AGE DEPENDENT SPECIES 2 STEADY STATE SPECIES

PLANKTON BCF 10.0 COMPOUND DIFFUSIVITY = 0.4550E-05

STEADY STATE SPECIES

S P E C I E S 1 PLG INVT

RESPIRATION RATE PER DAY	0.1020E+00
GROWTH RATE PER DAY =	0.1000E-01
TOXICANT ASSIMILATION EFF.	0.3000E+00
BIOCONCENTRATION FACTOR	0.1000E+02
FOOD ASSIMILATION EFF.	0.3000E+00
FRACTION DRY WEIGHT =	0.2000E+00
RESPIRATION TEMP COEF,RHO	0.0000E+00

S P E C I E S 2 BNTH INVT

RESPIRATION RATE PER DAY	0.2000E-01
GROWTH RATE PER DAY =	0.1000E-01
TOXICANT ASSIMILATION EFF.	0.3000E+00
BIOCONCENTRATION FACTOR	0.1000E+02
FOOD ASSIMILATION EFF.	0.3000E+00
FRACTION DRY WEIGHT =	0.2000E+00
RESPIRATION TEMP COEF,RHO	0.0000E+00

S P E C I E S 3 FISH

3 AGE CLASSES OF 366. DAYS EACH AND BIRTH 0.DAYS AFTER START OF RUN

RESPIRATION COEFFICIENTS:	BETA =0.3800E-01
	GAMMA =0.2000E+00
	RHO =0.0000E+00
	OMGA =0.1100E+02
	DLTA =0.1000E+00
	PHI =0.4050E-01
	XNU =0.1000E-01
FOOD ASSIMILATION EFF.	0.8000E+00
FRACTION DRY WEIGHT	0.2500E+00
TOXICANT ASSIMILATION EFF.	=0.8000E+00

AGE CLASS	INITIAL WT. (GM)	GROWTH RATE (1/DAY)	BIOCONCENTRATION FACTOR (L/G)
1	0.1000E+01	0.7000E-02	0.1000E+02
2	0.1296E+02	0.3000E-02	0.1000E+02
3	0.3886E+02	0.1000E-02	0.1000E+02

$$$ 0 OF THE SPECIES MIGRATE $$$

****

1 SPATIAL COMPARTMENTS CONSIDERED

****

C O M P A R T M E N T 1

ANNUAL TEMPERATURE PROFILE DESCRIBED BY A STRAIGHT LINE FUNCTION WITH THE FOLLOWING BREAKS:

TIME	TEMP	TIME	TEMP	TIME	TEMP	TIME	TEMP
9999.0	15.0						

S P E C I E S 1

STEADY-STATE SPECIES WITH PREDATOR-PREY INDEX OF 1

PREY	FRACTION OF TOTAL CONSUMPTION
0	1.000

INITIAL CONCENTRATION (UG/G) = 0.000

S P E C I E S 2

STEADY-STATE SPECIES WITH PREDATOR-PREY INDEX OF 2

BENTHIC SPECIES ASSUMED TOCONSUME DETRITUS

INITIAL CONCENTRATION (UG/G) 0.000

S P E C I E S 3

AGE CLASS 1 PREDATOR-PREY INDEX 3

PREY	FRACTION OF TOTAL CONSUMPTION
1	0.500
2	0.500

INITIAL CONCENTRATION (UG/G) 0.000

AGE CLASS 2 PREDATOR-PREY INDEX 4

PREY FRACTION OF TOTAL CONSUMPTION

```
                1                       0.500
                2                       0.500

             INITIAL CONCENTRATION (UG/G)      0.000

             AGE CLASS  3     PREDATOR-PREY INDEX  5

           PREY             FRACTION OF TOTAL CONSUMPTION
             1                          0.500
             2                          0.500

             INITIAL CONCENTRATION (UG/G)      0.000

        WATER COLUMN SEGMENTS INCLUDED IN COMPARTMENT  1 ARE:

                1

        BED SEGMENTS INCLUDED IN COMPARTMENT  1 ARE:

                2
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TIME STEP= 2.0 RUN TIME= 366. PRNTINTERVAL= 30. JULIAN DATE AT START= 0.

****

CHEMICAL CONCENTRATIONS FOR SEGMENT 1

DISS. CONC. UG/L	PART. CONC. UG/G	TIME DAYS	DISS. CONC. UG/L	PART. CONC. UG/G	TIME DAYS	DISS. CONC. UG/L	PART. CONC. UG/G	TIME DAYS
0.1000E-01	0.0000E+00	366.						

CHEMICAL CONCENTRATIONS FOR SEGMENT 2

DISS. CONC. UG/L	PART. CONC. UG/G	TIME DAYS	DISS. CONC. UG/L	PART. CONC. UG/G	TIME DAYS	DISS. CONC. UG/L	PART. CONC. UG/G	TIME DAYS
0.1400E+00	0.2770E+00	366.						

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                    FOOD CHAIN MODEL

      AGE CLASS 1      EXCRETION RATE  0.1528E-01
      AGE CLASS 2      EXCRETION RATE  0.1264E-01
      AGE CLASS 3      EXCRETION RATE  0.1188E-01
*************************************************************************************************

                              YEAR 0  DAY   30.

         $$$$$$$$$$$$$$$$$$$$ SPATIAL COMPARTMENT 1 $$$$$$$$$$$$$$$$$$$$

                              S P E C I E S   1
                   STEADY-STATE CONCENTRATION =0.5101E+00 *

                              S P E C I E S   2
                   STEADY-STATE CONCENTRATION =0.1089E+01

                              S P E C I E S   3
  AGE CLASS  CONCENTRATION    AGE CLASS  CONCENTRATION     AGE CLASS  CONCENTRATION     AGE CLASS  CONCENTRATION
     1        0.1085E+01         2         0.7868E+00          3        0.6613E+00

                   AVERAGE CONCENTRATION FOR SPECIES   3   0.8445E+00
*************************************************************************************************

                              YEAR 0  DAY   60.

         $$$$$$$$$$$$$$$$$$$$ SPATIAL COMPARTMENT 1 $$$$$$$$$$$$$$$$$$$$

                              S P E C I E S   1
                   STEADY-STATE CONCENTRATION =0.5101E+00

                              S P E C I E S   2
                   STEADY-STATE CONCENTRATION =0.1089E+01

                              S P E C I E S   3
  AGE CLASS  CONCENTRATION    AGE CLASS  CONCENTRATION     AGE CLASS  CONCENTRATION     AGE CLASS  CONCENTRATION
     1        0.1509E+01         2         0.1239E+01          3        0.1099E+01

                   AVERAGE CONCENTRATION FOR SPECIES   3   0.1282E+01
*************************************************************************************************

                              YEAR 0  DAY   90.

         $$$$$$$$$$$$$$$$$$$$ SPATIAL COMPARTMENT 1 $$$$$$$$$$$$$$$$$$$$

                              S P E C I E S   1
                   STEADY-STATE CONCENTRATION =0.5101E+00
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* All Concentrations are μg/g(wet weight)

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                     STEADY-STATE CONCENTRATION =0.1089E+01

                              S P E C I E S   3
  AGE CLASS  CONCENTRATION      AGE CLASS  CONCENTRATION      AGE CLASS  CONCENTRATION      AGE CLASS  CONCENTRATION
      1        0.1670E+01           2        0.1498E+01           3        0.1387E+01

                     AVERAGE CONCENTRATION FOR SPECIES   3   0.1518E+01
**********************************************************************************************************************

                              YEAR 0  DAY  120.

          $$$$$$$$$$$$$$$$$$$$ SPATIAL COMPARTMENT 1 $$$$$$$$$$$$$$$$$$$$

                              S P E C I E S   1
                     STEADY-STATE CONCENTRATION =0.5101E+00

                              S P E C I E S   2
                     STEADY-STATE CONCENTRATION =0.1089E+01

                              S P E C I E S   3
  AGE CLASS  CONCENTRATION      AGE CLASS  CONCENTRATION      AGE CLASS  CONCENTRATION      AGE CLASS  CONCENTRATION
      1        0.1731E+01           2        0.1645E+01           3        0.1578E+01

                     AVERAGE CONCENTRATION FOR SPECIES   3   0.1651E+01
**********************************************************************************************************************

                              YEAR 0  DAY  150.

          $$$$$$$$$$$$$$$$$$$$ SPATIAL COMPARTMENT 1 $$$$$$$$$$$$$$$$$$$$

                              S P E C I E S   1
                     STEADY-STATE CONCENTRATION =0.5101E+00

                              S P E C I E S   2
                     STEADY-STATE CONCENTRATION =0.1089E+01

                              S P E C I E S   3
  AGE CLASS  CONCENTRATION      AGE CLASS  CONCENTRATION      AGE CLASS  CONCENTRATION      AGE CLASS  CONCENTRATION
      1        0.1752E+01           2        0.1730E+01           3        0.1704E+01

                     AVERAGE CONCENTRATION FOR SPECIES   3   0.1729E+01
**********************************************************************************************************************

                              YEAR 0  DAY  180.

          $$$$$$$$$$$$$$$$$$$$ SPATIAL COMPARTMENT 1 $$$$$$$$$$$$$$$$$$$$

                              S P E C I E S   1
                     STEADY-STATE CONCENTRATION =0.5101E+00

                              S P E C I E S   2
                     STEADY-STATE CONCENTRATION =0.1089E+01
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                              S P E C I E S   3
 AGE CLASS  CONCENTRATION    AGE CLASS  CONCENTRATION    AGE CLASS  CONCENTRATION    AGE CLASS  CONCENTRATION
     1       0.1756E+01          2        0.1779E+01          3      0.1787E+01

                    AVERAGE CONCENTRATION FOR SPECIES   3   0.1774E+01
*****************************************************************************************************************

                              YEAR 0  DAY  210.

          $$$$$$$$$$$$$$$$$$$$ SPATIAL COMPARTMENT 1 $$$$$$$$$$$$$$$$$$$$

                              S P E C I E S   1
                    STEADY-STATE CONCENTRATION =0.5101E+00

                              S P E C I E S   2
                    STEADY-STATE CONCENTRATION =0.1089E+01

                              S P E C I E S   3
 AGE CLASS  CONCENTRATION    AGE CLASS  CONCENTRATION    AGE CLASS  CONCENTRATION    AGE CLASS  CONCENTRATION
     1       0.1754E+01          2        0.1807E+01          3      0.1843E+01

                    AVERAGE CONCENTRATION FOR SPECIES   3   0.1801E+01
*****************************************************************************************************************

                              YEAR 0  DAY  240.

          $$$$$$$$$$$$$$$$$$$$ SPATIAL COMPARTMENT 1 $$$$$$$$$$$$$$$$$$$$

                              S P E C I E S   1
                    STEADY-STATE CONCENTRATION =0.5101E+00

                              S P E C I E S   2
                    STEADY-STATE CONCENTRATION =0.1089E+01

                              S P E C I E S   3
 AGE CLASS  CONCENTRATION    AGE CLASS  CONCENTRATION    AGE CLASS  CONCENTRATION    AGE CLASS  CONCENTRATION
     1       0.1749E+01          2        0.1822E+01          3      0.1880E+01

                    AVERAGE CONCENTRATION FOR SPECIES   3   0.1817E+01
*****************************************************************************************************************

                              YEAR 0  DAY  270.

          $$$$$$$$$$$$$$$$$$$$ SPATIAL COMPARTMENT 1 $$$$$$$$$$$$$$$$$$$$

                              S P E C I E S   1
                    STEADY-STATE CONCENTRATION =0.5101E+00

                              S P E C I E S   2
                    STEADY-STATE CONCENTRATION =0.1089E+01
```

S P E C I E S 3

AGE CLASS	CONCENTRATION	AGE CLASS	CONCENTRATION	AGE CLASS	CONCENTRATION	AGE CLASS	CONCENTRATION
1	0.1743E+01	2	0.1831E+01	3	0.1904E+01		

AVERAGE CONCENTRATION FOR SPECIES 3 0.1826E+01

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YEAR 0 DAY 300.

$$$$$$$$$$$$$$$$$$$$ SPATIAL COMPARTMENT 1 $$$$$$$$$$$$$$$$$$$$

S P E C I E S 1
STEADY-STATE CONCENTRATION =0.5101E+00

S P E C I E S 2
STEADY-STATE CONCENTRATION =0.1089E+01

S P E C I E S 3

AGE CLASS	CONCENTRATION	AGE CLASS	CONCENTRATION	AGE CLASS	CONCENTRATION	AGE CLASS	CONCENTRATION
1	0.1736E+01	2	0.1835E+01	3	0.1920E+01		

AVERAGE CONCENTRATION FOR SPECIES 3 0.1830E+01

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YEAR 0 DAY 330.

$$$$$$$$$$$$$$$$$$$$ SPATIAL COMPARTMENT 1 $$$$$$$$$$$$$$$$$$$$

S P E C I E S 1
STEADY-STATE CONCENTRATION =0.5101E+00

S P E C I E S 2
STEADY-STATE CONCENTRATION =0.1089E+01

S P E C I E S 3

AGE CLASS	CONCENTRATION	AGE CLASS	CONCENTRATION	AGE CLASS	CONCENTRATION	AGE CLASS	CONCENTRATION
1	0.1729E+01	2	0.1836E+01	3	0.1931E+01		

AVERAGE CONCENTRATION FOR SPECIES 3 0.1832E+01

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YEAR 0 DAY 360.

$$$$$$$$$$$$$$$$$$$$ SPATIAL COMPARTMENT 1 $$$$$$$$$$$$$$$$$$$$

S P E C I E S 1
STEADY-STATE CONCENTRATION =0.5101E+00

S P E C I E S 2
STEADY-STATE CONCENTRATION =0.1089E+01

S P E C I E S 3

AGE CLASS	CONCENTRATION	AGE CLASS	CONCENTRATION	AGE CLASS	CONCENTRATION	AGE CLASS	CONCENTRATION
1	0.1721E+01	2	0.1836E+01	3	0.1938E+01		

AVERAGE CONCENTRATION FOR SPECIES 3 0.1832E+01

****

YEAR 1 DAY 24.

$$$$$$$$$$$$$$$$$$$$ SPATIAL COMPARTMENT 1 $$$$$$$$$$$$$$$$$$$$

S P E C I E S 1
STEADY-STATE CONCENTRATION =0.0000E+00

S P E C I E S 2
STEADY-STATE CONCENTRATION =0.0000E+00

S P E C I E S 3

AGE CLASS	CONCENTRATION	AGE CLASS	CONCENTRATION	AGE CLASS	CONCENTRATION	AGE CLASS	CONCENTRATION
1	0.0000E+00	2	0.1108E+01	3	0.1320E+01		

AVERAGE CONCENTRATION FOR SPECIES 3 = 0.8096E+00