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A model for predicting the bioaccumulation of hydrophobic organic chemicals in aquatic food-webs: application to Lake Ontario

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ABSTRACT

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A simple model is presented for estimating concentrations of hydrophobic organic substances in various organisms of aquatic food-webs from chemical concentrations in water and sediments. The model is applied to the Lake Ontario food-web and shown to be in satisfactory agreement with field data. Model confidence is determined by Monte-Carlo simulation. Since the model only requires basic data to characterize the organisms of the food-web, chemical properties and environmental conditions, the model is an easy-to-apply and practical tool for the management of organic contaminants on an "ecosystem" level.

INTRODUCTION

For water quality management in rivers and lakes, it is important to be able to predict the impacts of chemical discharges in terms of chemical concentrations and toxic effects in aquatic organisms. In this paper, we present a steady-state model for estimating concentrations of hydrophobic organic substances in various organisms of aquatic food-webs, including fish, benthos, macrophytes, aquatic plants and others, from chemical concentrations in the water and sediments. The model combines the toxicoki-

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netics of chemical uptake, elimination and bioaccumulation in individual organisms and the trophodynamics of food-webs to estimate chemical concentrations in different organisms of food-webs. This food-web model differs from simple four-level generic food-chain models (e.g. Thomann, 1989; Clark et al., 1990) by incorporating multiple feeding interactions, including benthic and pelagic food-chains, and its ability as a generic model to apply to food-webs on a site-specific basis. The model is relatively simple and requires only few input data, which makes it easy to apply for practical use. We will demonstrate the applicability of this model for water quality management by applying it to more than 60 organochlorines in the Lake Ontario food-web and comparing model predicted and observed data.

BIOAVAILABILITY

In any model of the uptake and bioaccumulation of organic chemicals in aquatic organisms, one of the most important components is the concentration of the chemical in the water that can be absorbed by the organism from the water (e.g. via the gills in fish). In particular for very hydrophobic chemicals, the concentration of absorbable or bioavailable chemical is often only a fraction of the total chemical concentration in the water. This fraction is usually referred to as the Bioavailable Solute Fraction (BSF). or simply the bioavailability (Landrum et al., 1985; McCarthy and Jimenez, 1985; Black and McCarthy, 1988; Gobas et al., 1989a).

The bioavailability of organic chemicals in natural waters is largely determined by the interaction of the chemical with particulate organic matter in the water, which results in the formation of chemical aggregates or complexes that are too large to permeate through biological membranes (e.g. the gill membrane). It is generally believed that only chemicals in true solution are bioavailable. The bioavailability can thus be defined as the ratio of the truly dissolved chemical concentration in the water C_{WD} (μg/l) and the total chemical concentration in the water C_{WT} (μg/l), i.e. BSF equals C_{WD}/C_{WT}. A simple mass balance of the chemical in the water shows that:

$$V_{WT} \cdot C_{WT} = V_W \cdot C_{WD} + M_{OM} \cdot C_{OM} \quad (1)$$

where V_{WT}, V_W are the volumes (l) of respectively the total volume (i.e. water and organic matter) and the water only and M_{OM} is the mass (kg) of particulate organic matter in suspension. C_{OM} is the chemical concentration (μg/kg) in the organic matter. Since usually the fraction of particulate organic matter in natural waters ranges from approximately 10^{-5} to 10^{-7} (kg/kg), V_{WT} and V_W are approximately equal. C_{OM} and C_{WD} are related through the organic matter/water partition coefficient K_{OM} (l/kg), i.e.

C_{OM} equals $K_{OM} \cdot C_{WD}$ (Karickhoff, 1984). DiToro (1985) showed that, within experimental error, $K_{OM} \cdot d_{OM}$ equals the dimensionless 1-octanol–water partition coefficient K_{OW}. d_{OM} is the density of the organic matter (kg/l). It thus follows that the BSF can be expressed as

$$BSF = 1/(1 + (K_{OW} \cdot [OM]/d_{OM})), \quad (2)$$

where [OM] is the concentration (kg/l) of organic matter in the water, i.e. M_{OM}/V_W. Under most natural conditions, Eq. 2 may give a reasonable estimate of the fraction of the chemical concentration in the water that is available for chemical uptake in aquatic organisms.

BIOACCUMULATION IN AQUATIC MACROPHYTES

Uptake and bioaccumulation of chemicals in submerged aquatic macrophytes and phytoplankton are predominantly the result of chemical exchange between the organism and the water (Geyer et al., 1984; Mallhot, 1987; Gobas et al., 1991). Growth or population growth (for phytoplankton) can also be a factor influencing the concentration in the organism, since an increase in the organism's weight or volume has a "diluting" effect on the chemical concentration in the organism. The following model represents this:

$$dC_A/dt = k_1 \cdot C_{WD} - k_2 \cdot C_A - k_G \cdot C_A, \quad (3)$$

where C_A (μg/kg) is the chemical concentration in the organism and C_{WD} (μg/l) is the bioavailable concentration in the water. k_1 (l/kg · day) and k_2 (1/day) are the rate constants for respectively chemical uptake from the water and chemical elimination to the water. k_G (1/day) is the first order rate constant for growth. This model has the following steady-state solution:

$$BCF = C_A/C_{WD} = k_1/(k_2 + k_G), \quad (4)$$

where the ratio of the concentration in the organism and that in the water is often referred to as the bioconcentration factor BCF. Unless macrophytes are in a rapid growth phase (e.g. at certain times during the year), k_G is small compared to k_2, thus simplifying BCF to k_1/k_2. Since lipids are usually the predominant site for bioaccumulation of hydrophobic substances, BCF can be satisfactorily approximated by K_{OW}, giving

$$BCF = C_A/C_{WD} = k_1/k_2 = L_A \cdot K_{OW}, \quad (5)$$

where L_A is the lipid content (kg/kg) of the macrophytes (Geyer et al., 1984 for phytoplankton, Gobas et al., 1991 for aquatic plants).

BIOACCUMULATION IN ZOOPLANKTON

Due to their small size and large area/volume ratio, uptake and bioaccumulation of organic chemicals in zooplankton are predominantly the result of chemical exchange between the organism and the water (Clayton et al., 1977). Equation 5, which describes a similar process for aquatic macrophytes, may therefore also applies to zooplankton, but the lipid content of macrophytes and zooplankton are usually different.

BIOACCUMULATION IN BENTHIC INVERTEBRATES

It is often convenient to view the uptake and accumulation of hydrophobic organic substances in benthic invertebrates as the result of an equilibrium partitioning of the chemical between the lipids of the organism, the organic carbon fraction (OC) of the sediment, and the interstitial (or pore) water (Shea, 1988; Gobas et al., 1989b):

$$C_B \cdot d_L / L_B = C_S \cdot d_{OC} / OC = K_{LW} \cdot C_P, \quad (6)$$

where C_B is the chemical concentration in the benthic invertebrate (μg/kg wet weight), C_S is the concentration in the sediments (μg/kg dry weight), C_P is the truly dissolved chemical concentration in the pore water (μg/l water), L_B is the lipid fraction of the benthos (kg lipid/kg organism), d the density of the lipids of the benthos (kg/l), OC is the organic carbon fraction of the sediments (kg organic carbon/kg ~~organism~~ sediment), d_{OC} is the density of the organic carbon fraction of the sediments (kg/l) and K_{LW} is the dimensionless lipid water partition coefficient. An interesting aspect of this model is that C_B/C_S should be approximately similar for organic chemicals, namely $L_B \cdot d_{OC}/OC \cdot d_L$, or simply L_B/OC since d_L and d_{OC} are approximately the same. Thus, if for example, L_B is 6% and OC is 2%, then C_B is approximately 3 times higher than C_S.

Although this model is simple and physiologically more detailed models can be derived, Eq. 6 has been shown to be in better agreement with actual field data than the more detailed models (Gobas et al., 1989b; Landrum et al., 1992).

BIOACCUMULATION IN FISH

Fish absorb chemicals directly from the water, i.e. via the gills, and through the consumption of food, i.e. via the GI-tract (Bruggeman et al., 1981). Other uptake routes such as chemical absorption via the skin are usually insignificant. Chemical loss or elimination can occur via the gills to the water, via egestion of faecal matter or as a result of metabolic

transformation. Fish growth can have a considerable effect on bioaccumulation factors and concentrations in fish, in particular for chemicals of high K_{OW} (Thomann and Connolly, 1984; Clark et al., 1990). To incorporate fish growth into the model and to allow for a simple steady-state solution to be applied, the effect of growth can be introduced in terms of a rate constant k_G, i.e. $dV_F/V_F \cdot dt$, with units of 1/day. The following equation combines these processes in an overall flux equation, describing the net flux of chemical into the fish as the sum of all of the uptake and loss fluxes:

$$dC_F/dt = k_1 \cdot C_{WD} + k_D \cdot C_D - (k_2 + k_E + k_M + k_G) \cdot C_F, \quad (7)$$

where C_{WD} is the dissolved chemical concentration in the water (μg/l), C_D is the chemical concentration in the food (μg/kg) and C_F is the chemical concentration in the fish (μg/kg fish). V_F is the weight of the fish (kg). The k's are first order rate constants: k_1 for uptake from the water via the gills (l/kg · day); k_2 for elimination via the gills to the water (1/day); k_D for chemical uptake from food (in kg food/kg fish/day); k_E for elimination by faecal egestion (1/day); and k_M for metabolic transformation of the chemical (in 1/day). The steady-state mass balance equation is

$$C_F = (k_1 \cdot C_{WD} + k_D \cdot C_D)/(k_2 + k_E + k_M + k_G), \quad (8)$$

where $k_1/(k_2 + k_E + k_M + k_G)$ is usually referred to as the bioconcentration factor and $k_D/(k_2 + k_E + k_M + k_G)$ is the biomagnification factor.

From Eq. 8 it follows that to estimate steady-state chemical concentrations in fish, values are required for k_1, k_2, k_D, k_E, k_M and k_G for different chemicals and fish species.

Gill uptake rate constant

The rate at which chemicals are absorbed by fish via the gills is expressed by the gill uptake rate constant k_1 (l/kg · day). The gill uptake rate is the combined process of the gill ventilation rate G_V (l/day) and the diffusion rate of the chemical across the gills (Gobas and Mackay, 1987). The extent to which chemicals that enter the gill compartment by gill ventilation are actually absorbed by the organism is usually expressed by the gill uptake efficiency E_W. k_1 then follows as

$$k_1 = E_W \cdot G_V/V_F. \quad (9)$$

Studies of the relationship between k_1 and K_{OW} and between E_W and K_{OW} in various fish species have shown that (i) k_1 and E_W increase with K_{OW} if log K_{OW} is low (< 4.5 to 5), (ii) k_1 and E_W are constant if log K_{OW} is large (between 5 to 7), and (iii) k_1 and E_W drop with increasing K_{OW} for chemicals with extremely high K_{OW} (log K_{OW} above 7) (McKim et al., 1985; Gobas et al., 1986; Gobas and Mackay, 1987). Based on these

observations, a two-phase resistance model has been suggested, which assumes that gill uptake involves chemical transport in aqueous and in lipid phases (Gobas and Mackay, 1987). Two transport parameters, i.e. Q_W and Q_L with units of l/day represent the transport rates in the aqueous and the lipid phases of the fish. The resulting equations for k_1 and E_W are

$$1/k_1 = (V_F/Q_W) + (V_F/Q_L)/K_{OW}, \quad (10)$$

$$1/E_W = (G_V/Q_W) + (G_V/Q_L)/K_{OW}. \quad (11)$$

In essence, Eqs. 10 and 11 demonstrate that gill uptake tends to be controlled by transport in the lipid phases if the chemical's K_{OW} is low. But with increasing K_{OW}, chemical transport in the aqueous phases of the fish becomes more important and ultimately dominates the kinetics, resulting in a constant k_1 and E_W with K_{OW}. This model satisfactorily describes the behaviour of k_1 and E_W for most hydrophobic organic chemicals but it does not explain the drop of k_1 and E_W with K_{OW} for chemicals with extremely high K_{OW}. It is believed that the observed drop for high K_{OW} substances is not due to reduced gill uptake but the result of a reduced bioavailability and/or experimental errors associated with the difficult water concentration measurements (Gobas and Mackay, 1987).

Equation 10 demonstrates that, to estimate k_1, data are required for K_{OW}, V_F and Q_W and Q_L. The following relationship between Q (in l/day) and V_F (in kg) has been derived from experimental data to estimate Q_W (Gobas and Mackay, 1987):

$$Q_W = 88.3 \cdot V_F^{0.6(\pm 0.2)}. \quad (12)$$

Because of insufficient data, a similar weight dependent relationship for Q_L cannot be derived at present. However, from the available data it appears that Q_L is approximately 100 times smaller than Q_W (Gobas and Mackay, 1987). In particular for chemicals with a high bioconcentration potential (i.e. high K_{OW}), $V_F/(Q_L \cdot K_{OW})$ is small compared to V_F/Q_W and an accurate value for Q_L is not needed.

Equations 10 and 12 provide a simple method to estimate k_1 from K_{OW} and the weight of the fish. For example, Q_W for a 0.1-kg fish is 22.2 l/day and Q_L is approximately 0.222 l/day, thus giving a k_1 of 222 $l \cdot kg^{-1} \cdot day^{-1}$ for a chemical with a log K_{OW} of 6.

Gill elimination rate constant

The rate at which chemicals are being eliminated by fish via the gills is expressed by the gill elimination rate constant k_2 (1/day). Models for the chemical elimination from the fish to the water via the gills are closely related to models for the chemical uptake rate constant since elimination is

in essence the reverse process of gill uptake. The ratio of k_1 and k_2 is the chemical's partition coefficient between the fish and the water, which can be approximated by K_{OW}, i.e. k_1/k_2 equals $L_F \cdot K_{OW}$, where L_F is the lipid content of the fish, i.e. the ratio of the lipid weight V_L (kg) and wet weight V_F (kg) of the fish, V_L/V_F. If Eq. 10 is substituted in the expression for the fish–water partition coefficient, it follows that

$$1/k_2 = (V_L/Q_W) \cdot K_{OW} + (V_L/Q_L), \tag{13}$$

where Q_W and Q_L are the same as in Eqs. 10 and 11. Equation 13 predicts that k_2 is approximately constant if K_{OW} is low, and drops with increasing K_{OW} for chemicals of higher K_{OW}.

Metabolic transformation rate constant

The rate at which chemicals are being metabolized in fish is expressed by the metabolic transformation rate constant k_M (1/day). Presently, there are few models that can be used to estimate k_M for organic substances in fish or other organisms. This is a serious knowledge gap, in particular when the purpose of the model is to estimate the bioaccumulation tendency of new chemicals for which no information regarding metabolic transformation exists.

For persistent chemicals, which usually have the greatest bioaccumulation tendency, it is often possible to estimate an appropriate value for k_M from experimental data of the metabolic transformation rate in fish. If, for example, the chemical's half-life $t_{1/2}$ in fish is 3 years, a k_M of $0.693/t_{1/2}$ or 0.00063 day^{-1} can be estimated. If this value is small compared to k_2 or k_E, then its precise value becomes irrelevant and it can be assumed to be 0 without affecting the model calculations significantly.

Dietary uptake rate constant

The rate at which chemicals are absorbed by fish from the diet, i.e. via the GI-tract, is expressed by the dietary uptake rate constant k_D (kg food/kg fish/day). The dietary uptake rate is the combined process of the food ingestion rate F_D (kg food/day) and the diffusion rate of the chemical across the intestinal wall and the faecal egestion rate F_E (Gobas et al., 1988, 1993; Clark et al., 1990). The extent to which chemical in the diet is actually absorbed by the organism can be expressed by the ~~gill~~ dietary uptake efficiency E_D, which is related to k_D by

$$k_D = E_D \cdot F_D/V_F. \tag{14}$$

Although there is a considerable variability in the data, it has been shown that E_D is constant at approximately 50% for chemicals with a log K_{OW} up to 6 to 7, and tends to drop with increasing K_{OW} for

chemicals with log K_{OW} exceeding 6 to 7 (Gobas et al., 1988). These observations can be explained by a two-phase resistance model for dietary uptake, which assumes that dietary uptake involves transport in aqueous and in lipid (or membrane) phases (Gobas et al., 1988):

$$1/E_D = A \cdot K_{OW} + B, \quad (15)$$

where A and B are constants relating to the transport rates of the chemical in aqueous and lipid phases of the fish. By non-linear regression of available experimental data A was found to be $5.3(\pm 1.5) \cdot 10^{-8}$ and B is $2.3(\pm 0.3)$.

Based on studies by Weininger (1978), a simple bioenergetics-based model can be used to estimate the feeding rate F_D as a function of temperature T (°C) and the fish's body weight:

$$F_D = 0.022 \cdot V_F^{0.85} \cdot \exp(0.06 \cdot T). \quad (16)$$

Equations 14 to 16 provide a simple method to estimate k_D from K_{OW}, the weight of the fish and temperature. For example, a 0.1-kg fish at 10°C has a feeding rate of approximately 5.7 g food/day or 0.0057 kg food/day. If the food contains a chemical with a log K_{OW} of 6, E_D is approximately 42% and k_D is 0.024 kg food/kg fish/day.

Faecal egestion rate constant

The rate at which chemicals are being eliminated by the egestion of faecal matter, i.e. via the GI-tract, is expressed by the faecal elimination rate constant k_E (kg faeces/kg fish/day). Available data indicate that the faecal egestion rate is approximately 3 to 5 times lower than the ingestion rate (Gobas et al., 1989a, 1993). We thus suggest that:

$$k_E = 0.25 \cdot k_D. \quad (17)$$

k_E is dependent on K_{OW} and the feeding rate in a similar manner as k_D. The approximately 4 times lower value of k_E is due to food digestion, causing the egestion rate (in 1/day) to be smaller than the feeding rate (1/day). In addition, faecal matter may have a lower affinity for hydrophobic chemicals than the more organic-rich food phase, which further reduces k_E relative to k_D (Gobas et al., 1993). This drop in gastro-intestinal flow and chemical binding affinity causes a concentration and fugacity increase in the GI-tract (i.e. magnification), thus providing the concentration gradient between the GI-tract and the fish which can result in a concentration in the fish that exceeds that in the consumed food (i.e. biomagnification) if gill elimination and metabolic transformation are small (Gobas et al., 1988). The ratio k_D/k_E is the predominant factor in the model that causes biomagnification in the food-web.

Growth

The following generalized growth equations have been suggested by Thomann et al. (1992) and are believed to give an adequate representation of the magnitude of fish growth:

$$k_G = 0.00251 \cdot V_F^{-0.2} \quad \text{for temperatures around 25°C,} \tag{18}$$

$$k_G = 0.000502 \cdot V_F^{-0.2} \quad \text{for temperatures around 10°C.} \tag{19}$$

FOOD-WEB TRANSFER AND ACCUMULATION

The models discussed above describe chemical bioaccumulation in individual organisms. However, as a result of the feeding relationships, the chemical concentration in the predator is related to that in its prey. The trophodynamics therefore play an important role in the transfer of chemicals through the food-chain and the accumulation of chemicals in the organisms of the food-web (Thomann and Connolly, 1984; Oliver and Niimi, 1988). In terms of describing and modelling this process we can

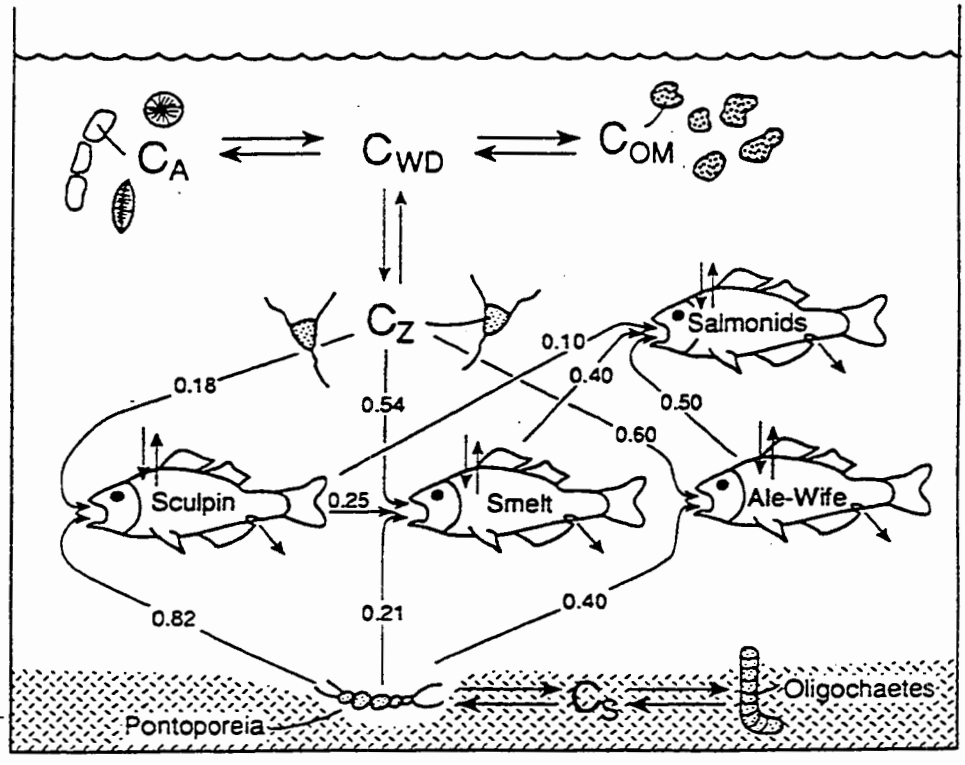

Fig. 1. Conceptual model illustrating chemical transfer in the Lake Ontario food-web.

combine the submodels for individual organisms to form food-webs if feeding relationships can be defined. This is exemplified in Fig. 1, which illustrates chemical transfer in the Lake Ontario food-web resulting from feeding interactions and direct exchange with the water. This model assumes that chemical uptake in phyto- and zooplankton are predominantly from the water and that uptake from food consumption is insignificant. This assumption, which distinguishes our model from other attempts to model contaminants in food-chains (Connolly and Pedersen, 1988; Thomann, 1989; Thomann and Connolly, 1989), is based on the rapid organism–water exchange (due to small size of the organism) which reduces the effect of dietary magnification. Food-web accumulation of organic chemicals therefore occurs predominantly in fish. To include feeding interactions in the model, we can add food-preference factors P to Eq. 8 to give

$$C_F = \left(k_1 \cdot C_{WD} + k_D \cdot \sum P_i \cdot C_{D,i}\right)/(k_2 + k_E + k_M + k_G), \quad (20)$$

where $\sum P_i \cdot C_{D,i}$ represents the composition of the fish's diet. P_i is the fraction of the fish's diet that consists of component i with concentration of $C_{D,i}$. If experimental data for P_i are not available, it may in some cases be possible to estimate P_i from prey densities (Legovic, 1989). If, for example, the fish's diet consists of 30% phytoplankton, 60% benthic invertebrates and 10% small fish, then P_i are respectively 0.3, 0.6 and and $C_{D,i}$ is respectively C_A, C_B and C_F for small fish.

MODEL APPLICATION

To test the food-web model, we applied the model to the Lake Ontario food-web because: (i) there is an extensive and reliable collection of data on chemical concentrations in the most important species in Lake Ontario (Oliver and Niimi, 1988); (ii) biomonitoring studies suggest that concentrations of PCBs and other organochlorines in the Lake Ontario food-web are at or close to steady-state: from 1977 to 1988, there were no significant changes in the concentrations of PCBs and other organochlorines in Lake Ontario rainbow smelt and slimy sculpins, and PCB concentrations in age 4 + lake trout fell only from 5 to 3.5 ppm (Borgmann and Whittle, 1991; Environment Canada, 1991); and (iii) data collection was on a whole-lake basis, which accounts for spatial differences.

The model considers phytoplankton, zooplankton (i.e. *Mysis relicta*), two benthic invertebrate species (i.e. Oligochaetes (*Tubifex tubifex*) and *Pontoporeia affinis*), and four fish species, i.e. sculpins (*Cottus cognatus*), alewifes (*Alosa pseudoharengus*), smelt (*Osmerus mordax*) and a composite group of 60 large size salmonid species, including lake trout (*Salvelinus namaycush*),

rainbow trout (*Oncorhynchus mykiss*) and coho salmon (*Oncorhynchus velinus namaycush*). To compare model predictions to field observations, the model was parameterized with data for the lipid contents and weights of the individual organisms that were taken from Oliver and Niimi (1988). Data for feeding preferences were taken from Flint (1986). Based on experimental observations that approximately 50% of the total concentration of PCBs in Lake Ontario is in a sorbed state (Mackay et al., 1992), a value of $2.5 \cdot 10^{-7}$ kg/l was chosen for the organic matter content of Lake Ontario water, which represents a C_{WD} that is 50% of C_{WT} for a chemical with a log K_{OW} of 6.6. The data that were used to parameterize the model are listed in Table 1. A simple Monte-Carlo simulation (MCS) with a sample size of 10000 was performed to estimate the variability introduced into the model calculations by the variability in observed water and sediment concentrations and fish weights. The MCS was limited to these three parameters because data of the variability of other model parameters were unavailable. The MCS assumed normal distributions, because experimental variability was reported to be normally distributed, and reports the variability of the predicted concentrations in terms of a standard deviation.

Typical results of the model-data comparison are graphically illustrated in Figs. 2 and 3. Figure 2 includes data for 63 organic substances, including PCB congeners, DDT, DDE, chlorobenzenes, mirex, octachlorostyrene, hexachlorobutadiene, lindane and others. Table 2 summarizes predicted and observed concentrations and standard deviations of total PCBs in various organisms of the Lake Ontario food-web and Fig. 3 further illustrates the agreement with observed data. Considering the variability in the experimental data, there are no significant differences ($P < 0.05$) between observed and predicted concentrations for total PCBs in fish and benthic invertebrates. The only exception is that observed concentrations in phyto- and zooplankton are higher than predicted. The reason for this is unknown, but it is possible that sampling difficulties and small sample sizes ($n = 3$ for phytoplankton and $n = 2$ for zooplankton) contribute to the poor fit. The apparent underestimation of the observed concentrations in phyto- and zooplankton does not appear to affect the quality of fit for the fish species. This may also be an indication that actually observed concentrations for phyto- and zooplankton may have exceeded their actual values.

A sensitivity analysis of the water and sediment concentrations showed that contaminant concentrations in all fish species are more sensitive to changes in sediment concentration than to changes in the water concentration. Consequently, the predicted variability in the concentrations of the fish species largely reflects the variability in the sediment concentrations. This suggests that, in general, Lake Ontario fish are more responsive to sediment than to water concentrations. The reason for this is that the

TABLE 1

A summary of the input parameters that are used in the Lake Ontario food-web model calculations. Data are from Flint (1986) and Oliver and Niimi (1988)

Environmental properties:
Mean water temperature: 8°C
Organic content of the water: 0.00000025 kg/l
Organic carbon content of the sediments: 2%
Density of lipids: 0.9 kg/l
Density of organic carbon: 0.9 kg/l
Metabolic transformation rate constant: 0 day^{-1}

Chemical characteristics [a]*:*
Octanol–water partition coefficient: $10^{6.6}$
Total water concentration: 1.1 (±0.52) ng/l
Sediment concentration: 570 (±240) ng/g dry weight

Species characteristics:
Phytoplankton:
Lipid content 0.5%

Zooplankton: Mysids (*Mysis relicta*)
Lipid content 5.0%

Benthos 1: *Pontoporeia* (*Pontoporeia affinis*)
Lipid content 3.0%

Benthos 2: Oligochaetes (*Tubifex tubifex*)
Lipid content 1.0%

Fish 1: Sculpin (*Cottus cognatus*)
Weight: 5.4 g; lipid content: 8.0%
Diet: 18% zooplankton, 82% *Pontoporeia*

Fish 2: Alewife (*Alosa pseudoharengus*):
Weight: 32 g; lipid content: 7.0%
Diet: 60% zooplankton, 40% *Pontoporeia*

Fish 3: Smelt (*Osmerus mordax*)
Weight: 16 g; lipid content: 4.0%
Diet: 54% zooplankton; 21% *Pontoporeia*; 25% sculpins

Fish 4: Salmonids (*Salvelinus namaycush*, *Oncorhynchus mykiss*, *Oncorhynchus velinus namaycush*)
Weight: 2410 (±770) g; lipid content: 16%
Diet: 10% sculpin, 50% alewife, 40% smelt

[a] Chemical data are for total PCBs only. Water and sediment concentration data for PCB congeners and other substances are reported in Oliver and Niimi (1988).

sediment is at a higher chemical activity (or fugacity) than the water. As a result, chemical uptake through the dietary benthic food-chain provides a more important source of chemical uptake in fish than the water. Conse-

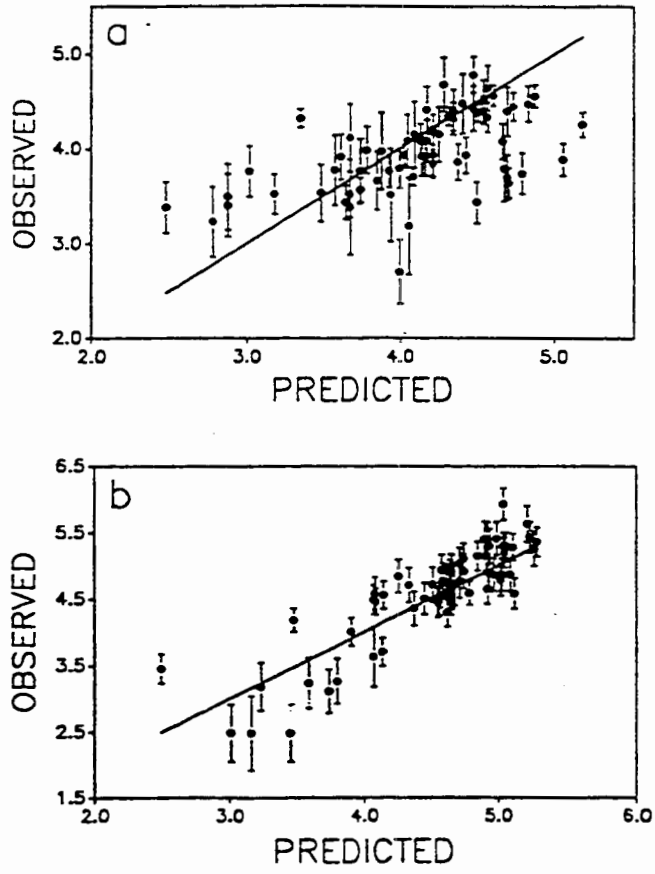

Fig. 2. Logarithms (10 base) of observed vs predicted concentrations (ng/kg) of various organic chemicals in (a) *Pontoporeia* and (b) salmonids of the Lake Ontario food-web. The solid line represents the ideal fit. Error bars reflect standard deviations of the observed data.

quently, the chemical concentrations in the biota of the Lake Ontario aquatic food-web can be expected to reflect chemical concentrations in the sediments rather than concentrations in the water.

CONCLUSIONS

This study presents a model for the chemical distribution and transfer of chemicals in aquatic food-webs, which combines a series of models of the chemical uptake, elimination and bioaccumulation in fish, aquatic macrophytes, benthos and phyto- and zooplankton. Each of these "sub-models" has been tested individually and represents the current state of understand-

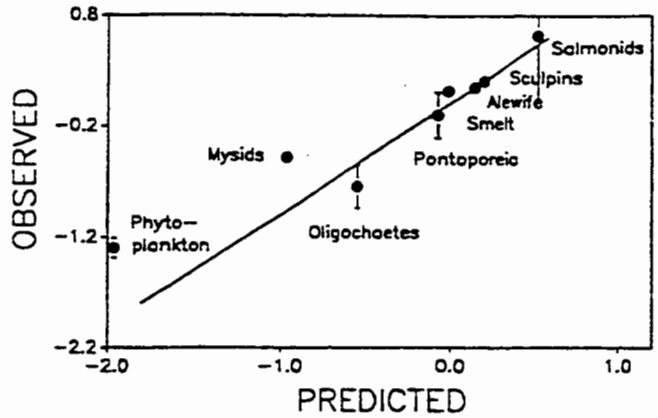

Fig. 3. Logarithms (10 base) of observed vs predicted concentrations (ng/kg) of total PCBs in various organisms of the Lake Ontario food-web. The solid line represents the ideal fit. Error bars reflect standard deviations of the observed data.

ing regarding the mechanism of chemical bioaccumulation. The food-web model is shown to be in good agreement with observed data from Lake Ontario.

This ability to predict chemical distribution and food-web transfer of organic substances in real food-webs provides an important tool for the management of contaminants on a "eco-system" level. The model is simple, in that it only requires basic data regarding the types of species of the food-web, weights, lipid contents and trophic interactions. Thus with little effort, predictions of chemical concentrations in various organisms

TABLE 2

A comparison of model predicted and observed concentrations ($\mu g/g$) of total PCBs in various organisms of the Lake Ontario food-web. The observed data are from Oliver and Niimi (1988). Standard deviations are reported in brackets and reflect the variability introduced into the model predictions by the reported variability in water and sediment concentrations and fish weights (i.e. for the predicted values) and the variability in the observed data (i.e. for the observed values)

Species	Predicted	Observed
Phytoplankton	0.011 (±0.005)	0.05 (±0.012)
Mysids	0.11 (±0.05)	0.33 (±0.12)
Pontoporeia affinis	0.86 (±0.36)	0.79 (±0.48)
Oligochaetes	0.29 (±0.12)	0.18 (±0.1)
Sculpin	1.6 (±0.65)	1.6
Alewife	0.99 (±0.35)	1.3
Smelt	1.4 (±0.5)	1.4
Salmonids	3.5 (±1.3)	4.3 (±3.2)

can be made from concentrations in water and sediments. The model predictions are believed to be accurate within a factor of 2 to 3, which may to a large degree reflect the variability in sediment concentrations of Lake Ontario.

Recently, models for the physical distribution of chemicals have been developed, which successfully can estimate contaminant concentrations in water and sediments from chemical loadings (Mackay, 1989; Mackay et al., 1992). The combination of these fate models with food-web models will provide a capability to assess on an "eco-system" level the chemical exposure of biota as a result of chemical discharges.

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ADDENDUM

A copy of the food-web computer model can be requested from the author in writing. Please enclose a formatted 5.25 or 3.5 inch disk in MS-DOS or MS-DOS compatible format.

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