NOAA Technical Memorandum ERL GLERL-35

AN EQUILIBRIUM MODEL FOR THE PARTITIONING OF SYNTHETIC ORGANIC COMPOUNDS: FORMULATION AND CALIBRATION

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Ann Arbor, Michigan
May 1981

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AN EQUILIBRIUM MODEL FOR THE PARTITIONING OF SYNTHETIC ORGANIC COMPOUNDS: FORMULATION AND CALIBRATION*

Brian J. Eadie

An equilibrium toxic organic distribution model has been designed. This simple model, needing only information on the contaminants, water solubility, and vapor pressure, yields useful information on the distribution of environmentally persistent organic contaminants.

The model was calibrated for total DDT in three ecosystems: a representative coastal regime, Lake Michigan, and a global system. There are some discrepancies between model output and available data; while the model calibrated well for the coastal regime and the Lake Michigan ecosystem, it failed for the global ecosystem. This is presumably because of the uneven application of DDT and the large biomass of terrestrial plants, which are relatively uncontaminated. Owing to its low vapor pressure, DDT has not and will not come to a global equilibrium.

The Lake Michigan model was also run for four other organic contaminants, which span several orders of magnitude in solubility and vapor pressure. These will be discussed, as will sensitivity of the model to input parameters.

1. INTRODUCTION

In August 1979, the Great Lakes Environmental Research Laboratory (GLERL) initiated a research program entitled "The Cycling of Toxic Organic Substances in the Great Lakes Ecosystem." This research was partially supported by the Office of Marine Pollution Assessment (OMPA) under Section 202 of PL 92-532, which states that NOAA should initiate "a comprehensive and continuing program of research with respect to the possible long-range effects of pollution, overfishing, and man-induced changes of ocean ecosystems."

GLERL's approach consists of a series of models designed to simulate ecosystems at different scales of time and space and to improve these models through research on various important processes. This report describes one of these models.

2. MODEL DESCRIPTION

Conceptually, this is a simple model that assumes that the ecosystem under consideration is in equilibrium with the toxic organic contaminant.

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*GLERL Contribution No. xxx.

It is recognized that the equilibrium assumption is naive, but for persistent organic contaminants in well-mixed environments, the approach does yield worthwhile information.

The environment or ecosystem under consideration is divided into compartments, such as atmosphere, water, sediments, biota, etc. At equilibrium, the toxic organic contaminants' "escaping tendency" or fugacity from each compartment is equal. Mackay (1979) clarifies the concept through the following analogy:

> Fugacity is to mass diffusion as temperature is to heat diffusion. Mass (or heat) always diffuses from high to low fugacity (or temperature). Diffusion directions are not obvious from concentrations such as g mol m^{-3} (or cal m^{-3}), but they are obvious when expressed in atm (or °C). The insights into heat diffusion provided by temperature can be obtained for mass by using fugacity.

Fugacity has units of pressure and, at the very low concentrations encountered with trace organic contaminants, it is linearly proportional to concentration. In Mackay's (1979) terms,

$$C = Zf, \tag{1}$$

where C = concentration (g mol m^{-3})
Z = fugacity capacity (g mol m^{-3} atm^{-1}), and
f = fugacity (atm).

The fugacity capacity (Z) for each ecosystem compartment must be estimated. In this work each was calculated in the following manner:

Vapor phase (atmosphere)--for an ideal gas, fugacity is exactly equal to partial pressure (P). At the concentrations with which this model deals, the vapor phase will be close to ideal. Thus, from

$$PV = nRT$$

$$fV = nRT,$$

from equation (1)

$$\frac{CV}{Z} = nRT$$

and $CV = n$ (number of g mols)

$$Z = CV\,(nRT)^{-1} = RT^{-1}\ (\approx 40\text{-}45)$$

where $R = 82 \times 10^{-6}$ and

T = °K.

The fugacity capacity in the vapor phase is independent of compound characteristics.

Liquid phase (water)--the ratio of contaminant vapor pressure (P) to solubility (S) is the Henry's Law constant (H). From

$$H = PS^{-1} = C \text{ vapor } (C \text{ dissolved})^{-1} = fCd^{-1},$$
$$f = HCd$$

and combining with equation (1), it follows that $Z = 1 \; H^{-1}$.

Sorbed phases (particulates, sediments, etc.)--if the equilibrium partition coefficient (K_p) is defined as the ratio of sorbed concentration ($\mu g \; g^{-1}$) to water concentration ($g \; m^{-3}$), then

$$C \text{ sorbed} = K_p \; C \text{ dissolved}$$

since

$$f = HCd = \frac{HCs}{K_p} \; ;$$

then substituting equation (1)

$$Z = K_p H^{-1}.$$

The K_p is calculated from the contaminant's octanol-water partition coefficient (K_{ow}) as discussed below.

Biotic phases (plankton, fish, benthos, etc.)--there have been several attempts at correlating concentration in fish based on the contaminant's K_{ow} (Vieth et al., 1979; Chiou et al., 1977; Thomann, 1979). Mackay (1979) assumes that the biotic phases act as passive substrates for sorption. Although there is considerable evidence for bioaccumulation and biomagnification up the food chain, this equilibrium approach (which is based on mass, not surface area) appears to be reasonable.

Thus

$$Z = K_p H^{-1}.$$

2.1 Estimation of the Equilibrium Partition Coefficient

K_p, the equilibrium partition coefficient is defined as follows:

$$K_p = \frac{\text{Contaminant concentration in the sorbed phase (ppm)}}{\text{Contaminant concentration in the dissolved phase (ppm)}} \qquad (2)$$

Karickhoff et al. (1979) and others have shown that K_p is primarily a function of the octanol-water partition coefficient of the contaminant (K_{ow}) and the organic carbon content of the substrate. For neutral, hydrophobic organic contaminants, this result agrees with intuition; the contaminant preferentially dissolves (partitions) more favorably into those substrates that are highest in organic carbon content. K_p can be described as

$$K_p = K_{oc} * \frac{\text{percent substrate organic carbon}}{100} ,$$

where K_{oc} is the partition coefficient normalized to organic carbon content (Means et al., 1979).

Life is never quite so simple; there are several other variables that appear to affect K_p; among them are substrate surface area (Karickhoff et al., 1979), concentration of substrate (O'Connor and Connolly, 1980), and the nature of the substrate organic matter. These complications appear to be second order, and the approximation based on K_{oc} (described below) will be used in this preliminary model.

K_{oc} has been shown to be well correlated to the octanol-water partition coefficient (K_{ow}) of the contaminant. Figure 1 illustrates two of the most recent of these correlations (which therefore employ the most data). The Smith and Bomberger (1979)/Chiou et al. (1977) line was derived from their individual correlations of K_{oc} with solubility and K_{ow} with solubility, respectively. These will be described in more detail below. The dashed line was used in this model. (Log K_{oc} = 1.05; Log K_{ow} - 0.500.)

K_{ow} is a relatively simple laboratory measurement, and values of K_{ow} are available in the literature (Leo et al., 1971). K_{ow} can also be approximated directly from the molecular structure of the compound by the "Hansch method," described in Hansch (1980) and supported by numerous references. That article, along with Tulp and Hutzinger (1978), discusses the limits of this approach, generically termed structure-activity relationships, and the extension of the technique into the estimation of toxicity. Although not included in the current version of our model, this approach is certainly promising and will be pursued by our laboratory in future modeling efforts.

A third technique for estimating K_{ow} is the relationship developed between K_{ow} and solubility. Chiou et al. (1977) derived the relationship

$$\log K_{ow} = 5.00 - 0.670 \log S,$$

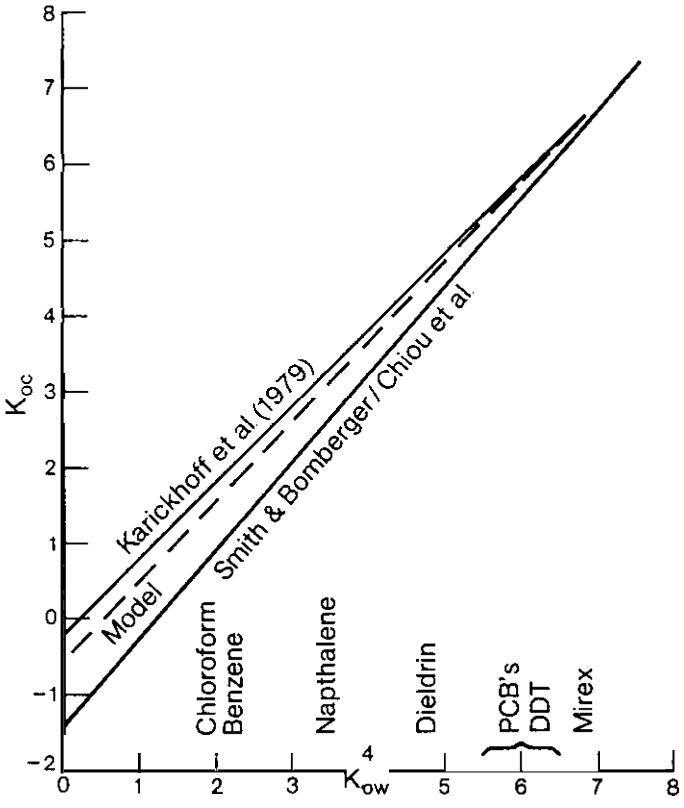

Figure 1.--The relationship between K_{oc} and the octanol-water partition coefficient, K_{ow}. For Karickhoff *et al.*, log K_{oc} = log K_{ow} - 0.21 (r^2 = 1.00, n = 10). The Smith and Bomberger/Chiou *et al.* line was derived from their correlations of K_{oc} and K_{ow} versus solubility, respectively (n > 33). Sample compounds are listed on the abscissa and illustrate the properties of a range of contaminants. The dashed line was used in the model.

where S = aqueous solubility in micromols per liter

$r^2 = 0.970$, $N = 33$, log K_{ow} range = 1.26-6.72.

This relation is shown in figure 2, along with a relation generated by Smith and Bomberger (1979), which relates K_{oc} directly with solubility. Although statistics are not provided, the scatter of data indicates a poorer correlation than was found by Chiou et al. (1977), which is to be expected since the nature of the substrate is now part of the variability. Recall that the subject models parameterization of K_{oc} is

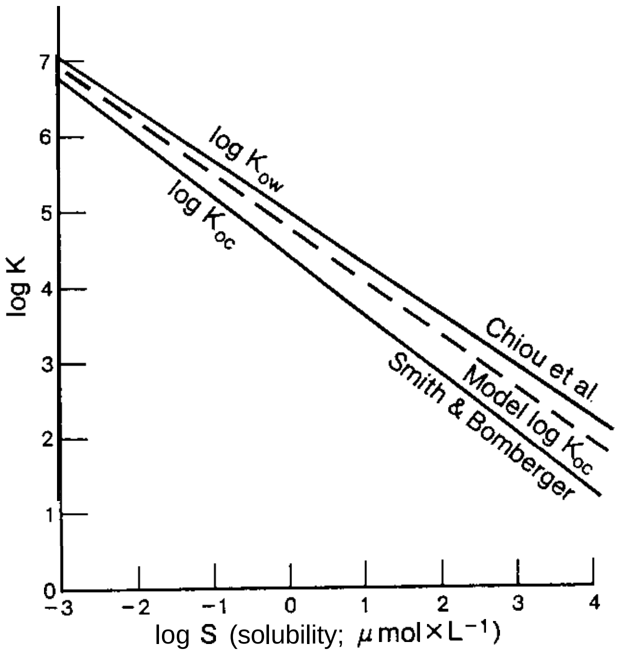

Figure 2.--*The relation between partitioning and solubility. For Chiou et al., r^2 = 0.97, n = 33. The dashed line compromise was used in the model.*

$$\log K_{oc} = 1.05 \log K_{ow} - 0.500.$$

In our model, K_{ow} is calculated from Chiou's equation. Our calculations can also be presented in terms of $\log K_{oc} = f(S)$ as follows:

$$\log K_{ow} = 5.00 - 0.670 \log S$$

and $$\log K_{oc} = 1.05 \log K_{ow} - 0.500.$$

Substituting $$\log K_{oc} = 4.75 - 0.704 \log S,$$ plotted as the dashed line in figure 2,

K_p is then calculated from K_{oc} as

$$K_p = K_{oc} * \frac{\text{percent substrate organic carbon}}{100}$$

2.2 Biotic Phases

As mentioned earlier, $Z = K_pH^{-1}$ is used for all sorbed phases including biotic compartments. Figure 3 illustrates the problem with this approach. The above formulation, using 50 percent organic carbon (dry weight) for fish, yields a bioconcentration function that differs from the results of four other syntheses of real data. The bioconcentration factor (BCF) correlations presented in figure 3 were considered, and an information item was included in the model output indicating the concentration of contaminant in large fish based on

$$\log BCF = \log K_p = 0.80 \log K_{ow} - 0.50,$$

which is approximately midway between the values obtained by Vieth _et_ _al_. and Chiou _et_ _al_.

2.3 Benthic Organisms

Difficulty was encountered when the passive sorption concept was applied to benthic organisms. The sparse environmental data indicate that contaminant concentrations in benthic organisms (dry weight) are approximately twice those of dry sediments. Since the organic carbon concentration of a benthic organism is 10-40 times as high as that of the sediments, and the model is based on K_p, which is linearly dependent on organic carbon content, the benthos values predicted by the model are too high by an order of magnitude. At this level of model development, the benthic organisms have been left out, although they are considered a prime target for further research since benthos are exposed to long-term high concentrations of contaminants in the surficial sediments.

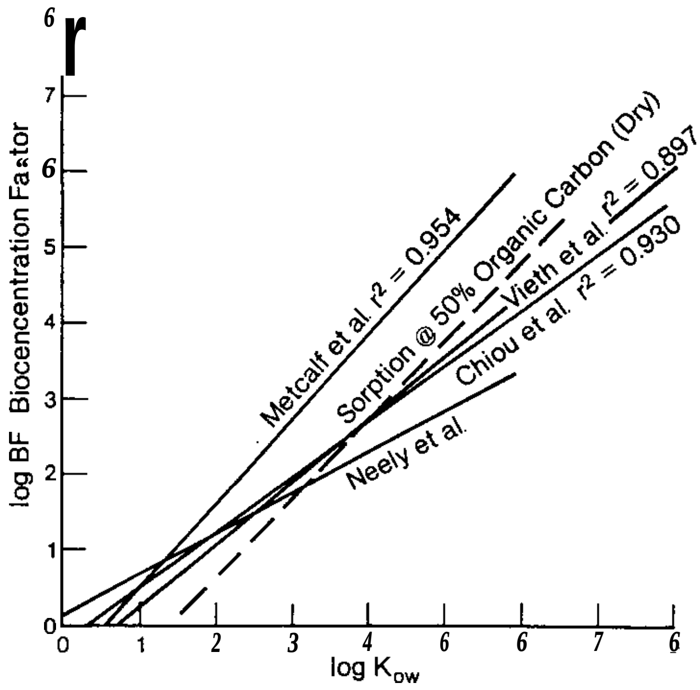

Figure 3.--*Bioconcentration factors in fish. The solid lines are syntheses of experimental data on fish (minnows through trout). The dashed tine assumes equilibrium sorption as the only factor influencing bioconcentration. A compromise equation, approximately midway between those of Vieth and Chiou, was used for calculating bioconcentration in the model.*

2.4 Calculating the Distribution of Contaminants Within the Ecosystem

Once the Z values for each environmental compartment have been calculated, the concentration in each compartment is calculated in the following manner:

At equilibrium $f_1 = f_2 = f_i$, i = compartment, and the total mass of contaminant (M) equals

$$M = \Sigma C_i V_i ,$$

where V_i = volume of the ith compartment and from $C = fZ$ [equation (1)],

$$M = \Sigma f_i Z_i V_i ,$$

$$M = f_i \Sigma V_i Z_i, \text{ and}$$

$$f_i = M(\Sigma\ V_i Z_i)^{-1}.$$

The terms on the right are either input (M, V_i) or calculated from inputs [Z_i = f(solubility, vapor pressure, K octanol-water)]. The mass in each compartment is

$$M_i = f_i Z_i V_i$$

and the concentration is

$$C_i = f_i Z_i.$$

The total mass of a contaminant in the ecosystem (M) is rarely known; therefore, for an initial run, an arbitrary value may be used (e.g., 1.0). Model output will then give relative concentrations in each compartment, and if data exist for any compartment, the value of M can be scaled up by

$$\frac{C_i(\text{data})}{C_i(\text{model output})},$$

which will yield approximate concentrations in all compartments.

2.5 Description of an Ecosystem

As developed in the previous section, the volume (V_i) of each environmental compartment needs to be input. This is not too difficult for the large, physically distinct compartments of atmosphere, water, and sediments (except for estimating the mixing depths of the atmosphere and sediments), but how does one estimate the dry weight volume of any biotic compartments? It turns out that, although concentrations of a contaminant are high in biota, the mass of the contaminant in these phases is bound to be small for large lakes and marine systems, and the model is insensitive to order-of-magnitude errors in these compartment volumes.

Three model ecosystems were run; they are described below. They are (ECOL), a 1-m^2 horizontal area, 100-m-deep water body; (LKMi), an approximation of Lake Michigan; and (ECOALL), a representation of a global ecosystem.

All volumes are calculated on a dry-weight basis, and comparative data should be carefully examined and corrected to a dry-weight basis.

2.6 Compartmentalization of ECOL

Atmosphere (10-km mixed depth)

$$V = 1\ \mathrm{m}^2 \times 10{,}000\ \mathrm{m} = 10^4\ \mathrm{m}^3\ .$$

Water

$$V = 1\ \mathrm{m}^2 \times 100\ \mathrm{m} = 10^2\ \mathrm{m}^3\ .$$

Sediment (2-percent organic carbon, 5-cm mixed depth)

$$V = 1\ \mathrm{m}^2 \times 5\ \mathrm{cm} \times 0.5\ (\mathrm{porosity}) = 2.5 \times 10^{-2}\ \mathrm{m}^3\ .$$

Suspended matter (1.5 mg l^{-1}, ρ = 1.5 g m^{-3}, 15-percent organic carbon)

$$V = \frac{1.5\ \mathrm{g}}{\mathrm{m}^3} \times 10^2\ \mathrm{m}^3 \times \frac{1\ \mathrm{cm}^3}{1.5\ \mathrm{g}} \times \frac{\mathrm{m}^3}{10^6\ \mathrm{cm}^3} = 1 \times 10^{-4}\ \mathrm{m}^3\ .$$

Biota (1 μg l^{-1} chlorophyll a ≈ 50 μg C l^{-1} total plankton, ρ = 1.0 g/cm^3).

$$V = 50\ \frac{\mathrm{mg\ C}}{\mathrm{m}^3} \times 10^2\ \mathrm{m}^3 \times \frac{2.5\ \mathrm{mg\ org.\ matter}}{\mathrm{mg\ org.\ carbon}} \times$$

$$\frac{1\ \mathrm{cm}^3}{10^3\ \mathrm{mg}} \times \frac{\mathrm{m}^3}{10^6\ \mathrm{cm}^3} = 1.25 \times 10^{-5}\ \mathrm{m}^3\ .$$

The above values are representative of Lake Michigan or a coastal marine ecosystem.

2.7 Compartmentalization of LKM_i

Lake Michigan

Surface area (5.8×10^{10} m^2).

Average depth (86 m).

Atmosphere (10-km mixed depth)

$$V = 5.8 \times 10^{14} \text{ m}^3.$$

Water

$$V = 5.8 \times 10^{10} \times 86 \simeq 5 \times 10^{12} \text{ m}^3.$$

Suspended matter (1.5 mg l^{-1}; ρ = 1.5 g cm^{-3}, 10-percent organic carbon)

$$V = 1.5 \frac{\text{g}}{\text{m}^3} \times 5 \times 10^{12} \text{ m}^3 \times \frac{1 \text{ cm}^3}{1.5 \text{ g}} \times \frac{\text{m}^3}{10^6 \text{ cm}^3} = 5 \times 10^6 \text{ m}^3$$

Phytoplankton cell density $\simeq$ 1500 cells ml^{-1} (Tarapchak and Stoermer, 1976)

$\simeq$ 100 pg $cell^{-1}$ (Stoermer and Ladewski, 1978)

$$V = 1500 \frac{\text{cells}}{\text{cm}^3} \times 5 \times 10^{18} \text{ cm}^3 \times \frac{100 \times 10^{12} \text{ g}}{\text{cell}} \times 1 \text{ cm}^3 \times \frac{\text{m}^3}{10^6 \text{ cm}^3} = 7.5 \times 10^5 \text{ m}^3.$$

Zooplankton (30 mg m^{-3}, ρ = 1)

$$V = \frac{30 \text{ mg}}{\text{m}^3} \times 5 \times 10^{12} \text{ m}^3 \times \frac{1 \text{ cm}^3}{\text{g}} \times \frac{\text{g}}{1000 \text{ mg}} \times \frac{\text{m}^3}{10^6 \text{ cm}^3} = 1.5 \times 10^5 \text{ m}^3.$$

Forage fish (10^5 MT, $\rho = 1 \text{ g cm}^{-3}$, 40-percent organic carbon)

$$V = 10^5 \text{ MT} \times \frac{10^6 \text{ g}}{\text{MT}} \times \frac{1 \text{ cm}^3}{\text{g}} \times \frac{1}{5}\frac{\text{g day}}{\text{g wet}} \times \frac{\text{m}^3}{10^6 \text{ cm}^3} = 2 \times 10^4 \text{ m}^3.$$

Top predators; salmonids (1.6×10^3 MT, $\rho = 1 \text{ g cm}^{-3}$)

$$V = 1.6 \times 10^3 \text{ MT} \times \frac{10^6 \text{ g}}{\text{MT}} \times \frac{1 \text{ cm}^3}{\text{g}} \times \frac{1}{5}\frac{\text{g dry}}{\text{g wet}} \times \frac{\text{m}^3}{10^6 \text{ cm}^3} \times 3.2 \times 10^2 \text{ m}^3.$$

Sediment (5-cm mixed depth, 2-percent organic carbon)

$$V = 5.8 \times 10^{10} \text{ m}^2 \times 5 \text{ cm} \times \frac{\text{m}}{10^2 \text{ cm}} \times \frac{1 \text{ g dry}}{2 \text{ g wet}} \approx 1.5 \times 10^9 \text{ m}^3.$$

2.8 Compartmentalization of ECOALL

Earth (Mclellan, 1968)

Surface area (land) ($1.5 \times 10^{14} \text{ m}^2$).

Surface area (water) ($3.6 \times 10^{14} \text{ m}^2$).

Augmented depth (3.8×10^3 m).

Atmosphere (10-km depth)

$$V = 5.1 \times 10^{14} \text{ m}^2 \times 10^4 \text{ m} = 5.1 \times 10^{18} \text{ m}^3.$$

Water

$$V = 3.6 \times 10^{14} \text{ m}^2 \times 3.8 \times 10^3 \text{ m} \approx 1.4 \times 10^{18} \text{ m}^3.$$

Suspended matter ($2 \text{ } \mu\text{g l}^{-1}$, 10-percent organic carbon)

$$V = \frac{2 \text{ mg}}{\text{m}^3} \times \frac{\text{cm}^3}{\text{g}} \times \frac{\text{m}^3 \text{ g}}{10^3 \text{ mg}} \times \frac{}{10^6 \text{ cm}^3} \times 1.4 \times 10^{18} \text{ m}^3 = 2.8 \times 10^9 \text{ m}^3.$$

Plant biomass

Aquatic (1.8×10^{15} g C; Whittaker and Likens, 1973).

$$V = 1.8 \times 10^{15}\ \text{g C} \times \frac{2.5\ \text{g biomass}}{\text{g C}} \times \frac{1\ \text{cm}^3}{\text{g}} \times \frac{\text{m}^3}{10^6\ \text{cm}^3} = 4.5 \times 10^9\ \text{m}^3.$$

Terrestrial (1.9×10^{12} MT; Woodwell *et al.*, 1971)

$$V = 1.9\ 10^{18}\ \text{g} \times \frac{}{\text{g}} \times 1\ \text{cm}^3\ \frac{\text{m}^3}{10^6\ \text{cm}^3} = 1.9 \times 10^{12}\ \text{m}^3.$$

Animal biomass

Aquatic (0.45×10^{15} g C; Whittaker and Likens, 1973).

$$V = 0.45 \times 10^{15}\ \text{g C} \times \frac{2.5\ \text{g biomass}}{\text{g C}} \times \frac{1\ \text{cm}^3}{\text{g}} \times \frac{\text{m}^3}{10^6\ \text{cm}^3}$$

$$= 1.1 \times 10^9\ \text{m}^3.$$

Terrestrial (0.5×10^9 MT; Woodwell *et al.*, 1971).

$$V = 0.5 \times 10^{15}\ \text{g} \times \frac{1\quad{}^3}{\text{g}} \times \frac{\text{m}^3}{10^6\ \text{cm}^3} = 5 \times 10^8\ \text{m}^3.$$

Sediments

Aquatic (1-cm mixed depth, 50-percent dry, 1-percent organic carbon).

$$V = 3.6 \times 10^{14}\ \text{m}^2 \times 0.01\ \text{m} \times 0.5 = 1.8 \times 10^{12}\ \text{m}^3.$$

Terrestrial (1-cm mixed depth, 2-percent organic carbon).

$$V = 1.5 \times 10^{14}\ \text{m}^2 \times 0.01\ \text{m} = 1.5 \times 10^{12}\ \text{m}^3.$$

3. MODEL CALIBRATION

The minimum input that the model requires is a description of the ecosystem in terms of volume and the fugacity capacity values (Z), which are calculated from solubility, vapor pressure, and temperature. For the synthetic organics that are of initial interest, the solubilities are so low (microgram per liter range) that measured values often range over an order of magnitude. The same range exists for vapor pressures. This allows for a small amount of "tuning" if we have reliable environmental data for one or more of our ecosystem compartments.

Another tuning factor is the percent organic carbon of sorption substrates since partitioning is linearly related to this value. Reliable numbers are usually available for percent organic carbon of sediments or suspended matter, but most ecosystems are heterogeneous and an average value needs to be estimated.

The final input variable is the total amount of contaminant in the ecosystem, a number rarely available. As mentioned earlier, this can be scaled by first running the model with an input of 1.0 and then multiplying this input (for the second run) by the ratio of the contaminant concentration (data) in any compartment to the model output for that compartment.

These calibration knobs are straightforward and are constrained within generally acceptable limits. Sensitivity to these calibration terms will be discussed in the following section, which describes model output for several representative compounds.

4. MODEL ANALYSIS

The most extensive model analysis has been done with total DDT (DDT plus decomposition products, mostly DDE and DDD), for which a reasonable amount of environmental data is available. The first run was with the global system, ECOA11. Accepted values for solubility (1.2×10^{-3} ppm) and vapor pressure (1.6×10^{-7} mm Hg) were input, along with the estimated value for total world DDT production of $\sim 2.5 \times 10^{12}$ g (Woodwell _et al._, 1971). Model output concentrations, shown in table 1, were close to those summarized in Woodwell, with the notable exception of land plant data. Results from this run indicate that DDT is stored primarily in terrestrial plants (60 percent) and water (36 percent). The mass of DDT stored in land plants is in excess of that estimated by Woodwell _et al._ (1971) by a factor of 1000. The sediment (land) values output from the model (4.0 g m^{-2}) are in the middle of their agricultural soils range data (0.15-11), but are much higher than for unsprayed forests (0.0004-0.004), which accounts for most of the land plant biomass. The global ecosystem has not been uniformly exposed to DDT, and the equilibrium assumption leads to an inaccurate distribution pattern. Presumably, this is because of DDT usage patterns and the compound's low vapor pressure. The model's atmospheric concentration (0.17×10^{-8} g m^{-3}) is within the data range of $0.1\text{-}10 \times 10^{-8}$ g m^{-3}, but represents less than 0.1 percent of atmospheric saturation ($\sim 3 \times 10^{-6}$ g m^{-3}).

The second model ecosystem considered was the simple 1-m^2 coastal representation. A single run for DDT was made simply by scaling the DDT mass in this system to that in the global system by the volume ratio of the atmospheres ($0.10 \times 10^{5}\ 0.51^{-1} \times 10^{-19} = 1.96 \times 10^{-15}$), yielding 1.4×10^{-5} g

TABLE 1.--*Comparison of model output and summarized data for the global system. DDT concentrations are in ppm.*

Compartment	Data[1]	Model
Atmosphere	1-100 x 10^{-9}	1.7 x 10^{-9}
Water	--	6.5 x 10^{-7}
Land Plants	10^{-4}-10^{-1}	0.81
Aquatic Plants	0.1-1	0.81
Land Animals	1.	1.
Aquatic Animals	1.	1.
Land Sediment	0.1-10	4.0
Aquatic Sediment	--	2 x 10^{-2}

[1] Data synthesized in Woodwell et al., 1971 order of magnitude.
[2] Model output DDT Mass = 2.5 x 10^{12} g; appendix 1.
[3] Units of g m^{-2}; model assumes 1-cm thickness.

in the system. In this case, DDT more realistically resides in the sediments (91 percent), for the same approximate concentration in the biota (1-3 ppm). This single output is listed below; other model outputs discussed in this report are listed in appendix 1.

The final ecosystem calibrations and sensitivity testing were performed on the Lake Michigan ecosystem. Data were summarized for Lakes Michigan and Ontario from the International Joint Commission (International Joint Commission, 1977, 1978, 1980) and Sonzogni et al. (1981), and ranges are compared to 10 model outputs in figure 4. The variations in the 10 outputs are described in table 2 below; for clarity only those variables that were altered are listed.

In the initial runs, the concentrations in the sediments were too high. The discrepencies were eventually reduced by lowering the percent organic carbon in the sediments from 2 percent to 1 percent. The solubility was increased by a factor of 10 and kept at that level for the last 5 runs because the octanol-water partition coefficient (calculated from the solubility) for this solubility was closer to measured K_{ow} (5.5-6.2).

These 10 runs also show that a two-order-of-magnitude change in solubility (runs 1-4) or vapor pressure (runs 8-10) has very little impact on the concentrations of contaminant in sediments and biota. The insensitivity to these 2 input variables is important because reported values for contaminants often range over a factor of 10 or more.

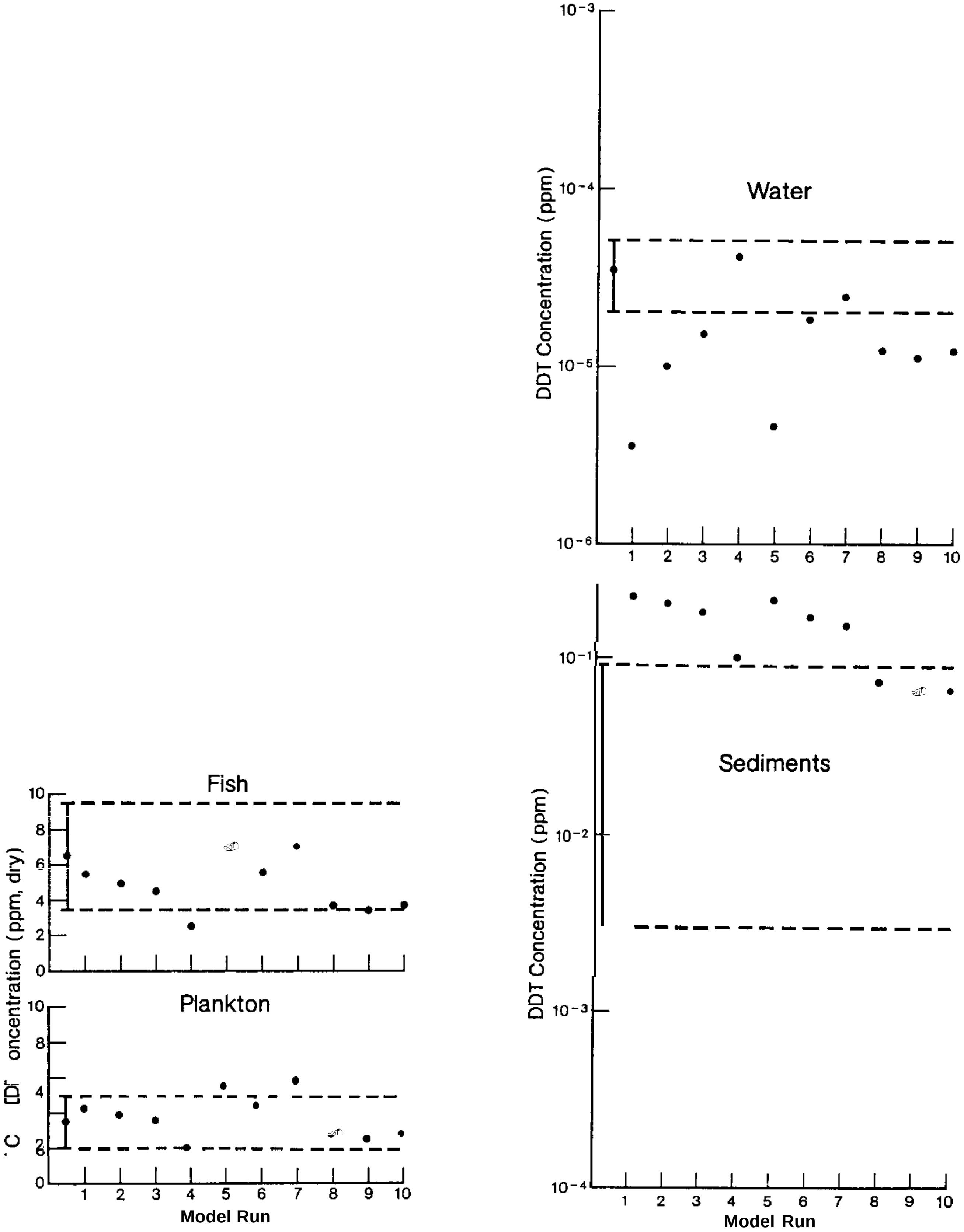

Figure 4.--*Model output versus DDT data for Lake Michigan. See table 2 for input variables, appendix 1 for total outputs. Dot with error bars connecting to dashed lines represent data mean ± standard deviation. Individual dots represent model output for each run.*

TABLE Z.--*Input variables for the 10 calibration and sensitivity runs. Only changes are listed; subsequent runs used the last listed value. Outputs are in appendix 1.*

Model Run	Solubility	Vapor present	DDT Mass (g)	Sed. org. C (%)
1	1.2×10^{-3}	1.6×10^{-7}	1×10^{6}	2.0
2	6.0×10^{-3}			
3	1.2×10^{-2}			
4	1.2×10^{-1}			
5	1.2×10^{-3}			1.5
6	1.2×10^{-2}			
7				1.0
8			5×10^{5}	
9		1.6×10^{-8}		
10		1.6×10^{-6}		

The final model exercise was to take the calibrated Lake Michigan ecosystem (the reduction of sediment organic carbon from 2 percent to 1 percent) and to examine other organic contaminants. Unfortunately, data for comparison are sparse.

This exercise yields two important pieces of information (shown in table 3). First, the model appears to work well for contaminants other than DDT (runs 11 and 12), and second, the model yields useful information on the relative distribution of contaminants even when environmental data are not available (runs 13 and 14).

The mirex run (#12) was a particularly interesting exercise. Mirex is not known to be a problem in Lake Michigan, but is known to be a contaminant in Lake Ontario. Not having a Lake Ontario ecosystem (which is similar in relative volume distribution to Lake Michigan), I scaled up the estimated mass of mirex in Ontario (688 kg; Holdrinet et al., 1978) to Michigan as follows:

$$\text{g mirex} = 6.88 \times 10^{5} \times A \times S \times \frac{100}{P} \times C ,$$

TABLE 3.--*Model outputs* for *selected contaminants*.

Model run	Compound	Fish	Concentrations (PPM)		Water
			Plankton	Sediments	
11*	Dieldrin	0.12	0.095	2.4×10^{-3}	3.1×10^{-6}
Data		0.2±0.2	0.14±0.10	$1.8 \pm 1.2 \times 10^{-3}$	$3.7 \pm 2.9 \times 10^{6}$
12†	Mirex	0.35	0.28	7×10^{-3}	2.3 x 18
Data		1.0±1.0	--	$7.5 \pm 8.3 \times 10^{-3}$	--
13†	Naphthalene	552.	447.	11.	1.0
14†	Benzene	24.	19.	0.5	1.0

*Contaminant mass scaled to known approximate concentrations.

†Compartment concentrations are reported as a ratio to the water concentration.

where A = area ratio of Lake Michigan to Ontario = 3.03,

S = 5/3; mixed sediment thickness in model
mixed sediment used by Holdernet *et al.*,

P = percent of mirex in sediment (62 percent from model),

C = 3; mirex only in 1/3 of Lake Ontario sediment, model assumes equilibrium,

$$g \text{ mirex} = 1.7 \times 10^{7} \text{ g}.$$

This mass gave concentrations in fish and sediments in agreement with reported data.

5. RUNNING THE MODEL

The information necessary to run this model consists of the contaminants' solubility in water, its vapor pressure, and a description of the ecosystem. The program is interactive and will prompt the user to supply information. We have created three procedure files for the three ecosystems described in this report. They are shown below. Ecosystem files are LKMI, ECOALL, and ECOL (also listed below). To generate a new procedure file, simply create a new file, then change the LKMIs to the new file name in the procedure file (e.g., RUNMI).

The model is initiated by typing in (e.g.) CALL, RUNMI.

Procedure Files

```
/COPY,RUN1
SET. FUGMOD1.
GET,SUBS1 .
GET. TAPE7=ECO1.
XEDIT,FUGMOD1,I=SUBS1.
REWIND,LGO.
REWIND,TAPE6.
MAP,OFF.
FTN,I=FUGMOD1,L=0.
LGO.
REPLACE,TAPE7=ECO1 .
REWIND,TAPE6.
COPY,TAPE6, OUTPUT.
 EOI ENCOUNTERED.
```

```
/COPY,RUMMI
GET,FUGMOD1.
GET,SUBS1.
GET,TAPE7=LKMI.
XEDIT,FUGMOD1,I=SUBS1.
REWIND,LGO.
REWIND,TAPE6.
MAP,OFF.
FTN,I=FUGMOD1, L=O.
LGO.
REPLACE,TAPE7=LKMI.
REWIND,TAPE6.
COPY,TAPE6,OUTPUT.
 EOI ENCOUNTERED.
```

```
/COPY,RUNALL
GET,FUGMOD 1 .
GET,SUBS1.
GET,TAPE7=ECOALL.
XEDIT,FUGMOD1,I=SUBS1.
REWIND,LGO.
REWIND,TAPE6.
MAP, OFF.
FTN,I=FUGMOD1,L=0.
LGU.
REPLACE,TAPE7=ECOALL.
REWIND,TAPE6.
COPY,TAPE6,OUTPUT.
 EOI ENCOUNTERED.
```

Ecosystem Files

```
/COPY,ECO1
ATMOSPHERE(10 KM)       .100E+05-.100E+01
WHTER       (100 M)     .100E+03-.200E+01
DETRITUS    1.5PPM; 5 X .1 OOE-03 .500E+01
BIOTA       1PPB CHL A .125E-04 . 400E+02     .
SEDIMENTS    5CM;2%C   .250E-01  .200E+01
 EOI ENCOUNTERED.
```

```
GET,LKMI
/COPY, LKMI
ATMOSPHERE(1 0 KM)       .580E+15-.100E+01
WATER       (86 M)       .490E+13-.200E+01
DETRITUS    1.5PPM1 0%C .500E+07 . 1 00E+02
SEDIMENTS 5CM; 2. 0%OC .150E+10.200E+01
PHYTO       1500CEL/ML . 750E+06 .400E+02
ZOOPLANK    (30G/M3)     .150E+06 .400E+02
FORAG  FISH(1E5  MT) .200E+05  .500E+02
SALMONOIDS(1.6E3  MT) .320E+03 .500E+02
CALIBRATION OF LAKE MICHIGAN
 EOI ENCOUNTERED.
```

```
/COPY,ECOALL
ATMOSPHERE (10 KM)         . 51 0E+19-.100E+01
WATER          (3800 M)    .140E+19-.200E+01
DETRITUS 2PPB; 1 0%C       .280E+10 . 1 00E+02
PLANTS         HQUHTIC     . 450E+1 0 . 400E+02
PLANTS         LHND         190E+13 ,400E+02
ANIMALS        HQUHTIC     :110E+10 .500E+02
ANIMALS        LAND         500E+09 .500E+02
SEDIMENTS AQUATIC          : 180E+13 .IOOE+OI  .
SEDIMENST LAND             .150E+13 .200E+01
CALIBRATION O F GLOBAL ECOSYSTEM 2
```

If there is an ecosystem file, the model is run as follows:

```
/CALL,RUNMI
 XEDIT 3.1.00
      END
FUGMOD1 II A LOCAL FILE
 ENTER THE COMPOUND NAME (20 CHARACTERS)
? MIREX
 ENTER THE COMPOUNDS MOLECULAR WEIGHT
? 546
 ENTER TOTAL MASS OF COMPOUND IN SYSTEM (G) OR 1.0
? 2.1E6
 IS THERE A FILE DESCRIBING THE ECOSYSTEM ? ; YES=1 ,NO=2
  1
 ENTER ECOSYSTEM FILE NUMBER, NUMBER OF COMPARTMENTS
? 7,8
 ENTER A TITLE FOR THIS RUN (80 CHARACTERS)
? TEST
 ENTER THE SYSTEM TEMPERATURE (C)
? 15
 ENTER THE COMPOUND'S WATER SOLUBILITY (G/M3)
? .7E-4
 ENTER THE COMPOUNDS VAPOR PRESSURE (MM HG)
   1E+5


TEST


                                MIREX


 MOLECULAR WEIGHT = 546

 SYSTEM TEMPERATURE =  15.0 C

 WATER SOLUBILITY  =  .700E-04 (G/M3)

 VAPOR PRESSURE = . 1 00E-05 (MM HG)

 LOG(10)  (OCTANOL-WATER COEFFICIENT)  =  7.608

 TOTAL MASS OF COMPOUND I N SYSTEM =  .385E+04   MOL   688 kg x 3   = LK Ont Mass x  3

 EQUILIBRIUM FUGACITY  =  .530E-13 (ATM)

 HENRYS CONSTANT  =  .1 03E-01 (ATM M3/MOL)



 #   COMPARTMENT            VOL(M3)                           CONC(PPM)   MASS(MOL)
=====================================================================================

 1 ATMOSPHERE(1 0 KM)      .58E+15    .42E+02    .34E+02    .12E-08    .13E+04
 2 WATER      (86 M)       .49E+13    .97E+02    .66E+00    .28E-08    .25E+02
 3 DETRI TUS   1. 5PPtll 0%C  .50E+07    .30E+09    .21E+01    .87E-02    .79E+02
 4 SEDIMENTS 5CM; 1 .0%OC  .15E+10    .30E+08    .62E+02    .87E-03    .24E+04
 5 PHYTO      1500CEL/ML   .75E+06    .12E+10    .12E+01    .35E-01    .48E+02
 6 ZOOPLANK   (30G/M3)     .,5E+06    .12E+10    .25E+00    .35E-01    .95E+01
 7  FORAG FISH(1E5 MT)     .20E+05    .15E+10    .41E-01    .43E-01     16E+01
 8 SALMONOIDS(1 . 6E3 MT)  .32E+03  .  15E+10    .66E-03    .43E-01    :25E-01

   TOP AQUATIC PREDATOR                                     .54E-02
```

If there is no ecosystem file, the model is run as follows:

```
CALL,RUNMI
 XEDIT 3.1.00
       END
FUGMOD1 IS A LOCAL FILE
 ENTER THE COMPOUND NAME (20 CHARACTERS)
? TOTAL DDT
 ENTER THE COMPOUNDS MOLECULAR WEIGHT
? 356
 ENTER TOTAL MASS OF COMPOUND IN SYSTEM (G)  ❑ R 1.0
? 1
 IS THERE A FILE DESCRIBING THE ECOSYSTEM ?;YES=1,NO=2
?2

Z'S ARE CALCULATED AS FOLLOWS
VAPOR PHASE ; Z = 1/RT
LIQUID PHASE ; Z  =  1/H
SORBED ❑ R BIOTIC PHASE;Z = KP/H
KP = KOC * % ORGANIC CARBON/100
KOC = 1.05 . XLKOW - 0.50

FOR Z CLASSIFICATION , ENTER
- 1 . FOR VAPOR PHASE (ATM)
-2. FOR LIQUID PHASE
%SUBSTRATE ORGANIC CARBON FOR SORBED OR BIOTIC PHASE

 ENTER A TITLE FOR THIS RUN (80 CHARACTERS)
? EXAMPLE
 ENTER THE SYSTEM TEMPERATURE (C)
? 155
 ENTER THE COMPOUND'S WATER SOLUBILITY (G/M3)
? .12E-2
 ENTER THE COMPOUNDS VAPOR PRESSURE (MM HG)
?.16E-6
 ENTER THE NUMBER OF ECOSYSTEM COMPARTMENTS


NAME (IN QUOTES),INFO (IN QUOTES) ARE 10 CHARACTERS MAX

ENTER COMPARTMENT 1  NAME , INFO , VOL (M3) , Z CLASS (-1. ,  -2.  , %OC.)
? "ATMOSPHERE" , " (7.555KM) ", 1E6 , - 1
ENTER COMPARTMENT 2  NAME , INFO , VOL (M3) , Z CLASS (-1. ,  -2.  ,  %OC.)
? "WATER" , " (170 M) " , 6.3E3 ,   -2
ENTER COMPARTMENT 3 NAME , INFO , VOL (M3) , Z CLASS r:-1.,-2.,%OC.)
? "SEDIMENTS" , " (1CM;4%C) " , 4E1 ,   4


EXAMPLE


                              TOTAL DDT


 MOLECULAR WEIGHT = 356

 SYSTEM TEMPERATURE  =  15.0C

 WATER SOLUBILITY  =  .120E-02 (G/M3)

 VAPOR PRESSURE  =  .160E-06 (MM HG)

 LOG(10)  (OCTANOL-WATER COEFFICIENT)  =  6.656
```

```
TOTAL MASS OF COMPOUND I   N SYSTEM =   .281E-02 MOL

EQU ILIBRIUMFUGAC ITY =   . 355E-13 (ATM)

HENRYS CONSTANT  =   . 625E-04 (ATM M3/MOL)


#    COMPARTMENT              VOL(M3)          Z            %          CONC(PPM)   MASS(MOL)
_________        _______________________________________________________________________________

1 ATMOSPHERE (7.55KM)        10E+07       .42E+02      .53E-01      .53E-09      .15E-05
2 WATER        (1 70 M)     :63E+04       .16E+05      .13E+00      .20E-06      .36E-05
3 SEDIMENTS (1CM; 4%C)      .40E+02       .20E+10      .10E+03      .25E-01      .28E-02

  TOP AQUATIC PREDATOR                                               .68E-01
EO I ENCOUNTERED.
```

The input ecosystem file is in temporary local storage and can be retained by copying to a permanent file.

```
GET,LKMI
./COPY,LKMI
ATMOSPHERE(7.55KM)     .100E+07-.100E+01
WATER        (,70 M)   .630E+04-.200E+01
SEDIMENTS ( 1CM; 4%C)  .400E+02 .400E+01
EXAMPLE
```

6. ACKNOWLEDGMENTS

Partial funding for this work was provided by the Office of Marine Pollution Assessment (OMPA).

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Appendix 1 - Model Runs

The following section lists the model inputs and outputs for the runs discussed in this report.

Global Ecosystem Run

```
                                TOTAL DDT

 MOLECULAR WEIGHT  =  356

 SYSTEM TEMPERATURE  =   15.10 C

 WATER  SOLUBILITY  = .120E-02  (G/M3)

 VAPOR PRESSURE  =  .160E-06 (MM HG)

 LOG ( 10) (OCTANOL-WATER COEFFICIENT)  =  6.656

 TOTAL MASS OF COMPOUND IN SYSTEM =   .720E+10 G MOL

 EQUILIBRIUM FUGACITY =    .115E-12 (ATM)

 HENRYS  CONSTANT  = .625E-04  (ATM  M3/MOL)


 #    COMPARTMENT              VOL(M3)        Z           %        CONC(PPM)   MASS(MOL)
================================================================================================

 1 ATMOSPHERE (10 KM)       .   51E+19  .42E+02     .34E+00      .17E-08     .25E+08
 2 WATER         (3800 M)   .14E+19     .16E+05     .36E+02      .65E-06     .26E+10
 3 DETPITUS   2PPB; 1 0%C   .28E+10     .49E+10     .22E-01      .20E+00      .16E+07
 4 PLHNTS     AQUATIC       .45E+10     .20E+11     .   14E+00  .81E+00      .10E+08
 5 PLHNTS     LAND          .19E+13     .20E+11     .60E+02      .81E+00     .43E+10
 6 ANIMALS    AQUATIC       .11E+10     .25E+11     .43E-01   .   10E+01     .31E+07
 7 ANIMALS    LAND          .50E+09     .25E+11     .20E-01      .10E+01     .14E+07
 8 SEDIMENTS AQUATIC        .18E+13     .49E+09      14E+01      .20E-01     .10E+09
 9 SEDIMENST  LAND          .15E+13     .99E+09     :24E+01      .40E-01     .17E+09

   TOP AQUATIC PREDATOR                                          .22E+00
```

DDT Calibration for the Lake Michigan Ecosystem (See Table 2).

Run 1

```
CALIBRATION ❑ F LAKE MICHIGAN

                                   TOTAL DDT

   MOLECULAR WEIGHT  =  356

   SYSTEM TEMPERATURE =   15.0C

   WATER SOLUBILITY =    .120E-02 (G/M3)

   VAPOR PRESSURE =    .160E-06 (MM H G ,

   LOG(10)  (OCTANOL-WATER COEFFICIENT)  =   6.656

   TOTAL MHSS OF COMPOUND IN SYSTEM = .100E+07 G MOL

   EQUILIBRIUM FUGACITY  =  .614E-12 (ATM)

   HENRYS CONSTANT =   . 625E-04 (ATM M3/MOL)


   #   COMPARTMENT               VOL(M3)                  %        CONC(PPM)   MASS(MOL)
 ==========================================================================================

   1 ATMOSPHERE (10 KM)        .58E+15     .42E+02     .15E+01     .93E-08     .15E+05
   2 WATER       (86 M)        .49E+13     .16E+05     .48E+01     .35E-05     .48E+05
   3 DETRITUS   1.5PPM10%C     .50E+07     .49E+10     .15E+01      11E+01     .15E+05
   4 SEDIMENTS 5CM;2.0%OC      .15E+10     .99E+09     .91E+02     :22E+00     .91E+06
   5 PHYTO      1500CEL/ML     .75E+06     .20E+11     .91E+00     .43E+01     .91E+04
   6 ZOOPLANK   (306/M3)       .15E+06     .20E+11     .18E+00     .43E+01     .18E+04
   7  FORAG FISH(1E5 MT)       .20E+05     .25E+11     .30E-01     .54E+01     .30E+03
   8 SALMONOIDS (1. 6E3 MT)    .32E+03     .25E+11     .49E-03     .54E+01     .49E+01

     TOP AQUATIC PREDATOR                                          .12E+01
```

Run 2

```
#    COMPARTMENT                  VOL(M3)        Z           %        CONC(PPM)   MASS(MOL)
===========================================================================================

 1 ATMOSPHERE(10 KM)             .58E+15     .42E+02     .85E+00     .52E-08     .85E+04
 2 WATER       (86 M)            .49E+13   .   80E+05    .14E+02     .99E-05     .14E+06
 3 DETRITUS   1.5PPM10%C         .50E+07  .  80E+10   .  14E+01     .99E+00     .14E+05   .
 4 SEDIMENTS 5CM; 2. 0%OC        .15E+10     .16E+10     83E+02     .20E+00     .83E+06
 5 FHYTO       1500CEL/ML        .75E+06     .32E+11    :83E+00     .39E+01     .83E+04
 6 ZOOPLANK   (30G/M3)           .15E+06     .32E+11     .17E+00     .39E+01     .17E+04
 7  FORAG FISH(1E5 MT)            20E+05_.__.40E+11     .28E-01     .49E+01     .28E+03   .
 8 SALMONOIDS(1.6E3 M      T      >.32E+03 .40E+11 .44E-03     .49E+01     .44E+01

   TOP AQUAT I C: PREDATOR                                            .14E+01
```

Run 3

```
#    COMPARTMENT                  VOL(M3)        Z           %        CONC(PPM)   MASS(MOL)
===========================================================================================

 1 ATMOSPHERE(10 KM)             .58E+15     .42E+02     .64E+00     .39E-08     .64E+04
 2 WATER       (86 M)             49E+13     .16E+06     .21E+02     .15E-04     .21E+06
 3 DETRITUS 1.5PPM10%C           :50E+07     .98E+10     .13E+01     .91E+00     .13E+05
 4  SEDIMENTS 5CM;2.0%OC         .15E+10     .20E+10     .77E+02   .  18E+00     .77E+06
 5 FHYTO       1500CEL/ML        .75E+06     .39E+11     .77E+00     .36E+01     .77E+04
 6 ZOOPLANK   (30G/M3)           .15E+06     .39E+11     .15E+00     .36E+01     .15E+04
 7  FORAG FISH(1E5 MT)           .20E+05     .49E+11     .26E-01     .45E+01     .26E+03
 8 SALMONOIDS(1.6E3 MT)          .32E+03     .49E+11     .41E-03     .45E+01     .41E+01

   TOP AQUATIC PREDATOR                                               .14E+01
```

Run 4

```
#    COMPARTMENT                  VOL(M3)                    %        CONC(PPM)   MASS(MOL)
===========================================================================================

 1 ATMOSPHERE (10KM)             .58E+15     .42E+02   .  18E+00     .11E-08     .18E+04
 2 WATER       (86 M)            .49E+13     .16E+07     .57E+02     .41E-04     .57E+06
 3 DETRITUS 1.5PPM10%C           .50E+07     .19E+11     .70E+00     .50E+00     .70E+04
 4 SEDIMENTS 5CM;2. 0%OC         .15E+10   .   39E+10    .42E+02     .10E+00     .42E+06
 5 FHYTO 1500CEL/ML              .75E+06     .77E+11     .42E+00     .20E+01     .42E+04
 6 ZOOPLANK   (30G/M3)           .15E+06   .   77E+11    .84E-01     .20E+01     .84E+03
 7 FORAG FISH(1E5 MT)            .20E+05     .97E+11     .14E-01     .25E+01     .14E+03
 8 SALMONOIDS(1.6E3 MT)          .32E+03     .97E+11     .22E-03     .25E+01     .22E+01

   TOP AQUATIC PREDATOR                                               .12E+01
```

Run 5

```
::   COMPARTMENT                VOL(M3)                          %       CONC(PPM)   MASS(MOL)
==================================================================================================

1 ATMOSPHERE (10 KM)       .58E+15     .42E+02     .20E+01     .12E-07     .20E+05
2 WATER       (86 M)       .49E+13     .16E+05     .62E+01     .45E-05      62E+05
3 DETRITUS  1.5PPM10%C     .50E+07     .49E+10     .20E+01     .14E+01     :20E+05
4 SEDIMENTS SC:“; 1 .5%OC  .15E+10     .74E+09     .88E+02     .21E+00     .88E+06
5 PHYTO       1500CEL/ML   .75E+06     .20E+11     .12E+01     .56E+01     .12E+05
6 ZOOPLANK    (30G/M3)     .15E+06      20E+11     .24E+00     .56E+01     .24E+04
7 FORAG FISH(1E5 MT)       .20E+05     .25E+11     .39E-01     .70E+01     .39E+03
8 SALMONOIDS(1.6E3 MT?     .32E+03     .25E+11     .63E-03     .70E+01     .63E+01

   TOP AQUATIC PREDATOR                                        .15E+01
```

Run 6

```
#    COMPARTMENT                VOL(M3)                          %       CONC(PPM)   MASS(MOL)
==================================================================================================

1 ATMOSPHERE (1 0 KM)      .58E+15     .42E+02     .79E+00   .  49E-08     .79E+04
2 WATER       (86 M)       .49E+13     .16E+06     .25E+02   .    18E-04   .25E+06
3 DETRITUS  1.5PPM10%C     .50E+07     .98E+10     .16E+01     .11E+01     .16E+05
4 SEDIMENTS 5CM;1.5%OC     .15E+10     .15E+10     .71E+02   .  17E+00     .71E+06
5 PHYTO       1500CEL/ML   .75E+06     .39E+11     .95E+00     .45E+01     .95E+04
6 ZOOPLANK    (30G/M3)   .   15E+06    .39E+11     .19E+00     .45E+01     .19E+04
7 FORAG FISH(1E5 MT)       .20E+05     .49E+11     .32E-01     .56E+01     .32E+03
8 SALMONOIDS (1 .6E3 MT)   .32E+03     .49E+11     .51E-03     .56E+01     .51E+01

   TOP AQUATIC PREDATOR                                        .18E+01
```

Run 7

```
#    COMPARTMENT                VOL(M3)                          %       CONC(PPM)   MASS(MOL)
==================================================================================================

1 ATMOSPHERE (10 KM)       .58E+15     .42E+02     .10E+01     .64E-08      10E+05
2 WATER       (86 M)       .49E+13   .  16E+06     .33E+02     .24E-04     :33E+06
3 DETRITUS  1.5PPM10%C     .50E+07     .98E+10     .21E+01     .15E+01     .21E+05
4 SEDIMENTS SC”; 1. 0%OC   .15E+10     .98E+09     .62E+02     .15E+00     .62E+06
5 PHYTO       1500CEL/ML   .75E+06     .39E+11     .12E+01     .59E+01   .  12E+05
6 ZOOPLANK    1.3 0G/M3)   .15E+06     .39E+11     .25E+00     .59E+01     .25E+04
7 FORHG FISH(1E5MT)        .20E+05     .49E+11     .41E-01     .74E+01   .  41E+03
8 SALMONOIDS il. 6E3 M T ; .32E+03     .49E+11     .66E-03     .74E+01     .66E+01

   TOP AQUATIC PREDATOR                                        .23E+01
```

Run 8

```
#   COMPARTMENT                  VOL(M3)      Z                      CONC(PPM)   MASS(MOL)
==========================================================================================

1  ATMOSPHERE(10 KM)           .58E+15     .42E+02     .10E+01     .32E-08     .52E+04
2  WATER       (86 M)          .49E+13     .16E+06     .33E+02     .12E-04     .17E+06
3  DETRITUS  1.5PPM10%C        .50E+07     .98E+10     .21E+01     .74E+00     .10E+05
4  SEDIMENTS 5CM;1.0%OC        .15E+10     .98E+09     .62E+02     .74E-01     .31E+06
5  PHYTO     1500CEL/ML        .75E+06     .39E+11     .12E+01     .29E+01     .62E+04
6  ZOOPLANK   (30G/M3)         .15E+06     .39E+11     .25E+00     .29E+01     .12E+04
7  FORAG FISH(1E5 MT)          .20E+05     .49E+11     .41E-01     .37E+01     .21E+03
8  SALMONOIDS(1.6E3 MT)        .32E+03     .49E+11     .66E-03     .37E+01     .33E+01

   TOP AQUATIC PREDATOR                                            .12E+01
```

Run 9

```
#   COMPARTMENT                  VOL(M3)      Z           %          CONC(PPM)   MASS(MOL)
                                                                       X 10
==========================================================================================

1  ATMOSPHERE(10 KM)           .58E+15     .42E+02     .95E+01     .29E-08     .48E+04
2  WATER       (86 M)          .49E+13     .16E+05     .30E+02     .11E-05     .15E+05
3  DETRITUS  1.5PPM10%C        .50E+07     .98E+09     .19E+01     .67E-01     .95E+03
4  SEDIMENTS 5CM;1.0%OC        .15E+10     .98E+08     .57E+02     .67E-02     .28E+05
5  PHYTO     1500CEL/ML        .75E+06     .39E+10     .11E+01     .27E+00     .57E+03
6  ZOOPLANK   (30G/M3)         .15E+06     .39E+10     .23E+00     .27E+00     .11E+03
7  FORAG FISH(1E5 MT)          .20E+05     .49E+10     .38E-01     .34E+00     .19E+02
8  SALMONOIDS(1.6E3 MT)        .32E+03     .49E+10     .61E-03     .34E+00     .30E+00

   TOP AQUATIC PREDATOR                                            .11E+00
```

Run 10

```
#   COMPARTMENT                  VOL(M3)      Z           %          CONC(PPM)   MASS(MOL)
==========================================================================================

1  ATMOSPHERE(10 KM)           .58E+15     .42E+02     .11E+00     .32E-09     .53E+03
2  WATER       (86 M)          .49E+13     .16E+07     .34E+02     .12E-04     .17E+06
3  DETRITUS  1.5PPM10%C        .50E+07     .98E+11     .21E+01     .74E+00     .10E+05
4  SEDIMENTS 5CM;1.0%OC        .15E+10     .98E+10     .63E+02     .74E-01     .31E+06
5  PHYTO     1500CEL/ML        .75E+06     .39E+12     .13E+01     .30E+01     .63E+04
6  ZOOPLANK   (30G/M3)         .15E+06     .39E+12     .25E+00     .30E+01     .13E+04
7  FORAG FISH(1E5 MT)          .20E+05     .49E+12     .42E-01     .37E+01     .21E+03
8  SALMONOIDS(1.6E3 MT)        .32E+03     .49E+12     .67E-03     .37E+01     .33E+01

   TOP AQUATIC PREDATOR                                            .12E+01
```

Run **11**

```
CALIBRATION: NEW COMPOUND

                              DIELDRIN

 MOLECULAR WEIGHT = 377

 SYSTEM TEMPERATURE  =   15.0C

 WATER SOLUBILITY  =   .240E+00  (G/M3)

 VAPOR PRESSURE = .100E-06(MM HG)

 LOG(10)(OCTANOL-WATER COEFFICIENT)   =   5.131

 TOTAL MASS OF COMPOUND IN SYSTEM =   .500E+05 G MOL

 EQUILIBRIUM FUGACITY =    .169E-14 (ATM)

 HENRYS CONSTANT  =   .207E-06 (ATM M3/MOL)


 ::   COMPARTMENT             VOL(M3)                           CONC(PPM)   MASS(MOL)
=========================================================================================

 1  ATMOSPHERE(10 KM)        .58E+15     .42E+02     .83E-01     .27E-10     .41E+02
 2 WRTER        (86  M)      .49E+13     .48E+07     .80E+02     .31E-05      40E+05
 3  DETRITUS  1.5PPM10%C     .50E+07     .37E+11     .63E+00     .24E-01      32E+03
 4  SEDIMENTS5CM;1.0%OC      .15E+10     .37E+10     .19E+02     .24E-02     .95E+04
 5  PHYTO        1500CEL/ML  .75E+06     .15E+12     .38E+00     .95E-01     .19E+03
 6  ZOOPLANK    (30G/M3)     .15E+06     .15E+12     .76E-01     .95E-01     .38E+02
 7  FORAG FISH(1E5 MT)       .20E+05     .19E+12     .13E-01     .12E+00     .63E+01
 8 SALMONOIDS(1.6E3 MT)      .32E+03     .19E+12     .20E-03     .12E+00     .10E+00

   TOP AQUATIC PREDATOR                                          .62E-01
```

Run 12

CALIBRATION

```
                              MIREX

MOLECULAR WEIGHT = 546

SYSTEM TEMPERATURE =   15.0 C

WATER SOLUBILITY =   .700E-04 (G/M3)

VAPOR PRESSURE =    .100E-05 (MM HG)

LOG(10)(OCTANOL-WATER COEFFICIENT) =   7.608

TOTAL "ASS OF COMPOUND IN SYSTEM =.311E+05 MOL

EQUILIBRIUM FUGHCITY =   .429E-12  (ATM)

HENRYS CONSTANT = .103E-01 (ATM M3/MOL)


#    COMPARTMENT                VOL (M3)       Z           %          CONC(PPM)   MASS(MOL)
==========================================================================================

1 ATMOSPHERE(10 KM)          .58E+15     .42E+02     .34E+02     .99E-08   .  11E+05
2 WATER        (86 M)        .49E+13     .97E+02     .66E+00     .23E-07     .20E+03
3 DETRITUS   1.5PPM10%C      .50E+07     .30E+09     .21E+01     .70E-01     .64E+03
4 SEDIMENTS 5CM;1.0%OC       .15E+10     .30E+08     .62E+02     .70E-02     .19E+05
5 PHYTO      1500CEL/ML      .75E+06     .12E+10     .12E+01     .28E+00     .39E+03
6 ZOOPLANK   (30G/M3)        .15E+06     .12E+10     .25E+00     .28E+00     .77E+02
7  FORAG FISH(1E5 MT)        .20E+05     .   15E+10  .41E-01     .35E+00     .13E+02
8 SALMONOIDS(1.6E3 MT)       .32E+03     .   15E+10  .66E-03     .35E+00     .21E+00

  TOP AQUATIC PREDATOR                                            .44E-01
EOI ENCOUNTERED.
```

Run 13

```
ALIBRATION; N E W COMPOUND

                                                 NHPHTHALEN

"CLECULHR  WEIGHT  =  128

SYSTEM TEMPERATURE =   15.0 C

WATER SOLUBILITY  =   . 330E+02 (G/M3)

VAPOR PRESSURE  =   .230E+00  (MM  HG)

LOG(10)(OCTANOL-WATER COEFFICIENT> =   3. 384

TOTAL MASS O F COMPOUND I N S Y S T E M  = . 100E+01  G MOL

EQUILIBRIUM FUGACITY  =   .348E-16  (ATM)

HENRYS CONSTANT =   . 117E-02 (ATM M3/MOL)


:    COMPARTMENT                 VOL(M3)          Z            %          CONC(PPM)   MASS(MOL)
=================================================================================================

1  ATMOSPHERE(10 KM?          .58E+15       .42E+02      .85E+02      .19E-12      .85E+00
2  WATER       (86  M)        .49E+13       .85E+03      .15E+02      .38E-11      .15E+00
3  DETRITUS 1.5PPM10%C        .50E+07       .96E+05      .17E-02      .43E-09      .17E-04
4 SEDIMENTS SCM; 1.0%OC       .15E+10       .96E+04      .50E-01      .43E-10      . SUE-03
5  PHYTO 1  5   0 OCEL/ML     .75E+06       .39E+06      . 1 OE-02    .17E-08      .10E- 04
6  ZOOPLANK   (30G/M3)        .15E+06       .39E+06      .20E-03    .  17E-08      .20E-05
7 FORAGFISH(1E5 M T ?         .20E+05       .48E+06      .34E-04      .21E-08      .34E-06
8  SALMONOIDS(1.6E3 MT)       .32E+03       .48E+06      .54E-06      .21E-08      .54E-08

   T O P AQUATIC PREDATOR                                             .31E-08
```

Run 14

```
CALIBRATI ON :NEW COMPOUND

                                  BENZENE

 MOLECULAR WEIGHT = 78

 SYSTEM TEMPERATURE =   15.10 C

 WATER SOLUBILITY  =   . 178E+04 (G/M3)

 VAPOR PRESSURE =  .988E+02 (MM HG)

 LOG(10)(OCTANOL-WATER COEFFICIENT) =  2.080

 TOTAL MASS OF COMPOUND IN SYSTEM =  .100E+01 G MOL

 EQUILIBRIUM FUGACITY =  .393E-16 (ATM)

 HENRYS CONSTANT =  .570E-02 (ATM M3/MOL)


 #   COMPARTMENT                VOL(M3)       Z            %          CONC(PPM)   MASS(MOL)
=========================================================================================

 1  ATMOSPHERE(10 KM)          .58E+15     .42E+02     .97E+02      .13E-12     .97E+00
 2 WRTER        (86 M)         .49E+13     .18E+03     .34E+01      .54E-12     .34E-01
 3  DETRITUS    1. 5PPM10%C    .50E+07     .85E+03     .17E-04      .26E-11     .17E-06
 4  SEDIMENTS   SCM; 1.0%OC    .15E+10     .85E+02     . SUE-03     .26E-12      50E-05
 5  PHYTO       1500CEL/ML     .75E+06     .34E+ "4    .1JJF-04     .10E-10     :1 "E-06
 6  ZOOPLANK    (30G/M3)       .15E+06     .34E+04     .20E-05      .10E-10     .20E-07
 7   FORAG FISH(1E5 MT)        .20E+05     .42E+04     .33E- 06     .13E-10     .33E-08
 8  SALMONOIDS(1.6E3 MT)       .32E+03     .42E+04     .53E-08      .13E-10     .53E-10

    TOP AQUATIC PREDATOR                                            .39E-10
```

Procedure File

```
GET,RUNMI
/COPY,RUNMI
GET,FUGMOD1.
GET,SUBS1.
GET,TAPE7=LKMI.
XEDIT,FUGMOD1,I=SUBS1.
REWIND,LGO.
REWIND,TAPE6.
MAP,OFF.
FTN. I=FUGMOD1,L=0.
LGO.
REPLACE,TAPE7=LKMI.
REWIND,TAPE6.
COPY ,TAPE6,OUTPUT.
  EOI  ENCOUNTERED.
```

```
/GET,SUBS1
/COPY,SUBS1
B
READP $FUGI $FUGO ZIN
E
 EOI ENCOUNTERED.
```

Main Program

```
/GET,FUGMOD1
/COPY,FUGMOD1
      PROGRAM MOD (INPUT, OUTPUT, TAPE6, TAPE5=INPUT, TAPE7)
C
C   MAIN PROGRAM FOR FUGACITY MODEL 1 (NO DECOMPOSITION)
C
C   FOR INFORMATION SEE MACKAY(1979);ES&T 13,OCT,79; 1218-1223
C
      COMMON /DATA/MW,TC,SG,VPM,XLKOW,C,NC,CNAME,F,H
      COMMON /ID/ V(20),Z(20), ID(20),CM(20),PCM(20),CC(20),NAME(20)
C
      no   10 I = 1,20
      V (I) = 0.
      Z(I) = 0.
      ID(I) = 0
     CM(I)  =  0.
      PCM(I) = 0 .
      CC(I) = 0.
   10 NAME(I) = 0
C
      CALL FUGI
C
C
C   CALCULATE THE FUGACITY
C
      SUMF = 0.
      DO 40 I = 1,NC
   40 SUMF = SURF + V(I).Z(I)
      F = C/SUMF
C   F = EQUILIBRIUM FUGACITY
C
C   CALCULATE THE COMPOUNDS DISTRIBUTION AT EQUILIBRIUM
C
      SUMM = 0.
      no   50 I = 1,NC
      CM(I) = F •  V(I) . Z(I)
   SO SUM" =SUMM + CM(I)
C
C CM(I) = MASS(MOL) IN EACH COMPARTMENT ;SUMM = C
C
C   CALCULATE FERCENTRGE DISTRIBUTION
C
      DO 60 I = 1,NC
   60 PCM(I)=100. •  CM(I)/SUMM
C
C   CALCULATE COMPARTMENT CONCENTRATIONS
C
      no 70 I = 1,NC
   70 CC(I) = CM(I) * MW /V(I)
C
      CALL FUGO
C
      STOP
      END
 EOI ENCOUNTERED.
```

Subroutines

```
/GET,SFUGI
./COPY,SFUGI
      SUBROUTINE FUGI
      COMMON /DATA/ MW,TC,SG,VPM,XLKOW,C,NC,CNAME,F,H
      COMMON /ID/ V(20),Z(20),ID(20),CM(20),PCM(20),CC(20),NAME(20)
      COMMON /CK/ ICHK,CO I 20)
C
C   SUBROUTINE CONTROLS INTERACTIVE INPUT TO FUGACITY MODELS
C
      PRINT • *"ENTER THE COMPOUND NAME (20 CHARACTERS)"
      READ (5, 11) CNAME
   11 FORMAT(2A10)
      PRINT • 9"ENTER THE COMPOUNDS MOLECULAR WEIGHT"
      READ •, MW
      PRINT ..."ENTER TOTAL MASS OF COMPOUND IN SYSTEM (G) OR 1.0"
      READ • .C
      C = C / MW
      PRINT •,"IS THERE A FILE DESCRIBING THE ECOSYSTEM ?; YES=1,NO=2"
      READ • vICHK
      IF (ICHK.EQ.2) GO TO 100
      PRINT • ."ENTER ECOSYSTEM FILE NUMBER , NUMBER OF COMPARTMENTS"
      READ • rN:NC
C
      REWIND N
      DO 10 I = 1,NC
   13 FORMAT(2A10,2E9.3)
   10 READ(N,13) NAME(I),ID(I),V(I),CO(I)
C
  100 CALL CREATZ
C
  101 CONTINUE
C  THIS HAS DEFINED THE ECOSYSTEM AND COMPARTMENT PROPERTIES
C
      RETURN
      END
 EOI ENCOUNTERED.
```

```
/GET,ZIN
/COPY,ZIN
      SUBROUTINE CREATZ
      COMMON/DATA/ MW,TC,SG,VPM,XLKOW,C,NC,CNAME,F,H
      COMMON/ID/ V(20),Z(20),ID(20),CM(20),PCM(20),CC(20),NAME(20)
      COMMON /CK/ ICHK,CO(20)
      DIMENSION SYSTEM(8)
I-
:   ROUTINE CHLCULRTES Z'S ;FUGACITY CAPACITIES
C
      IF(ICHK.EQ.1) GO TO 16
      WRITE(5,22)
   22 FORMAT(" "/
     1"Z'S HRE CHLCULHTED AS FOLLOWS"/
     2"VAPOR PHASE ; Z = 1/RT"/
     3"LIQUID PHASE ; Z = 1/H"/
     4"SORBED OR BIOTIC PHASE;Z = KP/H"/
     5"KP = KOC  •  % ORGANIC CARBON/100"/
     6"KOC = 1. 05 • XLKOW - 0.50"/
     ⌨❾      ")
C
      WRITE(5, 52:)
C
   52 FORMAT("FOR Z CLASSIFICATION, ENTER",'
     1"-1. FOR VAPOR PHASE(ATM)"/
     2"-2. FOR LIQUID PHASE"/
     3"% SUBSTRATE ❑ RGHNIC CARBON FOR SORBED OR BIOTIC PHASE"/
     4"    ")
   16 CONTINUE
      PRINT *,"ENTER A TITLE FOR THIS RUN (80 CHARACTERS)"
      READ(5,31)   (SYSTEM(J),J=1,8)
   31 FORMAT(8A10)
C
      PRINT . . "ENTER THE SYSTEM TEMPERRTURE (C)"
      READ *,TC
      PRINT *,"ENTER THE COMPOUND'S WATER SOLUBILITY(G/M3)"
      READ *,SG
      PRINT ● v "ENTER THE COMPOUNDS VAPOR PRESSURE (MM HG)"
      READ *,VPM
C
      R G  = 82.0 . 1E-06
      TK  =  TC + 273.
      RT  =  RG . TK
      VPA  =  VPM/760.
      SM  =  SG/MW
      H  =  VPH  / SM
      XLKOW  =  5.00 - 0.670*ALOG10(SM * 1000)
C
      IF(ICHK .EQ.1) GO  TO  77
C
      PRINT ●  , "ENTER THE NUMBER OF ECOSYSTEM COMPARTMENTS"
      READ *,NC
      REWIND 7
      PRINT "8
   98 FORMAT(/,"NAME < I N QUOTES),  INFO(IN QUOTES) HRE 10 CHRRRCTERS MAX
     1",/)
      DO  41  I  =  1,NC
      PRINT 99 ,  I
   99 FORMAT("ENTER COMPARTMENT",I3,1X," N H M E,I N F O,VOL(M3),Z CLASS
     1 (-1.  ,  -2. ,  %OC.)")
      READ *,NAME(I),ID(I),V(I),CO(I)
      IF(CO(I)  .GT.  0.)  Z(I)  =  10**(1.05*XLKOW-0.50)*.01*CO(I)/H
      IF(CO(I) .EQ. -1.) Z(I)   =   1./RT
     IF(CO(I)  .EQ.  -2.) Z(I)   =   1./H
   11 FORMAT(2A10,2E9.3)
   41 WRITE(7,11)  NAME(I),ID(I),V(I),CO(I)
```

```
/GET,SFUGO
/COPY,SFUGO
       SUBROUTINE FUGO
       COMMON /DATA/ MI.,,. TC,SG,VPM,XLKOW,C, NC:, CNAME,F,H
       COMMON /IO/ V(20), Z(20), ID(20), CM(20), PCM(20), CC(20), NAME(20)
C
C  SUBROUTINE FOR DATA OUTPUT FROM FUGACITY MODELS
C
       WRITE(6,200)CNAME
       WRITE(6,201)MW
   200 FORMAT(30X,2A10)
   201 FORMAT(//," MOLECULAR WEIGHT =",I4,/)
       WRITE(6,202)TC
   202 FORMAT(" SYSTEM TEMPERATURE =", F6.1, " C" ,/)
       WRITE(6,203)SG
   203 FORMAT(" WATER SOLUBILITY =", E|0.3, "  (G/M3)", /)
       WRITE(6,204)VPM
   204 FORMAT(" VAPOR PRESSURE =" , E10.3, "  (MM HG) ", /)
       XLKOW = ALOG1 0(XLKOW)
       WRITE(6,205)XLKOW
   205 FORMAT("LOG(1 03  (OCTANOL-WATER COEFFICIENT) =",F7.3. /)
       WRITE(6,206)C
   206 FORMAT(" TOTAL MASS OF COMPOUND | N SYSTEM =", E |0.3, " MOL", /)
       WRITE(6,207)F
   207 FORMAT(" EQUILIBRIUM FUGACITY =", E10. 3, " (ATM) ", /)
       WRITE(6,208)H
   208 FORMAT (" HENRYS CONSTANT =",E10.3, "  (ATM M3/MOL) ", /)
       WRITE(6,209)
   209 FORMAT(///," ::    COMPARTMENT                  VOL(M3)
      1"    %        CONC(PPM)   MASS(MOL)",/)
       WRITE(6,210)
       DO 12 | = 1,NC
    12 W RITE(6,211) I,NAME(I),ID(I),V(I),Z(I),PCM(I),CC(I),CM(I)
   210 FORMAT("======================================================",
      1"====================",/)
   211 FORMAT(I2,1X,2A10,5(E10.2,1X))
C
C  BIOMAGNIFICATION CALCULATION
       XZ = 10**(0.80*XLKOW- a.50)/H
       CX = F . XZ . MW . 5
C  CONVERTED TO DRY WEIGHT BY 5X
       WRITE(6,212) CX
   212 FORMAT(/,3X,"TOP AQUATIC PREDATOR",33X,E10.2)
       RETURN
       END
  EO] ENCOUNTERED.


C
       GO TO 44
       no  45 I = 1,NC
       IF(CO(I) .GT. 0) Z(I) = 10**(1. 05*XLKOW-0.50)*. 01*CO(I)/H
       IF(CO(I).EQ.-1) Z(I) = 1./RT
    45 IF(CO(I).EQ.-2.) Z(I) = 1./H
C
    44 PRINT 66
    66 FORMAT(/)
       WR|TE(7,31)   (SYSTEM(J),J=1,8)
       PRINT 31,   (SYSTEM(J),J=1 , 8;
       PRINT 66
       XLKOW = 10 ** XLKOW
       RETURN
       END
 EOI ENCOUNTERED.
```